

Commentary

Nanofiltration for circularity: Fit-for-purpose design and evaluation

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Nanofiltration—a technology that selectively extracts critical materials from streams—can help secure resources while minimizing wasteful and unsustainable extraction practices. However, next-generation nanofiltration membranes must be designed with a fit-for-purpose framework in mind to fully harness its capabilities in resource conservation and minimize trade-offs.

Nanofiltration as potential driver for circularity

Rapid population and economic growth require an unprecedented level of material supply. This presents a major challenge that can only be effectively addressed through sustainable practices, particularly by implementing enhanced circularity. The high consumption rate of critical materials not only jeopardizes their supply chains but is also detrimental to the environment.¹ For instance, the rising demand for batteries has created instability in the supply of lithium, an essential element for low-carbon energy technologies. To meet the long-term material demand, it is crucial to shift away from linear economic systems that rely on resource extraction, single-use consumption, and disposal, which result in pollution and worsen climate change. Embracing circular economic systems that prioritize material recycling and reuse is crucial to reduce strain on supply chains, enhance resource security, and mitigate climate change by lowering greenhouse gas emissions. Notably, the [United Nations](#) has recognized sustainable production and consumption as one of the key sustainable development goals, guiding societies toward embracing circularity.

The realization of a circular economy necessitates technological advancements that facilitate precise separations. Efficient extraction of critical materials from diverse sources—for example, ores, minerals, electronic waste, wastewater, produced water, and brines—is essential to achieving a circular economy.² The variable and complex nature of these sources, and the plethora of crit-

ical resources that can include water, metals, rare earth elements, nutrients, and pharmaceuticals, requires adaptable and versatile separation technologies. One such candidate is nanofiltration (NF), which can achieve energy-efficient, modular, chemical-free, and customized separation, provided it is suitably engineered.³ NF technology employs a nanoporous membrane that serves as a molecular filter, distinguishing between various species present in the mixture. In contrast with reverse osmosis membranes that reject most ions and uncharged molecules, NF membranes allow some solutes to pass through the nanopores, offering the opportunity to differentiate between them and recover those that are critical.

Nanofiltration holds significant potential as a catalyst for promoting circularity within various industries.^{3,4} Currently, NF is utilized for water softening, removal of organic compounds from surface and groundwater, wastewater treatment in the textile, leather, and paper sectors, as well as in the production of biopharmaceuticals (e.g., purifying antibiotics) and food processing (e.g., concentrating and demineralizing lactose, concentrating maple syrup, and dealcoholizing beer). However, to fully unleash the potential of NF for a circular economy and sustainable manufacturing, it is necessary to optimize the membrane properties to enhance the differentiation between similar solutes and increase membrane stability, especially under the harsh operational conditions existing in some streams containing critical materials. Given the wide array of critical mate-

rials and streams, relying solely on a single type of NF membrane is not a feasible solution. Even within a target application (e.g., lithium recovery), there can be a high variability in terms of the competing species, mineral scalants, foulants, and pH level present, depending on the source (e.g., brines and produced waters from different locations).

Designing fit-for-purpose membranes is essential to unlock the versatility of NF for circularity ([Figure 1](#)). For instance, successful desalination of antibiotics demands an open-structure membrane with an engineered pore size distribution that allows salt ions and water molecules to pass at a high rate and retain valuable antibiotics. Recovering lithium from unconventional sources, on the other hand, requires precise control over membrane-ion interactions and confinement to differentiate between lithium ions and other competing ions. Although both applications fall under the NF category, the required membrane features differ significantly. To enable next-generation NF membranes, it is crucial to advance our understanding of the fundamental principles underlying the design and fabrication of single-species selective membranes and follow a fit-for-purpose strategy informed by the specific requirements for the targeted stream.

Fit-for-purpose design of nanofiltration membranes

The membrane design strategy for upcoming NF applications can vary significantly, depending on the specific application at hand. Therefore, to achieve optimal membrane design that is tailored for each



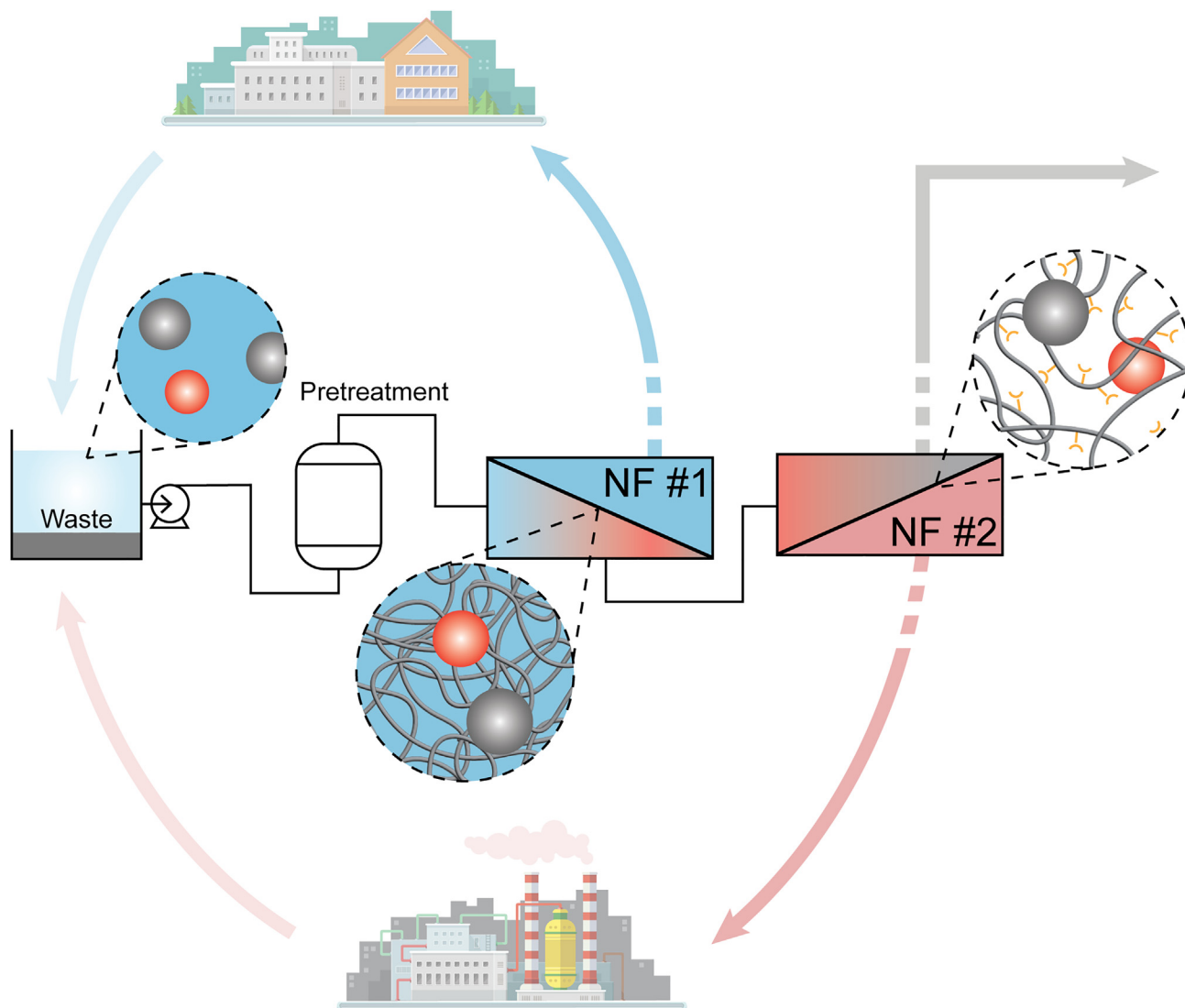


Figure 1. Circularity enabled by nanofiltration

Schematic showing the use of nanofiltration to increase the circularity of water (blue) and valuable solutes (red) while minimizing waste (gray). A first nanofiltration membrane (NF #1) concentrates solutes to recover water from the waste stream and a second nanofiltration membrane (NF #2) separates the valuable solutes (red) to reuse them and discards the waste (gray). The recovered water increases the municipal water supply, and the valuable solutes are reused in industry. After being reused some of the water and valuable solutes end up in a waste stream that can be treated again. Some examples of valuable solutes are nutrients and critical metals.

specific purpose, it is essential to have a comprehensive understanding of the transport mechanisms encompassing both the target species and the competing species. Particularly, acquiring a detailed understanding of how water molecules, ions, and neutral solutes traverse membrane materials is of utmost significance for applications aiming to differentiate between similar species like lithium mining from brines, nutrient recovery from wastewater, and purification of antibiotics. Similar to reverse osmosis membranes, where it has been recently shown that wa-

ter transport is governed by a pore-flow mechanism with a pressure gradient as the driving force,⁵ the water transport in NF is also likely to be governed by a similar mechanism, since NF membranes have a looser and more porous active layer structure. On the other hand, ion and neutral solute transport in NF is governed by a combined contribution of diffusion, advection, and electromigration, following the partitioning of ions and neutral solutes into the membrane.⁶ However, unraveling the transport mechanism of molecules when dealing with complex

streams and membrane designs is not trivial. For example, in ultra-permeable NF membranes, advection is likely to play an important role in neutral solute and ion transport, and in streams with similar competing species, coupling mechanisms can govern the transport. Overall, an improved understanding of the transport mechanisms, particularly in the presence of similar competing species and harsh conditions, is needed for achieving fit-for-purpose membrane design and effective optimization strategies.

After selecting a robust membrane design strategy based on transport rate and mechanisms, it is imperative to conduct a fit-for-purpose optimization. During the optimization process, it is necessary to identify and prioritize the key features that significantly influence membrane performance for resource recovery from a particular stream. Key features include membrane properties, such as surface charge, average pore size, cross-linking density, as well as solution properties, such as ionic composition, pH, and temperature. These properties play a vital role in determining the separation performance of the membrane for a specific application. For instance, the recovery of lithium from brines necessitates membranes with a specific surface charge and an optimal average pore size that selectively facilitate the passage of Li^+ ions while impeding the transport of Mg^{2+} ions. On the other hand, in the context of mining critical metals from hydrometallurgical battery recycling streams, the utilization of a membrane with exceptional stability in highly acidic environments is of utmost importance. Additionally, such a membrane should possess tailored properties to facilitate the accurate separation of the target metal ions. Most studies focus on a limited number of such features without providing a justification for their selection, potentially overlooking other influential factors. To address this limitation, we propose embracing machine learning techniques to guide experimental investigations by assessing the sensitivity of each feature. By leveraging machine learning algorithms, the process of discovering optimized membranes can be accelerated and made more efficient. Further, by systematically evaluating the impact of various features, we can gain insights into their significance and make informed decisions regarding feature selection for membrane optimization.⁷

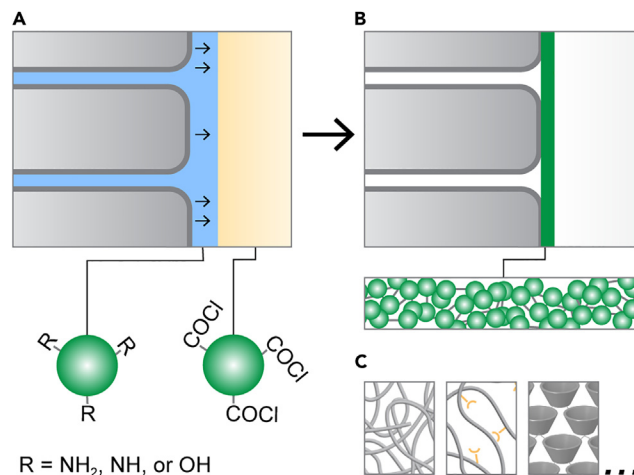


Figure 2. Interfacial polymerization is a versatile, robust technique for the preparation of NF membranes

(A–C) (A) Schematic representation showing the preparation thin-film composite nanofiltration membranes by interfacial polymerization. In this method, monomers in the aqueous phase diffuse to the water/organic interface. At this interface, the amine or hydroxyl functional groups of the monomers react with the acyl chloride functional groups of the monomers in the organic phase. If one or more of the monomers possess three or more reactive sites, this chemical reaction results in the formation of a densely crosslinked polyamide or polyester film, as depicted in (B). The monomers, additives, and reaction conditions control the properties of the polyamide selective layer. (C) The schematic representation showcases three distinct selective layers that can be generated through interfacial polymerization, each exhibiting unique characteristics. On the left, a densely packed structure with small pores (or free volume) is depicted, indicating a barrier that restricts the passage of solutes. In the middle, an open structure is shown, featuring functional units that selectively interact with specific solutes, enhancing their separation. On the right, preferentially aligned cavities are displayed, forming well-defined pores across the selective layer, enabling precise control over molecular transport. These illustrations represent only a glimpse of the diverse range of structures attainable through interfacial polymerization, denoted by the three dots, emphasizing the broad scope of possibilities in this technique.

Addressing the challenge of enabling NF for resource recovery applications, which aims to enhance the circularity of critical materials, necessitates collective and collaborative efforts. To foster collaboration and knowledge sharing within the nanofiltration membrane community, it is essential to establish an open and comprehensive membrane database. A model similar to the one utilized in reverse osmosis⁸ should be implemented, where researchers can report their findings and contribute to a centralized repository of membrane data. This database would serve as a valuable resource for researchers and practitioners, facilitating the development of machine learning models and supporting the advancement of membrane technology.

Designing NF membranes with tailored properties for specific applications requires advancements in material engineering and membrane synthesis. In contrast to reverse

osmosis, a universal NF membrane material does not exist. Implementing NF to improve the circularity of critical materials will require a portfolio of membrane materials. More challenging applications requiring resilience in harsh environments or precise solute-solute selectivity can benefit from novel materials and novel synthesis techniques.

Promising innovations for fit-for-purpose designs

Interfacial polymerization, characterized by the formation of a film at the interface of two immiscible solvents containing mutually reactive monomers, presents significant potential as a synthesis platform for the efficient and scalable production of next-generation NF membranes. The inherent self-limiting nature of this process yields continuous thin films that serve as selective barriers, with their properties easily controlled through simple synthesis parameters and additives. Moreover, the extensive use of this technique in large-scale reverse osmosis

membrane production for over four decades has led to accumulated expertise that can expedite the upscaling of customized interfacial polymerization-based NF membranes for resource recovery applications. The high tunability of interfacial polymerization enables the fabrication of readily scalable, purpose-specific NF membranes.

Typically, interfacial polymerization produces thin selective layers by the reaction of two monomers, one with either amine or hydroxyl groups and one with acyl chloride groups, at the interface of two immiscible liquids (Figures 2A and 2B). By fine-tuning the interface during the reaction and selecting appropriate monomers, improvements can be made in water permeance and solute-solute selectivity (Figure 2C). For instance, surfactant molecules can be utilized to generate crumpled structures with a larger effective surface area to enhance

water transport⁹ or to increase the uniformity of sub-nanometer pores in the polyamide layer for precision separations.¹⁰ Alternatively, contorted monomers can be employed to enhance the microporosity of the selective layer for high water flux applications.¹¹ To improve the sustainability of the manufacturing process and bypass complex synthesis protocols commonly associated with contorted molecules, bio-derived alternatives can be explored.¹² Lastly, the use of cavitands as interfacial polymerization monomers provides improved control over the nanopores in the selective layer, thereby facilitating the permeation of molecules conducive to the container-shaped molecule's cavity, while rejecting those that are not conducive.¹³ The cavitands can also be functionalized to promote their arrangement at the interface to produce films with aligned pores, further enhancing their performance.¹⁴

There are promising NF membrane materials beyond interfacial polymerization-derived selective layers, such as block copolymers, metal and covalent organic frameworks, zeolites, and 2D nanoporous materials. NF membranes made from these materials may offer performance advantages compared to interfacial polymerization based polymeric membranes, and their research and development could lead to significant breakthroughs in NF technology. For instance, the remarkable ability to precisely control confinement and functionalities on crystalline materials like metal-organic frameworks enables discrimination between monovalent ions with selectivities comparable to those exhibited by biological ion channels¹⁵—an achievement unprecedented in polymeric systems. However, efforts to reduce the cost and increase the processability of these materials are needed to show that they can be manufactured at scale.¹⁶ A recent example is the synthesis of solution-processable metal-organic framework nanosheets that can be cast using a doctor blade, similar to polymeric solutions, into large-area (>200 cm²) ultrathin membranes with remarkable homogeneity and sufficient flexibility.¹⁷

Resource recovery applications typically involve handling substantial volumes of materials, making it crucial to consider the intended scale of the application early in the material discovery process. Hence, it is imperative to demonstrate that up-

coming fit-for-purpose NF membranes can be produced at an industrial scale and a reasonable cost, which can be determined by techno-economic analysis.¹⁸ This is of paramount importance for their successful adoption and to enhance the circularity of critical materials. While research on materials that pose uncertainties in scaling up holds value in unraveling new transport mechanisms and improving the understanding of existing ones, it is equally important to undertake parallel efforts to demonstrate the feasibility of processing such materials into membranes at a scalable level. Collaborations between academia and industry are necessary to take lab-scale efforts demonstrating the scale-up potential of emerging membrane materials to the next level, where continuous production can be achieved.

The future of fit-for-purpose NF membranes

Our need of circularity for a sustainable future has opened many opportunities for NF to become a driver for circularity, contributing to water management and to the agricultural, energy, and pharmaceutical industries. In the agricultural industry, NF is expected to play a crucial role in water management and sustainable farming practices. An efficient treatment of agricultural wastewater will enable the reuse of valuable nutrients and irrigation water and facilitate the removal of harmful substances, such as pesticides and heavy metals, from agricultural runoff. In the energy sector, NF offers promising solutions for improving energy efficiency and sourcing critical materials needed for a wide range of technologies, such as energy storage. Similarly, in the pharmaceutical industry, NF can increase circularity by enabling the recovery and purification of valuable compounds from its wastewaters. However, additional efforts in both fundamental and applied research are imperative to attain optimal customization of NF membranes and processes for their respective applications, ensuring an optimal fit-for-purpose performance.

On the fundamental side, a deeper understanding of the underlying solute and water transport mechanisms is needed to inform and guide the design of next-generation NF membranes, encompassing material selection and membrane

synthesis. Interdisciplinary collaborations will pave the way for more precise and targeted strategies to fulfill the requirements of emerging separations, such as achieving enhanced solute-solute selectivity and facilitating improved tunability and stability of NF membranes. On the application side, optimization and evaluation within a fit-for-purpose framework, informed by a techno-economic analysis, is required to properly guide the development of NF processes that reduce energy consumption in current applications and enable new ones. Techno-economic analysis plays a pivotal role in assessing the economic viability of fit-for-purpose NF membranes and should garner greater attention among membrane scientists—particularly when designing the next generation NF membranes. By establishing a clearly defined research pathway for fit-for-purpose NF, a future marked by circular and sustainable manufacturing, enabled through the adoption of NF technology, can be anticipated.

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DECLARATION OF INTERESTS

The authors declare no competing interests.

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