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Supporting Information

Tailored design of nanofiltration membranes for water treatment based on synthesis–property–performance relationships

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S1: Calculation of water/solute selectivity and solute/solute selectivity

Water/solute selectivity (A/B):

The transport of water and solutes through NF membrane can be described using the solution-diffusion model.[1,2]

$$J_w = A(P - \Delta\pi_m) \qquad (1)$$

$$J_S = B\Delta C \qquad (2)$$

$$\Delta C = f_{cp}(C_f - C_p) \qquad (3)$$

Here, J_w is the water flux (L/m^2/h), A is the water permeability coefficient (L/m^2/h/bar); P is the applied hydraulic pressure (bar); $\Delta\pi_m$ is the osmotic-pressure difference across the membrane active layer (bar); J_S is the solute flux (kg/m^2/h); B is the solute permeability coefficient of the membrane (L/m^2/h); ΔC is the solute concentration difference across the membrane (kg/L); C_f and C_p (kg/L) are the solute concentrations of the feed and permeate water, respectively; and f_{cp} is the concentration polarization factor. Since the experimental conditions reported in the publications about membrane fabrication often do not contain sufficient information to accurately determine f_{cp}, the concentration polarization effect was assumed negligible (f_{cp}=1).

Generally, the observed solute rejection rate (R) was reported in literature to evaluate membrane separation performance.

$$R = 1 - \frac{C_p}{C_f} \qquad (4)$$

Combining the above equations leads to

$$R = \frac{A/B(P - \Delta\pi_m)}{A/B(P - \Delta\pi_m) + 1} \qquad (5)$$

$$A/B = \frac{R}{(1 - R)(P - \Delta\pi_m)} \qquad (6)$$

Eq. (5) indicates that the solute rejection is not only determined by the membrane intrinsic properties but also affected by the driving force ($P - \Delta\pi_m$). The experimental conditions are often very different among the numerous studies, so it is more appropriate to utilize water/solute selectivity (A/B) rather than the reported solute rejection to evaluate the membrane separation capability.

Solute/solute selectivity:

The separation factor (α) of solute X1 to solute X2 is a typical adopted parameter to characterize solute/solute selectivity in a membrane separation process, and can be calculated using the following equation:[3,4]

$$\alpha(X1/X2) = \frac{C_{X1,p}/C_{X2,p}}{C_{X1,f}/C_{X2,f}} \qquad (7)$$

Here, $C_{X1,p}$ and $C_{X2,p}$ are the solute X_1 concentration and the solute X_2 concentration in permeate water, respectively; $C_{X1,f}$ and $C_{X2,f}$ are the solute X1 concentration and the solute X2 concentration in feed solution, respectively. The above equation can be further extended to

$$\alpha(X1/X2) = \frac{1 - R_{X_1}}{1 - R_{X_2}} \qquad (8)$$

For example,

$$\alpha(NaCl/Na_2SO_4) = \frac{1 - R_{NaCl}}{1 - R_{Na_2SO_4}} \qquad (9)$$

$$\alpha(NaCl/MgCl_2) = \frac{1 - R_{NaCl}}{1 - R_{MgCl_2}} \qquad (10)$$

S2. Calculation of the required hydraulic pressure and membrane area

Investment and operating cost of membrane process are two parameters that engineers are very concerned about, which can be expressed to some extent by the required hydraulic pressure and membrane area during operation.

Equation 1 have presented how to calculate water flux according to the solution-diffusion model. Concentration polarization has a significant effect on the properties of the feed solution at membrane-water interface. For RO, Equation 1 can be modified using film theory as follows:[5]

$$J_w = A[P - \Delta\pi_{av}\exp\left(\frac{J_w}{k_f}\right)] \tag{11}$$

Here, k_f is the mass transfer coefficient (L/m^2/h) averaged for all feed solutes, $\Delta\pi_{av}$ the average osmotic pressure (bar) throughout the filtering process and can be calculated by:[6]

$$\pi_{av} = \frac{\pi_f ln(\frac{1}{1-R})}{R} \tag{12}$$

where π_f is the initial osmosis pressure (bar) of the feed water, which is proportional to the concentration of salt in the feed, Y is the water recovery.

Thus, the required hydraulic pressure (P, bar) can be calculated by:

$$P = \frac{J_w}{A} + \pi_{av}exp(\frac{J_w}{k_f}) \tag{13}$$

The required membrane area (S, m^2) at a constant applied hydraulic pressure and a given water flow rate can be calculated by:

$$S = \frac{Q}{J_w} \tag{14}$$

where Q is the water flowrate (L/h).

To calculate J_w, we need to solve the Equation 13 using the Newton-Raphson method, with an error criterion of $|(J_w)_{k+1} - (J_w)_k| < \frac{1}{2} \times 10^{-6}$, and all the calculation were conducted using MATLAB R2020b.

In order to reduce the amount of calculation, the above process is simplified and considered under an idealistic approach.[7,8] For example, pressure drop in the feed channel, pump inefficiencies, and energy recovery device inefficiencies were neglected in our calculation process. We focus mainly on the effect of membrane properties on the change of membrane system, such as the required hydraulic pressure and membrane area. Of course, these simplifying assumptions do not prevent us from reaching correct conclusions.

Detailed parameters used for the required hydraulic pressure and membrane area is provided in Table S1.

Table S1. Parameters used for the calculation of required hydraulic pressure and membrane area.

Mass transfer coefficient	k_f	100 L/m^2/h
Feed concentration	C_f	0.5-4.0 g/L
Feed osmotic pressure	π_f	C_f*1 bar (approximate)
Water recovery	R	0.15
Average water flux	J_w	40 L/m^2/h
Water flowrate	Q	100 L/h
Pressure set for membrane area calculation	P	6 bar

The calculation results of the required hydraulic pressure and membrane area with increasing water permeability were showed in Table S2 and Table S3.

Table S2. The required hydraulic pressure at a constant membrane area with increasing water permeance.

Water permeance (A, L/m^2/h/bar)	Required hydraulic pressure (P, bar) with different salt concentration			
	0.5 g/L	1.0 g/L	2.0 g/L	4.0 g/L
5	8.81	9.62	11.23	14.47
6	7.47	8.28	9.90	13.13
7	6.52	7.33	8.95	12.18
8	5.81	6.62	8.23	11.47
9	5.25	6.06	7.68	10.91

10	4.81	5.62	7.23	10.47
20	2.81	3.62	5.23	8.47
30	2.14	2.95	4.57	7.80
40	1.81	2.62	4.23	7.47
50	1.61	2.42	4.03	7.27
60	1.47	2.28	3.90	7.13
70	1.38	2.19	3.80	7.04
80	1.31	2.12	3.73	6.97
90	1.25	2.06	3.68	6.91
100	1.21	2.02	3.63	6.87

Table S3. The required membrane area at a constant hydraulic pressure with increasing water permeance.

Water permeance (A, L/m^2/h/bar)	Required membrane area (S, m^2) with different salt concentration			
	0.5 g/L	1.0 g/L	2.0 g/L	4.0 g/L
5	3.78	4.32	5.83	14.70
6	3.17	3.64	4.97	12.71
7	2.74	3.16	4.36	11.29
8	2.41	2.81	3.91	10.23
9	2.16	2.53	3.55	9.41
10	1.96	2.31	3.27	8.76
20	1.08	1.34	2.03	5.84
30	0.81	1.05	1.65	4.89
40	0.68	0.91	1.46	4.42
50	0.62	0.83	1.36	4.14
60	0.57	0.78	1.29	3.96
70	0.55	0.75	1.24	3.83
80	0.53	0.73	1.21	3.73
90	0.51	0.71	1.18	3.66
100	0.50	0.70	1.16	3.60

S3. Commercialization prospect of different NF membrane fabrication methods.

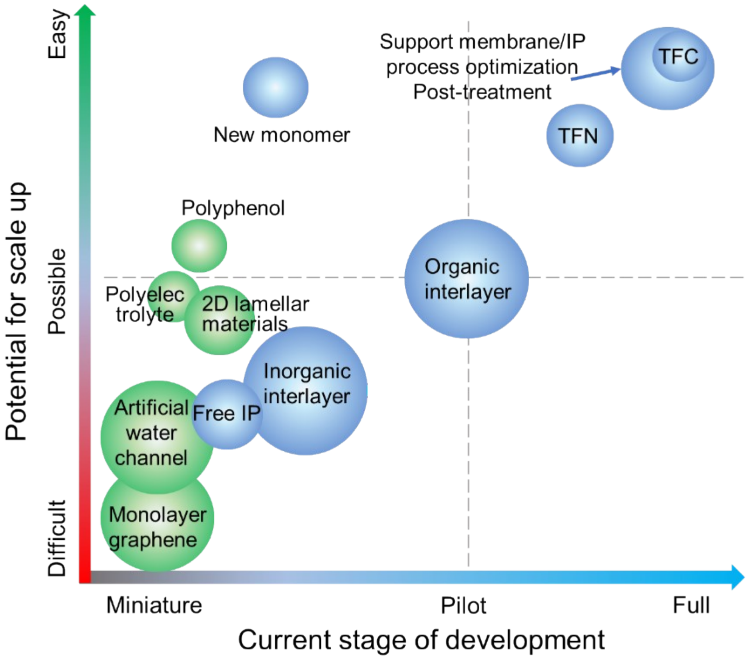

Fig. S1. Comparison of the current stage of development, and potential for scale up and performance enhancement of different membrane fabrication methods based on comprehensive discussion in this review. The horizontal axis classifies different technologies into full scale, pilot scale, and miniature scale. The vertical axis represents the potential for scale up of these fabrication technologies, comprehensively considering the technical difficulties and potential cost of production. The size of the sphere represents the potential performance enhancements of a particular technology, where a larger sphere indicates a great potential to improve NF membrane performance, including enhanced reliability, reduced cost, and energy consumption, and/or improved water quality. (see references[9,10])

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