Investigation of the Performance of an Optimized Tree-Type Cylindrical-Shaped Nanoporous Filtering Membrane for Varying Operational Parameter Values

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Abstract

The performance of an optimized tree-type cylindrical-shaped nanoporous filtering membrane proposed in the former study is analytically investigated for varying operational parameter values. Across the membrane thickness, this membrane has two-leveled tree-structured pores including one trunk pore and the multiple branch pores. The physical properties of the surfaces of all the pores are identical. The branch pore is for filtration, while the radius of the trunk pore is optimized for achieving the lowest flow resistance of the membrane. The calculation results show that in a liquid-particle separation, the influence of the number N of the branch pores in each pore tree on the lowest flow resistance of the membrane in the optimum condition strongly depends on the radius R_{b,1} of the branch pore; When R_{b,1} is over 10 nm, this influence is normally very significant; In a liquid-liquid separation, the performance of the membrane mainly depends on the radius R_{b,1}, which should normally be no more than 3 nm or even more less depending on the liquid-pore wall interaction, although both a smaller N value and a greater value of the ratio of the depth of the branch pore to the membrane thickness helps to improve the separation.

Keywords

- Membrane
- Nanopore
- Filtration
- Separation
- Optimization

Highlights

- The performance of the proposed membrane in liquid-particle separation in wide cases;
- The capability of the liquid-liquid separation of the membrane in wide cases.

1. Introduction

Nanoporous filtering membranes have been in fast progress because of their super purification capability and their important applications in purification of water and seawater, hemofiltration, drug delivery and DNA analysis et al. [1-5]. They are also capable of liquid-liquid separation because of the different liquid-pore wall interactions [6]. These membranes not only should satisfy the requirement of super purification but also should have the satisfactory flux and mechanical strength. These are not easily realized because the size of the filtration pores of these membranes should be as small as on the nanometer scale while the membrane thickness should be sufficiently large to maintain the mechanical strength.

People have been trying to find the methods to improve the overall performance of nanoporous filtering membranes including manufacturing very thin membranes by graphene, taking the filtration pore as conical, and taking the membrane as consisted of both nanopores and micropores [7-9].

For improving the performance of such membranes, the author developed an optimized cylindrical-shaped nanoporous filtering membrane composed of...
two kinds of concentric pores across the membrane thickness i.e. the filtration pore and the flow resistance-reducing pore [10]; the radius of the latter pore is optimized for yielding the lowest flow resistance or the highest flux of the membrane. By this way, the mechanical strength of the membrane can be improved with a relatively thick membrane. Later, the author developed a tree-type cylindrical-shaped nanoporous filtering membrane based on the principle of transportation in nanotube tree [11]. Across the thickness of this membrane there are two-leveled tree-structured pores i.e. one trunk pore and the four branch pores. The branch pore is for filtration, and the trunk pore is larger for collecting the flow out of its branch pores and also reducing the flow resistance of the membrane. In this membrane, there is a small angle \( \theta \) between the axis of the trunk pore and the axes of its branch pores. In a recent research [12], the geometrical structures of this tree-type membrane were optimized by taking \( \theta = 0^\circ \), using various branch pores in each pore tree, and optimizing the radius of the trunk pore for yielding the lowest flow resistance of the membrane. It was found that the increase of the number \( N \) of the branch pores in each pore tree significantly reduces the flow resistance of the membrane and thus improves the flux of the membrane [12], and the membrane has the capability of a liquid-liquid separation for a very low value of the radius of the branch pore in spite of the value of \( N \) if the mixed liquids have greatly different interactions with the pore wall [12].

The present paper further analytically investigates the performance of the nanoporous filtering membrane proposed in Ref. [12] in the liquid-particle and liquid-liquid separations by widely varying operational parameter values. Important calculation results were obtained regarding the dependence of the lowest flow resistance of this membrane in the optimum condition on the operational parameters and the dependence of the liquid-liquid separation capability of this membrane on the operational parameters. Conclusions were drawn concerning the choice of the operational parameter values of this membrane for a liquid-particle separation or a liquid-liquid separation.

2. Studied membrane

The studied membrane is exemplarily shown in Figures 1(a) and (b). Across the thickness of this membrane are manufactured two-leveled tree-structured cylindrical pores which are evenly distributed within the membrane. In each pore tree, there is one trunk pore with the radius \( R_{b,2} \) and the pore depth \( l_2 \); there are also multiple branch pores with the number \( N \) with the radius \( R_{b,1} \) on the nanometer scale and the pore depth \( l_1 \) (In the figure, as an example \( N=4 \)). The branch pore is for filtration, and the trunk pore is for reducing the flow resistance of the membrane. The physical properties of the surfaces of all the pores are identical. The thickness of the membrane is \( l = (l_1 + l_2) \).

3. Analysis

The liquid flow within the membrane in Figures 1(a) and (b) is studied by using the developed flow equation for a nanoscopic fluid flow. Detailed analysis for this membrane has been presented in Ref. [12]. For brevity, only necessary contents are repeated here.

In each pore tree, the \( N \) branch pores with the pore depth \( l_j \) is equivalent to the straight cylindrical pore with the radius \( R_{b,j} \) and with the pore depth \( l_j \). When neglecting the liquid-pore wall interfacial slippage, \( R_{eq} \) is solved from the following equation [12]:

\[
\frac{N \cdot Cy(R_{b,1}) S(R_{b,1})}{Cy(R_{eq})} - \frac{Cy(R_{eq})}{Cy(R_{b,1})} = 0
\]

where \( R_{b,1} = R_{b,1} / R_{eq} \), \( R_{eq} = R_{eq} / R_{eq} \), \( R_{eq} \) is the critical radius of the pore for the filtered liquid to become continuum across the pore radius, \( Cy(R) = \eta_\text{eff} (R) / \eta \), \( Cy(R) = \rho_\text{eff} (R) / \rho \), and \( \eta_\text{eff} \) and \( \eta_\text{eff} \) are respectively the average density and the effective viscosity of the filtered liquid across the pore radius, \( S \) is the parameter describing the non-continuum effect of the filtered liquid across the pore radius \( (1 \leq S < 0) \), and \( \rho \) and \( \eta \) are respectively the bulk density and the bulk viscosity of the filtered liquid at the environmental temperature and pressure.

The radius \( R_{b,2} \) of the trunk pore is optimized for yielding the lowest flow resistance of the membrane. The equation for calculating this optimum \( R_{b,2} \) value was presented in Ref. [12]. The lowest dimensionless flow resistance of the membrane is calculated as: \( I_{f,\text{min}} = (R_e / R_{eq})^2 F_{\text{min}} \), where

\[
R_{eq} = R_e / R_{eq} ; \quad R_e \text{ is a constant reference radius, } R_{eq} = R_{eq} / R_{eq} ; \quad \text{and} \quad F_{\text{min}} \text{ is [12]:}
\]

\[
F_{\text{min}} = \begin{cases} 2 \left( \lambda_e (1 - \lambda_e) Cy(R_{eq}) \right)^{-1} Cq(R_{eq}) S(R_{eq}) & \text{for } R_{b,2} \geq R_{eq} \\ Cy(R_{eq}) \left( Cq(R_{eq}) S(R_{eq}) \right)^{-1} & \text{for } R_{b,2} < R_{eq} \end{cases}
\]

where \( \lambda_e = l_e / l \).

For evaluating the capability of the liquid-liquid separation of the membrane, the two parameters \( r_m \) and \( r_s \) are here used. \( r_m \) is the ratio of the dimensionless flow resistance \( I_f \) of the membrane for the liquid with a medium-level interaction with the pore wall to that \( (I_{f,\text{min}}) \) for the liquid with a weak interaction with the pore wall when the radius \( R_{b,2} \) of the trunk pore is optimized for yielding the lowest flow resistance of the membrane for the liquid with a weak interaction with the pore wall. \( r_s \) is the ratio of the dimensionless flow resistance \( I_f \) of the membrane for the liquid with a strong interaction with the pore wall to that \( (I_{f,\text{min}}) \) for the liquid with a weak interaction with the pore wall when the radius \( R_{b,2} \) of the trunk pore is optimized for yielding the lowest flow resistance of the membrane for the liquid with a weak interaction with the pore wall. The mixed liquids may have greatly different interactions with the pore wall, and the values of \( r_m \) and \( r_s \) can measure the capability of the membrane in separating these liquids from one another.

In calculating the values of \( r_m \) and \( r_s \), the dimensionless flow...
resistance $I_f$ of the membrane for the liquid with medium-level or strong interactions with the pore wall is calculated as: $I_f = (R_l/R_{eq})^2 F$, where $F$ is [12]:

$$F = \frac{\lambda_0Cy(R_{eq})}{Cq(R_{eq})} \left(\frac{R_{b,2}}{R_{eq}}\right)^2 + \frac{(1-\lambda_0)Cy(R_{b,2})}{Cq(R_{b,2})} \left(\frac{R_{b,2}}{R_{eq}}\right)^2$$

(3)

where $R_{b,2} = R_{b,1}/R_{eq}$.

4. Calculation

For investigating the performance of the membrane in Figure 1, the lowest flow resistances ($I_{f,min}$) of the membrane in the optimum condition respectively for weak, medium-level and strong liquid-pore wall interactions were calculated when both $R_{b,1}$ and $N$ were widely varied. The values of $R_m$ and $R_s$ were also calculated when the operational parameter values were widely varied.

In the calculations, for whichever liquid-pore wall interaction, $Cq(R)$ was generally expressed as [12]:

$$Cq(R) = \begin{cases} 1, & \text{for } R \geq 1 \\ m_1 + m_2 R + m_3 R^2 + m_4 R^3, & \text{for } 0 < R < 1 \end{cases}$$

(4)

where $R$ is $R_{b,1}$, $R_{eq}$ or $R_{b,2}$ (same in the following equations), $m_1$, $m_2$, $m_3$ and $m_4$ are respectively constants.

$Cy(R)$ was generally expressed as [12]:

$$Cy(R) = \begin{cases} 1, & \text{for } R \geq 1 \\ a_0 + a_1 R + a_2 R^2, & \text{for } 0 < R < 1 \end{cases}$$

(5)

where $a_0$, $a_1$ and $a_2$ are respectively constants.

$S(R)$ was generally expressed as [12]:

$$S(R) = \begin{cases} -1, & \text{for } R \geq 1 \\ [n_0 + n_1 (R-n_2)^{n_3}]^{n_4}, & \text{for } n_1 < R < 1 \end{cases}$$

(6)

where $n_0$, $n_1$, $n_2$ and $n_3$ are respectively constants.

For weak, medium-level and strong liquid-pore wall interactions, the values of $R_{eq}$ were respectively taken as 3.5, 10 and 20 nm [12]. For different types of the liquid-pore wall interaction, the values of the other parameters are respectively shown in Tables 1(a-c).

Table 1(a)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong</td>
<td>1.8335</td>
<td>-1.4252</td>
<td>0.5917</td>
</tr>
<tr>
<td>Medium</td>
<td>1.0822</td>
<td>-0.1758</td>
<td>0.0936</td>
</tr>
<tr>
<td>Weak</td>
<td>0.9507</td>
<td>0.0492</td>
<td>1.6447E-4</td>
</tr>
</tbody>
</table>

5. Results and discussion

Figure 2 plots the numerically solved values of the ratio $R_{eq}/R_{b,1}$ against $N$ respectively for weak, medium-level and strong liquid-pore wall interactions. The ratio $R_{eq}/R_{b,1}$ is found to be weakly dependent on the radius $R_{b,1}$ of the branch pore; it is significantly influenced by both the number $N$ of the branch pores in each pore tree and the liquid-pore wall interaction. The plotted $R_{eq}/R_{b,1}$ values in Figure 2 are valuable for designing the membrane in Figure 1, as the optimum ratio of $R_{eq}$ to $R_{b,1}$ is calculated as: $(R_{eq}/R_{b,1})_{opt} = (R_{eq}/R_{b,1})(R_{eq}/R_{b,2})_{opt}$ [12].

Figures 3(a-c) respectively plot the values of the dimensionless lowest flow resistances $I_{min}$ of the membrane for different $R_{b,1}$ and $N$ respectively for the weak, medium and strong liquid-pore wall interactions when $R_s = 10nm$, $\lambda_0 = 1\times10^{-3}$, and the ratio $R_{eq}/R_{b,1}$ is optimum. For each liquid-pore wall interaction and a given $N$ value, the value of $I_{min}$ is rapidly reduced with the increase of the radius $R_{b,1}$ of the branch pore. The figures evidently show the significant benefits of the increase of the number ($N$) of the branch pores in each pore tree in reducing the flow...
resistance of the membrane and thus improving the flux of the membrane. The figures give the indication that in engineering application the values of $R_{b,1}$ and $N$ both should be as large as possible for yielding the highest flux of the membrane.

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Figure 4(a) plots the values of $r_m$ against $R_{b,1}$ for different $N$ when $\lambda_0 = 1 \times 10^{-3}$. Only when $R_{b,1}$ is no more than 1 nm, the values of $r_m$ are over 10 so that the membrane in Figure 1 is possible to be used for separating the two liquids which respectively have weak and medium interactions with the pore wall. In this case, $R_{b,1}$ is so small that the flux of the membrane might be quite small. The influence of the parameter $N$ on the value of $r_m$ is so weak that it is negligible.

Figure 4(b) plots the values of $r_m$ against $\lambda_0$ for different $N$ when $R_{b,1} = 0.5nm$. Although both the increase of $\lambda_0$ and the reduction of $N$ increases the value of $r_m$ and thus slightly improves the capability of the liquid-liquid separation of the membrane, they can not radically influence the liquid-liquid separation performance of the membrane, which is actually determined by the radius $R_{b,1}$ of the branch pore as shown in Figure 4(a).

![Figure 4(a)](image1)

![Figure 4(b)](image2)

Fig. 4. Values of $r_m$.

![Figure 3](image3)

Fig. 3. Plots of the dimensionless lowest flow resistances of the membrane for different $R_{b,1}$ and $N$ respectively for the weak, medium and strong liquid-pore wall interactions when $R_{b} = 10nm$, $\lambda_0 = 1 \times 10^{-3}$, and the ratio $R_{b,2}/R_{b,1}$ is optimum.
Figure 5(a) plots the values of $r_s$ against $R_{b,1}$ for different $N$ when $\lambda_0 = 1 \times 10^{-3}$. It is shown that if the membrane in Figure 1 is used for separating the two liquids which respectively have weak and strong interactions with the pore wall, the radius $R_{b,1}$ may be no more than 3 nm. In this case, the influence of the parameter $N$ on the separation performance of the membrane is negligible. The comparison between Figure 5(a) and Figure 4(a) shows that for a given low $R_{b,1}$ and the same operating condition, $r_s$ is much greater than $r_m$. This means that the liquid-liquid separation performance of the membrane is significantly better if the difference between the interactions of the two mixed liquids with the pore wall is significantly increased. The comparison also suggests that in the liquid-liquid separation, the interactions of the mixed liquids with the pore wall are at best largely different so that a considerably larger value of $R_{b,1}$ can be used for improving the flux of the membrane.

Figure 5(b) plots the values of $r_s$ against $\lambda_0$ for different $N$ when $R_{b,1} = 0.75 \text{nm}$. Same as in Figure 4(b), both the parameters $\lambda_0$ and $N$ can not radically influence the value of $r_s$, which is mainly determined by the radius $R_{b,1}$ as shown in Figure 5(a), though the appropriate choices of their values can further slightly improve the liquid-liquid separation performance of the membrane due to the increased $r_s$ values.

6. Conclusions

The paper analytically investigates the performance of the optimized tree-type cylindrical-shaped nanoporous filtering membrane proposed in Ref. [12] in the liquid-particle and liquid-liquid separations by widely varying the operational parameter values. Conclusions are drawn as follows:

(1) For any kind of liquid-pore wall interaction, the value of the dimensionless lowest flow resistance $I_{f,\min}$ of the membrane is rapidly reduced with the increase of the radius $R_{b,1}$ of the branch pore when the ratio of the trunk pore radius $R_{b,2}$ to its branch pore radius $R_{b,1}$ is optimum. The influence of the number $N$ of the branch pores in each pore tree on the value of $I_{f,\min}$ is increased with the increase of $R_{b,1}$, and it is also increased with the weakened liquid-pore wall interaction.

(2) Relatively big values of the number $N$ of the branch pores in each pore tree have significant benefits in reducing the flow resistance of the membrane and thus improving the flux of the membrane, especially when the radius $R_{b,1}$ of the branch pore is comparatively big and the liquid-pore wall interaction is weak.

(3) The capability of the liquid-liquid separation of the membrane is determined by the radius $R_{b,1}$ of the branch pore. A very small $R_{b,1}$ value around 1 nm or even more less is required for achieving a good performance of the membrane in a liquid-liquid separation. Both the ratio $\lambda_0$ of the depth of the branch pore to the membrane thickness and the number $N$ of the branch pores in each pore tree can not radically influence the liquid-liquid separation performance of the membrane, though the increase of $\lambda_0$ and the reduction of $N$ both further slightly improves this performance of the membrane.

(4) The performance of the liquid-liquid separation of the membrane is better if the difference between the interactions of the two mixed liquids with the pore wall is greater.

Nomenclature

$a_0$, $a_1$, $a_2$ = respectively constant, Eq. (5)

$C_q(\bar{R}) = \rho_{\text{eff}}\, (\bar{R}) / \rho$

$C_y(\bar{R}) = \eta_{\text{eff}}\, (\bar{R}) / \eta$

$F_{\text{min}} =$function, Eq.(2)

$F =$function, Eq.(3)

$I_f = (\bar{R}_f / \bar{R}_{eq})^2 F$

$I_{f,\min} =$dimensionless lowest flow resistance of the membrane,

$(\bar{R}_f / \bar{R}_{eq})^2 F_{\text{min}}$

$l =$thickness of the membrane
$l_1$ = depth of the branch pore

$\rho_0$, $\eta_0$, $m_0$, $m_1$, $m_2$, $m_3$, respectively constant, Eq.(4)

$n_0$, $n_1$, $n_2$, $n_3$, respectively constant, Eq.(6)

$N$ = number of the branch pores in each pore tree

$R_{b,1}$ = radius of the branch pore

$R_{b,2}$ = radius of the trunk pore

$R_{eq}$ = radius of the straight cylindrical pore equivalent to the $N$ branch pores in transportation

$R_{cr}$ = critical radius of the pore for the filtered liquid to become continuum across the pore radius

$R_m$ = ratio of the dimensionless flow resistance $I_f$ of the membrane for the liquid with a medium-level interaction with the pore wall to that ($I_{f,\text{min}}$) for the liquid with a weak interaction with the pore wall when the radius $R_{b,2}$ of the trunk pore is optimized for the liquid with a weak interaction with the pore wall

$R_s$ = ratio of the dimensionless flow resistance $I_f$ of the membrane for the liquid with a strong interaction with the pore wall to that ($I_{f,\text{min}}$) for the liquid with a weak interaction with the pore wall when the radius $R_{b,2}$ of the trunk pore is optimized for the liquid with a weak interaction with the pore wall

$R_r$ = constant reference radius

$\lambda_{opt} = l_1 / l$

$\theta$ = angle between the axis of the trunk pore and the axes of its branch pores

$\rho$, $\eta$ = respectively the bulk density and the bulk viscosity of the filtered liquid at the environmental temperature and pressure

References


