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Modelling the Separability Process of Oil-Water Molecular Motion for Stable and Efficient Wettability Process

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Abstract

The molecular motions of oil-water particles are extremely complex and unpredictable during oil-water separation. This is due to the complexity of the dynamic forces that impacts oil-water molecular behaviour during separation. Most often membrane fouling and degradation are reported due to poor membrane design used in oil-water separation. For over decades now, several efforts have been used to improve membrane efficiency during oil-water separation. To design an efficient or stable wettability surface membrane scientists and engineers must model the molecular behaviours of the parameters or variables that impacts efficient or stable wettability process. The modelling process must also consider membrane flow momentum and velocity of flow that impacts the molecular motion of oil-water particles during oil-water separation. In this paper, the tool of stochastic mechanics and fluid dynamics are used to model the molecular interaction of oil-water particles during separation. The following facts were theoretically revealed and validated. It was revealed that an increase in membrane pressure led to an increase in energy and momentum which impacts the molecules of oil-water during separation. It was also revealed that the change in membrane pressure affects the backward flow process of oil molecules and forward flow of water in the hydrophobic membrane. It was observed that an increase in momentum led to an increase in membrane flow rate. It was also revealed that as membrane energy decreases, the rate of flow of pure water in the membrane channel increases as the system gain momentum. Membrane performance was observed to be more efficient surface energy and momentum were at critical limit during operation. At the critical limit, there was an increase the backward flow of oil molecules with an increase forward flow of water molecules in the hydrophobic membrane. At the critical limit in momentum and pressure, membrane fouling and degradation were minimized since the required momentum and pressure was needed for stable and efficient operation.

Keywords: molecular interaction, oil-water molecules, momentum and change in pressure.

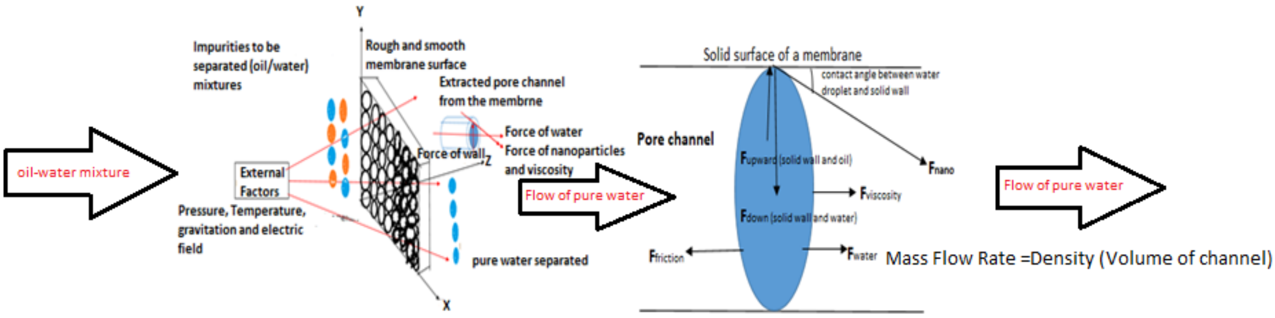
1. INTRODUCTION

Nanostructured membranes used in oil/water separation are based on membrane dynamic forces which are internal and external forces. These forces are reported to have an impact in the functionality of a membrane system during oil-water separation [1-4]. There are complexity and uncertainty when dealing with these dynamics forces during oil-water separation as they affect membrane molecular behaviour and membrane performance during oil-water separation [1-5]. Most developed membrane system focused on limited membrane dynamic forces without taking into consideration all the external and internal factors that impacts oil-water molecules and membrane performance during oil-water separation [1-6]. These membranes technologies are inefficient with poor controllability during oil-water separation since the molecular behaviours of oil-water particles are not computed proportional during oil-water separation [1-14].

Membrane technologies are impacted by several parameters that are critical and most developed membrane technology only focused on limited parameters leading to the current design problem of inefficient membrane performance during oil-water separation [1-6]. Membrane technologies used in oil-water separation are affected by several dynamic forces that impacts the molecular behaviour of oil-water during separation. These dynamic forces are nanoparticle (Fnano), force of viscosity (Fviscosity), force of water (Fwater), force of solid surface and water (Fdown), force on solid surface and oil (Fupward) and force of friction (Ffriction) [8]. There are other forces such as temperature, pressure, electric field, and gravitation are the main external forces being using in modelling and designing of the current membrane technology [8] which also affect membrane performance during oil-water separation. In most developed membrane technologies used in oil-water separation, membrane channel flow rates are impacted by the external and internal forces. These forces play a vital role in impacting performance, since they impacts the molecular behaviour of oil-water but most membrane studies focused on the internal parameters, without critically looking at other dynamic forces such as momentum and change in membrane pressure that impacts the molecular behaviours of oil-water molecules. Therefore, to design a membrane system that is more efficient or stable during oil-water separation process, these dynamic forces such as momentum and change in membrane pressure must be investigated. To design a membrane surface that is more efficient with stable performance during oil-water separation, membrane flow momentum and change in pressure during increase and decrease in momentum must be model for optimal wettability during oil-water separation. The membrane change in moment and pressure change are modelled by taking into consideration their direct impact on surface energy driven separability and other membrane dynamic forces that impacts the molecular behaviours of oi-water molecules. For membrane external forces, the application of linear momentum conservation which describes the summation of external forces on the control system volume which is equal to the practical rate of time of change in momentum within the control system was investigated and it impacts on wettability revealed.

2. METHODOLOGY

For the design of a stable and efficient wettability surface, it is important to theoretically modelled membrane dynamics forces, membrane internal forces and external forces during oil-water separation by understanding their impacts on the molecular behaviours of oil-water. Figure 1 (a) shows a schematic illustration of 3-D porous membrane technology used in the designed membrane technology as revealed by [8]. The morphology (rough or smooth) of the surface, which imposed the frictional force, played a significant role on how the spherical water molecules flew through the membrane surface during separation process. The major forces being modelled during oil-water separation as shown in Fig.1 being the reaction force from the water droplet, which is observed to be perpendicular to the solid surface of the membrane as shown in Fig.1. The molecular behaviour of oil-water particles has direct impacts on these forces during oil-water separation. There are other forces that impacts oil-water separation such as the force of nano-particle (Fnano) to lower the surface energy on the channel, force of viscosity (Fviscosity), force on water to due applied pressure (Fwater), force on solid wall and water (Fdown), force on wall and oil (Fupward) and force of friction (Ffriction) and the total external factors [8]. These forces are shown in the schematic in Fig. 1.



Dynamic factors = flow of oil, flow of water, motion of oil, motion of liquid, mass flow rate of water through the membrane, flow velocity, pressure, density and temperature

Figure 1. Schematic diagrams of nanostructured membrane showing external factors, impurities (oil/water mixture) and pure water being separated in a membrane channel and the forces on water molecules.

Figure 1 shows the main forces on a water droplet during oil-water separation. During the process of oil/water separation, it is not only the force of water, force on wall and force from nanoparticle that impact the flow of water through the membrane. The viscosity of water is also impacted by shear stress, temperature and membrane dynamics forces during oil-water separation. In most cases, the viscosity of water on a membrane surface was modelled by the contact angle of water on the membrane surface as defined by Thomas Young in the 1805s. Thomas Young model described contact angle of a liquid drop on an ideal solid surface as the mechanical equilibrium of the droplet under the action of three interfacial forces (tensions) on the surface, and these forces are liquid-vapor, solid-vapor, and solid-liquid interfacial tensions, where θ is the contact angle. The young's model has undergone several modifications based on several ignored parameters as reported by [8]. In the current study the developed model by [8] was modified by taking into consideration more membrane flow momentum and change in pressure which impacts molecular dynamics activities of oil-water molecules which the Young models and [8] did not take into consideration during oil-water process given as

$$F_{Total} = F\cos\theta + F_{viscosity} + F_{upward(solid\ and\ oil)} - F_{down\ (solid\ and\ water)} + F_{\frac{water}{pressure}} + \sum \vec{F}\ external \quad [1]$$

The model given by equation (1) is affected by several dynamic factors and external factors which are considered as major forces during oil-water separation. In modelling the dynamic and external forces that impacted oil-water molecules during separation, the flow of fluids (oil and water) must be describe during oil-water separation. The aerodynamics motion and hydrodynamics (motion of liquids) must be analysed according to the physical reality during oil-water separation. The mass flow rate of oil and water during flow through the membrane must analysed. The flow velocity, pressure, density and temperature function in a membrane system must be analysed during oil-water separation. This analysis is possible by looking at the volume flow of water flow during oil-water separation which can be translated to velocity using dimensional analysis. In the process of mathematical modelling, the mobility of oil-water molecules must be analysed based on the physical reality of the system during operating.

The summation of membrane external forces on the control volume being the membrane channel is equal to the time rate of change of momentum within the control volume, plus the net momentum flux across the control surfaces. Assuming that the control membrane volume is connected to the inlet of the oil-water mixture and connected to the outlet where pure water is collected and at another outlet where pure oil is collected. Therefore, there is a dynamic' momentum flux, or momentum flux produced by the system and therefore the control volume and the net momentum flux is existing and it greatly influenced the molecular behaviours of oil-water molecules since separation of oil-water takes place in the control volume. The total sum of the external forces can be computed by using dimensional analysis which relates control volume to velocity and the expression for the external force is given as

$$\frac{\partial}{\partial t}\int \rho\vec{V}\,dV \;+\; \int \rho\vec{V}\left(\vec{V}\,.\,n\right)dS = \sum \vec{F}\,external \qquad [2]$$

Where V is the velocity in m/s, ρ density of separated oil-water, $(\vec{V}.n)dS$ is the mass flow rate through dS into the control volume, membrane external force is affected by velocity of oil-water molecules in the membrane channel. It is therefore important to analyse the velocity in the membrane. If the flow of water must be steady with a fixed control volume during oil-water separation, momentum equation can be applicable in the study. The momentum of flow is affected by velocity and the membrane surface area. By simplifying all the momentum, momentum flow and defined force from Newton's second law, the integral equation of momentum is given as

$$\frac{d}{dt}\iiint \rho\vec{V}dv \;+\; \oiint \rho(\vec{V}.\hat{n})\vec{V}\,dA = \oiint -p\hat{n}dA$$
$$+\;\iiint \rho\vec{g}\,dv +\; F_{viscous} \qquad [3]$$

The integral mass equation given by (3) can be application in any defined finite control volumes as applicable in this study. A pressure integral surface equation can be converted using the Gradient Theorem which impacts the molecular behaviour of oil-water molecules given as

$$\oiint \rho(\vec{V}.\hat{n})\left(u\,\hat{\imath} \;+\; v\,\hat{\jmath} \;+\; w\,\hat{k}\right)dA \;=\; i\iiint \nabla.\;\left(\rho\,\vec{V}u\right)dv$$
$$+\,j\,\iiint \nabla.\;\left(\rho\,\vec{V}\,v\right)dv \;+\; k\,\iiint \nabla.\;\left(\rho\,\vec{V}w\right)dv \qquad [4]$$

The defined momentum equation given by the Gradient theorem affect the velocity distribution of oil-water molecules and discharge produced by the membrane being pure clean water in the forward direction through the exit and backward direction where pure oil was also collected as shown in Fig. 2.

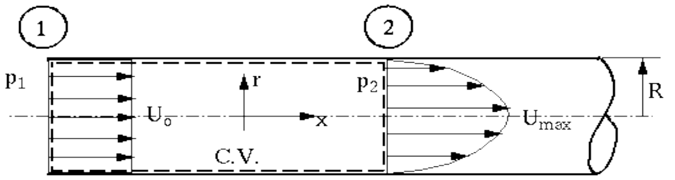


Figure 2. Schematic diagrams of velocity and velocity distribution in a channel during viscous flow

The flow rate through the membrane channel dQ can be computed by assuming the velocity along the membrane surface x the area of the strip. By considering that the rate of flow of fluids through the channel strip of thickness dr and integrating the rate of flow through the strip gives $dQ = \frac{S_3}{2\mu}\partial P\left[\frac{r^2}{4} - r\right]x\;d(2\pi r S_3)$. Simplifying the expression yields

$$Q = \frac{2\pi S_3}{\mu}\partial P\left[\frac{r^4}{16} - \frac{r^3}{3}\right] \qquad [5]$$

The flow rate through the membrane surface is affected by pressure change ∂P which impacts fluid molecular motion and fluid viscosity μ and and S3 obtained from the speed formula as given by equation (6). The derived model of flow rate and change in momentum during oil-water separated were tested with the models of surface energy driven wettability derived by Sob et al [8] given as,

$$P.A_1 = F_{Total} = \frac{surface_{energy}.A_3}{S_3} = \frac{d_{energy}.A_3}{S_3} \qquad [6]$$

where $A_1 = pr^2$ is membrane cross-sectional area at inlet, $A_3 = 2prS_3$ is surface area of the channel over which liquid flow, r is the radius of the channel which takes into consideration the random hydrophobic nanoparticles that are coated on the membrane surface which lower surface energy to improve membrane wettability. Equations (1-6) are solved simultaneously using Engineering Equation Solver software (F-Chart Software, Madison, W153744, USA) and the results are presented and discussed below.

3. RESULTS AND DISCUSSION

The proposed models derived in this paper were tested with the following data ρ = 1000 kg/m3, h = 6.626 x 10-34 J.s, μ = 0.000720 m2/s, S1 = 0.3 m, Vvol = 0.12 m3, t2 = 150 sec, t3 = 120 sec, A1 = 0.08 m, A2 = 0.04 m, F = 100 KN. ρ = 1000, S1 = 0.3, V = 200 m/s, t2 = 3 sec, t3 = 1 sec, σ = 0.002, A1 = 0.08 m, A2 =0.0 4 m, F = 100 KN. ρ = 1000 kg/m3, h = 6.626 x 10-34 J.s, μ = 0.000720 m2/s, S1 = 0.3 m, Vvol = 120 litres, t2 = 150 sec, t3 = 120 sec, A1 = 8 cm, A2 = 4 cm, F = 100 KN. ρ = 1000, h = 6.626 x 10-34 μ = 0.000720 N.s/m2, S1 = 0.3 m, $V_{Vol} = 0.12\,m^3$, V = 200 m/s, t2 = 3 sec, t3 = 1 sec, A1 = 0.08 m, A2 = 0.04 m, F = 100 KN. ρ = 1000 kg/m3, S1 = 0.3 m, Vvol = 0.12 m3, t2 = 150 sec, t3 = 120 sec, A1 = 0.08 m, A2 =0.0 4 m, F = 100 KN. The obtained results are presented and discussed.

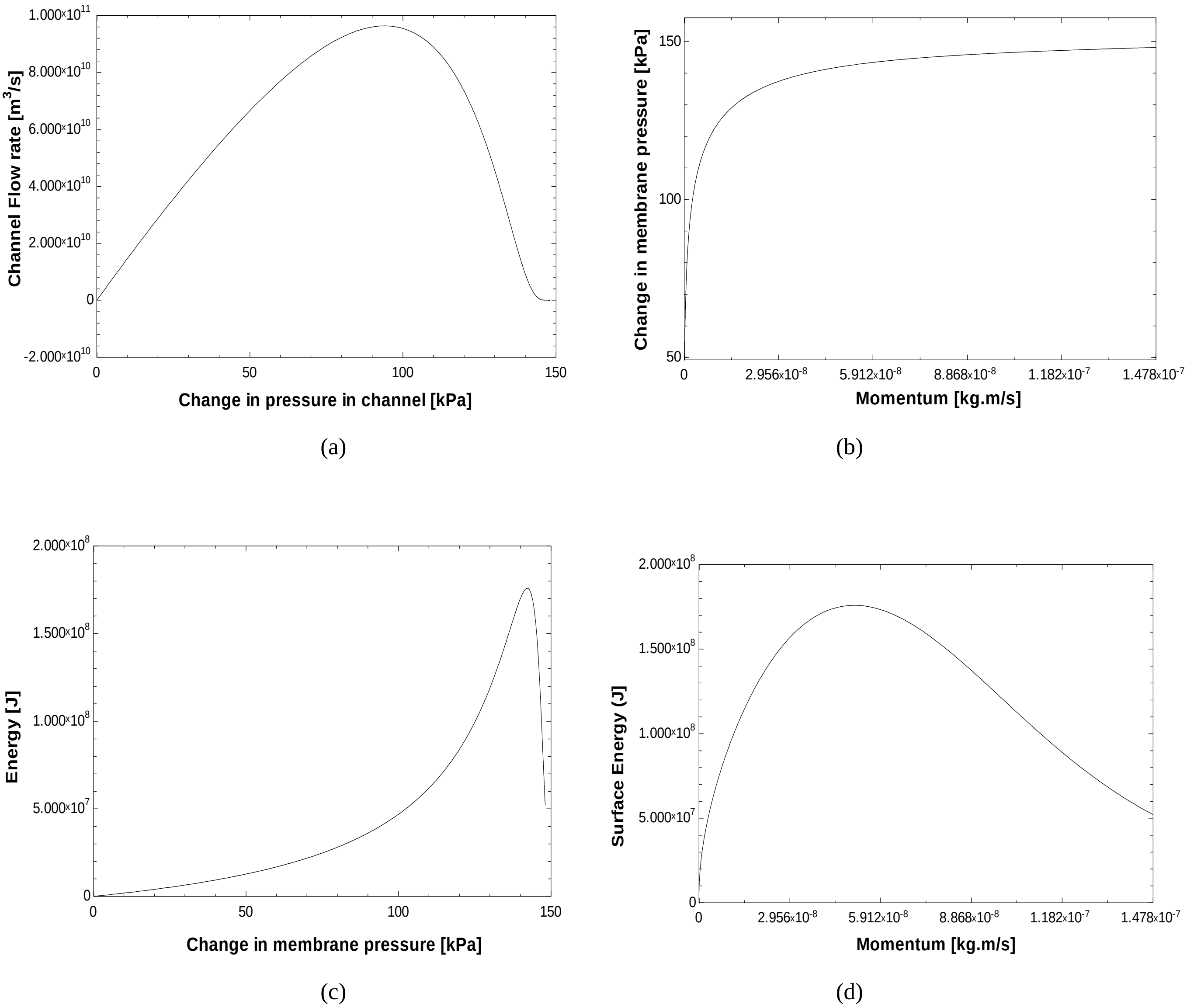
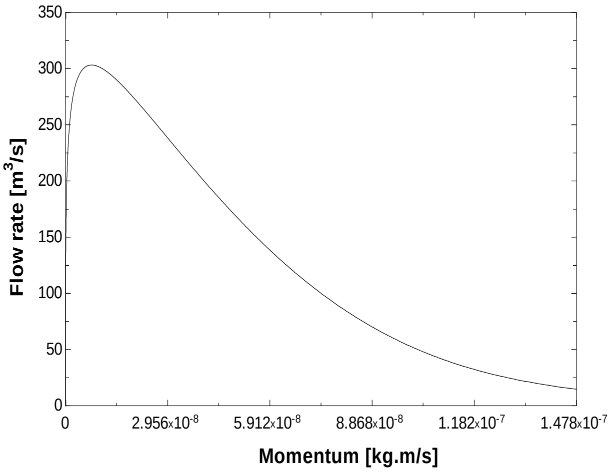


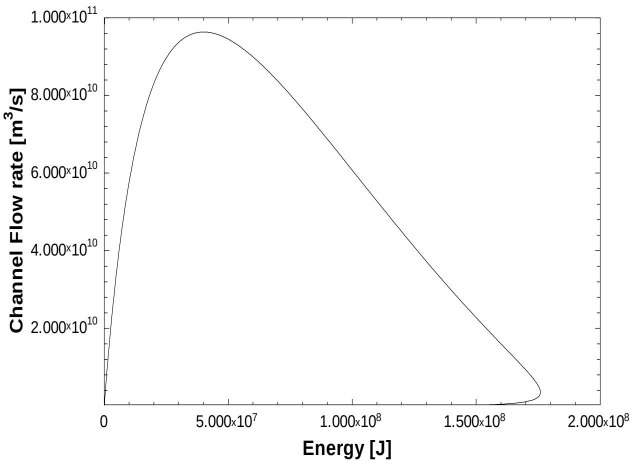
Figure 3. (a) channel flow rate [m3/s] against change in pressure in channel (b) Change in pressure [kPa] against momentum [kg.m/s] (c) Energy [J] against change in membrane pressure [kPa] and (d) surface energy [J] versus momentum [kg.m/s]

Figure 3 (a-d) revealed the relationship between membrane momentum of flow on pressure change, flow rate and energy during varying molecular motion of oil-water molecules during separation. It is observed as shown in Fig.3 (a) that, the change in pressure waves in the membrane channel during oil-water separation led to an increase in membrane flow rate during oil-water separation. As the change in membrane pressure increases during oil-water separation, the flow momentum begins to build-up in the membrane channel. It increased to an optimal momentum depending on the change in pressure that took place during oil-water separation as it impacts oil-water molecules as shown in Fig.3 (b). The change in membrane pressure and momentum impacts oil-water molecules and membrane surface energy driven separability as shown in Fig. 3 (c-d). It is revealed from Fig. 3 (a-d) that an increase in membrane pressure led to an increase in energy surface and momentum, which negatively affected oil-water molecules during separation. The change in membrane pressure affects the backward flow process of oil and forward flow process of water in the hydrophobic membrane.

Water flow through the membrane surface due to low surface energy of water molecules as impacted by hydrophobic nanoparticles, and at the same time there is a backward flow motion of oil molecules. The produced membrane is phobic to water molecules; therefore, the flow momentum and pressure change improve the efficiency in the system during oil-water separation as shown in Fig. 3 (a-b). It was also revealed in Fig.3 (c-d) that continuous increase in change in membrane pressure during oil-water separation impacts oil-water molecules and it did not always lead to continuous increase in membrane surface energy. There is a critical change in membrane pressure and momentum flow when the membrane surface energy starts decreasing due to the molecular behaviours of oil-water molecules and this led to an increase in membrane flow rate of pure water due to the fact that lower surface energy the molecular speed of water through the membrane surface. Therefore, the hydrophobic force from the nanoparticles was overcome by the change in membrane pressure and momentum leading to a steady drop surface energy that increase membrane efficiency. Other internal factors such as dynamic viscosity, drag force, fluid resistance, maximum velocity and shear stress might also play a significant role in membrane performance as change in pressure and momentum impacts the molecular dynamic of oil-water molecules. These factors are provoked by change in membrane pressure and flow momentum during membrane oil-water separation. The fluid momentum depends on the fluid viscosity which impacts membrane parameters such as membrane shear stress and drag force decreased that increased the membrane surface energy and impacts oil-water separation. It should be noted that the membrane performance and efficiency during oil-water separation also depend on the characterisation of membrane pore sizes and the characterisation of nanoparticles on the membrane surface that reduced surface energy to improve membrane efficiency and stability during of oil-water separation. The impacts of membrane change in pressure and momentum impacted flow rate in the channel as shown in Fig. 4 (a-b).



(a)



(b)

Figure 4. (a) Flow rate [m3/s] against momentum [kg.m/s] (b) Flow rate [m3/s] against Energy [J]

Figure. 4 (a-b) revealed the relationship between membrane flow rate, flow momentum and surface energy. It is observed that an increase in momentum led to an increase in membrane flow rate during oil-water separation. This is because an increase in momentum impacts the molecular dynamics of oil-water molecules as the molecules begin to vibrate at high speed with high vibration energy. At this high vibration energy their molecular interaction is easily manipulated by nanoparticles due to their high surface volume ration. At their high surface volume ratio, the coated hydrophobic nanoparticles have more impact on their vibration energy as the surface energy of water become more lower than oil and water can easily flow through the membrane channel. It is also shown in Fig. 4 (b) that as membrane energy decreases the channel flow rate in the membrane increases to an optimal level where the membrane flow rate start decreasing. Both obtained results in Fig. 4(a-b) revealed a smooth transition in membrane momentum and energy as the membrane flow rate increases and later decreases.

To increase performance during oil-water separation, the flow energy in a membrane channel should be increased and at the same time the surface energy due to coated nanoparticles in the membrane must be low. Membrane performance was observed to increase when surface energy and flow momentum where at their critical range. At this critical range, there was an increase the backward flow of oil molecules with an increased in forward flow of water molecules in the hydrophobic membrane. The critical ranges are observed in Fig. 4 (b-c) with a smooth transition of momentum and energy as membrane channel flow rate are impacted. The obtained results revealed in this study are compared with other results of membrane performance during oil-water separation [7] as shown in Fig.5

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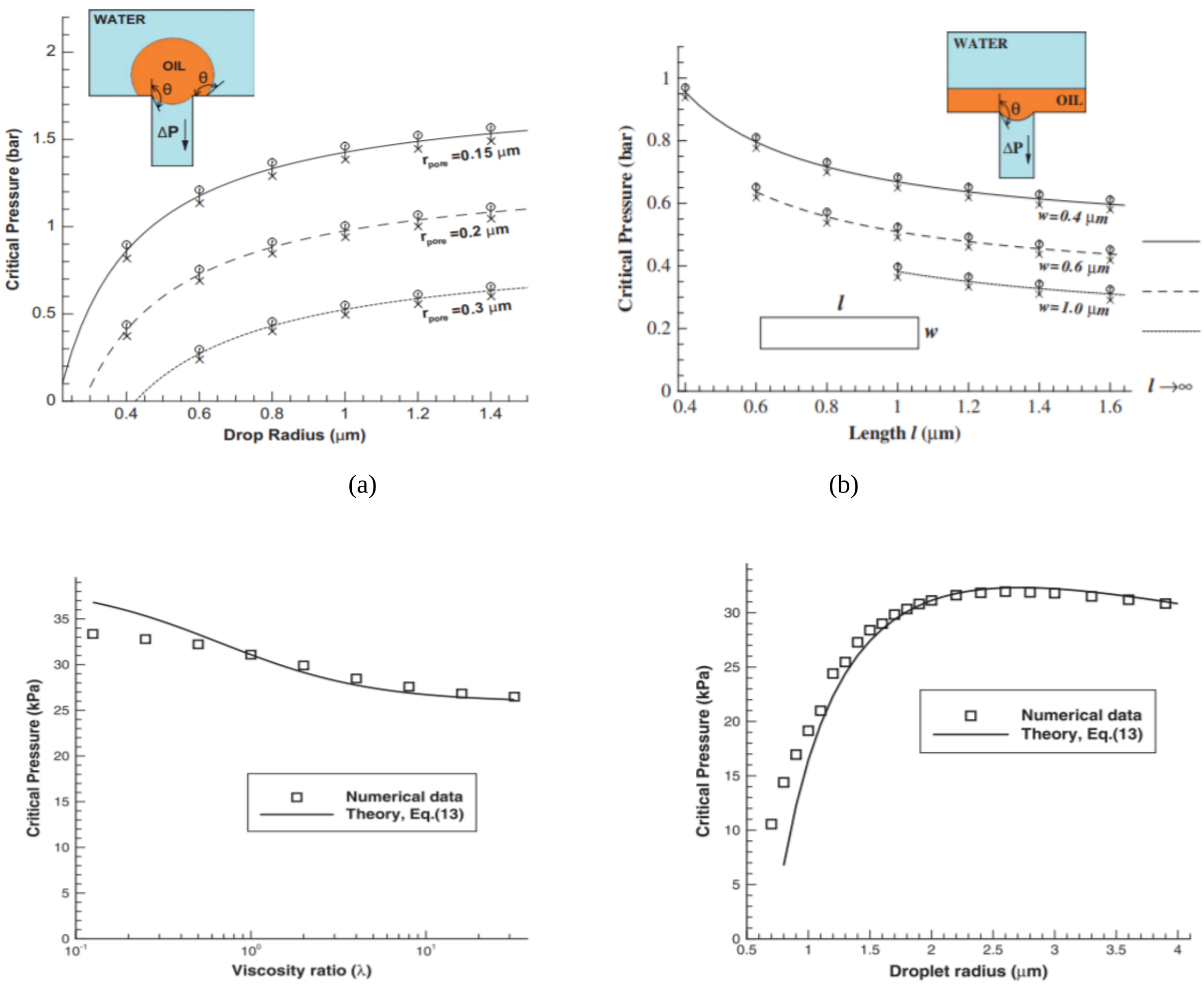

(a) (b)

(c) (d)

Figure.5 Critical pressure against drop in radius, length and viscosity ratio, image courtesy by Tohid Darvishzadeh [7]

The results obtained in Fig. 5 revealed simulated and empirical obtained data during membrane change in pressure and flow viscosity as reported by [7]. The obtained results were in line with the numerical and analytical predictions based on the Young–Laplace equation during oil-water separation. It was revealed that when an applied pressure is close to the critical pressure, the net force on membrane interface is small, as a results longer time in simulation was needed to capture the molecular motion of oil-water during separation as revealed in Fig. 5 (a-b). The results in Fig.5 (a) also revealed the increase in critical pressure and increase in droplet radius during oil-water separation. It was also revealed that the critical pressure in the membrane decreases monotonically with increasing viscosity ratio during oil-water separation as shown in Fig. 5(c). This is because a larger viscosity ratio during oil-water separation results in higher shear stress on the droplet, which leads to larger deformation and consequently permeation at lower transmembrane pressures as reported by [7]. The results in Fig.5 as reported by [7] validate the obtained results in this paper. Previous research studies in membrane wettability mainly focused on transmembrane pressure drop and flux permeation without critically looking at other factors such as membrane momentum of flow which is impacted transmembrane change in pressure and flow rate which has been investigated in the current research findings.

4. CONCLUSION AND RECOMMENDATION

The aim of the current study was to design a membrane surface for optimal performance during oil-water separation by looking at the molecular dynamics of oil-water molecules during separation. To achieve the objective, it was important to model parameters that impact oil-water molecules during separation are ignored by other researchers, such as membrane flow momentum, membrane pressure change, and membrane surface energy which impacts behaviour of oil-water molecules during separation. The application of membrane linear membrane was one of the rational in the current study since it describes the summation of external forces on the control system volume which impacts the molecular behaviours of oil-water molecules during separation. The following facts were theoretically revealed and validated. It was revealed that the change in pressure led to an increase in membrane flow rate during oil-water separation. This was impacted by momentum of fluid flow which begins to build-up pressure in the channel. The change in membrane pressure and momentum impacts surface energy and surface energy driven separability.

It was also revealed that the change in membrane pressure affects the backward flow process of oil and forward flow process of water in the hydrophobic membrane. This was reported to have impacted the membrane surface energy and the efficiency of the designed hydrophobic membrane. Critical parameters in momentum, change in membrane pressure and surface energy driven separability were also revealed in the current study. It was revealed that, as the membrane energy decreases the membrane channel flow rate increases to an optimal level where the membrane flow rate start decreasing. It was also revealed that, to increase performance and purity of the separated oil-water molecules, the flow energy in a membrane channel should be increased and at the same time the surface energy in the membrane surface are low due to the coated nanoparticles.

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