Numerical simulation of heat and mass transfer in direct membrane distillation in a hollow fiber module with laminar flow

Numerical simulation of heat and mass transfer in direct contact membrane distillation in a hollow fiber module with laminar flow

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Abstract

The heat and mass transfer processes in direct contact membrane distillation (MD) under laminar flow conditions have been analyzed by computational fluid dynamics (CFD). A two-dimensional heat transfer model was developed by coupling the latent heat, which is generated during the MD process, into the energy conservation equation. In combination with the Navies-Stokes equations, the thermal boundary layer build-up, membrane wall temperatures, temperature polarization coefficient (TPC), local heat transfer coefficients, local mass fluxes as well as the thermal efficiency, etc. were predicted under counter-current flow conditions. The overall performance predicted by the model, in terms of fluxes and temperatures, was verified by single hollow fiber experiments with feed in the shell and permeate in the lumen.

Simulations using the model provide insights into counter-current direct contact MD. Based on the predicted temperature profiles, the local heat fluxes are found to increase and then decrease along the fiber length. The deviation of the membrane wall temperature from the fluid bulk phase on the feed and the permeate sides predicts the temperature polarization (TP) effect. The TP coefficient decreases initially and then increase along the fiber length. It is also found that the local Nusselt numbers (*Nu)* present the highest values at the entrances of the feed/permeate sides. Under the assumed operating conditions, the feed side heat transfer coefficients h_f are typically half the h_p in the permeate side, suggesting that the shell-side hydrodynamics play an important role in improving the heat transfer in this MD configuration. The model also shows how the mass transfer rate and the thermal efficiency are affected by the operating conditions. Operating the module at higher feed/permeate circulation velocities enhances transmembrane flux; however, the thermal efficiency decreases due to the greater heat loss at a higher permeate velocity. The current study suggests that the CFD simulations can provide qualitative predictions on the influences of various factors on MD performance, which can guide future work on the hollow fiber module design, module scale-up and process optimization to facilitate MD commercialization.

Key words: membrane distillation, computational fluid dynamics, heat transfer, single fiber module, thermal efficiency

1. Introduction

Membrane distillation (MD), a thermally-driven process that integrates mass and heat transfers for high-quality water production, is an emerging technology for seawater desalination. Amongst the four typical MD configurations, direct contact membrane distillation (DCMD) attracts the most attention as no external devices are needed for permeate condensation. With the spike in energy prices in recent years, the MD process has become a potential substitution for the conventional desalination technologies such as reverse osmosis (RO), provided there is access to waste heat. However, there remain several major obstacles to the widespread commercialization of MD process, which include the relatively low permeate flux and low thermal efficiency of MD modules [1].

To properly understand the complicated combination of mass and heat transfers in the MD process, the temperature distributions adjacent to the membrane surfaces along the module length should be fully described. Unfortunately, it is impossible to attain temperature information via the most widely used non-intrusive experimental approaches such as the flow visualization with dye, Particle Image Velocimetry (PIV) and Direct Observation through the Membrane (DOTM), etc. These observational techniques are not able to provide sufficient flow and thermal field information in the boundary layers [2]. To acquire heat transfer coefficients in the MD process, some researchers [3] have replaced the membranes with aluminum film and others [4-8] have conducted mathematical modeling using semi-empirical correlations and resistance-in-series model to predict the temperature distributions.

However, the efficacy of these semi-empirical correlations has been questioned recently. This is mainly because the correlations used were developed based on non-porous and rigid tube-shell heat exchangers which are not coupled with mass transfer [1]. Also, the variations of the temperature distribution along the module length have been ignored by

treating the hollow fiber module as a whole heat transfer unit. In the radial direction, the temperature distributions have been simplified as mean fluid temperatures and membrane surface temperatures calculated based on boundary layer development, and these mean values were used to explain the temperature polarization effect [4, 9, 10]. Since the heat transfer coefficients, especially under low permeate flux, are strongly affected by the accuracy and applicability of these semi-empirical correlations, efforts have been made to modify the model parameters to improve the accuracy of the empirical correlations [11].

Basically, the empirical correlations and conservation equations used in earlier studies provided simplified one dimensional solutions. To further improve model applicability and accuracy, computational fluid dynamics (CFD) simulations involving Navier-Strokes equations in two dimensional (2D) and three dimensional (3D) domains have been employed to provide more reliable and comprehensive information on flow fields. For example, Charfi et al. [12] have used numerous submodels, such as the Ergun model, Knudsen-molecular diffusion model, momentum/energy and mass transport equations, in their CFD modeling to study the heat and mass transfer in the sweeping gas membrane distillation process. However, this model is rather complicated for industrial applications due to its high computational workload.

Commonly used simplifications for numerical simulation of the mass transfer process include estimating the mass transfer coefficients using empirical equations [13], assuming a constant mass flux condition [14], or applying Henry's law constant to describe the equilibrium state of the targeted compound partitioning between water and the membrane phases [14]. Zhang et al [15, 16] suggested treat the transfer processes associated with the membrane and two surrounding fluids as a conjugate problem, and they have simulated the heat and mass transfer in membrane-based ventilators without considering phase changes. More widely used CFD models ignored the permeate flow and only focused on the mass/heat transfer in the bulk feed flow and /or simplify the transfer model across the membranes [2]. In summary, there has been no report on CFD modeling of all three simultaneous heat transfer steps taking place in the feed, permeate and membrane,

respectively, in the DCMD process.

The present work describes CFD simulations that couple the Navies-Stokes equations with the energy conservation equation in a two-dimensional domain to describe the hydrodynamic and thermal conditions in a single hollow fiber module with laminar flow for DCMD process. A newly developed heat transfer model, which allows the latent heat transfer due to the evaporation/condensation processes during the MD process, but ignores the transmembrane mass flux itself, has been used to estimate the heat transfer coefficients at different fluid conditions, temperature profiles, temperature polarization coefficients (TPC), mass flux distribution, heat loss and MD thermal efficiency. The aim of this work is to provide a deeper insight into the heat and mass transfer phenomena in the DCMD process and to guide further optimization of MD operation for performance enhancement.

2. Theory

2.1 Governing transport equations and boundary conditions

In general, the DCMD process can be described by three steps: 1) vapor evaporates on the feed side at the membrane surface; 2) vapor crosses the membrane; 3) vapor condenses on the permeate side near membrane surface. The transmembrane mass flux is the key issue in the MD process. However, it should be noted that the transmembrane mass flux of a single fiber has a negligible contribution to both the feed and permeate when compared to the operating feed flow rate. For example, the typical transmembrane mass flow rate in the current study is around 7.50×10^{-6} kg·s^{-1}, which is three orders of magnitude lower than the feed flow rate Q_f =4.22×10^{-3} kg·s^{-1}. Thus, in this study, a simplified heat transfer model was established for the DCMD process by ignoring the influence of the transmembrane mass flux in the conservation equations, but combining the latent heat incurred by evaporation/condensation into the heat transfer process.

In a steady-state heat transfer process under laminar flow, the overall governing transport

equations for the feed, permeate and membrane are as follows:

The continuity equation:

$$\nabla \cdot (\rho \vec{v}) = 0 \tag{1}$$

The momentum transport equation:

$$\nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} \tag{2}$$

where $\bar{\bar{\tau}}$ is the stress tensor, which can be expressed as:

$$\bar{\bar{\tau}} = \mu \left[\left(\nabla \vec{v} + \nabla \vec{v}^T \right) - \frac{2}{3} \nabla \cdot \vec{v} I \right] \tag{3}$$

The energy conservation equation:

$$\nabla \cdot (\vec{v} \rho c_p T) = \nabla \cdot (k \nabla T) + S_h \tag{4}$$

where k is the heat conductivity ($W \cdot m^{-1} \cdot K^{-1}$), S_h ($W \cdot m^{-3}$) is the boundary condition which serves as a heat-source term for the feed or permeate on the membrane surface, and indicates the amount of latent heat generated by evaporation at the hot-side membrane surface and subsequently released through condensation at the cold-side membrane surface. It can be written as:

$$S_h = \begin{cases} \dfrac{q_{MD}}{\delta r} \cdot \dfrac{R_{mo}}{R_{mi}} & \text{for } r = R_{mi} \\ -\dfrac{q_{MD}}{\delta r} & \text{for } r = R_{mo} \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where q_{MD} is the latent heat flux on the feed side membrane surface, r is the radial direction, δr is the chosen grid thickness in the r direction. This is shown in Fig.1 which illustrates a two-dimensional domain where the heat and mass transfer processes occur. R_{mi} and R_{mo} are the inner and outer radii of the fiber, respectively. The feed and permeate flow in counter-current mode on the shell and lumen sides, respectively.

For the MD modules with varying length L (in the range 0.25-1.02 m), other boundary conditions are applied:

- Entrance of feed and permeate: Re_f=500~2000, T_{fi} = 327.2 K, Re_p= 200~2000, T_{pi} = 294.0 K
- Outlet of feed and permeate: outlet pressure is 0.0 Pa (gauge pressure)
- Membrane wall: no-slip condition, conjugate heat conduction:

$$q_f\big|_{r=R_{mo}} = q_m\big|_{r=R_{mo}},\ q_m\big|_{r=Rmi} = q_p\big|_{r=R_{mi}}$$

$$T_f\big|_{r=R_{mo}} = T_m\big|_{r=R_{mo}},\ T_f\big|_{r=R_{mi}} = T_m\big|_{r=R_{mi}} \tag{6}$$

where Re_f, Re_p, T_{fi}, T_{pi} are Reynolds number and inlet bulk temperature of feed and permeate respectively.

2.2 Mass and heat transfer analysis in MD

2.2.1 Mass transfer

The transmembrane mass flux N_m can be written as:

$$N_m = C\Delta P = C(P_{fm} - P_{pm}) \tag{7}$$

where C is the intrinsic mass transfer coefficient of the membrane, P_{fm} and P_{pm} are the saturated vapor pressures at the membrane wall temperatures T_{fm} and T_{pm}, respectively. To obtain the C value for the heat transfer simulation in MD, researchers have reported various approaches, such as the combined Knudsen diffusion, molecular diffusion and Poiseuille flow transition model [17], Knudsen diffusion model [8, 11] and Monte Carlo simulation method [18]. Although C is claimed to be dependent on the operating temperature and pressure, it can be assumed to be constant under certain operating conditions and membrane properties in many simplified cases [19]. Therefore, here we

have adopted a similar simplified model with a constant *C*, which is equal to 2.0×10^{-7} $kg\cdot m^{-2}\cdot s^{-1}\cdot Pa^{-1}$calculated from the single-fiber module tests [20].

2.2.2 Heat transfer

The saturated vapor pressure at the membrane wall temperature T_m is obtained from the Antoine equation [21]: .

$$P = exp\left(23.238 - \frac{3841}{T_m - 45}\right) \tag{8}$$

As the mass and heat transfer are closely correlated in a MD system, the latent heat flux N_e generated can be written as:

$$q_{MD} = N_m \cdot \Delta H_{T_{fm}} \tag{9}$$

where $\Delta H_{T_{fm}}$ is the latent heat of the fluid adjacent to the membrane surface on the feed side (T_{fm}).

a) Heat transfer coefficients

To investigate the heat transfer process, an analysis of local heat transfer coefficients (Nusselt number) along the fiber length was required. Usually, the Nusselt number (*Nu*) is calculated based on various empirical correlations [1], and only one particular *Nu* value is obtained under given membrane and operating conditions. However the local *Nu* of the developing flow cannot be revealed through these correlations. In general, the calculated *Nu* value is either under- or over-estimated as compared with the actual situations. Fortunately, it is possible to track the changes in *Nu* (and local heat transfer coefficients) along the membrane surface in this study, as the whole temperature profile can be obtained via numerical simulation. *Nu* is defined as [22]:

$$Nu = \frac{h \cdot d}{k} = \frac{q \cdot d}{k \cdot (T_b - T_m)} \tag{10}$$

where h, d, k, q, and T_b are heat transfer coefficient, hydraulic diameter, thermal conductivity, heat flux, and local bulk temperature of fluids, respectively.

The local bulk temperature is defined as:

$$T_b = \frac{\int_S \rho u T \mathrm{d}S}{\int_S \rho u \mathrm{d}S} \tag{11}$$

where ρ, u and S are density, velocity and cross-sectional area of the feed-side or permeate-side, respectively. u is the velocity which normalizes to S. q and h are defined as:

$$q = k\left(\frac{\partial T}{\partial r}\right)_m = h\left(T_b - T_m\right) \tag{12}$$

$$h = \frac{q}{T_b - T_m} = \frac{k\left(\frac{\partial T}{\partial r}\right)_m}{T_b - T_m} \tag{13}$$

In the MD process, the universal heat flux q can be rewritten as the heat transferred through liquid films (feed side q_f or permeate side q_p) or latent heat plus heat conduction across membrane (q_m). q_f and q_p can be written as:

$$q_f = h_f \Delta T_f = h_f(T_f - T_{fm}),\ q_p = h_p \Delta T_p = h_p(T_{pm} - T_p) \tag{14}$$

where h_f and h_p are the heat transfer coefficients at the feed and permeate sides, T_f and T_p are the bulk temperatures of feed and permeate, respectively.

b) Temperature polarization coefficient (TPC)

As a main concern in MD process, the temperature polarization (TP) describes the temperature differences between the bulk and membrane surface and hence leads to a decrease of driving force (temperature difference) across the membranes [10]. Using TPC to define the temperature polarization coefficient, it is written as:

$$TPC = \frac{T_{fm} - T_{pm}}{T_f - T_p} \tag{15}$$

c) Local transmembrane mass flux

To reveal the relationship between mass transfer and the membrane temperature, local transmembrane mass flux N_m can also be rewritten in terms of transmembrane temperature difference[10]:

$$N_m = C\frac{\mathrm{d}P}{\mathrm{d}T}\Big|_{T=T_m}(T_{fm} - T_{pm}) \tag{16}$$

where the gradient dP/dT is given by Antoine equation (Eq.(8)):

$$\frac{\mathrm{d}P}{\mathrm{d}T} = 3841\frac{exp\left(23.238 - \dfrac{3841}{T_m - 45}\right)}{(T_m - 45)^2} \tag{17}$$

Then the second derivative $\mathrm{d}^2P/\mathrm{d}T^2$ can be written as:

$$\frac{\mathrm{d}^2P}{\mathrm{d}T^2} = \frac{exp\left(23.238 - \dfrac{3841}{T_m - 45}\right)}{(T_m - 45)^3}\left(\frac{14753281}{T_m - 45} - 7682\right) \tag{18}$$

In the temperature range of T_m=273~373K, dP/dT is a monotonically increasing function because $\mathrm{d}^2P/\mathrm{d}T^2$ is greater than zero; also, since dP/dT is greater than zero, Eq.(16) indicates that the transmembrane mass flux N_m and membrane temperature T_m have a positively increasing relation, which means a higher operating temperature will be favorable for a higher transmembrane mass flux. Thus, the distributions of N_m can be clearly explained by the temperature distributions.

d) MD thermal efficiency η_h

As mentioned previously, the total heat flux transferred in the MD process has two components, the latent heat of evaporation and conductive heat across the membrane, and

the latter is considered as heat loss. The thermal efficiency η_h is the fraction of the heat transfer that contributes to the evaporation as defined below:

$$\eta_h = \frac{N_m \Delta H_{T_{fm}}}{q_f} = \frac{N_m \Delta H_{T_{fm}}}{N_m \Delta H_{T_{fm}} + \frac{k_m}{b}\left(T_{fm} - T_{pm}\right)\frac{d_m}{d_o}} \tag{19}$$

In order to maximize the MD thermal efficiency, the conductive heat loss should be minimized. Here, we define N_{HL} as the equivalent transmembrane mass flux loss:

$$N_{HL} = \frac{\frac{k_m}{b}\left(T_{fm} - T_{pm}\right)\frac{d_m}{d_o}}{\Delta H_{T_{fm}}} \tag{20}$$

Then the thermal efficiency in MD can be seen as the ratio of the actual transmembrane mass flux and the theoretical mass flux without heat loss:

$$\eta_h = \frac{N_m}{N_m + N_{HL}} \tag{21}$$

2.3 Computational domain and algorithm

By assuming the single-fiber modules have a cylindrical structure, a series of 2D axial-symmetric single-fiber domains were built. The quad mesh was adopted for grid generation in this model. To optimize the grid configuration, in the *r* direction, a grid scale of 5×10^{-6} m was chosen for the bulk permeate and the membrane, and progressively increasing grid scales from 5×10^{-6} to 2×10^{-4} m were set for the bulk feed (shell-side); while in the *x* direction, a grid scale of 1×10^{-4}m was employed universally. As an example, the grid configuration for a 0.25 m long module is shown in Fig.2, which illustrates the whole geometry and locally amplified regions in the 2D domain.

In the current MD system, the effect of the hollow fiber membrane surface roughness on the wall boundary conditions was ignored as it has a magnitude of 10^{-8} m, which is far smaller than the grid scale.

The simulations were carried out using the software Fluent 6.3, with SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm for pressure-velocity coupling and QUICK (Quadratic Upstream Interpolation for Convective Kinetics) algorithm for discretization of the conservation equations. A computational accuracy of 10^{-5} was chosen for convergence.

3. Experimental

This section describes measurements and experiments used to validate the CFD simulation model.

3.1 Materials

In general, the properties of a polymeric membrane can be expressed as:

$$\Phi_m = \Phi_{PVDF} \cdot (1-\varepsilon) + \Phi_v \cdot \varepsilon \tag{22}$$

where general variable symbol Φ_{PVDF} and Φ_v are the properties (density, specific heat, and thermal conductivity) of the membrane material and vapor, respectively, ε is the porosity of the membrane. In the present study, a hydrophobic polyvinylidene fluoride (PVDF) membrane was used and its porosity was measured experimentally to be 0.83. Other relevant properties of the PVDF hollow fiber membrane and testing fluids are listed in Tables 1 and 2, respectively.

3.2 DCMD experimental set-up

The DCMD experimental setup for the single fiber module tests is similar to that used in our previous work [20]. Both the feed and permeate solutions were cycled through the hollow fiber module in countercurrent mode. On the shell side, the feed solution (synthetic seawater: 3.5 wt% sodium chloride (NaCl) with conductivity around 60 ms·cm^{-1}) was heated (T_{fi} = 327.2 K) and circulated by a peristaltic pump (u_{fi}= 0.06022 m·s^{-1}, Reynolds number Re_f=836). On the lumen side, the permeate (pure water, with conductivity around 0.5 μs·cm^{-1})

was cooled down to T_{pi} = 294.0 K by a cooling circulator and cycled by another peristaltic pump (u_{pi}= 0.4171 m·s^{-1}, Re_p=460). The distillate was collected in an overflow tank sitting on a balance (±0.1 g). Based on these operating conditions, laminar conditions were applied to the conservation equations during the simulations.

Single-fiber modules, which contained only one straight fiber with various lengths ranging from 0.25 m to 1.02 m, were made to investigate the fiber length effect. These lab-scale MD modules were fabricated by potting the PVDF hollow fiber membranes into Teflon housings. The specifications of the PVDF hollow fibers and modules are listed in Table 3.

4. Results and discussion

4.1 Comparison between experimental data and simulation results

Firstly, the simulated average bulk temperatures were compared with the experimental results to verify the validity of the newly-built heat transfer model. The experimental data and the simulation results are listed in Table.4, where T_{fo}, and T_{po} are bulk temperatures at the exits of the feed side and the permeate side, respectively. The simulation conditions were the same as that listed in Section 3.2. It can be seen that the simulation data agrees well with the experimental values. The relative errors are lower than 1%, which testify to the reliability of the newly-developed numerical method.

4.2 Temperature profiles inside the module

The temperature profiles inside a 0.25 m-long module are obtained from the CFD simulations. Fig.3 shows the temperature distributions along the *x* and *r* direction. The build-ups of the thermal boundary layers along the flow directions (*x* direction) can be observed clearly. On the shell side, the thickness of the boundary layer reaches nearly 1/3

of the flow channel at the feed outlet; while on the lumen side, the thermal boundary layer fills the entire channel at the permeate exit. The temperature profile across the membrane from the feed to the permeate shows a dramatic drop, which indicates that the membrane resistance might play a major role in the heat transfer process.

4.3 Heat transfer in MD process

4.3.1 Local heat flux and driving force for modules with various lengths

Fig.4 shows the relationships between the local heat flux q_f and the bulk feed temperature difference ΔT_f ($=T_f-T_{fm}$), that is the local driving force for heat transfer in the bulk feed, versus the dimensionless module length x/L. For all four modules of various lengths (L = 0.25 m, 0.34 m, 0.84 m and 1.02 m, respectively), the ΔT_f increases along the flow direction (x) as shown in Fig. 4. This is because T_{fm} decreases gradually along the fiber length as the cold permeate flows counter-currently on the opposite side, while T_f is not affected much by the thermal boundary layer. Also, the shorter modules (i.e., L=0.25 m and 0.34 m) show larger temperature gradients than the longer ones at the same dimensionless length, because there is less heat transfer and thus the permeate temperature is lower due to smaller membrane surface with the same flow conditions at the entrances, making T_{fm} drop more severely in shorter modules. Note that the temperature profiles have negligible differences when the modules are very short (i.e., L=0.25m and 0.34 m).

It is also observed that in Fig. 4 that the local heat flux q_f for various modules decreases firstly when entering the modules and subsequently increases after a certain length. In the entrance region there is a high local heat transfer coefficient h_f due to the thin thermal boundary layer, though the temperature difference ΔT_f is low. Their product (q_f=h_f*ΔT_f, Eq. (13)) can still reach a relatively high value because of the much larger magnitude of h_f. However, as the flow develops and the thermal boundary layer builds up along the fiber

length, the continuous increase of ΔT_f and the decrease of h_f result in an initial decrease then a gradual increase of q_f after a certain length. In addition, the shorter modules show higher local heat fluxes at the same dimensionless length compared to the longer ones. This is due to the thinner thermal boundary layers incurred from the developing flows.

Similarly for the permeate side, Fig. 5 depicts the trends of the local heat flux q_p and the temperature difference ΔT_p ($=T_{pm}-T_p$), the local driving force for heat transfer in the bulk permeate, versus the dimensionless module length x/L. As discussed for Fig. 4, ΔT_f increases along the fluid flow direction in a countercurrent flow pattern; while the ΔT_p curves show more complicated trends for modules with different lengths as shown in Fig.5: (a) in shorter modules (L=0.25 m and 0.34 m), where the thermal boundary layers are still developing at the exit, the ΔT_p curves have similar shapes as the ΔT_f along the flow direction; (b) in longer modules (L=0.84 m and 1.02 m), where the thermal boundary layers are fully developed before approaching the exit, the ΔT_p increases initially at the entrance region and slightly decreases as the bulk temperature approaches the wall temperature after the flow is fully developed. This is consistent with the results of the temperature distribution shown in Fig. 3, which shows the thickness of the fully-developed thermal boundary layer exceeds the width of the flow channel at the permeate outlet. Hence, the temperature difference ΔT_p shows an initial increase and a subsequent decrease along the flow direction.

In terms of $q_{p,,}$ although it shows a similar trend as q_f (in Fig. 4), the magnitude of q_p (in Fig.5) is larger than q_f because the permeate side has a smaller contact area (inner membrane wall) than the feed side (outer membrane wall). With a fixed local heat transfer rate (q*A) imposed at the same location in the radial direction, q_p is larger than $q_{f.}$

4.3.2 Heat transfer coefficients for modules with various lengths

To investigate the effect of module length on the MD heat transfer coefficient *h*, a series of numerical simulations for Nu_p and Nu_f have been conducted. Fig.6 plots the local Nusselt numbers as a function of the dimensionless module length *x/L*. It is found that both the Nu_p and Nu_f curves for different modules present similar trends: the highest values appear at the entrances of the feed/permeate sides and then decrease along the flow directions until reaching a plateau. It is also observed that the shorter modules (L=0.25 and 0.34 m) tend to have relatively higher Nu_p and Nu_f values than the longer ones (L=0.84 and 1.02 m) due to their developing boundary layer status in the flow channels. Since the value of *Nu* indicates the thickness of the thermal boundary layer, the lower average *Nu* value of the longer modules at the same dimensionless length implies more significant temperature polarization (TP) effects and hence a higher heat transfer resistance for the MD system.

4.3.3 Heat transfer coefficients at various flow conditions

To investigate the effect of flow conditions on the heat transfer coefficient *h* or *Nu*, two sets of simulations have been conducted by varying the following parameters: (1) Re_p (i.e., Reynolds number of the permeate flow velocity) was varied from 200 to 2000 while holding the feed/permeate inlet temperatures and Re_f (i.e., Reynolds number of the feed flow velocity) constant; (2) Re_f was varied from 500 to 2000 while holding the feed/permeate inlet temperatures and Re_p constant. Fig.7 and 8 plot the profiles of *Nu* (Nu_p & Nu_f) as functions of Re_p and Re_f, respectively.

Under a given Re_p, Fig. 7 shows that the Nu_p decreases after entering the module until an asymptotic value is reached. For different Re_p, both Nu_p and the entrance length increase significantly with increasing Re_p because of the relatively thin thermal boundary layer at a higher flow condition. Interestingly, although Re_f was kept constant, Nu_f still decreases slightly with increasing Re_p. This implies that the thermal boundary layer on the feed side thickens due to a lower local membrane surface temperature caused by a higher permeate

flow velocity. Also, as the transmembrane heat flux is carried away faster by a higher permeate velocity (Re_p), it is anticipated that a higher Re_p will lead to more conductive heat loss. More discussion of the correlation between heat loss and flow conditions is given in Section 4.4.

Similarly, Fig 8 shows that Nu_f increases with increasing Re_f, while in contrast, Nu_p does not show visible changes with increasing Re_f. The sensitive response of the Nu_f to the flow conditions implies that the major heat transfer resistance of fluids is at the feed side rather than the permeate side. This can be further explained by the distributions of heat transfer coefficients h shown in Fig.9, which plots the local heat transfer coefficients h_f and h_p as functions of the dimensionless module length x/L. Although Nu_f is generally higher than Nu_p as shown in Figs. 7 and 8, the h curves in Fig. 9 clearly illustrate that the major heat transfer resistance of the fluids is on the feed side. The local heat transfer coefficient on the feed side h_f is typically less than half of that on the permeate side h_p under the chosen operating conditions. This suggests that, to enhance the performance of the MD system with constant membrane properties, improvement of the feed-side hydrodynamics is one of the key factors.

4.4 Temperature polarization coefficient (TPC)

To evaluate the temperature polarization (TP) effect in a single-fiber module system, numerical simulations on the TPC [defined by Eq. (15)] distributions along the module length for various modules were performed, and the results are shown in Fig. 10. It is observed that the TPC firstly decreases and then increases along the fiber length. The TPC value varies between 0.63 and 0.73, in which the highest value is reached at the entrance of the feed or permeate side where the thermal boundary layer is the thinnest (refer to the boundary profiles in Fig.3). The U shapes of these TPC curves can be explained based on the results in Fig.4 and 5, in which the local temperature difference on the permeate side ΔT_p ($=T_{pm} - T_p$) shows an initial increase and then a subsequent decrease along its flow

direction (the negative x direction), while on the feed side ΔT_f ($=T_f - T_{fm}$) increases continuously along the opposite direction. In addition, Fig. 10 also shows that shorter modules (L=0.25 and 0.34 m) are less vulnerable to the TP effects and hence have higher TPC than the longer configurations (L=0.84 and 1.02 m). Overall, the deviation of the membrane wall temperature from the fluid bulk phase at the feed and the permeate sides leads to the observed distribution trend of the TPC along the x direction, which is consistent with the temperature distribution and local heat transfer analysis in Sections 4.2 and 4.3.

4.5 Mass transfer in MD process

4.5.1 Local mass flux for modules with various lengths

Fig.11 plots the distributions of the local transmembrane mass flux N_m along the dimensionless fiber length x/L for modules with different lengths (note that N_m is defined based on the outer membrane area of the fiber). These N_m curves, which have similar shapes to the q_f and q_p distributions in Fig.4 and 5, illustrate that the local mass fluxes decrease initially and then increase slowly with increasing x/L. This complicated trend can be explained by the opposite build-ups of the thermal boundary layers on the feed and permeate sides, where the thinnest boundary layers occur at the respective entrance regions. Since the feed heat transfer plays a more significant role in its entrance region due to the much higher temperature, a high N_m occurs at the feed inlet and then decreases as the flow develops. After a certain length the N_m will start to increase gradually as the transmembrane temperature difference (refer to Fig.10) increases with x/L. Therefore, this countercurrent flow pattern in MD leads to a characteristic U shape for the local mass flux N_m distributions along the dimensionless length x/L for various modules. However, the shorter modules (L=0.25 and 0.34 m) present rather flat U shapes due to the developing flows on both sides.

It is also noted that the local fluxes decrease with increasing module length at the same dimensionless length, which is consistent with our previous experimental results [20]. This is mainly due to the decrease in the local driving forces and the build-up of thermal boundary layers as channel length increases. Although the longer modules with larger membrane area can contribute to more water production, an optimized module length should be chosen for industrial applications based on an acceptable magnitude of the local driving force and hence a more even distribution of N_m. Fortunately, the trends of the N_m distribution curves are adaptable by adjusting the flow conditions (e.g., circulation flow rates) to achieve better module performance. Further investigations of the N_m curves at various hydrodynamic conditions (*Re*) are discussed in the following Section.

4.5.2 Local mass flux N_m at various flow conditions

To investigate the relationship between the transmembrane mass flux and the flow conditions, Fig.12 shows the distributions of N_m along the dimensionless module length *x/L* (*L*=0.25 m) with varying *Re*. Clearly, these N_m curves present similar trends to those shown in Fig.11. It also shows that the mass flux increases with increasing feed/permeate flow velocities (Re_f & Re_p). The maximum mass flux can be achieved at the highest circulation velocities (Re_f=Re_p=2000) under laminar flow conditions. This is because a higher feed or permeate flow velocity can effectively reduce the thickness of the thermal boundary layer and maintain higher temperate differences across the membrane to increase the mass flux.

4.6 MD thermal efficiency η_h at various flow conditions

Since the thermal efficiency (Eq. (19) and (21)) is a key criterion to evaluate module performance in MD systems, the effect of operating conditions on thermal efficiency η_h has also been investigated. Fig.13 shows the simulation results of the distributions of local thermal efficiencies η_h at different Re_f and Re_p using a 0.25 m-long hollow fiber module. It

is observed that the η_h increases significantly with decreasing permeate flow velocity (Re_p) while holding the feed flow velocity (Re_f=836) and other operating conditions constant. This may be due to the increase of the membrane wall temperature T_{pm} with a lower permeate flow velocity. Therefore, the overall thermal efficiency η_h increases as a smaller transmembrane temperature difference leads to reduced conductive heat loss. Based on the curves in Fig.13, the average thermal efficiency η_h varies from 0.43 to 0.48 with Re_p increases from 200 to 2000 (constant Re_f=836).

In contrast, the thermal efficiency curves increase with increasing Re_f under given permeate flow velocity (Re_p=460). Although the conductive heat loss increases with an increase of the membrane wall temperature T_{fm} caused at a higher feed flow velocity, η_h still presents a growing trend. This is attributed to the exponential increase (Eq.(8)) of the evaporation rate that is the numerator in Eq. (19). However, the effect of Re_f on the average thermal efficiency η_h is fairly modest ($0.45 - 0.46$).

This analysis shows that the flow conditions on the lumen side play a more critical role in the energy efficiency. For example, a reasonably high thermal efficiency and low conductive heat loss are achieved with a high Re_f (2000) and a low Re_p (200) chosen in this study (Fig. 13); while the mass fluxes N_m are generally low under these operating conditions due to the low transmembrane temperature gradient (Fig. 12). Combined with the discussions in Sections 4.5.2 & 4.6, a trade-off is evident between the mass flux and MD thermal efficiency, and therefore between capital and operating costs.

5. Conclusions

A two-dimensional heat transfer model has been established for the DCMD process. Based on single-fiber module tests, the validity of the CFD model was verified. Using this model, numerical simulations of the thermal boundary layer build-up, membrane wall

temperatures, TPC, local heat transfer coefficients, local mass fluxes as well as the thermal efficiency, etc. along the hollow fiber module length have been conducted and the results are discussed in details.

Based on the temperature profiles gained from the CFD simulations, the local heat fluxes are found to increase and then decrease along the flow directions. The deviation of the membrane wall temperature from the fluid bulk phase at the feed and the permeate sides leads to the temperature polarization (TP) effect. The TPC decreases initially and then increase along the fiber length.

The local *Nu* presents the highest values at the entrances of the feed/permeate sides. The feed side heat transfer coefficients h_f are typically half that of h_p on the permeate side under the chosen operating conditions, suggesting that the hydrodynamics on the feed side may play an important role in improving the heat transfer in the MD system.

In addition, the mass transfer rate and the thermal efficiency are affected by the operating conditions. Operating the module at higher feed/permeate circulation velocities enhances the transmembrane flux; however, the thermal efficiency decreases due to the greater heat loss at a higher permeate velocity.

A thorough consideration of the heat transfer parameters (q, *TPC*, *Nu* *and* η_h), water production/mass transfer (N_m), module configurations, membrane properties and systematic energy recovery and/or consumption is needed to optimize the MD process. Our current study shows that CFD simulations can provide useful qualitative predictions of the influences of various factors on MD performance, which can guide future work on the hollow fiber module design, module scale-up and process optimization to facilitate MD commercialization.

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Nomenclatures

A	membrane area, m^2
C	intrinsic mass transfer coefficient of the membrane ($kg \cdot m^{-2} \cdot s^{-1} \cdot Pa^{-1}$)
c_p	specific heat capacity of material ($J \cdot kg^{-1} \cdot K^{-1}$)
d	hydraulic diameter (m)
E_t	Tensile modulus (MPa)
h	heat transfer coefficient of fluid
k	thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)
L	length of module or hollow fiber (m)
$LEPw$	Liquid entry pressure of water (bar)
N_m	transmembrane mass flux ($kg \cdot m^{-2} \cdot s^{-1}$)
Nu	Nusselt number
P	water vapor pressure (Pa)
Pr	Prandtl number
q	heat flux ($W \cdot m^{-2}$)
q_{MD}	transmembrane latent heat flux ($J \cdot m^{-2} \cdot s^{-1}$)
Re	Reynolds number
R_{mi}, R_{mo}	inner, outer radii of hollow fiber (m)
S	cross-sectional area of feed-side or permeate side (m^2)
S_h	source term of energy transport equation ($J \cdot m^{-3} \cdot s^{-1}$)
v	velocity of feed or permeate ($m \cdot s^{-1}$)
x, r	axial, radial direction in cylindrical coordinate (m)

Greek letters

ΔH_T	latent heat of vaporization of water at temperature T ($J \cdot kg^{-1}$)
η_h	energy efficiency
$\bar{\bar{\tau}}$	stress tensor ($kg \cdot m^{-1} \cdot s^{-1}$)

μ	viscosity (Pa·s)
ρ	Density (kg·m^{-3})
ε	Membrane porosity (%)
δ_b	Strain at break (%)
δ_m	Membrane thickness (μm)

Suffix

b	bulk average value
f	feed
fi, *fo*	entrance, outlet of feed
fm	on feed-side membrane surface
m	membrane, or membrane surface
p	permeate
pi, *po*	entrance, outlet of permeate
pm	on permeate-side membrane surface

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