Evaluation of hollow fiber-based direct contact and vacuum membrane distillation systems using aspen process simulation

Guan, Guoqiang; Yang, Xing; Wang, Rong; Field, Robert; Fane, Anthony Gordon

2014

Guan, G., Yang, X., Wang, R., Field, R., & Fane, A. G. (2014). Evaluation of hollow fiber-based direct contact and vacuum membrane distillation systems using aspen process simulation. Journal of Membrane Science, 464, 127-139.

https://hdl.handle.net/10356/79612

https://doi.org/10.1016/j.memsci.2014.03.054

Evaluation of Hollow Fiber-based Direct Contact and Vacuum Membrane Distillation Systems using Aspen Process Simulation

Guoqiang Guan[a, b, c], Xing Yang [b, c], Rong Wang[*, b, c], Robert Field[d], Anthony G. Fane[b, c]

[a] *School of Chemistry and Chemical Engineering, Southern China University of Technology, Guangzhou, 510640, P. R. China*

[b] *School of Civil and Environmental Engineering, Nanyang Technological University, 639798, Singapore*

[c] *Singapore Membrane Technology Centre, Nanyang Technological University, 639798, Singapore*

[d] *Department of Engineering Science, University of Oxford, Oxford, OX1 3PJ, UK*

[*] To whom correspondence should be addressed. Tel. +65 6790 5327, Email address: rwang@ntu.edu.sg

Abstract

Among four membrane distillation (MD) configurations, direct contact MD (DCMD) and vacuum MD (VMD) exhibit attractive characteristics from different perspectives and have great potential in treating reverse osmosis (RO) brine. Aiming at establishing a quick approach to predict the key output parameters associated with MD module performance and process efficiency, Aspen plus was employed to conduct systematic evaluation for both DCMD and VMD. Due to the lack of built-in MD operation models in Aspen Plus, one dimensional transport models were developed and complied as user customized units to simulate the hollow fiber-based DCMD and VMD modules. The corresponding programming was coded in FORTRAN language. The mathematical models for DCMD and VMD were verified by comparing the simulations results with the experimental and literature data, respectively.

By incorporating the boundary-layer effect into the newly-established transport models, steady-state simulations of the respective DCMD and VMD flowsheets were carried out. The results showed that the DCMD presented much lower process efficiency than VMD in terms of permeation flux and specific energy consumption per kg distillate generated, even though it is considered as the simplest and most commonly employed configuration. With the same module specifications and operating conditions at equivalent energy cost, the VMD system demonstrated a minimal 2.5-fold higher average vapor flux (*e.g.*, water recovery capacity) when compared to DCMD. The fundamental difference between the two configurations was revealed through MD mass- and heat- transfer analysis. Based on simulated temperature profiles, it was found that the VMD configuration presented a much higher driving force (transmembrane temperature difference) and negligible conductive heat loss to the membrane, which is a promising feature for achieving high thermal efficiency.

Keywords: direct contact membrane distillation; vacuum membrane distillation; desalination; transport model; specific energy consumption; process simulation

1. Introduction

It has been reported that over 48 million tons of fresh water per day is provided by more than 4900 desalination plants worldwide, among which 60% are operated using reverse osmosis (RO) technology [1, 2]. However, an enormous amount of high-salinity brine is discharged as RO by-product. The environmental impact of costal brine disposal on the ecological system was analyzed in prior studies [3-8], which suggest that a low cost and environmental friendly approach of brine treatment is urgently needed. As an alternative solution for desalination, membrane distillation (MD) is a thermal process for water production that is driven by a vapor pressure difference across hydrophobic porous membrane and its performance is not significantly affected by the brine salinity. Therefore, MD has a great potential in treating RO brine to maximize water recovery and reduce the amount of concentrate for disposal [9, 10]. Also, its mild operating conditions and the capability of utilizing low-grade heat, such as power plant waste heat, solar and geothermal energy [11-14], have made MD an energy competitive technology for brine concentration [14-17] compared to other pressurized membrane processes such as RO, nanofiltration, etc.

In MD, with one surface of the membrane in direct contact with the hot aqueous feed solution [18], various methods can be employed to create a vapor pressure gradient across the membrane to drive water permeation. The permeate side of the membrane may be a cooling liquid in direct contact with the membrane (DCMD), a condensing surface separated from the membrane by an air gap (AGMD), a sweeping gas (SGMD), or a vacuum (VMD) [19]. Among all configurations, DCMD is the most studied and has the simplest operation [20]; while VMD is least studied and requires highly skilled system maintenance. Specifically, the DCMD system can be easily implemented with basic equipment but exhibits low thermal efficiency due to massive conductive heat loss across the membrane. The operation of VMD is rather complex due to the involvement of extra vacuum pumps and condensing devices, but is more thermally efficient with negligible conductive heat loss across the membrane as well as mass-transfer resistance at the permeate side. In a word, from different perspectives both DCMD and VMD

configurations exhibit promising features for industrial applications on brine concentration [12, 14]. Nevertheless, to date there is only a handful literature available on the comparison of the DCMD and VMD systems [21], not to mention systematic energy evaluation associated with their distinctly different configurational features.

In MD, the energy consumption is closely related to the distillate collection methods applied in downstream and module performance. To reveal the performance of hollow fiber-based MD modules, which are generally preferred in DCMD and VMD [18, 22, 23] due to their larger membrane area per unit volume, a good understanding on both microscopic transport mechanisms across the membrane and the macroscopic heat and mass transfer within the module is essential. The former describes the inherent vapor diffusion mechanisms across the membrane driven by vapor pressure difference; while the latter determines the overall thermal efficiency in relation to the inlet/outlet flow conditions and process driving force. It is widely reported that the microscopic vapor transport across the porous membrane matrix in MD is mainly governed by three mechanisms, *i.e.*, Knudsen diffusion, Poiseuille and molecular flow [24]. Extensive prior studies show that the overall membrane distillation coefficient of either DCMD [25-27] or VMD [28, 29] system can be determined based on the contribution from individual transport mechanisms and the measurable membrane structural parameters such as pore size, porosity and tortuosity, etc [24, 30-32]. Hence, the permeation flux can be well-predicted at known fluid properties and transmembrane temperature difference [24, 30, 31]. However, the flow hydrodynamics, which is strongly affected by the module configuration and operating parameters, plays an important role in determining the actual driving force (*e.g.*, transmembrane temperature difference) and overall heat and mass transfer efficiency [10, 33-35]. With known inlet flow conditions, quick solutions of the outlet parameters can be obtained via a comprehensive analysis of the macroscopic heat and mass transfer process, including the solute transport/diffusion through both the bulk feed/permeate streams and through the boundary layers. The latter is subjected to the temperature polarization effect in the liquid boundary layers [24], which have been well-studied using the empirical equations correlated with

Nusselt number for predicting membrane wall temperatures and mass- and heat-transfer coefficients in both DCMD [36, 37] and VMD [38-41] . Overall, despite the availability of the well-established models for transmembrane vapor transport and validated empirical correlations to analyze the polarization effects in the boundary layers, a comprehensive approach is needed to accurately predict MD module performance by solving material- and energy-transport equations in MD modules. Although computational fluid dynamics (CFD) was able to obtain detailed macroscopic flow information in MD modules [42-46], the establishment of complex grid structure and iteration of a full/large scale module is rather difficult and time-consuming for industrial applications. To evaluate MD process performance, a simplified numerical model was used to simulate the DCMD desalination system [15], in which the tubular module was divided into multiple serial-connected cells and then the material and energy balance equations were iteratively solved in each cell. Later on, a similar simplified DCMD model was built and solved using Matlab solver [47]. With the aid of process simulation tools such as Aspen Plus, an Aspen customized operation unit was established based on the one dimensional (1-D) transport model for DCMD module and then integrated into steady-state flowsheet simulation for module design and process optimization [49]. However, thus far there is still a lack of modeling work for the transport model describing the spatial variation in VMD modules except for a specially designed configuration, in which fibers are coaxially arranged [50]. Overall, a comprehensive model associated with general MD heat- and mass-transfer analysis is needed for obtaining quick numerical solutions of transport equations, which can help predict the key parameters (e.g., local permeation flux and temperature profiles) and their variations along the fiber length in both DCMD and VMD modules. In a word, a handy modeling approach is to be developed to assess module performance, energy efficiency as well as process operability.

Therefore, for the first time this study attempts to develop a general one dimensional (1-D) transport model for hollow fiber-based MD module, with a specific focus on the deviation of the governing transport equations for DCMD and VMD configurations due to their different permeate-side transport

mechanisms. Then, the DCMD and VMD transport models corrected by the boundary conditions corrections are individually programmed and compiled as user customized units built in Aspen, so as to conduct steady-state flowsheet simulations. A systematic evaluation of DCMD and VMD systems is carried out in terms of module performance associated with specific energy consumption and permeation flux in different operation scenarios. The temperature profiles along the fiber length are investigated to highlight the fundamental difference between the applications of two MD configurations in RO brine processing.

2. Theory and methodology

2.1 Transport models in MD hollow fiber module

2.1.1 Module specifications and feeding pattern

In the current simulated flowsheets for both DCMD and VMD, a membrane module with the same specifications was used: N pieces of hydrophobic porous hollow fibers with an effective length of L regularly packed into an adiabatic shell, as depicted in Fig.1 (a). The inner diameters of fibers and shell were denoted as d_1 and d_2, respectively.

In the simulated hollow fiber module, the hot brine is in direct contact with the membrane wall and is fed into the lumen side; while the permeate is collected from the shell side of the membrane. The selection of flow pattern is based on following two considerations 1) In the MD process there is no significant difference for shell- or lumen-side feeding when similar hydrodynamic conditions are maintained on both sides [22]; 2) In the VMD configuration, the introduction of vacuum pressure at the shell side will help to avoid severe membrane deformation/collapse.

2.1.2 Modeling assumptions

As mentioned previously, a transport model is to be established to correlate the local permeation rate with the overall MD module performance. The following assumptions are made for the current modeling study:

1) The module shells are well-insulated with no heat loss to the environment.
2) All hollow fibers are ideally identical and regularly packed into the shell. Thus, with an ideal mixing and homogenous flow assumed, the boundary conditions and governing equations for one single fiber can be used to correlate the performance of the whole fiber bundle. In the current model, only symmetric feature of a hollow fiber is considered [51].
3) The radial flow velocity and temperature distributions in the shell-side bulk flow (i.e., external flow surrounding the fibers) can be ignored due to the even flow distribution created by regular fiber arrangement and high packing density.
4) No-slip condition is assumed within the boundary layer adjacent to membrane walls. Thus no axial flow occurs within the stagnant zone of the boundary layer, which correlates to polarization effects in MD.
5) With sufficiently large length-to-diameter ratio of the fiber (e.g., $L/d > 5$) in an MD module, the entrance effects for both shell and lumen sides can be ignored in the current model.
6) The MD vapor flux J_M (magnitude of 10^{-3} $kg \cdot m^{-2} \cdot s^{-1}$) has a negligible contribution to either the feed or permeate bulk flows when compared to the operating feed flow rate [45, 52]. Thus, the calculation of lumen- and shell-side hydraulic pressure drop is similar to shell-and-tube heat exchanger. The variation of fluid properties caused by the transmembrane flux is considered insignificant.

2.1.3 General transport model for MD hollow fiber module

As mentioned previously, a transport model is to be established to correlate the local permeation rate with the overall MD module performance. Based on assumption #3, which indicates negligible radial flow distribution at the shell (permeate) and lumen (feed), the flows on both sides of the membrane

module can be simplified as one dimensional axial flow. The coordinates of the simulated module are shown in Fig.1 (a).

1) General transport equations at the lumen side in MD

In a sufficiently thin element of a hollow fiber along the *z* direction, as shown in Fig.1 (b), the feed brine flows into a location at *z* and out at *z*+Δ*z*. With the continuous generated vapor (permeate) flowing out from the circumferential area of this membrane element, the material balance at location *z* can be written as:

$$\frac{\pi}{4}d_1^2(\rho_1 v_1)|_z - \frac{\pi}{4}d_1^2(\rho_1 v_1)|_{z+\Delta z} - \pi d_1 \Delta z J_M = 0 \tag{1}$$

Similarly, the momentum and energy balance equations are given as:

$$\frac{\pi}{4}d_1^2\phi_{z,1}|_z - \frac{\pi}{4}d_1^2\phi_{z,1}|_{z+\Delta z} = 0 \tag{2}$$

and

$$\frac{\pi}{4}d_1^2 e_{z,1}|_z - \frac{\pi}{4}d_1^2 e_{z,1}|_{z+\Delta z} - \pi d_1 \Delta z J_{H,1} = 0 \tag{3}$$

where the ρ and v are the fluid density and flow velocity, ϕ_z and e_z are the *z*-components of the combined momentum-flux tensor and energy vector, respectively [53]; the J_M and J_H are the permeation flux and heat flux, respectively. It is noted that the corresponding temperature in the general transport equations for fluid properties is the bulk temperature *T* at the respective side of the module.

When divided by the local flow volume (¼ π d_1^2 Δ*z*) and the limit taken as Δ*z* approaches zero, Eqs (1) − (3) can be rewritten, respectively, as:

$$\frac{d}{dz}(\rho_1 v_1) = \frac{4}{d_1}J_M \tag{4}$$

$$\frac{d\phi_{z,1}}{dz} = 0 \tag{5}$$

and

$$\frac{de_{z,1}}{dz} = \frac{4}{d_1} J_{H,1} \tag{6}$$

Based on assumption #6, the hydraulic pressure drop along the fiber lumen, Δp_1, is calculated as [54]:

$$\Delta p_1 = \frac{f_1(\rho_1 u_1)^2}{2\rho_1} \left(\frac{L}{d_1}\right) \left(\frac{\mu_1}{\mu_{W,1}}\right)^{-0.14} \tag{7}$$

where f is dimensionless Darcy fiction factor, $f = \frac{Re}{64}$, and (μ/μ_{W1}) is the correction factor of the fluid wall viscosity.

With the negligible variation of axial flow velocity and diffusive heat transfer of forced convective flow at the lumen side, the energy balance equation (Eq. (6)) can be rewritten as:

$$\rho_1 v_1 \hat{c}_{P,1} \frac{dT_1}{dz} + v_1 \frac{dp_1}{dz} = \frac{4}{d_1} J_{H,1} \tag{8}$$

where the terms on the left represent the convective energy and flowing work, respectively; the right side of Eq. (8) indicates the heat source; $\hat{c}_P$ is the average heat capacity. The detailed derivations of the above energy balance equation can be found in appendix A1 (Eqs (a1)-(a3)).

2) General transport equations at the shell side in MD

In a sufficiently thin element on the shell side, as shown in Fig.1 (c), the permeate fluid flows through the free volume between the shell and membrane surface. Assumed all fibers are evenly arranged, each control element can be treated as a heat and mass source of the shell-side fluid. Thus, the mass balance equation can be given as:

$$\frac{\pi}{4}d_2^2(\rho_2 v_1)|_z - \frac{\pi}{4}d_2^2(\rho_2 v_2)|_{z+\Delta z} + N\pi d_1 \Delta z J_M = 0 \tag{9}$$

where *N* is the number of fibers. Similarly, the combined momentum and energy balance equations can be written as:

$$\frac{\pi}{4}d_2^2\phi_{z,2}|_z - \frac{\pi}{4}d_2^2\phi_{z,2}|_{z+\Delta z} = 0 \tag{10}$$

$$\frac{\pi}{4}d_2^2 e_{z,2}|_z - \frac{\pi}{4}d_2^2 e_{z,2}|_{z+\Delta z} + N\pi d_1 \Delta z J_{H,2} = 0 \tag{11}$$

With the same approach applied at the lumen side, the general balance equations for the shell side are derived as:

$$\frac{d(\rho_2 v_2)}{dz} = -\frac{4Nd_1}{d_2^2}J_M \tag{12}$$

$$\frac{d}{dz}\phi_{z,2} = 0 \tag{13}$$

$$\frac{d}{dz}e_{z,2} = -\frac{4Nd_1}{d_2^2}J_{H,2} \tag{14}$$

Coupling the lumen-side correlations (*i.e.*, Eqs. (4), (7) and (8)) with the shell-side balance equations (*i.e.*, Eqs. (12)-(14)), the axial profiles of the temperature and permeation flux can be obtained in both DCMD and VMD simulations. Since the difference between DCMD and VMD occurs from the permeate collection, the specific shell-side transport equations of the respective process will be further derived in the following sections.

2.1.4 Specific shell-side (permeate) transport equations in DCMD

Similar to that in a shell-and-tube heat exchanger, the shell-side hydraulic pressure drop of a DCMD module can be correlated by:

$$\Delta p_2 = \frac{f_2 G_2^2}{2\rho_2}\left(\frac{L}{d_{e,2}}\right)\left(\frac{\mu_2}{\mu_{W,2}}\right)^{-0.14} \tag{15}$$

where $d_{e,2}$ means the hydraulic diameter of the shell side.

Based on assumption #6 in Section 2.1.2, which indicates insignificant variation of fluid density and flow velocity, the shell-side energy equation (i.e., Eq. (14)) for the current DCMD system can be simplified as (detailed derivation can be found in Appendix A1, Eqs (a1)-(a3)):

$$\rho_2 v_2 \hat{c}_{P,2} \frac{dT_2}{dz} + v_2 \frac{dp_2}{dz} = -\frac{4Nd_1}{d_2^2} J_{H,2} \tag{16}$$

With experimentally measured inlet temperatures of lumen- ($T_{1,0}$) and shell-side ($T_{2,0}$) fluids, which were operated in a counter-current mode, the boundary conditions for the ordinary differential equations (ODEs) are given as:

$$\begin{aligned} T_1|_{z=0} &= T_{1,0} \quad v_1|_{z=0} = v_{1,0} \\ T_2|_{z=L} &= T_{2,0}\text{'} \; v_2|_{z=L} = v_{2,0} \end{aligned} \tag{17}$$

Thus, the combination of lumen- and shell -side energy balance equations (Eqs. (8) and (16)) with corresponding boundary conditions (Eq. (17)) is adopted to correlate DCMD system performance. It also indicates that the changes of the flow temperatures on both sides are dependent on the local heat flux along the fiber length.

2.1.4 Specific shell-side (permeate) transport equations in VMD

In VMD, the vapor generated at the shell-side is considered as compressible fluid. The relationship between the vapor pressure and operating temperature is correlated by the state of equation (EOS) for ideal gas:

$$\frac{1}{p_2}\frac{dp_2}{dz} = \frac{1}{\rho_2}\frac{d\rho_2}{dz} + \frac{1}{T_2}\frac{dT_2}{dz} \tag{18}$$

Due to the extremely low viscosity of the vapor, the term of viscosity dissipation in the momentum equation can be neglected. Hence, Eq. (13) is rewritten for the vapor phase in VMD as (detailed derivation can be found in Appendix A2, Eqs (a4)-(a7)):

$$\frac{dp_2}{dz} + v_2^2\frac{d\rho_2}{dz} + 2\rho_2 v_2\frac{dv_2}{dz} = 0 \tag{19}$$

The general MD energy balance equation (Eq. (14)) can also be simplified by ignoring the heat diffusion in VMD, as:

$$\begin{aligned}\rho_2 v_2 \hat{c}_{P,2}\frac{dT_2}{dz} + \left[p_2 - p^{\ominus} + \rho_2\hat{c}_{P,2}(T_2 - T^{\ominus}) + \frac{3}{2}\rho_2 v_2^2\right]\frac{dv_2}{dz} + \\ \left[\frac{1}{2}v_2^3 + \hat{c}_{P,2}(T_2 - T^{\ominus})v_2\right]\frac{d\rho_2}{dz} + v_2\frac{dp_2}{dz} = -\frac{4Nd_1}{d_2^2}J_{H,2}\end{aligned} \tag{20}$$

Similar to the DCMD system, the inlet operating conditions (*e.g.*, flowrate, operating temperatures, fluid properties as well as the vacuum pressure of the shell side $p_{2,0}$, etc) of the brine feed in a VMD module were predetermined experimentally. Thus, the boundary conditions for a VMD module can be expressed as:

$$\begin{aligned}T_1|_{z=0} = T_{1,0}\ \ v_1|_{z=0} = v_{1,0} \\ p_2|_{z=0} = p_{2,0}\text{'}\ v_2|_{z=0} = 0\end{aligned} \tag{21}$$

Combining the balance equations (Eqs. (12), (19) and (20)), EOS (Eq. (18)) and the corresponding boundary conditions (Eq. (21)), the VMD system can be simulated.

2.2 Heat/mass transfer fundamentals and boundary corrections in MD

As discussed in Section 2.1, the respective transport models for DCMD and VMD systems were derived. With the ODEs and known operating parameters, a correlation can be established between the module performance and transport characteristics of the membrane, *i.e.*, local heat and mass fluxes.

2.2.1 Transmembrane mass flux

As a thermally-driven process, the permeation flux of MD J_M is proportional to the driving force (*i.e.*, the actual vapor pressure difference across the membrane) and the mass transfer coefficient (also known as the MD coefficient):

$$J_M = C(p_{W,1} - p_{W,2}) \tag{22}$$

where the MD coefficient, C, can be determined using structural parameters of the membrane [24]. In a DCMD module, the local vapor pressures of both sides are obtained based on Antoine equation when the vapor-liquid phase equilibrium is reached at feed/permeate membrane wall temperatures T_{W1} and T_{W2}, respectively [55]. Similarly, in a VMD module the lumen-side vapor pressure, $p_{W,1}$, is calculated [55]; while the shell-side vapor pressure $p_{W,2}$ is equal to the operating vacuum pressure p_2.

However, due to the temperature polarization phenomenon [24], the wall temperatures T_W can be significantly different from the bulk temperatures T, which were used in the transport models in Section 2.1.3. Therefore, a boundary correcting factor should be incorporated to correlate the T_W and T.

2.2.2 Boundary correction in DCMD case

Assumed that the liquid boundary layers of both feed and permeate flows are sufficiently thin, and no axial flow occurs within the stagnant zone adjacent to the membrane walls, a schematic diagram of the local heat and mass transfer near the membrane surface is illustrated in Fig.2 (a).

As shown in Fig.2 (b)-(d), the enthalpy balance is depicted for three control volumes, *i.e.*, CV-1 and CV-2 for the liquid boundary layers (feed and permeate sides), and CV-M for the membrane. In the control volume of CV-1 shown in Fig.2 (b), the incoming enthalpy flow ($E_{1,\text{in}}$) consists of the inlet material enthalpy and heat flux from the bulk feed by neglecting the kinetic and potential energy:

$$E_{1,\mathrm{in}} = W_{P,1,\mathrm{in}} e^{L}|_{T_1} + J_{H,1} A \tag{23}$$

where e^L is the specific enthalpy of liquid, W_P is the local permeation rate and A is the local membrane surface area of the control volume CV-1. Similarly, the outgoing enthalpy flow includes the outlet material enthalpy and the heat transferred from the membrane:

$$E_{1,\mathrm{out}} = W_{P,1,\mathrm{out}} e^{V}|_{T_{W,1}} + J_{H,W1} A \tag{24}$$

Noted that water evaporates on the outgoing surface of CV-1, the specific enthalpy of vapor is used in Eq. (24).

Since there is no mass and enthalpy accumulated in steady-state transport, the assumption of the vapor-liquid phase equilibrium is still applicable on the membrane surface, *i.e.*, $e^V - e^L = \Delta h_V$. Since J_M can be expressed as $W_{P,1}/A$, Eqs. (23) and (24) are combined and rewritten to show the relationship between the heat and mass transfer as:

$$J_{H,1} = J_M \Delta h_V|_{T_{W,1}} + J_{H,W1} \tag{25}$$

From the heat transfer characteristic in volume CV-M shown in Fig.2 (c), it is noted that the heat fluxes on both membrane surface are approximately equal:

$$J_{H,W1} = J_{H,W2} = \frac{\kappa_m}{\delta}(T_{W,1} - T_{W,2}) \tag{26}$$

where κ_m and δ are the membrane thermal conductivity and wall thickness, respectively.

Similar to CV-1, an enthalpy balance equation is obtained for volume CV-2 shown in Fig. 2 (d):

$$J_{H,2} = J_M \Delta h_V|_{T_{W,2}} + J_{H,W2} \tag{27}$$

As the above enthalpy balance equations suggest the heat fluxes through the shell-side and lumen-side boundaries are not equal, the difference can be obtained by the subtraction of Eqs. (27) and (25) as:

$$J_{H,1} - J_{H,2} = J_M(\Delta h_V|_{T_{W,2}} - \Delta h_V|_{T_{W,1}}) \quad (28)$$

where the latent heat at both membrane surface is considered approximately equal in DCMD. Therefore, it is widely accepted that the enthalpy difference in the feed and permeate bulks is negligible in DCMD [24]. Both Eqs (25) and (27) can be expressed as a general classic correlation of heat and mass transfer [24]:

$$J_H = J_M \Delta h_V + \frac{\kappa_m}{\delta}(T_{W,1} - T_{W,2}) \quad (29)$$

where the latent heat Δh_V is determined at the averaged membrane temperature ($T_{W,1}$ +$T_{W,2}$)/2.

To solve the wall temperatures $T_{W,1}$ and $T_{W,2}$, the local heat fluxes at the feed and permeate sides (Eqs. (25) and (27)) can also be expressed as:

$$J_{H,1} = h_1(T_1 - T_{W,1}) \quad (30)$$

and

$$J_{H,2} = h_2(T_{W,2} - T_2) \quad (31)$$

where the heat transfer coefficients h_1 and h_2 can be correlated by the semi-empirical equations involving dimensionless groups, *e.g.*, Nusselt number, Reynolds number, Prandtl number and Graetz number, etc. The semi-empirical correlations used in this study were adopted from the open literature [19, 41].

2.2.3 Boundary correction in VMD case

In VMD the local heat- and mass-transfer profiles in the control volumes of CV-1 and CV-M are the same as those of DCMD. However, in the control volume of CV-2 at the shell side, the permeated vapor

flows out from the membrane but no condensation takes place. Thus, its enthalpy balance equation is given as:

$$W_{P,2}e_2^V|_{T_{W,2}} + J_{H,W2}A = W_{P,2}e_2^V|_{T_2} + J_{H,2}A \tag{32}$$

The heat flux on the shell side is derived as:

$$J_{H,W2} = \hat{c}_{P,2}(T_2 - T_{W,2})J_M + J_{H,2} \tag{33}$$

The vapor bulk temperature T_2 is approximate to the wall temperature $T_{W,2}$ for the negligible effect of the vapor boundary layer. Thus, the heat fluxes $J_{H,W2}$ at the permeate side wall temperature and $J_{H,2}$ of the bulk flow are considered equal. Based on the above derivations, in VMD the heat flux at the lumen side (feed) is completely different from the shell-side shown in Eq. (27), where the $J_{H,W2}$ is much larger than the $J_{H,2}$. Hence, the classic MD heat- and mass-transfer relationship (Eq. (29)) might not be applicable for the VMD configuration, whose membrane wall temperatures and corresponding heat and mass fluxes can be obtain by solving the combination of Eqs. (25), (26), (30), (31) and (33). A summary of equations for transport models in DCMD and VMD simulations, respectively, is given in Table 1.

2.3 Simulation of hollow fiber modules for DCMD and VMD configurations

2.3.1 User unit operation model for MD simulation in Aspen Plus

With the above-derived transport equations, a user unit operation model coded in FORTRAN language was developed to simulate the respective DCMD and VMD hollow fiber module in Aspen Plus. A computational algorithm, as shown in Fig.3, was established to simulate the module performance in the DCMD and VMD processes, respectively. The module dimensions and membrane properties were specified as solution parameters (inputs). The fluid properties of the brine and permeate were also assigned in the interface subroutines and the physicochemical characteristics were extracted from the Aspen™ Property database (supplied by Aspen Technology Inc. US). The transport equations

summarized in Table 1 were solved by the Shampine and Gordon solver [56] (FORTRAN source codes from the information on the website: http://www.sc.fsu.edu/~burkardt/f_src/ode/ode.html). The boundary correction equations (Table 1) were simultaneously solved to correlate the local heat and mass fluxes using the non-linear optimization programs of MINPACK, which was developed by the Operator of Argonne National Laboratory at University of Chicago. All programs in this algorithm were coded and compiled in Intel © Visual FORTRAN v11.1. The solved profiles of fluid temperature, permeation flux, pressure and flowrate served as the outputs of the algorithm to be packed and fed into the Aspen interface subroutines.

2.3.2 MD flowsheet simulations

In the current study the flowsheet simulations of both DCMD and VMD systems were developed to recover fresh water from RO brines using Aspen Plus. The same membrane material properties were used in the simulation as that in the MD verification experiments. Both DCMD and VMD simulated modules had the same specifications: 22 PDVF hollow fibers regularly packed into a PP tube with the inner diameter of 15 mm and an effective length of 200 mm. The total membrane area, A_M, was 180.9 cm^2. The simulated flow charts of DCMD and VMD processes are presented in Fig.4.

In Fig.4 (a) the DCMD flow chart shows that the feed (synthetic brine: 7.0 wt% sodium chloride (NaCl) solution as an initial concentration) is fed into the lumen side in batch mode until approaching the saturated concentration of 27 wt%; while the permeate is collected at the shell side of the module. Similar to the experimental conditions, circulating flows are employed at both sides to reduce the temperature polarization effects [57-59]. In Fig.4 (b) the output fluid for the VMD system is the water vapor under vacuum conditions. Therefore, an external condenser and compressor are included in the simulations. All heaters and coolers shown in the Fig.4 are built-in heat-exchanging units in Aspen plus; while the pumps and compressor are built-in pressure units. As communicating interfaces for the assigned process parameters and compiled subroutines described in Section 2.3.1, the user customized

units in Aspen plus are used to simulate the DCMD and VMD modules. The sequential modular strategy [60] is applied to solve the steady-state flowsheet simulation.

With available low-grade heat resources (*e.g.*, low grade waste heat, solar power, and geothermal energy), the major energy consumption of an MD system would be the pumping electricity required. The specific energy consumption *e* is defined as:

$$e = \begin{cases} \frac{P_{\text{Brine Pump}}+P_{\text{Permeate Pump}}}{\sum W_P} = \frac{P_{\text{Brine Pump}}+P_{\text{Permeate Pump}}}{A_m J_M} & \text{for DCMD} \\ \frac{P_{\text{Brine Pump}}+P_{\text{Compressor}}}{\sum W_P} = \frac{P_{\text{Brine Pump}}+P_{\text{Compressor}}}{A_m J_M} & \text{for VMD} \end{cases} \quad (34)$$

where the P means the required electricity for the pumps or compressor, the $\sum W_P$ indicates the totally generated distillate (permeate), and the A_m means the total membrane area.

2.3.3 DCMD experiments for model verification

In this study DCMD modules were fabricated to verify the transport models established in section 2.1. The hollow fiber modules packed with twenty six polyvinylidenefluoride (PVDF) fibers, which were specifically developed for MD applications. The fibers have an averaged outer diameter of 1.46 mm and wall thickness of 0.24 mm. The module housing is a polypropylene (PP) tube with an inner diameter of 0.012 m and length of 0.22 m. A DCMD system was built to perform MD tests and verify the simulation result for the DCMD model. In this experimental setup, both the feed and permeate solutions were cycled through the shell and lumen sides of the hollow fiber modules, countercurrently. On the lumen side, the feed stream (synthetic brine: 3.0 wt% sodium chloride (NaCl) solution as an initial concentration) was heated to a specified temperature (*e.g.*, 60 °C) and then fed into the module by a peristaltic pump. On the shell side, the permeate (pure water) was maintained at an inlet temperature of 30 °C by a chiller and cycled by another peristaltic pump. The permeate was collected via an overflow tubing for mass flux calculation. More details of the experimental settings can be found in the previous

work [33, 34]. It is noted that the current MD system was operated in batch mode, *i.e.*, no fresh feed supplement up to the saturation point of NaCl solution.

3. Results and discussion

3.1 Transport model verification

3.1.1 Model verification for DCMD

The transport models applied in the DCMD module were verified by the experimental results. The simulated outlet temperatures and the permeation flux were well agreed with the experimental values (relative error < 10 %), as presented in Fig.5. The currently established transport models showed a higher accuracy compared to the previous models [49] in predicting experimental outcomes.

3.1.2 Model verification for VMD

Using the published experimental results of a VMD system [1, 22], the VMD transport models described in Section 2 were validated. The results are listed in Table 2 in terms of the root mean square (RMS) errors. The comparison of the simulation results and published experimental data shows an averaged RMS error of 10 %, which is acceptable for industrial applications.

3.2 Process performance of DCMD and VMD systems

3.2.1 Effects of hydrodynamic conditions on MD performance

To simulate the process performance of batch-mode DCMD and VMD operation, the raw brine was concentrated from 7.0 wt% up to saturation at a feed inlet temperature of $T_{1,0}$ = 80 °C and permeate side $T_{2,0}$ = 30 °C. With the assumption of accessible low-grade heat resources, the effects of the flow conditions (represented by the Reynolds numbers of the feed and permeate flows, Re_1 and Re_2) on the permeation flux and specific energy consumption e in DCMD are shown in Fig. 6 (a) and (b), respectively.

In Fig. 6 (a), the permeation flux shows an initial rapid increase with increasing flow velocities (Re_1 and Re_2) on both sides at a relatively low *Re* range and then a fairly slow rise at a high *Re* range. The increasing trend is due to the reduction of transfer resistance on the thermal boundary layers with an improvement on the hydrodynamic conditions and enhancement of driving force with a higher outlet temperature at a higher Reynolds number. However, a further increase on the *Re* (>2000) will lead to a relatively slower flux enhancement on both sides due to a potential shift of controlling heat-transfer resistance from the liquid boundary layers to the membrane itself. Interestingly, compared to the permeate side, the permeation flux shows a more sensitive response to the feed side (lumen) Re_1, which has strongly affected the thickness of thermal boundary layer and the heat-transfer process because of a much higher operating temperature and hence a more dominant contribution to the vapor pressure difference (based on Antoine equation [55]).

In Fig. 6 (b), the feed-side (lumen) specific energy consumption *e* increases with increasing Re_1 – initially a relatively slow increase at a low Re_1 range and then a rapid increase after Re_1 reaches 2000. Although the overall pumping energy required and permeation flux are expected to increase simultaneously with increasing *Re*, the specific energy consumption still shows a continuously increasing trend. This is because of a much higher pressure drop along the fiber length (overall pumping energy required) incurred in the lumen due to the much smaller inner diameter (flow channel) of the fiber. Moreover, the pressure drop is proportional to the square of the flow velocity (*Re*); while the permeation flux is only correlated with the boundary correction described in section 2.3.1. Therefore, more rapid increase on the *e* value after reaching turbulence (Re_1 > 2000) can be explained by a slower increase on the denominator in Eq. (34) - permeation rate (Fig. 6(a), J_M vs. Re_1) due to the insignificant influence from the flow dynamics. On the contrary, the permeate-side (shell) specific energy consumption presents a slight increase because of the much smaller magnitude of pressure drop at the

shell side due to the larger hydraulic diameter. The increase on the Re_2 will result in a slight increasing trend on the *e* value, as the rise of permeation rate became much slower (Fig. 6(a), J_M vs. Re_2).

Clearly, the influence of the flow conditions on the specific energy consumption is more significant at the feed side (lumen) in DCMD. For instance, the specific energy consumption is more than 9 times higher at Re_1 = 3000 than that of Re_1 = 500; while at the permeate side (shell), the change is rather insignificant for the same *Re* range. The reason is that, compared to the shell side, the magnitude of the pressure drop at the lumen side is much higher due to the ten times narrower flow channel, which implies a ten times higher flow velocity (pumping energy) is required for achieving the same *Re*. Therefore, it is necessary to choose optimal operating conditions with compromised performance of specific energy consumption and permeation flux, *i.e.*, a rapid increase of *e* value occurred when Re_1 > 2000 and an acceptable J_M value at the shell side when Re_2 = 2000.

To increase the transmembrane vapor pressure difference in VMD, the operating vacuum pressure at the shell side (permeate, p_2) and feed flowrate (lumen side, Re_1) are two important variables. Their effects on the specific energy consumption *e* are analyzed based on simulation results, as shown in Fig. 7. It is found that the specific energy consumption slightly increases with increasing vacuum pressure p_2. This is due to two reasons: firstly, in VMD the energy required for external condensation-compression process (CCP) almost remains constant for a wide range of operating pressure; secondly, the increase of operating vacuum pressure at the permeate side (shell) has led to a decrease on the permeation flux (based on Eq. (22)). Therefore, a lower operating vacuum pressure is beneficial for reducing the specific energy consumption in VMD. Similar to the results of hydrodynamics shown in Fig. 6(a), the specific energy consumption increases with increasing feed side Re_1 – an initial slow increase at a low *Re* range and then a drastic rise occurs under turbulent conditions.

3.2.2 Comparison of energy consumption in DCMD and VMD

To compare the energy consumption under equivalent operating conditions, the initial vacuum pressure $p_{2,0}$ (at z = 0) in the VMD simulation was kept at 4.25 kPa, which is equal to the permeate vapor pressure at an inlet temperature of 30 °C in DCMD. The feed-side inlet temperature and permeate-side flow conditions were fixated at $T_{1,0}$ = 80 °C and Re_2 = 456 in both MD systems. The feed-side Re_1 was selected as the variable to investigate the permeation rate and specific energy consumption for both MD systems, as shown in Fig. 8 (a). The respective specific energy consumption of the DCMD and VMD configurations are shown in Fig. 8 (b) as a function of the permeation flux under equivalent operating conditions.

It is observed in Fig. 8 (a) that the both permeation flux J_M and specific energy consumption e curves show general increasing trends with increasing Re_1 for DCMD and VMD systems. Similar to the explanations for Fig. 6, this is due to a more rapid increase of overall energy required than the simultaneous improvement on the permeation flux caused by an increase of Re_1. However, compared to VMD, achieving the same amount of flux increase has a more dramatic impact on the specific energy consumption in the DCMD system (upper curve in Fig. 8(b)), *i.e.*, a much higher energy cost is required to gain the same enhancement on the permeation flux. At the lowest e value of 0.25 kWh·t^{-1}, the permeation flux of the VMD configuration (lower e curve in Fig. 8(b)) is at least 2.5-fold higher than that of DCMD. Furthermore, combined with the results in Figs. 6 and 7, it is observed in Fig. 8(b) that a fifty-fold rise on the energy consumption is incurred in DCMD with only 15% flux increase (from 0.003 to 0.0035 kg m^{-2} s^{-1}); while with an initial 150 % flux increase in VMD (*i.e.*, from 0.003 to 0.0075 kg m^{-2} s^{-1}) the e curve presents invisible changes with increasing Re_1. However, a further increase on the Re_1 would also cause a rather significant increase on the energy required in VMD when the design permeation rate is higher than 0.0075 kg m^{-2} s^{-1} till reaching a plateau value of 0.009 kg m^{-2} s^{-1} at Re_1 = 2000. Overall, the VMD system has shown the capacity to achieve higher thermal efficiency at optimal operating conditions and a lower energy cost. In another word, due to much lower conductive heat loss

to the membrane, VMD has a great potential producing the same amount of distillate with much less heat consumption, which leads to the design of significantly smaller heat exchangers and subsequently a major reduction on the capital investment.

3.2.3 Temperature profiles in DCMD and VMD hollow fiber modules

With the same external operating conditions applied, the simulation results in Figs. 6-8 showed that the overall VMD performance was more advantageous than DCMD. To further reveal the heat-transfer fundamentals related to such significant difference between two configurations, the simulated temperature profiles (bulk temperatures T_1, T_2 and wall temperatures $T_{W,1}$, $T_{W,2}$) along the fiber length in the respective DCMD and VMD modules are shown in Fig. 9.

With a counter-current flow pattern in DCMD, the brine feed enters the lumen side of the module at location z = 0 m and exits at z = 0.2 m; while the permeate flows from the opposite direction. Fig.9 (a) shows that in DCMD the simulated local temperatures at the feed side (bulk temperatures T_1 and wall temperatures $T_{W,1}$) decrease along the fiber length. This is due to the heat contributed to evaporation and conductive heat loss. On the contrary, the permeate temperatures (bulk temperatures T_2 and wall temperatures $T_{W,2}$) at the shell side increase along its flow direction (enters at z = 0.2 m) because of the equal amount of condensation heat received from the vapor generated. The overall transmembrane temperature difference ($T_{W,1} - T_{W,2}$) increases along the fiber length in z direction of the DCMD module. This is because the permeate-side temperature has a greater increase for its mass flow (permeate); while the feed-side temperature presents a less significant decrease with higher flowrate. As observed from Fig. 9(a), the local temperatures adjacent to the membrane walls are lower than that of the bulks. This is due to the temperature polarization effect caused by of the liquid boundary layer under non-ideal flow conditions.

With the vacuum pressure applied at the permeate side of the VMD module, the simulated temperature profiles shown in Fig. 9(b) are rather different from that in DCMD. Although similar decreasing trends are observed for the feed-side local temperatures T_1 and $T_{W,1}$, the permeate-side temperatures T_2 and $T_{W,2}$ only show a slight decrease along the fiber length. Since initially there is almost no vapor presenting at the entrance of the shell side, the local bulk temperature of the vapor chamber T_2 at z = 0 m approaches the wall temperature $T_{W,2}$. As the brine feed flowing into the lumen and vacuum conditions applied at the shell, T_1 and $T_{W,1}$ decrease along the fiber as vapor is continuously produced. As vapor diffusion takes place, the permeate bulk temperature T_2 is affected by the upstream and transmembrane vapor – with continuous mixing from the upstream vapor, the bulk phase shows a slightly higher temperature than the membrane surface ($T_{W,2}$). The permeate- and feed-side wall temperatures $T_{W,2}$ and $T_{W,1}$ are overlapped due to negligible conductive heat loss across the membrane matrix in VMD.

To associate the heat- and mass-transfer mechanisms with module performance in both DCMD and VMD, the distributions of local driving force (transmembrane vapor pressure difference, Δp) along the fiber length are shown in Fig. 10. Consistent with the temperature profiles in Fig. 9(a), the Δp distribution (lower curve) in the DCMD module shows a significant increase along z direction. On the contrary, in VMD the Δp distribution (upper curve) shows a slight decreasing trend along the flow direction z. This can be explained by the decreasing temperature profiles (T_1 and $T_{W,1}$) in Fig. 9(b), which have resulted in a decreasing vapor pressure difference with a constant operating vacuum pressure. Overall, the average driving force of the VMD configuration is two times higher than that of DCMD.

4. Conclusions

As one of the potential solutions for fresh water recovery from high salinity brines, MD has shown promising prospects with the utilization of low-grade energy. In this paper, one dimensional (1-D) transport models with the boundary correction were established to evaluate the performance of DCMD

and VMD hollow fiber systems. The models were programmed in FORTRAN language to serve as customized operation units in Aspen plus, which were further integrated into the steady-state DCMD and VMD flowsheet simulations for reverse osmosis (RO) brine processing.

The comparison of the DCMD and VMD module performance indicated that the VMD configuration demonstrated more competitive characteristics in terms of specific energy consumption, *i.e.*, more significant increase of permeation rate (minimum 2.5-fold) was achieved at the same energy cost. The module performance was further analyzed by the mass- and heat-transfer fundamentals based on the simulated temperature distributions which showed that VMD exhibited a much higher driving force and a significantly lower conductive heat loss than DCMD. This study has provided a handy modeling approach to evaluate the potential of RO brine treatment using different MD configurations, by establishing the correlations between the MD transport phenomena and module performance to assess overall process energy efficiency.

Acknowledgements

This work was funded by the project (#0901-IRIS-0203) from Environmental and Water Industry Programme Office (EWI) of Singapore. Authors would also like to thank Dr. Filicia Wicaksana and Dr. Hui Yu from Singapore Membrane Technology Centre for their inspiring discussions.

Appendix

A1) Derivation of energy balance equations for DCMD case

The general energy transport equation from the thin shell balance is given as:

$$\frac{d}{dz}e_{z,i} = S_i = \begin{cases} \frac{4}{d_1}J_{H,1} & \text{for } i = 1 \text{ (lumen side)} \\ -\frac{4Nd_1}{d_2^2}J_{H,2} & \text{for } i = 2 \text{ (shell side)} \end{cases} \tag{a1}$$

Substituting the definition of e_z, Eq. (a1) is rewritten as:

$$\frac{d}{dz}\left[\frac{1}{2}\rho_i v_i^2 v_i + \rho_i \hat{c}_{P,i}(T_i - T^{\ominus})v_i + (p_i - p^{\ominus})v_i - \mu_i v_i \frac{dv_i}{dz} - \kappa_i \frac{dT_i}{dz}\right] = S_i \tag{a35}$$

where $\hat{c}_P$ is the average heat capacity; μ and κ are the viscosity and thermal conductivity of the fluid, respectively. The temperature ($T^{\ominus}$) and pressure ($p^{\ominus}$) at the standard state are 273.15 K and 100 kPa, respectively.

Compared to the changes of fluid temperature and pressure in Eq. (a2), the variation of the flow velocity in the axial direction of the module is also ignored. Thus, with negligible diffusive heat transfer of the forced convective flow, the energy balance equation can be simplified as:

$$\rho_i v_i \hat{c}_{P,i}\frac{dT_i}{dz} + v_i \frac{dp_i}{dz} = \begin{cases} \frac{4}{d_1}J_{H,1} & \text{for } i = 1 \text{ (lumen side)} \\ -\frac{4Nd_1}{d_2^2}J_{H,2} & \text{for } i = 2 \text{ (shell side)} \end{cases} \tag{a36}$$

A2) Derivation of shell-side momentum and energy balance equations for VMD case

The general momentum balance equation is given as:

$$\frac{d}{dz}\phi_{z,2} = 0 \tag{a37}$$

Substituting the definition of $\phi_{z,2}$ into the shell-side momentum balance equation, Eq. (a4) is rewritten as:

$$\frac{d}{dz}\left(p_2 - 2\mu_2\frac{dv_2}{dz} + \rho_2 v_2^2\right) = 0 \tag{a38}$$

For VMD, the compressibility of vapor leads to the axial changes of density, velocity and pressure. Thus, with neglecting second-order derivation of velocity, Eq. (a5) can be revised as:

$$\frac{dp_2}{dz} + v_2^2\frac{d\rho_2}{dz} + 2\rho_2 v_2\frac{dv_2}{dz} = 0 \tag{a39}$$

The shell-side energy balance equation can also be simplified with neglectful heat diffusion term of $\kappa_2\frac{dT_2}{dz}$ from Eq. (a2) as:

$$\begin{aligned}\rho_2 v_2\hat{c}_{P,2}\frac{dT_2}{dz} + \left[p_2 - p^{\ominus} + \rho_2\hat{c}_{P,2}(T_2 - T^{\ominus}) + \frac{3}{2}\rho_2 v_2^2\right]\frac{dv_2}{dz} + \\ \left[\frac{1}{2}v_2^3 + \hat{c}_{P,2}(T_2 - T^{\ominus})v_2\right]\frac{d\rho_2}{dz} + v_2\frac{dp_2}{dz} = -\frac{4Nd_1}{d_2^2}J_{H,2}\end{aligned} \tag{a40}$$

Nomenclature

A	Local membrane surface area of control volume, m^2
A_m	Total membrane area, m^2
C	Membrane distillation coefficient, kg m^{-2} Pa^{-1} s^{-1}
$\hat{c}_P$	Average heat capacity, J kg^{-1} K^{-1}
d	Inner diameter, m
d_e	Hydraulic diameter, m
e	Specific energy consumption, kWh t^{-1}
e_z	Z-component of combined energy vector, W m^{-2}
e^L	Specific enthalpy of liquid, J kg^{-1}
e^V	Specific enthalpy of vapor, J kg^{-1}
E	Enthalpy flow, W
f	Darcy fiction factor, dimensionless
Gr	Graetz number, dimensionless
h	Film heat transfer coefficient, W m^{-2} K^{-1}
J_H	Heat transfer flux, W m^{-2}

J_M	Mass transfer flux, kg m^{-2} s^{-1}
L	Length of membrane, m
N	Number of hollow fiber membranes
Nu	Nusselt number, dimensionless
p	Pressure, Pa
P	Required electricity, kWh
Pr	Prandtl number, dimensionless
Re	Reynolds number, dimensionless
T	Bulk temperature, °C
T_W	Membrane surface temperature, °C
v	Velocity of fluid, m s^{-1}
W	Mass flow rate, kg s^{-1}
W_P	Local permeative mass flow, kg s^{-1}
z	Axial distance, m
Δh_V	Latent heat, J kg^{-1}

Greek letters

δ	Thickness of membrane, m

ϕ_z	Z-component of combined momentum, kg m^{-1} s^{-1}
κ	Thermal conductivity, W m^{-1} K^{-1}
μ	Viscosity, Pa s
ρ	Density, kg m^{-3}

Subscripts

0	Inlet condition of MD module
1	Lumen side of membrane distillation module
2	Shell side of membrane distillation module
in	Inlet of the control volume
m	Membrane
out	Outlet of the control volume
W	Membrane wall

Superscript

$\ominus$	Standard state

References

[1] J.P.M.J.P. Mericq, S. Laborie, C. Cabassud, Vacuum membrane distillation of seawater reverse osmosis brines, Water Research, 44 (2010) 5260-5273.

[2] L. Zhang, L. Xie, H.L. Chen, C.J. Gao, Progress and prospects of seawater desalination in China, Desalination, 182 (2005) 13-18.

[3] F. Hajbi, H. Hammi, A. M'nif, Reuse of RO Desalination Plant Reject Brine, Journal of Phase Equilibria and Diffusion, 31 (2010) 341-347.

[4] A.M.O. Mohamed, M. Maraqa, J. Al Handhaly, Impact of land disposal of reject brine from desalination plants on soil and groundwater, Desalination, 182 (2005) 411-433.

[5] I. Muñoz, A.R. Fernández-Alba, Reducing the environmental impacts of reverse osmosis desalination by using brackish groundwater resources, Water Research, 42 (2008) 801-811.

[6] Y. Fernández-Torquemada, J.L. Sánchez-Lizaso, J.M. González-Correa, Preliminary results of the monitoring of the brine discharge produced by the SWRO desalination plant of Alicante (SE Spain), Desalination, 182 (2005) 395-402.

[7] T. Peters, D. Pintó, Seawater intake and pre-treatment/brine discharge — environmental issues, Desalination, 221 (2008) 576-584.

[8] E. Gacia, O. Invers, M. Manzanera, E. Ballesteros, J. Romero, Impact of the brine from a desalination plant on a shallow seagrass (Posidonia oceanica) meadow, Estuarine, Coastal and Shelf Science, 72 (2007) 579-590.

[9] C.M. Tun, A.G. Fane, J.T. Matheickal, R. Sheikholeslami, Membrane distillation crystallization of concentrated salts-flux and crystal formation, Journal of Membrane Science, 257 (2005) 144-155.

[10] G. Chen, X. Yang, R. Wang, A.G. Fane, Performance enhancement and scaling control with gas bubbling in direct contact membrane distillation, Desalination, 308 (2013) 47-55.

[11] C. Charcosset, A review of membrane processes and renewable energies for desalination, Desalination, 245 (2009) 214-231.

[12] Z.W. Ding, L.Y. Liu, M.S. El-Bourawi, R.Y. Ma, Analysis of a solar-powered membrane distillation system, Desalination, 172 (2005) 27-40.

[13] P.A. Hogan, Sudjito, A.G. Fane, G.L. Morrison, DESALINATION BY SOLAR HEATED MEMBRANE DISTILLATION, Desalination, 81 (1991) 81-90.

[14] J. Koschikowski, M. Wieghaus, M. Rommel, Solar thermal-driven desalination plants based on membrane distillation, Desalination, 156 (2003) 295-304.

[15] S. Al-Obaidani, E. Curcio, F. Macedonio, G. Di Profio, H. Al-Hinai, E. Drioli, Potential of membrane distillation in seawater desalination: Thermal efficiency, sensitivity study and cost estimation, Journal of Membrane Science, 323 (2008) 85-98.

[16] A. Criscuoli, M.C. Carnevale, E. Drioli, Evaluation of energy requirements in membrane distillation, Chemical Engineering & Processing: Process Intensification, 47 (2008) 1098-1105.

[17] J.P. Mericq, S. Laborie, C. Cabassud, Evaluation of systems coupling vacuum membrane distillation and solar energy for seawater desalination, Chemical Engineering Journal, 166 (2011) 596-606.

[18] E. Curcio, E. Drioli, Membrane distillation and related operations - A review, Separation and Purification Reviews, 34 (2005) 35-86.

[19] K.W. Lawson, D.R. Lloyd, Membrane distillation, Journal of Membrane Science, 124 (1997) 1-25.

[20] K.W. Lawson, D.R. Lloyd, Membrane distillation .1. Module design and performance evaluation using vacuum membrane distillation, Journal of Membrane Science, 120 (1996) 111-121.

[21] Z.W. Ding, L.Y. Liu, Z.M. Li, R.Y. Ma, Z.R. Yang, Experimental study of ammonia removal from water by membrane distillation (MD): The comparison of three configurations, Journal of Membrane Science, 286 (2006) 93-103.

[22] D. Wirth, C. Cabassud, Water desalination using membrane distillation: Comparison between inside/out and outside/in permeation, Desalination, 147 (2002) 139-145.

[23] A. Alkhudhiri, N. Darwish, N. Hilal, Membrane distillation: A comprehensive review, Desalination, 287 (2012) 2-18.

[24] R.W. Schofield, A.G. Fane, C.J.D. Fell, Heat and mass transfer in membrane distillation, Journal of Membrane Science, 33 (1987) 299-313.

[25] A.O. Imdakm, T. Matsuura, A Monte Carlo simulation model for membrane distillation processes: direct contact (MD), Journal of Membrane Science, 237 (2004) 51-59.

[26] A.O. Imdakm, T. Matsuura, Simulation of heat and mass transfer in direct contact membrane distillation (MD): The effect of membrane physical properties, Journal of Membrane Science, 262 (2005) 117-128.

[27] M. Khayet, A.O. Imdakm, T. Matsuura, Monte Carlo simulation and experimental heat and mass transfer in direct contact membrane distillation, International Journal of Heat and Mass Transfer, 53 (2010) 1249-1259.

[28] A.O. Imdakm, M. Khayet, T. Matsuura, A Monte Carlo simulation model for vacuum membrane distillation process, Journal of Membrane Science, 306 (2007) 341-348.

[29] S. Soukane, S. Chelouche, M.W. Naceur, A ballistic transport model for vacuum membrane distillation, Journal of Membrane Science, 450 (2014) 397-406.

[30] S. Bandini, A. Saavedra, G.C. Sarti, Vacuum membrane distillation: Experiments and modeling, Aiche J., 43 (1997) 398-408.

[31] M. Khayet, T. Matsuura, Pervaporation and vacuum membrane distillation processes: Modeling and experiments, Aiche J., 50 (2004) 1697-1712.

[32] R.W. Field, H.Y. Wu, J.J. Wu, Multiscale Modeling of Membrane Distillation: Some Theoretical Considerations, Industrial & Engineering Chemistry Research, 52 (2013) 8822-8828.

[33] X. Yang, R. Wang, L. Shi, A.G. Fane, M. Debowski, Performance improvement of PVDF hollow fiber-based membrane distillation process, Journal of Membrane Science, 369 (2011) 437-447.

[34] X. Yang, R. Wang, A.G. Fane, Novel designs for improving the performance of hollow fiber membrane distillation modules, Journal of Membrane Science, 384 (2011) 52-62.

[35] X. Yang, R. Wang, A.G. Fane, Chuyang Y.Tang, I.G. Wenten, Membrane module design and dynamic shear-induced techniques to enhance liquid separation by hollow fiber modules: a review, Desalination and Water Treatment, 51 (2013) 3604-3627.

[36] M. Gryta, M. Tomaszewska, A.W. Morawski, Membrane distillation with laminar flow, Separation and Purification Technology, 11 (1997) 93-101.

[37] M. Gryta, M. Tomaszewska, Heat transport in the membrane distillation process, Journal of Membrane Science, 144 (1998) 211-222.

[38] S.G. Lovineh, M. Asghari, B. Rajaei, Numerical simulation and theoretical study on simultaneous effects of operating parameters in vacuum membrane distillation, Desalination, 314 (2013) 59-66.

[39] J. Zhang, J.-D. Li, M. Duke, M. Hoang, Z. Xie, A. Groth, C. Tun, S. Gray, Modelling of vacuum membrane distillation, Journal of Membrane Science, 434 (2013) 1-9.

[40] J.I. Mengual, M. Khayet, M.P. Godino, Heat and mass transfer in vacuum membrane distillation, International Journal of Heat and Mass Transfer, 47 (2004) 865-875.

[41] M. Khayet, Membranes and theoretical modeling of membrane distillation: A review, Advances in Colloid and Interface Science, 164 (2011) 56-88.

[42] H. Yu, X. Yang, R. Wang, A.G. Fane, Analysis of heat and mass transfer by CFD for performance enhancement in direct contact membrane distillation, Journal of Membrane Science, 405- 406 (2012) 38- 47.

[43] M. Shakaib, S.M.F. Hasani, I. Ahmed, R.M. Yunus, A CFD study on the effect of spacer orientation on temperature polarization in membrane distillation modules, Desalination, 284 (2012) 332-340.

[44] X. Yang, H. Yu, R. Wang, A.G. Fane, Analysis on the effect of turbulence promoters in hollow fiber membrane distillation module via computational fluid dynamic (CFD) simulations, Journal of Membrane Science, 415-416 (2012) 758-769.

[45] H. Yu, X. Yang, R. Wang, A.G. Fane, Numerical simulation of heat and mass transfer in direct membrane distillation in a hollow fiber module with laminar flow, Journal of Membrane Science, 384 (2011) 107-116.

[46] X. Yang, H. Yu, R. Wang, A.G. Fane, Optimization of microstructured hollow fiber design for membrane distillation applications using CFD modeling, Journal of Membrane Science, 421-422 (2012) 258-270.

[47] S.S. Ibrahim, Q.F. Alsalhy, Modeling and Simulation for Direct Contact Membrane Distillation in Hollow Fiber Modules, Aiche J., 59 (2013) 589-603.

[48] L.-H. Cheng, P.-C. Wu, J. Chen, Modeling and optimization of hollow fiber DCMD module for desalination, Journal of Membrane Science, 318 (2008) 154-166.

[49] G. Guan, R. Wang, F. Wicaksana, X. Yang, A.G. Fane, Analysis of Membrane Distillation Crystallization System for High Salinity Brine Treatment with Zero Discharge Using Aspen Flowsheet Simulation, Industrial & Engineering Chemistry Research, 51 (2012) 13405-13413.

[50] S.B. Abdallah, N. Frikha, S. Gabsi, Simulation of solar vacuum membrane distillation unit, Desalination, 324 (2013) 87-92.

[51] J. Zhang, J.-D. Li, M. Duke, Z. Xie, S. Gray, Performance of asymmetric hollow fibre membranes in membrane distillation under various configurations and vacuum enhancement, Journal of Membrane Science, 362 (2010) 517-528.

[52] H. Yu, X. Yang, R. Wang, A.G. Fane, Analysis of heat and mass transfer by CFD for performance enhancement in direct contact membrane distillation, Journal of Membrane Science, 405 (2012) 38-47.

[53] R.B. Bird, W.E. Stewart, E.N. Lightfoot, Transport phenomena, 2nd. ed., John Wiley & Sons, Inc., New York, 2007.

[54] T. Lestina, R. Serth, Process heat transfer: principles and applications, 1st ed., Academic Press, Singapore, 2007.

[55] R.H. Perry, D.W. Green, J.O. Maloney, Perry's chemical engineers' handbook, McGraw-Hill Companies, Inc., New York, 1997.

[56] L.F. Shampine, Numerical solution of ordinary differential equations, 1st ed., Chapman & Hall, New York, 1994.

[57] L. Martinez-Diez, M.I. Vazquez-Gonzalez, Temperature and concentration polarization in membrane distillation of aqueous salt solutions, Journal of Membrane Science, 156 (1999) 265-273.

[58] A.G. Fane, R.W. Schofield, C.J.D. Fell, The efficient use of energy in membrane distillation, Desalination, 64 (1987) 231-243.

[59] G. Zuo, R. Wang, R. Field, A.G. Fane, Energy efficiency evaluation and economic analyses of direct contact membrane distillation system using Aspen Plus, Desalination, In Press, Corrected Proof (2011).

[60] B.J. Pangrle, E.G. Walsh, S.C. Moore, D. DiBiasio, Investigation of fluid flow patterns in a hollow fiber module using magnetic resonance velocity imaging, Biotechnol. Tech., 3 (1989).