Journal Pre-proof

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PII: S0376-7388(19)30531-9

DOI: <https://doi.org/10.1016/j.memsci.2019.117609>

Reference: MEMSCI 117609

To appear in: *Journal of Membrane Science*

Received Date: 20 February 2019

Revised Date: 19 September 2019

Accepted Date: 23 October 2019

Please cite this article as: A.E. Anqi, M. Usta, R. Krysko, J.-G. Lee, N. Ghaffour, A. Oztekin, Numerical study of desalination by vacuum membrane distillation – Transient three-dimensional analysis, *Journal of Membrane Science* (2019), doi: <https://doi.org/10.1016/j.memsci.2019.117609>.

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Numerical Study of Desalination by Vacuum Membrane Distillation – Transient Three-Dimensional Analysis

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ABSTRACT

The performance of vacuum membrane distillation (VMD) modules can be optimized through careful selection of design parameters. The present study examines how the addition of cylindrical filaments in the feed channel increases momentum mixing and the overall performance of VMD modules under different operating inlet conditions. Three-dimensional transient Computational Fluid Dynamics (CFD) simulations are conducted using Wall-Adapting Local Eddy-Viscosity (WALE) subgrid-scale Large Eddy Simulation (LES) turbulence model. Local concentration, temperature, and flux are coupled at the membrane surface to predict the rate of water vapor diffused through the membrane by Knudsen and viscous diffusion mechanisms. The predicted and measured vapor flux agrees reasonably well; validating the employed model. The small-scale eddies induced by the presence of spacer filaments promote mixing in the module, thus the temperature and concentration polarization is alleviated and the water vapor flux is immensely improved. The insertions of filaments in the feed channel increase the water permeate rate by more than 50% at higher feed flow rates and inlet temperatures. The

pressure drop by the spacer reduces the allowable module length by one order of magnitude, but the module length increases two folds at feed temperature 80°C. Even though the power consumption of the module containing the filaments is increased, the addition of filaments is strongly recommended since the required power for the process could be supplied from readily available low-grade heat source.

Keywords: VMD, 3-D transient CFD, Cylindrical spacer, Temperature polarization coefficient, Concentration polarization coefficient, Desalination.

1. INTRODUCTION

As the demand for purified water increases globally, desalination technologies continue to gain importance. Membrane Distillation (MD) is an emerging technology in this area, especially for the treatment of challenging feeds [1]. MD has shown potential advantages over competitors due to its ability to operate at lower feed channel temperatures and pressures as well as its ability to produce pure permeate regardless of feed water quality, including desalination brines [2]. MD also has increased resistance to fouling and scaling over the competition due to its operating conditions [3,4]. The low operating temperatures are especially attractive since it enables the potential to use readily available low-grade waste heat, solar energy, or low-enthalpy geothermal energy, to drive the system [5].

MD is a membrane separation process that takes advantage of hydrophobic microporous membranes by evaporating heated water at the membrane surface and passing water vapor through to the permeate side. The hydrophobicity of the membrane prevents the feed solution from entering the membrane pores thereby allowing only the pure vapor to pass through. Diffusion is achieved by the partial pressure difference resulting from a temperature gradient

1 between the two sides. Once the vapor passes through the membrane, it is condensed and
2 collected on the other side as pure liquid water.

3 There are different MD configurations that have been studied. These are direct contact MD
4 (DCMD), air gap MD (AGMD), sweeping gas MD (SGMD), vacuum MD (VMD), and material
5 gap or water gap MD (MGMD/WGMD). A more recent configuration from the feed side named
6 flashed-feed VMD has been proposed by Alsaadi et al. [6]. The current paper focuses on vacuum
7 membrane distillation (VMD) which utilizes a liquid feed mixture in the upstream, or feed side,
8 of the membrane and a vacuum vapor product in the downstream, or permeate, side. In order for
9 the process to perform effectively, the temperature at the feed side of the membrane surface must
10 be higher than the saturation temperature corresponding to applied vacuum pressure. The
11 performance of VMD systems has been shown to be dependent on both membrane properties and
12 feed channel operating conditions [7,8]. VMD has the ability to treat single component, binary or
13 multicomponent aqueous solution [9] at a competitive cost and low energy consumption [8].
14 Furthermore, VMD has salient features compared to other MD configurations such as high
15 permeate flux, low heat loss by conduction and low temperature polarization on the permeate
16 side [8].

17 VMD emerged as an active area of research with applications to desalination in the 1990s.
18 Schofield et al. [10–12] conducted theoretical and experimental studies through which they
19 observed the adverse effects of temperature polarization on MD performance. They also showed
20 that the application of vacuum pressure on the permeate side increases the temperature
21 polarization which limits the increase in flux [12]. Song et al. [13] performed an experiment to
22 study the effect of the feed concentration and temperature on the permeate production. They
23 noted that as the brine temperature was increased, the flux increased almost exponentially. They

also showed that a 10% increase in salt concentration resulted in a small reduction in flux. Izquierdo-Gil and Jonsson [14] theoretically and experimentally investigated the effects of operating conditions and membrane material on the permeate flux. They observed that the flux exponentially increases as the feed temperature rises. Similar effects of the feed temperature, concentration on the flux were reported by Lian et al. [15], Alsaadi et al. [6], and Zhang et al. [16].

Mericq et al. [17] experimentally investigated further distillation of seawater reverse osmosis brines by means of flat-sheet VMD. Although scaling of calcium crystals over the membrane surface occurred because of the highly concentrated reverse osmosis brines, it was found that the coupling of reverse osmosis and VMD increases the overall product recovery rate considerably. Lee et al. [18] performed one-dimensional simulations for heat and mass transfer in hollow fiber VMD and noticed a decrease in heat energy consumption as the feed temperature increases. Liu et al. [19] have conducted numerical simulations for hollow fiber VMD. The simulations considered momentum, energy and mass transport. The membrane was treated as a functional surface, but the concentration effect on the vapor pressure was not involved in the boundary condition equations of the membrane. Mengual et al. [20] conducted a comparison between the experimental results and the empirical correlations of heat transfer. The experimental results of the heat transfer deviate from the empirical correlations results, especially at the laminar flow regime. Zuo et al. [21] conducted an optimization study on four design and operation parameters including feed temperature, hollow fiber length, feed volume flow rate, and vacuum pressure of hollow fiber VMD modules utilizing a two-dimensional numerical approach. They reported that temperature significantly affects the permeate flux rate and that an optimized system can achieve a 38.1% reduction in the water production cost. Zhang et al. [22] employed three-dimensional

CFD simulations to study the effects of operating conditions and module dimensions on the heat transfer process in hollow fiber VMD. They found out that thermal efficiency is very sensitive to feed temperature and increasing fiber length decreases the thermal efficiency considerably. Two of the major challenges faced by MD are temperature and concentration polarization, especially temperature polarization [23]. As the liquid feed is evaporated and the vapor passes through the membrane surface, there is a reduction of temperature in the feed channel near the membrane surface. This effect is known as temperature polarization. Similarly, concentration polarization occurs when the concentration becomes elevated at the membrane surface as the vapor passes through the membrane. Each of these causes a reduction in mass transfer through the membrane. Insertion of spacer can attenuate temperature [16] and concentration [24] polarization in the feed channel. The placed spacer causes higher pressure drop in the feed channel. Kim et al. [25] have illustrated the increased trend in research of using spacers in the MD process and experimentally studied the spacer effect in DCMD. They reported permeate flux enhancement by 43% with spacers. Despite the available studies of the effect of spacer in membrane distillation configurations, there is no previous work to investigate the effect of the spacer in the feed channel of the VMD module. This can be attributed to the high potential of wetting in VMD [26].

Hitsov et al. [27] concluded CFD studies oversimplified the modeling of membrane distillation. These oversimplifications come from imposing empirical and semi-empirical relations to solve for heat and mass transfer. Empirical and semi-empirical relations fail to optimize the MD module because the relations are only valid for certain geometries or flow regimes [26,27]. Heat and mass transfer at the membrane surface are inter-coupled and should be solved simultaneously [3,26]. To the best knowledge of the authors, local water vapor flux, local

temperature, and local salt concentration have never been fully coupled and solved in previous VMD simulations.

The present study aims to conduct CFD simulations that fully and accurately couple and solve for the local water vapor, local temperature and local salt concentration at the membrane surface. The heat and mass transfer are considered without imposing predefined values of heat and mass transfer coefficients or fixed water vapor flux at the membrane surface. The simulations evaluate the effect of feed channel geometry and operating conditions on VMD system performance. Specifically, feed inlet velocity and inlet temperature are evaluated for a feed channel with and without cylindrical filaments. The filaments are added to the feed channel in order to enhance momentum mixing and reduce polarization effects. The effect of filaments on the pressure drop and the critical length for the onset of wetting are also determined for various operating conditions. To highlight the importance of selected parameters, the simulations are carried out for fixed membrane properties while the flow properties are varied. To compare the corresponding module performance for each set of parameters, the module-averaged concentration polarization, temperature polarization, mass flux, and the critical length for the wetting are evaluated.

2. MODEL DESCRIPTION

2.1. Governing Equations

The flow through the feed channel is modeled utilizing the finite volume method (FVM) to solve momentum, mass transport, and energy equations. For incompressible flows, the conservation of mass reduces to:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1)$$

The time-dependent conservation of momentum equation is written as:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad (2)$$

The equation governing the energy and solute mass transport through the feed channel is described by:

$$\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \frac{k_f}{\rho c_p} \frac{\partial^2 T}{\partial x_j \partial x_j} \quad (3)$$

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = D \frac{\partial^2 c}{\partial x_j \partial x_j} \quad (4)$$

In the above, ρ is the binary mixture density, p is pressure, ν is the kinematic viscosity, t is time, T is temperature, k_f is thermal conductivity of feed solution, c_p is specific heat, c is scalar salt concentration, and D is the diffusion coefficient. Although the density, ρ , is a function of salinity, it is assumed to be constant since the maximum local change in density is less than 3.9% in all cases studied.

2.2. Turbulence Model

In order to accurately characterize the complex transient, three-dimensional flow in the feed channel, large eddy simulations (LES) is employed. The LES model uses a filter to model the scales of motion smaller than the filter size and solves for the large eddies explicitly. The LES is used to provide time-dependent predictions to capture unsteady flow. The transient approach (LES) has two major advantages over time averaged solutions (Reynolds Averaged approach – RANS). First, LES provides more accurate solutions since the larger eddies are resolved and model dependent uncertainties are alleviated when compared to RANS. Second, time dependent solutions reveal a strong vortical structure in between two consecutive filaments. The LES has

different models for the sub-grid scales of motion which vary based on the application. Classical Smagorinsky formulation falls short in the regions where vorticity dominates the irrotational strain. Such behavior makes the Smagorinsky approach inaccurate at the vicinity of membrane surfaces in which the dominant deformation occurs. Wall adapting scheme basically adjust the calculation of strain rate by including the rotation rate tensor in the sub-grid scale viscosity formulation. This modification makes the model more sensitive to both strain and rotation rate of the small turbulent structures [28]. In this study, the Wall-Adapting Local Eddy-Viscosity (WALE) subgrid-scale model is used. The WALE model allows for resolution of the near wall flow-field which is important to the present simulation. The LES filtered momentum equation can be written as:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} \quad (5)$$

Closure is obtained by modeling the SGS stress tensor, τ_{ij} . The SGS model relates the SGS stresses to the large-scale strain rate tensor typically by using an eddy-viscosity model of the form:

$$\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_t \bar{S}_{ij} \quad (6)$$

For the WALE model, the eddy viscosity is defined as [28]:

$$\nu_t = (C_W \Delta)^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(\bar{S}_{ij}^d \bar{S}_{ij}^d)^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}} \quad (7)$$

where

$$S_{ij}^d = \frac{1}{2} (\bar{g}_{ij}^2 + \bar{g}_{ji}^2) - \frac{1}{3} \delta_{ij} \bar{g}_{kk}^2 \quad (8)$$

$$\bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial x_j} \quad (9)$$

2.3. VMD Model

In the MD process, the upstream of the hydrophobic microporous membrane is in contact with the liquid feed while the downstream is subject to a vacuum condition. The membrane hydrophobicity ensures that the liquid mixture cannot penetrate the cavities of the membrane whereas water vapor can. In order for this condition to be valid, the pressure of the fluid in contact with the membrane must not exceed the liquid entry pressure of the feed solution. The relationship between the membrane's maximum allowable pore size and operating conditions is given by the Young-Laplace equation [3,29,30]:

$$LEP = \frac{-2B\gamma_i \cos(\alpha)}{r_{max}} \quad (10)$$

where B is the geometric factor determined by pore structure, γ_i is the liquid surface tension for NaCl solution ($\gamma_i = 72 [mN/m] + 1.46 [mN L/m mol] c$), c is the salt concentration in mol/L [29,30], α is the liquid-solid contact angle, and r_{max} is the largest pore radius.

The driving force for the VMD process is the partial pressure difference between the feed and permeate sides of the membrane. This pressure difference is obtained by elevating the temperature on the feed side and applying a vacuum to the permeate side. The application of the

vacuum is what distinguishes VMD from other MD configurations. In the permeate channel, the applied vacuum eliminates the presence of any substances other than water vapor. This allows for the applied vacuum pressure to be taken as the actual vapor pressure for the downstream side of the membrane. The calculation of the vapor pressure on the feed side is not as straightforward since we are required to estimate the water vapor pressure in a non-ideal liquid mixture. The partial pressure of water vapor in the water liquid is the saturation pressure, P^0 , and is defined by the Antoine equation:

$$p_i = P^0 = \exp \left[A - \frac{B}{C + T} \right] \quad (11)$$

where T is the absolute temperature, A , B , and C are constants varying for different substances and it is readily available for water ($A = 23.1964$, $B = 3816.44$, $C = -46.13$) [31].

The partial pressure of water vapor in the non-ideal binary mixture is determined from

$$p_i = y_i p = X_i \alpha_i P_i^0 \quad (12)$$

where y_i and X_i are the vapor and liquid mole fractions of water, respectively, p is the total pressure, and P_i^0 is the saturation pressure of pure water from Eq. 11. The activity coefficient, α_i , has been determined through various means. Schofield [32] determined the activity coefficient of water in NaCl solutions from experimental data as

$$\alpha_{water} = 1 - 0.5X_{NaCl} - 10X_{NaCl}^2 \quad (13)$$

where X_{NaCl} is the mole fraction of NaCl. This study utilizes the activity coefficient approximated by Schofield since it is rooted in experimental measurements.

The Dusty Gas Model (DGM) as proposed by Lawson and Lloyd [3] is used in this study to model gas transport through porous membranes. The DGM defines the transport to take place by

a combination of several mechanisms and resistances. These are surface diffusion, Knudsen diffusion, molecular diffusion or viscous diffusion. The surface diffusion is negligible in the MD process due to the low surface area when compared to membrane pore area. Also, in the VMD process, the molecular diffusion resistance can be neglected since its contribution is determined by air trapped inside membrane cavities. This is unusual for the VMD technique because the applied vacuum on the permeate side ensures water vapor is the only substance contained within the membrane [33]. The degree to which each diffusion resistance is enacted can be determined by calculating the ratio of the pore size, r_p , to the mean free path, λ . From kinetic theory, the expression for the mean free path is given as [34,35]:

$$\lambda = \frac{k_B T}{\bar{p} \sqrt{2} \pi \sigma^2} \quad (14)$$

where σ is the collision diameter of the water molecules, $\bar{p}$ is the mean pressure within the membrane pores, T is the absolute temperature, and k_B is the Boltzmann constant.

Matsuura [34] defines a range of Knudsen number to determine which diffusion mechanism dominates. For the current study, both Knudsen and viscous mechanisms need to be considered. For Knudsen diffusion, the molar flux can be estimated as [7],

$$J_k = \frac{2}{3} \frac{\varepsilon_s r_p}{\tau R T \delta} \sqrt{\frac{8 R T}{\pi M_w}} (p_{wf} - p_v) \quad (15)$$

where r_p is the pore size, τ is the membrane tortuosity, δ is the membrane thickness, R is the gas constant, T is the temperature, M is the molecular weight of water, p_{wf} is the partial pressure of the water vapor at the upstream of the membrane, and p_v is the vacuum pressure at the downstream of the membrane.

The viscous diffusion can be characterized as a Poiseuille flow where molecule-molecule collisions occur due to larger membrane pore sizes. For this mechanism, the molar flux of the water vapor is calculated as

$$J_v = \frac{1}{8\mu_w} \frac{r_p^2 \varepsilon_s \bar{p}}{\tau RT \delta} (p_{wf} - p_v) \quad (16)$$

where μ_w is the viscosity of water vapor.

The total molar flux of water vapor, $J_t = J_k + J_v$, can be expressed as the sum of Knudsen flux, J_k , and viscous flux, J_v , [3,35,36]. The surface porosity, $\varepsilon_s = \varepsilon/\tau$, can be determined as a function of porosity and tortuosity [36]. The coefficients of the pressure differences in equations (15) and (16) represent the membrane permeability.

Since VMD is a thermally driven process, the heat transport through the membrane must also be considered since it will determine the partial pressure of water vapor in the feed side. In the case of VMD, the applied vacuum acts as an insulator and, as a result, conductive heat transfer can be neglected. The heat flux through the membrane is:

$$q''_m = N_t \Delta h_{fg} \quad (17)$$

$$\Delta h_{fg} = 3177800 - 2464.4T \quad (18)$$

where $N_t = J_t M_w$ is the local mass flux, M_w is the molecular weight of water, and Δh_{fg} is the enthalpy of water vaporization.

2.4. Geometry

The geometry used for this study is provided in Figure 1. Three-dimensional CFD simulations are employed on a channel featuring an active flat-sheet membrane surface to

investigate the sensitivity of the VMD performance to the feed channel operating conditions. The area of active membrane on one side is 10 cm^2 (rectangle sizes $10 \text{ cm} \times 1 \text{ cm}$ in stream-wise and span-wise directions, respectively) and the feed flow channel height, h , is 2 mm . Both the top and bottom surface of the channel are considered as a membrane which ends up to 20 cm^2 active surface area in total. Simulations for an empty channel are compared to those for a feed channel containing spacer filaments. A ladder-type spacer which causes no change in the bulk flow direction [37] is adopted in this study. The filaments in the ladder-type spacer come in two orientations: i) parallel and ii) perpendicular to the streamwise flow direction [37]. This results in a lower pressure drop compared to other types of spacers [24]. The filaments that are perpendicular to the streamwise flow direction have more influence on the boundary layer at the membrane surface than the filaments oriented in the flow direction. Therefore, a total of 8 filaments are added to the channel to induce mixing. A circular cross-section for filaments is a reasonable approximation [24], and these filaments can be held in the midplane of the channel by making thick filament joints [38] as supporting points. The filaments are placed perpendicular to the streamwise flow direction and spaced $5d$ apart. In order to reduce the mesh size, the filaments in the streamwise flow direction and thick joints are not considered in the computational domain. Such computational domains can be found in [39] and [24]. For further spacer geometry improvement, high fidelity simulations are needed to consider the effect of the thick joints. The filaments are placed far enough from the inlet and outlet to minimize boundary effects. A structured mesh is developed in OpenFoam v1706 which is employed as a meshing tool and an FVM solver.

Figure 1. Schematic of Flow Geometry (a) without and (b) with filaments

2.5. Boundary Conditions

The boundary conditions at the inlet and outlet are fixed averaged velocity, U_{ave} , and fixed pressure, respectively. Transitional periodicity is applied in the span-wise direction to represent larger modules. The membrane is treated as a permeable wall. At the membrane surface, local water flux, local temperature, and local concentration are coupled, and the following conditions are imposed for normal velocity, temperature, and concentration, respectively.

$$V_m = \frac{N_t}{\rho} \quad (19)$$

$$k_f \frac{\partial T}{\partial n} = \rho V_m \Delta h_{fg} \quad (20)$$

$$D \frac{\partial c}{\partial n} = V_m c \quad (21)$$

where V_m is the suction rate, N_t is the local mass flux, ρ is the density of water, k_f is the thermal conductivity of the feed solution, Δh_{fg} is the enthalpy of evaporation which is calculated from equation (18), D is the diffusivity of solute into the solvent, and n is the membrane surface

normal direction. The local mass flux, N_t , in the right-hand side of equation (19) is evaluated by combining Equations (11), (12), (13), (15) and (16). As a result, the boundary conditions for local water vapor flux, local temperature, and local concentration are fully coupled at the membrane surface and solved simultaneously by iteration.

For this study, the membrane properties are kept constant while the inlet temperature and velocity are varied. Values of these parameters and further details about flow properties are listed in Table 1 [40].

Table 1. Operating parameters and membrane properties

Parameter	Value
Pore radius, r_p	0.2 μm
Thickness, δ	179 μm
Porosity, ε	75%
Mean free path of water vapor molecule, λ	0.745 μm
Feed temperature, T_f	50°C, 80°C
Saturation temperature, T_{sat}	32.87°C (at 5 kPa)
Feed concentration, c_f	90 kg/m ³ [23]
Vacuum pressure, p_v	5 kPa
Reynolds number, $Re = U_{ave}h/\nu$	200, 1000

2.6. Mesh Study

To discretize the computational domain structured mesh is generated. Local mesh encryption is applied to the membrane surfaces which enables the accurate prediction of local temperature

and concentration. Meshing parameters are obtained from a previous study done by the present authors [41].

In order to ensure proper mesh discretization, a mesh convergence study is carried out. Simulations are conducted at the $Re = 1000, T = 80^\circ\text{C}$ case since it provides the most complex flow structures. The details of the mesh parameters for this study are shown in Table 2.

Table 2. Mesh convergence study details

Description	# of Cells	y_{min}^+	y_{max}^+	y_{avg}^+
M1	284040	0.012	0.226	0.111
M2	880992	0.007	0.186	0.088
M3	1959120	0.006	0.145	0.072
M4	3726888	0.004	0.136	0.065
M5	5011776	0.003	0.119	0.059

In order to assess the adequacy of each mesh, the drag coefficient calculated on the 5th filament in the stream-wise direction and the local mass flux through the membrane are examined. Figure 2a illustrates the drag coefficient on the filament for each mesh density as a function of non-dimensional time, $\tau_i = \frac{t U_{ave}}{d}$. The non-dimensional time is used to generalize the results. The results for each case are offset on the y-axis for visualization purposes. The drag coefficient is also time-averaged and listed on the y-axis next to the corresponding curve. Notice

that for the M1 and M2 mesh, the drag coefficient is oscillatory with time. As the mesh density is increased, the drag coefficient is more random as expected. The M4 and M5 mesh configurations show convergence on a drag coefficient. Figure 2b contains the same information as Figure 2a only now for the local mass flux. As with the drag coefficient, there is little change in the mass flux from the M4 mesh to the M5 mesh. Based on the mesh convergence, the M4 mesh is deemed sufficient and is utilized for the subsequent study.

Figure 2. Mesh convergence results for the M1 through M5 mesh configurations, (a) drag coefficient, C_d , history and (b) local mass flux, N_t ($\text{kg}/\text{m}^2\text{h}$), history. The time history is shown for non-dimensional time, τ_i . The average properties are indicated on y-axis.

2.7. Model Validation

Validation of the implemented mathematical model and numerical method was achieved by comparing experimental and numerical results for a channel without filaments, with matching operational conditions and membrane parameters, which are shown in Table 3. The experiments are carried out at King Abdullah University of Science and Technology (KAUST).

The experimental set-up consisted of the heater (VWR, USA), micro gear circulation pump (Cole Parmer, USA), pressure and temperature sensors, VMD module, chiller, vacuum vessel, balance (Mettler Toledo, USA), and vacuum pump (Vacuubrand, USA) as shown in Figure 3. The desired inlet feed temperature was maintained by a controller connected to the feed tank.

Figure 3. Experimental set-up of VMD process

The membrane module consists of feed and permeate channel which is separated by a flat sheet hydrophobic membrane. A polytetrafluoroethylene (PTFE) flat sheet membrane by Sterlitech Corporation, USA, is used. The membrane properties are listed in Table 3. The feed channel has a width of 1.5 cm, a length of 7 cm and a height of 0.3 cm. To accurately validate the simulations with the experimental data, the computational domain is matched with the physical feed channel in size.

The mean permeate flux (MPF) values obtained from experiments and simulations are listed in Table 3. In four cases, MPF values from the numerical simulations have a deviation of less than 6% from experimental results. Only one case has a deviation of 22.3%. Such accuracy indicates that coupling not only temperature and permeate flux but also concentration along the membrane surface is crucial for membrane transport model implementation.

Table 3. Model validation operating parameters and membrane properties.

Channel size: $W=1.5$ cm, $L=7$ cm, $h=3$ mm						
Membrane properties: $\varepsilon = 80\%$, $\delta = 100$ μm , pore size = 0.2 μm , $\tau = 1/\varepsilon$						
T_{in}	Re	Flow Rate (L/min)	Feed Velocity (m/s)	MPF (Exp.) (kg/m ² h)	MPF (CFD) (kg/m ² h)	Error %
50 °C	200	0.1	0.04	11.57	14.15	22.3
	602	0.3	0.11	16.93	17.86	5.5
	1000	0.5	0.19	19.7	20	1.5
80 °C	200	0.07	0.02	42.80	41.37	3.3
	1000	0.33	0.12	57.36	60.10	4.8

3. RESULTS AND DISCUSSION

The focus of this study is on the performance of VMD systems with cylindrical filaments in the feed channel under four different feed channel inlet conditions. The membrane properties and operating conditions are shown in Table 1. Contours, profiles, and averaged values for several performance parameters are examined for each condition. The contour plots are shown to provide visual interpretation and understanding of the flow-field and physics with the addition of filaments to the feed channel. This understanding is carried forward into detailed comparisons to the empty channel configuration. The latter can be used as the basis for performance evaluations and design trade studies.

3.1. Transient Flow Structures

Two important parameters used to evaluate membrane performance are the polarization coefficients. There are more multiple approaches to estimate the temperature polarization coefficient, as documented in Ref. [8], [22] and [42]. The present study uses the temperature polarization coefficient (TPC), θ , proposed by Khayet and Matsuura [7] to provide a quantitative evaluation of temperature polarization. The TPC is

$$\theta = \frac{T - T_{sat}}{T_f - T_{sat}} \quad (22)$$

where T is the local temperature at the membrane surface, T_{sat} is the saturation temperature for the applied vacuum pressure, and T_f is the bulk temperature determined at the feed inlet in this study, whereas Khayet and Matsura [7] calculated the bulk temperature along the stream-wise direction. The bulk temperature along the stream-wise direction is not used to avoid tedious calculation since it will not change the conclusion drawn about the temperature polarization in this work. The TPC varies from 0 to 1 with the best performance as the TPC approaches unity. Lower TPC's indicate degradation in system performance. If the membrane temperature reaches the equilibrium with the saturation temperature for the applied vacuum pressure, the membrane becomes dysfunctional [7].

Similarly, concentration polarization is evaluated using the concentration polarization coefficient (CPC) which is defined as

$$\varphi = \frac{c}{c_f} \quad (23)$$

where c is the concentration at the membrane surface and c_f is the bulk concentration in the feed channel. As with TPC, the ideal case is a CPC of unity. CPC values above unity indicate concentration elevation near the membrane surface. Elevated concentration polarization near the

1 membrane surface results in a decrease in the partial pressure and a corresponding decrease in
2 mass flux through the membrane. TPC and CPC are used throughout this study.

3 The flow-field within the membrane channel and resulting membrane performance in the
4 presence of filaments are transient and three-dimensional. Figure 4 illustrates the importance of
5 computing the unsteady characteristics of the flow using the LES simulation. Figure 4a through
6 4c show TPC on the top membrane surface adjacent to the filaments at three instances in time
7 (non-dimensional) ((a) $\tau_i = 493.2$, (b) $\tau_i = 575.4$, (c) $\tau_i = 657.6$). Figure 4d contains the time-
8 averaged TPC at the same location and Figure 4e shows TPC time history at two locations along
9 the membrane surface $x/d = 17.5$ and $x/d = 32.5$, x is the coordinate in the stream-wise
10 direction, and d is the diameter of filaments diameter.

Figure 4. Contours (a, b, c, d) and time history (e) of temperature polarization coefficient for non-dimensional time (a) $\tau_i = 493.2$, (b) $\tau_i = 575.4$, (c) $\tau_i = 657.6$, and (d) time-averaged at the top membrane surface. Time-history is shown for two different locations on the top membrane surface.

Through a comparison of Figure 4a – Figure 4c against Figure 4d, it is shown that the time-averaged solution does not accurately capture the transient behavior and can lead to incorrect module design decisions. The time-averaged solution (Figure 4d) indicates that the filaments only affect TPC in the membrane area immediately adjacent to it. This could lead to the conclusion that the filaments need to be tightly spaced to exhibit a benefit. However, the

unsteady results (Figure 4a through 4c) clearly show changes in TPC downstream of the filaments.

Figure 5a-5c shows CPC on the top membrane surface for the same three instances in Figure 4. The time-averaged CPC is shown in Figure 5d. The instantaneous images show that regions with high polarization are not stationary, but changes with time. The concentration polarization zones give an indication where fouling/scaling might occur. The concentration contours show similar trend that has an important value; meaning the regions for potential fouling/scaling vary in time. This would delay the occurrence of major fouling/scaling in the module. The steady simulations cannot capture such behavior.

Figure 5. Contours (a, b, c, d) concentration polarization coefficient ϕ , for non-dimensional time (a) $\tau_i = 493.2$, (b) $\tau_i = 575.4$, (c) $\tau_i = 657.6$, and (d) time-averaged at the top membrane surface.

The complex flow-field is further elucidated by observing the velocity and vorticity. Figure 6 shows instantaneous iso-surfaces of the stream-wise velocity as well as the x and y components of vorticity for the case with the inlet temperature of 80 °C. The left-hand side of the figure contains the results for Reynolds number of 200 and the right-hand side for Reynolds number of 1000.

Figure 6. Instantaneous iso-surfaces at non-dimensional time τ_i of the stream-wise velocity (first row), x-vorticity (second row), and y-vorticity (third row) for $Re = 200$ (left column) and $Re = 1000$ (right column) at $T = 80^\circ\text{C}$. The negative and positive vorticities are red and blue, respectively. The normalized vorticity, Ω , is obtained by $\omega/(U_{ave}/d)$.

Each case shows a different level of influence of the filaments. Figure 6a indicates that at lower Reynolds number the flow remains mostly two-dimensional whereas it is significantly three-dimensional at higher Reynolds number, as illustrated in Figure 6b. Once we take a closer look at the vorticity iso-surfaces, it is noticed that the vortical activity at lower flow speed is not so much dependent on the span-wise direction agreeing with the assertion made about secondary flows. As we compare the level and structure of the vorticity between Reynolds number of 200 and 1000 it is obvious that higher flow speeds induce secondary flow and more of scattered vortical structures. Also, the elevated vortical activity at higher Reynolds number extends up until to the next filament suggesting a strong transient behavior leading to more mixing.

3.2. Characterizing Flow Properties on the Membrane Surface

The pressure exerted on the membrane surface is an important parameter in VMD system design as it must be kept below the LEP as defined in Eq. 10 for the system to prevent membrane wetting. The instantaneous pressure is provided in Figure 7 as a differential pressure defined as

$$p_d = p_m - p_o \quad (24)$$

where p_m is the pressure on the membrane surface and p_o is the outlet pressure. The pressure results are interesting as they show a significant decrease in pressure with increasing temperature. This decrease in pressure is a result of the viscosity decrease due to the elevated temperature. Furthermore, higher flow rate yields to more pressure drop which increases the applied pressure on the membrane surface. Inclusion of filaments at higher inlet flow rates should be investigated rigorously to prevent membrane wetting.

Figure 7. Instantaneous contours of the differential pressure, p_d (Pa), on the top membrane surface at a non-dimensional time τ_i with the addition of filaments for (a) $Re = 200, T = 50^\circ\text{C}$ (b) $Re = 200, T = 80^\circ\text{C}$ (c) $Re = 1000, T = 50^\circ\text{C}$ (d) $Re = 1000, T = 80^\circ\text{C}$.

Figure 8 and Figure 9 show the instantaneous TPC and CPC, respectively. Each is provided as a contour plot comparing performance for the four different operating conditions. The left-hand side of each figure shows the coefficient for the lower temperature cases ($T = 50^\circ\text{C}$) while the right-hand side shows the higher temperature cases ($T = 80^\circ\text{C}$). The upper half of the figure provides the results for the lower Reynolds number ($Re = 200$), and the lower half contains the results for the higher Reynolds number cases ($Re = 1000$). In the low Reynolds number cases, TPC decreases in the flow direction between the cylindrical filaments as well as overall along the length (Figure 8a and Figure 8b) while CPC increases (Figure 9a and Figure 9b). Each of these indicates a decrease in performance. The decrease in coefficient is less pronounced in higher flow rate due to turbulent mixing. The presence of the cylindrical filaments improves the performance in the area directly near the filament as the flow is disturbed and velocity increased

around the cylinder. The increase in momentum mixing and the three-dimensional flow field is more readily observed in the higher Reynolds number cases. Figure 8c and Figure 8d, as well as Figure 9c and 9d, provide insight as to how the flow field shapes and reduces the polarization effects (increasing TPC and decreasing CPC). Additionally, it is shown that higher operating temperatures result in more polarization due to increased flux. Thus, higher temperature cases benefit more from the presence of filaments. Furthermore, at higher flow rates the flow becomes three-dimensional and such secondary flows contribute to the mixing results in more mitigation of both polarization mechanisms.

Figure 8. Instantaneous contours of the temperature polarization coefficient, θ , on the top membrane surface at a non-dimensional time τ_i with the addition of filaments for (a) $Re = 200, T = 50^\circ\text{C}$ (b) $Re = 200, T = 80^\circ\text{C}$ (c) $Re = 1000, T = 50^\circ\text{C}$ (d) $Re = 1000, T = 80^\circ\text{C}$.

Figure 9. Instantaneous contours of the concentration polarization coefficient on the top membrane surface at a non-dimensional time τ_i with the addition of filaments for (a) $Re = 200, T = 50^\circ\text{C}$ (b) $Re = 200, T = 80^\circ\text{C}$ (c) $Re = 1000, T = 50^\circ\text{C}$ (d) $Re = 1000, T = 80^\circ\text{C}$.

Figure 10 illustrates the instantaneous contours of TPC (top row) and CPC (bottom row) at three different span-wise locations and $Re = 200$ (left column), $Re = 1000$ (right column) for $T = 80^\circ\text{C}$. When low and high Reynolds numbers are compared it is noticed that the effect of secondary flows on the temperature and concentration distribution are visible thereof they do not vary much in the z -direction at lower flow speed whereas they do at higher flow speed. Concentration boundary layer thickness is low when compared to the temperature boundary layer due to the significant difference between Prandtl and Schmidt number of the feed solution. Higher flow speed mitigates the concentration and temperature polarization better due to induced momentum mixing and secondary flows.

Figure 10. Instantaneous slices on the x-y plane at a non-dimensional time τ_i with the addition of filaments of the (a) temperature polarization coefficient for $Re = 200$ (b) temperature polarization coefficient for $Re = 1000$ (c) concentration polarization coefficient for $Re = 200$ (d) concentration polarization coefficient for $Re = 1000$ at $T = 80^\circ\text{C}$.

Instantaneous contours of the local mass flux, N_t , along the top membrane surface are shown in Figure 11 for each of the conditions studied. The local mass flux is proportional to the suction rate and as expected increases in the area adjacent to the cylindrical filaments. The higher local mass flux increases with both increasing Reynolds number and increasing temperature. Note that there is a difference in scale between the right-hand and left-hand side of the graph. At the higher flow speed, the scattered distribution of higher and lower flux indicates that higher vortical activity attached to the membrane surface decrease the polarization locally and increase the flux in turn. The key contribution of transient simulations can be stated that it nicely articulates how the vortical activity is transported to the next consecutive filament. This keeps the permeate flux

level high between the filaments as well as adjacent to. The averaged mass flux values for all cases are illustrated in Figure 13.

Figure 11. Instantaneous contours of the local mass flux, N_t ($\text{kg m}^{-2}\text{h}^{-1}$), through the top membrane surface at a non-dimensional time τ_i with the addition of filaments for (a) $Re = 200, T = 50^\circ\text{C}$ (b) $Re = 200, T = 80^\circ\text{C}$ (c) $Re = 1000, T = 50^\circ\text{C}$ (d) $Re = 1000, T = 80^\circ\text{C}$.

Figure 12 shows the profiles of time-averaged temperature polarization, concentration polarization, local mass flux, and differential pressure along the membrane surface for all cases. It is noticed that in all properties except the differential pressure, the properties have similar values until the flow reaches to first filaments. Right after that filaments induce desirable momentum mixing and deviates the surface properties from the ones in the channel without filaments. TPC is more pronounced at lower Reynolds number and higher temperature, as shown in Figure 11a. So, the effect of filaments on the mitigation of polarization observed in these cases is more significant. As with the temperature polarization, concentration polarization is more

pronounced at lower flow speed and higher feed temperature because of higher permeate flux. Presence of filaments substantially mitigates the concentration polarization and $Re = 1000$; $T = 80^\circ\text{C}$ benefits the most from the filaments. As discussed before, temperature substantially changes the partial pressure of water vapor so that resulting vapor fluxes are differed by 2-3 folds between high and low feed temperatures, as illustrated in Figure 12c. Whether we consider relative or absolute improvement caused by the filaments, the higher temperature case takes advantage of the induced mixing more than lower temperatures. Due to membrane wetting risk, the examination of pressure exerted on the membrane surface is also important. As shown in Figure 12d, the differential pressure significantly increases with the inclusion of filaments. Note that y-axis on the graph is logarithmically scaled. In the spacer cases, a significant pressure drop is observed in the wake region of the last filament due to sudden expansion. Additionally, as discussed in Figure 7 above, the pressure drop is more significant at lower temperatures because of the temperature dependency of viscosity.

Figure 12. Profiles of (a) time-averaged temperature polarization coefficient, (b) concentration polarization coefficient, (c) local mass flux ($\text{kg m}^{-2}\text{h}^{-1}$), and (d) differential pressure versus stream-wise direction along a line located on top membrane surface at the mid-z location. The results are rendered with and without filaments for cases studied.

As it is aimed to increase the local mass flux ultimately, the examination of time-averaged local mass flux is achieved, and the results for all cases are illustrated in Figure 13. Based on the cases considered in this study, increasing the Reynolds number from 200 to 1000 increases the

flux in general and more significantly at higher temperatures. Introducing the filaments enhances the flux by 45% on average and 54.6% at maximum in $Re = 1000$; $T = 80^\circ\text{C}$ case. Such a result reveals that the filaments tremendously affect the local mass flux as they induce momentum mixing. Similar mass flux levels are reported by Alsaadi et al. [6].

Figure 13. Averaged water flux, N_t ($\text{kg m}^{-2}\text{h}^{-1}$), through the membrane for all 8 cases at $p_v = 5 \text{ kPa}$.

The power consumption and pressure drop are estimated in Table 4. The maximum used thermal power is in the case with filaments and at $Re = 1000$ and inlet temperature of 80°C while the lowest used thermal power is at $Re = 200$ and inlet temperature of 50°C . The pumping power consumption is very small compared with thermal power. The thermal power per volumetric permeate varies slightly with temperature and flow rate. It is lower in general for the empty channel compared to the channel filled with filaments. The variation is due to the temperature variation along the surface of the membrane and the dependence of latent heat vaporization on the temperature. The pumping power increased significantly when filaments are added in the feed channel. In order to produce fresh water efficiently in terms of power consumption, the empty feed channel performs better than placing spacers. However, this would require more membrane area which reduces the membrane module compaction. More

1 importantly, the thermal energy required for the process is the heat at a low temperature and is
2 considered as the low-grade heat. The thermal energy could be readily available from the waste
3 heat or from renewable sources at a low-cost. Hence, the remarkable increase in the permeation
4 rate per unit surfaces in these modules by using spacer filaments is viable. The spacers ought to
5 be considered in the design of modules even if the thermal energy requirement per permeation is
6 higher.

7 The maximum pressure drop per length is obtained in the module including filaments at
8 $Re = 1000$ and the inlet temperature of 50°C while the lowest pressure drop per length is
9 attained at $Re = 200$ and inlet temperature of 80°C . A critical module length is estimated by
10 limiting the pressure drop to 100 kPa as a conservative maximum tolerable pressure drop to
11 prevent wetting. With the absence of filaments, the membrane module length shows a significant
12 dependence on the operational conditions. It is worth mentioning that even with the lowest
13 possible membrane module length at $Re = 1000$ and inlet temperature 50°C the membrane
14 module can be wider or multiple membrane modules can be used in a parallel arrangement. This
15 could result in more demand for pumping power because of the increase in the feed flow rate.
16 However, it has been documented that the longer the membrane module the lower the thermal
17 efficiency [22]. By including filaments, the critical length for the onset of wetting is reduced
18 drastically for all flow rates and inlet temperature – an order of magnitude drops; highlighting
19 clearly the challenges of VMD modules consisting mixing promoters like spacers. This result
20 emphasizes the importance of design and optimization of modules using mixing promoters by
21 considering the entry pressure as one of the important factors. The second important observation
22 is that at any flow rate, with or without spacers, running the module at the higher temperature

- 1 nearly doubles the critical length of the module – so significant. The increase of temperature is
- 2 not only good for flux increase but is also good for mitigating wetting.

Table 4: Power consumption

	Empty channel				Channel with filaments			
	<i>Re</i> = 200		<i>Re</i> = 1000		<i>Re</i> = 200		<i>Re</i> = 1000	
	$T_{in} = 50^{\circ}\text{C}$	$T_{in} = 80^{\circ}\text{C}$	$T_{in} = 50^{\circ}\text{C}$	$T_{in} = 80^{\circ}\text{C}$	$T_{in} = 50^{\circ}\text{C}$	$T_{in} = 80^{\circ}\text{C}$	$T_{in} = 50^{\circ}\text{C}$	$T_{in} = 80^{\circ}\text{C}$
Thermal Power¹ (W)	12.6	40.8	16	58.7	16	58.1	20.8	91.1
Pumping Power² $\times 10^{-6}(\text{W})$	41	12	184	539	382	108	32732	9548
Vol. Permeate³ $\times 10^{-3}(\text{m}^3/(\text{m}^2\text{h}))$	19.26	62.15	23.38	89.04	23.57	86.31	30.56	137.65
Thermal Power/(Vol. Permeate) ($\text{Wm}^2\text{h}/\text{m}^3$)	654	657	684	659	678	673	681	662
Pumping Power/(Vol. Permeate) $\times 10^{-3}(\text{Wm}^2\text{h}/\text{m}^3)$	2.13	0.19	78.71	6.05	16.21	1.25	1070.97	69.36
Pressure drop per length $ \Delta P /\Delta x$ (kPa/m)	0.35	0.15	3.21	1.42	2.94	1.26	49.95	22.08
Critical module length⁴ (m)	285.21	647.41	31.2	70.21	34.04	79.16	2	4.53

¹ Thermal Power = feed mass flow rate $\times$ specific heat $\times$ temperature difference of feed inlet and outlet

² Pumping Power = feed pressure difference $\times$ feed volumetric flow rate

³ Vol. Permeate (volumetric Permeate) = N_t/ρ

⁴ Critical module length = 100 kPa / pressure drop per length

4. CONCLUSION

Three-dimensional transient laminar and turbulent flow simulations are carried out to investigate the effectiveness of filaments on the issue of concentration and temperature polarization and on the local mass flux through the membrane. The local water vapor flux, local temperature, and local concentration are fully coupled at the membrane surface without imposing empirical or semi-empirical relation for heat and mass transfer. To elucidate the effect of filaments more, different flow parameters such as feed temperature and flow rate are included in the study and time-averaged mass fluxes are compared between a channel with and without filaments for all four cases.

TPC and CPC are evaluated and it is found that the severity of both polarization increases with the higher temperature due to higher mass fluxes. Submerging filaments into the channel disrupts the flow and induces momentum and turbulent mixing resulting in the mitigation of polarization, but it creates an additional pressure drop across the module. The vortical structures are mostly two-dimensional and regular at $Re = 200$ whereas it is three-dimensional and scattered at $Re = 1000$. As with TPC and CPC, the local mass flux increases with the filaments and higher feed temperatures. The strong transient effects aid in mitigating the temperature and concentration polarization and enhancing the flux performance at higher flow rates. A great 54% increase in the permeation rate by the spacer at $Re = 1000$; $T = 80^\circ\text{C}$ comes with an expense of increased thermal power requirement. However, the thermal power increase of the process should not be a major concern since it is a low grade heat. As for the membrane wetting, the pressure applied on the membrane surface is examined and it is noticed that increasing the temperature decreases the pressure drop because of the change in the viscosity, but the inclusion of filaments increases the pressure drop significantly. The critical module length for the onset of

1 wetting decreases an order of magnitude in the module with filaments, but increases two folds
 2 when temperature changes from 50 to 80°C. Thus, it is important to monitor pressure increase
 3 while designing these systems. Further study is needed to optimize the spacer geometry using an
 4 accurate membrane modeling in the VMD process.

5 NOMENCLATURE

t	Time [s]
c	Concentration [kg/m ³]
Re	Reynolds number, $Re = U_{ave}h/\nu$
R	The gas constant [J/mol K]
LEP	Liquid entry pressure [Pa]
D	Diffusion coefficient [m ² /s]
B	Geometric factor [-]
T	Temperature [K]
p	Pressure [pa]
h	Channel height [m]
Δh_{fg}	Enthalpy of vaporization [J/kg]
y_i	Vapor mole fraction of water [-]
x_i	Coordinate directions
u_i	Velocity components [m/s]
r_p	Pore size
r_{max}	Largest pore size [m]
q_m	Heat flux through the membrane [W/m ²]
p_{wf}	Partial pressure of the water vapor at the upstream of the membrane [Pa]
p_v	Vacuum pressure [Pa]
p_o	Outlet pressure [Pa]
p_m	Pressure on the membrane surface [Pa]
p_i	Partial pressure [Pa]
p_d	Differential pressure [Pa]
$\bar{p}$	Mean pressure within the pore [Pa]
k_f	Thermal conductivity [W/m K]
k_B	Boltzmann constant [J/K]
c_p	Specific heat [J/Kg K]
c_f	Feed concentration [kg/m ³]
X_i	Liquid mole fraction of water
X_{NaCl}	Mole fraction of NaCl
V_m	Normal velocity to the membrane surface [m/s]
U_{ave}	Averaged velocity [m/s]

T_{sat}	Saturation temperature [K]	1
T_f	Feed temperature [K]	
P^0	Saturation pressure [Pa]	
M_w	Molecular weight of water [kg/mol]	
N_t	Local mass flux [kg/m ² h]	
J_v	Molar flux by viscous diffusion [mol/m ² s]	
J_t	Total molar flux [mol/m ² s]	
J_k	Molar flux by Knudsen diffusion [mol/m ² s]	

Greek Letters

α_i	Activity coefficient [-]
α_{water}	Activity coefficient of water
γ_i	Liquid surface tension [N/m]
ε_s	Surface porosity [-]
μ_w	Viscosity of water vapor [Pa s]
α	Liquid-solid contact angle [°]
δ	Membrane thickness [m]
ε	Porosity [-]
λ	Mean free path [m]
ν	Kinematic viscosity
π	Constant
ρ	Density [kg/m ³]
σ	Collision diameter [m]
τ_i	Non-dimensional time, $\tau_i = t U_{ave}/d$
τ	Tortuosity [-]
θ	Temperature polarization coefficient [-]
φ	Concentration polarization coefficient [-]

2

3 ACKNOWLEDGMENTS

4 The co-author Ali E. Anqi extends his appreciation to the Deanship of Scientific Research at
5 King Khalid University for the support he received through General Research Project under the
6 grant number (R.G.P.1/120/40). The research reported in this paper was also supported by King
7 Abdullah University of Science and Technology (KAUST), Saudi Arabia.

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HIGHLIGHTS:

- Transient three-dimensional simulations are conducted for VMD.
- Water flux, temperature and concentration are coupled at the membrane surface.
- Spacer is placed in the feed channel to enhance the membrane performance.
- Transient simulations reveal strong vortical structures in the feed channel.
- High feed flow rate and temperature increase permeate by 54% with spacer presence.

Conflict of Interest:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.