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# Model-guided design of high-performance membrane distillation modules for water desalination



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#### ARTICLE INFO

#### ABSTRACT

Keywords: Membrane distillation Hollow fiber membrane Module design Modeling Packing configuration The significance of geometrical and physical parameters of hollow fiber membrane modules in the membrane distillation process has not been fully evaluated. In this study, we develop a three-dimensional multi-physics model of a hollow fiber membrane module in order to investigate the effect of operating and design parameters on the module performance. The permeate flux and thermal efficiency of the system are considered as the characteristic parameters of the module, operated in direct contact membrane distillation mode (DCMD). The simulation results indicate that the permeate flux for the module can be enhanced by 54% when 1) the hollow fibers are in close-packed configuration, and 2) the interspacing parameter, the ratio of a fiber radius to the center-to-center distance between neighboring fibers, is adjusted properly. We identify the fiber interspacing parameter as a critical parameter for the module design. The permeate flux significantly drops when the interspacing parameter is equal to a value of 0.5, implying that the fibers are adjacent to each other. Moreover, the results indicate that, in our system, the time constant for the mass transfer process through the membrane is higher than that of heat transfer, meaning that the DCMD process for a hollow fiber membrane module under parallel flow condition is a mass transfer limited process.

#### 1. Introduction

Water scarcity induced by population growth and climate change has increased the demand for alternative methods of providing additional potable water [1,2]. Membrane-based separation technologies have been shown to be promising candidates for tackling the challenges related to water scarcity [3–7].

Membrane distillation (MD) is an emerging separation process for producing clean water through desalination of seawater and brackish water [2,8–10]. In MD, a hydrophobic membrane acts as a physical barrier between the feed and distillate streams. The membrane allows the water vapor to diffuse through the porous domains but hinders water transport. MD can be operated in three different modes: direct contact membrane distillation (DCMD), air gap membrane distillation (AGMD), and sweeping gas membrane distillation (SGMD) [11,12]. Of these operation modes, DCMD is the most frequently used method in desalination of water due to the simplicity of design and operation. [8,9,11,13].

MD has several advantages over other desalination methods. One distinct feature of the MD process is its theoretical, non-selective, 100% rejection value for non-volatile species. This unique characteristic makes MD an attractive process for removal of heavy metal ions from

the water supply [14–16]. Additionally, the driving force for the mass transfer in MD is not very sensitive to water salinity. It has been shown that the permeate flux only decreases 5% when the total dissolved solids (TDS) in the feed stream was increased from 35,000 mg/L to 75,000 mg/L [17,18]. Another important aspect of MD lies in its low processing pressure and temperature demand. The operability of MD at low temperatures (50–80 °C) allows for the coupling of the process with renewable and affordable energy resources such as solar and waste heat [5,19–21]. Moreover, compared to the pressure-driven processes, the low operating pressure in MD reduces the mechanical demands of the system and the fouling propensity of the membranes [17,22–27].

Although MD is a promising technology, it has not been fully developed for water desalination. The less-than-mature state of the technology is attributed to its lower permeate flux and energy efficiency compared to those of fully commercialized desalination processes such as reverse osmosis (RO) [28]. The main reason for low permeate flux and energy efficiency in the MD process is the lack of custom-made membranes and high-performance modules, designed and optimized explicitly for the MD operation [11]. Recently, it has been shown that a significantly high permeate flux can be obtained using MD when the membranes are specifically designed for that purpose [5-7,26,27,29-32].

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Nomenclature		h AH	Heat transfer coefficient (W m <sup><math>-2</math></sup> K <sup><math>-1</math></sup> ) The heat of evaporation (I mol <sup><math>-1</math></sup> )
Nomen $\gamma_w$ $\delta$ $\delta_a$ $\delta_w$ $\varepsilon$ $\theta$ $\lambda_{w-a}$ $\mu$ $\nu_r$ $\nu_{\theta}$ $\nu_z$ $\rho$ $\tau$ $\chi_a$ $\chi_m$ $\chi_p$ a $C_p$ $d_p$ $D_{eff}$ $D_H$ $D_{kn}$	clature Activity coefficient of water Membrane thickness (m) Collision diameter of air (m) Collision diameter of water molecules (m) Membrane porosity Temperature polarization Mean free path of water molecules in the air (m) Viscosity (Pa s) Fluid velocity in the radial direction (m s <sup>-1</sup> ) Fluid velocity in the angular direction (m s <sup>-1</sup> ) Fluid velocity in the angular direction (m s <sup>-1</sup> ) Fluid velocity in the axial direction (m s <sup>-1</sup> ) Density (kg m <sup>-3</sup> ) Tortuosity Physical properties of air Physical properties of the membrane Physical properties of the polymer Center to center distance of fibers (m) The specific heat capacity of water (J mol <sup>-1</sup> K <sup>-1</sup> ) Pore size (m) Effective diffusion coefficient (m <sup>2</sup> s <sup>-1</sup> ) Hydraulic diameter (m) Knudsen diffusion coefficient (m <sup>2</sup> s <sup>-1</sup> )	$\begin{array}{c} \Delta H_{lv} \\ J \\ k \\ k_a \\ k_m \\ k_p \\ L \\ M_a \\ M_w \\ Nu \\ P \\ P_w \\ q \\ R \\ Re \\ R_g \\ T_d \\ T_{d,in} \\ T_f \\ T_{f,in} \\ T_m \\ T_{mi} \end{array}$	Heat transfer coefficient $(W m^{-2} K^{-1})$ The heat of evaporation $(J mol^{-1})$ Permeate flux $(mol m^{-2} s^{-1})$ Water thermal conductivity $(W m^{-1} K^{-1})$ Air thermal conductivity $(W m^{-1} K^{-1})$ Membrane thermal conductivity $(W m^{-1} K^{-1})$ Polymer thermal conductivity $(W m^{-1} K^{-1})$ Fiber length $(m)$ Air molecular weight $(g mol^{-1})$ Water molecular weight $(g mol^{-1})$ Nusselt number The total pressure of the system (Pa) The partial pressure of the water (Pa) The heat of conduction $(W m^{-2})$ Hollow fiber diameter $(m)$ Reynolds number Gas constant $(J mol^{-1} K^{-1})$ Bulk temperature of distillate $(K)$ Distillate temperature at the inlet $(K)$ Bulk temperature of feed at the inlet $(K)$ Membrane temperature, inner surface $(K)$
$D_{kn}$ $D_t$ $D_{w-a}$	Total mass diffusion coefficient (m <sup>2</sup> s <sup>-1</sup> ) The molecular diffusion coefficient of water in the air (m <sup>2</sup> s <sup>-1</sup> )	$rac{T_{mo}}{V}$	Velocity vector

Apart from membrane structure and materials, proper module design is another important factor for achieving a high permeate flux [33–35]. Among all kinds of membrane modules, hollow fiber membrane modules are promising candidates for MD operation. Hollow fiber membrane modules offer the highest membrane packing density, reducing the capital cost of the process [29,36–40]. The packing density of these modules varies between 500 and 9000 m<sup>2</sup>/m<sup>3</sup>, exceeding the reported values of the spiral-wound modules ( $1200 \text{ m}^2/\text{m}^3$ ) [11]. Hollow fiber membrane modules also offer an excellent mass transfer coefficient, high mechanical strength, and a small footprint [41,42].

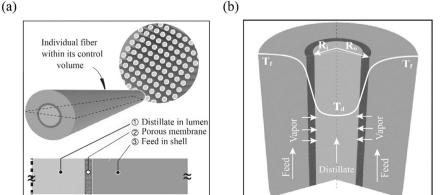
Computational Fluid Dynamics (CFD) has been one of the most popular methods for studying water desalination systems, especially membrane distillation [9,43–50]. However, there does not exist a threedimensional fully-coupled (momentum, heat, and mass transfer phenomena) mathematical model, capturing the importance of packing configuration, fiber-to-fiber interspacing, hollow fiber membrane properties, and process conditions for designing high-performance hollow fiber membrane modules.

In the present work, we develop a fully-coupled mathematical model to investigate the effect of different packing configurations of hollow fiber membrane modules, operating in the DCMD process, on module performance. Additionally, we identify the importance of the fiber interspacing parameter to the flux and energy efficiency of the simulated MD module. We studied the impact of various geometrical and process parameters on module performance to arrive at the optimal design and operating conditions. Here, we introduce the geometrical and operating conditions that permit the module to provide both high thermal efficiency and permeate flux. This model-guided approach enables the design of high-performance hollow fiber membrane modules.

#### 2. Mathematical modeling

The governing equations for the MD process include mass, momentum, and energy transfer equations. Fig. 1 shows an individual hollow fiber membrane in the bundle of fibers, as well as the configuration of feed and distillate streams. As shown in Fig. 1.b, the feed stream (saline water) flows in the shell side, whereas distillate (freshwater) concurrently flows through the core. The temperature gradient across the membrane results in a vapor pressure difference, which is the

> **Fig. 1.** The schematic of a hollow fiber membrane module. (a) An individual fiber within its control volume is divided into three subsystems: 1) distillate in the lumen, 2) porous membrane, and 3) feed in the shell (the cross-section representation is not to scale). (b) A schematic of the hollow fiber membrane cross-section, and representative temperature profile in the system.



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