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# Molecular Dynamic Simulations of Fibrous Distillation Membranes

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ABSTRACT

The rate of heat and mass transfer through distillation membranes is typically estimated using an over-simplified, straight-cylindrical-pore approach coupled with several empirical correction factors that are included to compensate for the simplicity of the approach. In the present work, we have calculated for the first time the rate of transport of heat and mass through three-dimensional virtual membranes from first principles without the need for any empirical correction factors. More specifically, molecular dynamic (MD) simulations are conducted in idealized 3-D geometries that resemble the microstructure of a nanofiber membrane. The SPC/E molecular model and coarse-grain Pea model are considered to simulate, respectively, water molecules and air. The fibers, on the other hand, are constructed as simple metal lattice, and their contact angle with water is controlled using a scaling factor from the Lorentz–Berthelot mixing parameters. A proof-of-concept study is presented to demonstrate the capabilities of the new modeling approach in predicting the effects of the membrane's microstructural properties on the desalination performance. While the simulations are conducted at scales 3–4 orders of magnitudes smaller than an actual electrospun membrane, the conclusions can be applied membranes with more practical dimensions.

## 1. Introduction

Scarcity of fresh water is a major global concern that is expected to worsen as the impact of global warming on our planet becomes more severe in the next decades. When a modest amount of energy is available, direct-contact membrane distillation (DCMD) is a method for producing freshwater by creating a temperature difference between the feed (warm salty water) and permeate (cold purified water) separated from one another by a hydrophobic membrane [1,2]. The temperature difference across the membrane, in turn, creates a vapor pressure gradient that serves as the driving mechanism for the transport of water vapor from the feed to the permeate through the pores of the membrane (see Fig. 1). Mass transfer through a DCMD membrane is directly related to fresh water production rate and should be maximized, while heat transfer should be minimized to maintain a temperature difference across the membrane [3]. Therefore, developing computational tools that allow one to predict the rate of heat and mass transport through a DCMD membrane can be very beneficial in optimizing the microstructure of such membranes.

Vapor transport through a membrane can generally be characterized using the concept of molecular diffusion through a straight cylindrical pore [1–8]. Such a model can be incorporated in a larger (continuum flow) numerical simulation that includes the feed and permeate flow and temperature fields outside the membrane [1,9–13]. This classical approach relies on predetermined empirical factors/relationships that compensate for the over-simplified description of the membrane's microstructure. Being empirical in nature, those correction factors can only be used in studying the particular membrane for which they were obtained [14].

To overcome the aforementioned limitations, the present study is devised to investigate how molecular dynamic simulations (MD) can be used to simulate vapor transport through a DCMD membrane without (or with minimal) use of case-dependent empirical factors. Creating a universally-applicable simulation method will allow for optimizing the microstructure of the membranes for different flow conditions. The present paper is, however, only a starting point in our path to this ambitious goal. The present research is in fact the first to consider MD simulations to predict the rate of mass and transfer through a DCMD membrane. Given the complicated internal porous structure of membranes produced via film extrusion, we have focused our study on

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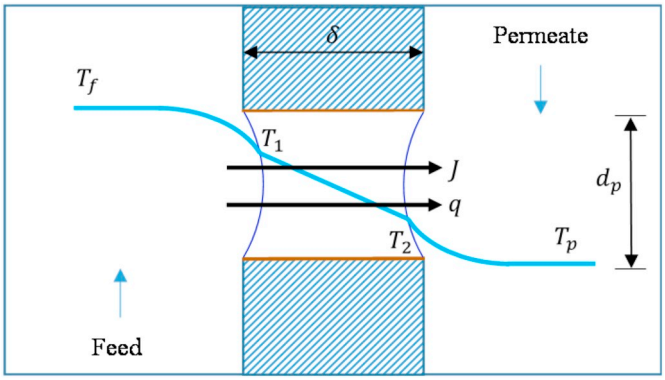


**Fig. 1.** Traditional approach to study distillation membranes where membrane pores are represented as a straight cylindrical hole with a length of δ and a diameter of $d_p$. The difference between the feed temperature $T_f$ and permeate temperature $T_p$ temperatures is the main driving force for vapor transport across the membrane.

membranes made of hydrophobic fibers (e.g., electrospun membranes [15,16]) known for their well-defined microstructures. While many membranes for DCMD are produced through solution-based electrospinning, there is a growing desire for using melt-electrospinning which provides a pathway for controlled fiber deposition [17,18]. Such controlled fiber deposition allows for predetermined pore geometry and uniformity compared to the random nature of solution electrospinning [15–18]. For the sake of simplicity, the virtual membranes are made of orthogonally-oriented fibers as might be prepared through melt-electrospinning methods. The fiber orientation in this study was kept constant while variables such as fiber diameter, hydrophobicity, and spacing were explored.

In the remainder of this paper, we first describe our approach toward MD simulations in Section 2, and then present a case where MD simulations are used to model vapor transport in a simplified virtual membrane in Section 3. The conclusions drawn from our study are given in Section 4.

## 2. Molecular Dynamic Simulations

MD is a molecular-level simulation approach based on integrating the equations of motion written for every atom in a substance over time [19]. The initial position and velocity of these atoms are used as the starting conditions in the integration process to predict future positions and velocities for the entire system [19–22]. In this work, the equations of motion are integrated using the Velocity–Verlet algorithm [23]. Using the principles of statistical mechanics, system properties (e.g., energy, temperature, and pressure) are then quantified and reported. The interaction between the molecules in an MD simulation is presented in terms of interatomic (bonded or non-bonded) potential energy [24]. The LAMMPS MD simulation code is used in our study for its flexibility and proven accuracy [25,26]. Certain assumptions have been considered to help speed up the otherwise computer-intensive MD calculations, as will be discussed later in this section.

An SPC/E water model is considered to model the interactions between water molecules [27,28]. The SPC model is proven to provide fairly accurate predictions for physical properties such as density, surface tension, and heat of evaporation, in good agreement with experimental results [27,28]. In this model, the total potential energy $U_{ij}^{SPC/E}$ of an interacting pair of particles $i$ and $j$ is.

$$U_{ij}^{\mathrm{SPC/E}} = U_{ij}^{\mathrm{disp}} + U_{ij}^{\mathrm{LRC}} + U_{ij}^{\mathrm{Coulomb}} \quad (1)$$

where the superscripts "disp", "LRC", and "Coulomb" stand for pair dispersion energy, long-range correction to the pair dispersion energy, and the Coulombic potential energy, respectively [25,26,28–30].

The traditional Lennard-Jones (LJ) intermolecular potential energy is considered for the pair dispersion energy [26]. The term $U_{ij}^{\mathrm{LRC}}$ is known as the long-range Coulombic potential which is calculated in the present work using the particle–particle particle–mesh (PPPM) method with an accuracy of $1 \times 10^{-4}$ [30].

Since the long-range interaction of the Coulombic term is highly important for the surface tension calculations of the SPC/E model, an Ewald sum is introduced to correct these interactions [25,29–33]. Moreover, for the LJ term, an empirical tail correction is introduced to recover the discrepancies caused by these long-term interactions in the Coulombic term [31–33]. The SHAKE algorithm is utilized to constrain the internal geometry of each water molecule with time [25]. In the flexible isosceles triangle model of SPC/E model, constant charges of −0.8476 e and 0.4238 e were considered for the oxygen and hydrogen atoms, respectively. For the intramolecular bonds in the SPC/E model, the harmonic bond was assumed to be $\frac{1}{2}k_b(r - r_0)^2$ with an amplitude of $k_b = 1000.0$ eV/A$^2$ and distance-parameter of $r_0 = 1.0$ $A$, while the angle bond can be written as $\frac{1}{2}k_\theta(\theta - \theta_0)^2$ with an amplitude of $k_\theta = 1000.0$ eV and angular-parameter of $\theta_0 = 109.47^\circ$ [34]. The open-source code of LAMMPS is used for the modeling of these bonds [26].

To examine the accuracy of the SPC/E model, we compared its predictions against those obtained from the TIP4P model (a four-site molecule), which is a more accurate water molecule model (but computationally much slower). We simulated a water droplet with an arbitrary diameter and temperature using both the SPC/E and TIP4P models with identical initial input parameters. Using the Laplace equation, surface tension values of 0.0635 N/m and 0.0748 N/m at $T = 300$ K were obtained from, respectively, the SPC/E and TIP4P simulations. From SPC/E there is an underestimation of about 12% in the surface tension compared to the experimental value of 0.072 N/m [35]. This is because the SPC/E model is non-polarizable [36], and there is also an overestimation of the diffusion constant where the hydrogen bonding is not sufficiently simulated in the SPC/E model [20,37].

The smallest computational domain considered for the simulations reported here is shown in Fig. 2 (larger domains are created by repeating the 4-fiber unit cell shown in the figure in the z-direction). To

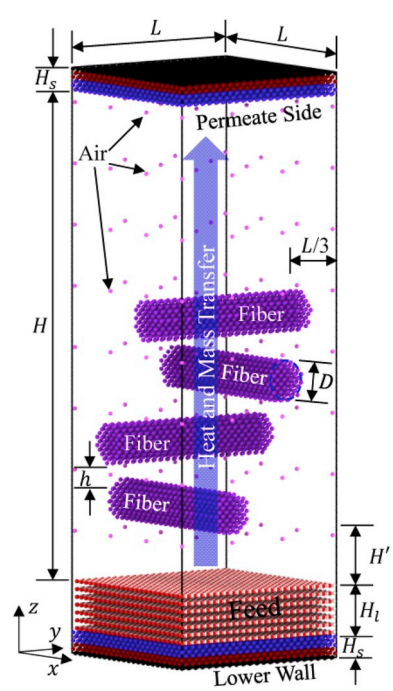


**Fig. 2.** Smallest simulation domain (unit cell) comprised of four fibers between two parallel boundaries with spacing $H$. Larger domains are created by repeating the 4-fiber unit cell in the z-direction.

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