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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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