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A ballistic transport model for vacuum membrane distillation

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ABSTRACT

Vacuum Membrane Distillation (VMD) as other membrane distillation (MD) techniques is receiving much attention for its ability to produce drinkable water at low cost. Aiming to analyze the VMD process and particularly mass transfer through porous membranes, a ballistic flow model is developed to predict fluxes out from high aspect ratio cylindrical pores. The model is based on the estimation of direct and indirect transmission probabilities by direct integration of species flux. A power law that uses the pore aspect ratio is developed to enable a quick estimation of the flux fraction exiting the pore. The flux entering the pore is calculated using Hertz–Knudsen–Schrage equation and depends on the values of the condensation and evaporation coefficients of the transferred species. Simulation results are compared to classical Knudsen diffusion predictions as well as to experimental data.

1. Introduction

Water scarcity around the world has led to water production from sea and brackish water. Production of drinking water by membrane processes is crucial as it stands energetically efficient compared to other processes. Over decades, reverse osmosis (RO) has been used as an attractive choice to purify water for both industrial and household usage. However, other processes for water purification exist among which MD represents an attractive choice. Indeed, MD requires low operating temperature and pressure compared to multi-stage flash distillation and RO.

MD is a thermally driven process [1,2] where low-grade waste heat or renewable energy can be used to produce drinking water. However, MD modules performance depends on the membrane transport properties. The driving force in MD process is the difference between the partial pressure of the transferred vapor between the feed and the permeate sides. This non-equilibrium state can be generated using various techniques that result in different MD configurations. A basic design would be represented by two independent containers (volumes), the permeate container and the feed container respectively, separated by a membrane. In direct contact membrane distillation (DCMD), a fluid in direct contact with the membrane flows in the permeate compartment at a lower temperature than the feed side. In air gap membrane distillation (AGMD), a stagnant gas resides in the permeate side between the membrane and the condensing liquid, while a cold gas flows in sweeping gas membrane distillation (SGMD) and vacuum prevails in vacuum membrane distillation (VMD) (see [3] for details). Most recent research efforts focused on DCMD [4], although all configurations are still at the laboratory or small pilot phase [2]. However, VMD is receiving much attention [5–10] as it shows promising in various applications including the separation of aqueous solutions and the elimination of gaseous and organic volatile compounds from water. VMD presents several advantages in sea water desalination [11,12], and suffers less from the polarization phenomenon at the membrane surface. Tang et al. [13] conducted VMD through PVDF hollow fiber membranes to separate NaCl from aqueous solutions, which suggests VMD as a viable alternative for the treatment of high salinity brine. Moreover, heat losses by conduction through the membrane are drastically reduced and are sometimes negligible. However, the risk of pore wetting remains significant in VMD [11].

Modeling and analysis of membrane distillation is still under intensive development and efforts are deployed towards an efficient VMD usage for desalination [11,14]. Experimental studies have been conducted and models have been established to determine the most important parameters that might affect VMD membrane modules, permeation flux and energy consumption [12]. For a given membrane, process sensitivity has been commonly attributed to feed temperature and feed rate as well as vacuum pressure and the solute concentration in the feed solution.

The dusty gas model (DGM), established for mass transfer in porous media [15,16], is commonly used to estimate the permeation flux through membranes in MD. Soni et al. [17] developed a mathematical model for transport phenomena in VMD and considered the temperature dependence on the fluid physical properties. Both experimental and modeling results show that the permeation flux increases when the pressure is dropped (higher vacuum) as well as when the feed rate is increased. Banat et al. [6] carried out a sensitivity analysis on the operating conditions.

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The authors showed that mass flux through the membrane is highly sensitive to the feed temperature, particularly at higher vacuum, while sensitive to vacuum pressure when the lowest feed temperatures are used. In a similar approach, Upadhyaya et al. [18] conducted a sensitivity analysis of VMD for desalination aiming to identify the most important parameters that influence mass transfer. Their results show that for the desalination process, mass flux is remarkably affected by membrane characteristics (thickness, tortuosity, porosity, pore diameter), while it remains sensitive to vacuum pressure and feed temperature. Analogously, Cabassud and Wirth [12] emphasized the important effect of membrane permeability and pointed out the ability of VMD to energetically compete with RO when choosing a proper membrane.

2. Knudsen diffusion in VMD

Flow in thin long tubes is commonly classified into different categories depending on the operating conditions. At relatively high pressures, where the media is considered as a continuum, molecule–molecule collisions dominate and the flow is described by ordinary diffusion. Indeed, a molecule traveling through the tube is more likely to hit another molecule than the tube side walls. As the pressure decreases, molecule–wall collisions become more frequent and the flow is often considered transitional and described by a combination of ordinary diffusion and Knudsen diffusion. When the medium becomes rarefied, molecule–wall collisions dominate the flow, and Knudsen diffusion takes place. The Knudsen number "*Kn*" enables assessing the prevailing regime. It is commonly expressed as the ratio of the mean free path λ to the medium characteristic length, commonly taken as the membrane pore diameter (d_p) in MD, viz.

$$Kn = \frac{\lambda}{d_p} \tag{1}$$

where the mean free path is usually expressed as [19]

$$\lambda = \frac{1}{\sqrt{2}(\pi d^2) n_m} \tag{2}$$

where (πd^2) represents the collision cross section and n_m the number of molecules. Using the ideal gas law, Eq. (2) is rewritten:

$$\lambda = \frac{k_B T}{\sqrt{2}(\pi d^2) P} \tag{3}$$

where k_B is the Boltzmann constant, T the absolute temperature and P the pressure. In MD applications the average pressure $\overline{P}$ and the average temperature $\overline{T}$ between the feed side and the permeate side of the membrane pore are used [3]. The Knudsen number is thus simply expressed as

$$Kn = \frac{k_B \overline{T}}{\sqrt{2}(\pi d^2) \overline{P} d_p} \tag{4}$$

Values of K_n higher than 10 indicate a Knudsen diffusion mechanism, while for values lower than 0.01 classical diffusion mechanism prevails. Therefore, a wide transition regime exists between these two upper and lower values where both type of mechanisms contribute to species transport [3].

The development of predictive models for vacuum membrane distillation is an ongoing process. Prediction of permeate fluxes of some species s is commonly approached by solving the following differential form of Knudsen diffusion [15]:

$$\mathfrak{J} = -\frac{4}{3} K \overline{v}_s \nabla C_s \tag{5}$$

where $\mathfrak{J}$ is the flux of species s (mol m^{-2} s^{-1}). $\overline{v}_s$ is the species average molecular speed (m s^{-1}) given by $\sqrt{8R_gT/\pi M_s}$, where R_g represents the ideal gas constant (8.314 J K^{-1} mol^{-1}), T the temperature (K) and M_s the molecular weight of species s (kg mol^{-1}). K is a parameter called permeability coefficient with the units of (m) that depends only on the pore geometry and the gas-surface scattering law. K is often measured experimentally but rarely known with precision [15]. For long cylindrical pores and diffuse scattering, K is assumed $R/2$ where R is the pore radius. C_s is the concentration of species s (mol m^{-3}).

The correction of the diffusion coefficient by the porosity (ε)/tortuosity (τ) factor and using the ideal gas law leads to the following form of Eq. (5):

$$\mathfrak{J} = -\frac{2R\varepsilon}{3\tau}\sqrt{\frac{8}{\pi R_g T M_s}}\nabla P_s \tag{6}$$

where P_s is the partial pressure of species s.

A linear approximation of the partial pressure gradient over the pore length L and multiplication by the molecular weight gives the mass flux J (Kg m^{-2} s^{-1}) of species s:

$$J = -\frac{2R\varepsilon}{3L\tau}\sqrt{\frac{8M_s}{\pi R_g T}}\Delta P_s \tag{7}$$

Although subject to accurate values of the porosity/tortuosity factor, Eq. (7) is commonly used to predict permeate fluxes without explicit knowledge of membrane pore geometry. However, in the present work, the ability of pore scale simulation to predict experimental data is assessed. Pore size calculations, of which the basic approach is detailed in the sequel, are carried out by integrating fluxes of species incoming from the liquid–vapor interface and summing up the re-emission contribution resulting from collisions with the pore side walls.

3. Ballistic model development

Since Knudsen early work [20], flow in rarefied media has been the focus of many research efforts. Steckelmacher [21] presents the evolution of flow models over seventy five years, providing an analysis and comparison of different advances in the area including those by Knudsen, Smoluchowski, Langmuir, Clausing… The main interest is clearly the prediction of the flux of species leaving the tube or the capillary and preferably the evaluation of the "direct" contribution from the pore inlet and the "indirect" contribution resulting from collisions with the pore sidewalls. The fraction of species that leaves the tube is often referred to the transmission probability or the Clausing factor as a reference to Clausing [22] who initially tackled the problem.

As recently stressed out by Shi et al. [23], Clausing developed an integral equation to calculate the indirect contribution but failed to predict the asymptotic limit when pore length becomes much larger than the diameter. The authors present a comparative analysis of Knudsen [20], Walsh [24] and Pollard and Present [25] respective works to develop an analytical approach consistent with the asymptotic behavior observed for very long tubes or very short tubes. They present an analytical expression for the indirect contribution with comparison to Monte Carlo simulations. At this point, accurate analytical expressions of transmission probabilities for cylindrical, conical and even bulged tubes are available [23]. However numerical approaches are required to investigate the effect of more complex pore structures on species transport. Although Monte Carlo simulations have been widely used to simulate Knudsen flow [23,26,27], ballistic transport has also been undertaken to predict transport with surface reaction mechanisms occurring in micro/nanosized features as encountered in semiconductor processing [28,29]. Most applications focused on pores (vias) of relatively moderate aspect ratios, even though recent