Mathematical Modeling and Simulation of Coupling Parameters Transfers of Steam in a Membrane-Type Solar Still AGMD

Mandiang Y*, Sene M and Thiam A

Laboratoire d’Energétique Appliquée (LEA), Ecole Supérieure Polytechnique (ESP) de Dakar, BP 5085 Université Cheikh Anta Diop (UCAD) de Dakar, Senegal

Abstract

Membrane distillation (MD) is a hybrid separation technique increasingly used in various fields such as desalination and the food industry. In this work, we present three theoretical models of flow and heat and mass transfers in membrane distillation unit air gap (AGMD). The results on the effect of membrane pore size have been analyzed for different mechanisms of mass transfer involved by estimating the flow of generated steam. A mathematical model was presented for determining exchanges and possible combinations.

Keywords: Membrane; Distillation; AGMD; Diffusion; Pore

List of Symbols

\( C_s \) mole fraction of NaCl
\( D \) diffusion coefficient, \( \text{m}^2\text{s}^{-1} \)
\( d_h \) half-width of the flow channel, \( \text{m} \)
\( g \) acceleration of gravity, \( \text{m.s}^{-2} \)
\( H_m \) membrane length, \( \text{m} \)
\( J \) length-averaged permeate flux at the hot side of the membrane, \( \text{kg.m}^{-2}.\text{s}^{-1} \)
\( K \) membrane Permeability, \( \text{m}^{-1}.\text{s}^{-1} \)
\( J_l \) local permeate flux at the hot side of membrane, in vapor phase, \( \text{kg.m}^{-2}.\text{s}^{-1} \)
\( K_m \) mass transfer coefficient, \( \text{J.m}^{-2}.\text{s}^{-1}.\text{K}^{-1} \)
\( M \) molar mass, \( \text{kg.mol}^{-1} \)
\( m \) mass, \( \text{kg} \)
\( m \) mass flow rate, \( \text{kg.s}^{-1} \)
\( p \) pressure, \( \text{Pa} \)
\( p_v \) water vapor pressure, \( \text{Pa} \)
\( R \) Universal gas constant, \( \text{J.kmol}^{-1}.\text{K} \)
\( r_p \) membrane pore size, \( \text{m} \)
\( r_{1,\text{h}} \) largest membrane pore, \( \text{m} \)
\( T \) temperature, \( ^\circ\text{C} \)
\( T_{ci} \) inlet temperature of cold solution, \( ^\circ\text{C} \)
\( T_{hi} \) inlet temperature of hot solution, \( ^\circ\text{C} \)
\( \bar{T} \) average temperature, \( ^\circ\text{C} \)
\( V \) velocity, \( \text{m.s}^{-1} \)
\( V_f \) velocity of feed solution, \( \text{m.s}^{-1} \)
\( V_{r} \) the velocity in radius direction, \( \text{m.s}^{-1} \)
\( w_a \) mass fraction of air in vapour
\( z \) coordinate along the solution flow

Greek Letters

\( \Delta p \) water vapor pressure difference, \( \text{Pa} \)
\( \delta \) Thickness or width, \( \text{m} \)
\( \varepsilon \) porosity of the membrane
\( \gamma_l \) surface tension of water, \( \text{N.m}^{-1} \)
\( \mu \) dynamic viscosity, \( \text{kg.m}^{-1}.\text{s}^{-1} \)
\( \rho \) density, \( \text{kg.m}^{-3} \)
\( \tau \) tortuosity

Subscripts

\( a \) Air
\( atm \) Atmosphere
\( Avg \) Average
\( c \) cold solution
\( f \) condensate film
\( f_p \) condensate film/cooling plate interface
\( g \) vapor/air gap
\( g_f \) air gap/condensate film interface
\( h \) hot solution
\( hi \) inlet of the hot channel

*Corresponding author: Mandiang Y, Laboratoire d’Energétique Appliquée (LEA), Ecole Supérieure Polytechnique (ESP) de Dakar, BP 5085 Université Cheikh Anta Diop (UCAD) de Dakar, Senegal. Tel: (+221) 33 864 51 96; E-mail: youssouf.mandiang@yahoo.com

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of the membrane results in the evaporation of water at the hot side of the wall and the flow of steam produced by the membrane to the vapour-air space. In porous materials filled with a gas mixture, there is a pressure difference on either side of the membrane creates a mass transfer flux. This flow is modeled in the porous medium by a bundle of cylindrical capillaries controlled by the laws of transfer as reported by Damak et al. [6]. Indeed, collisions between molecules, and between molecules and the capillary walls, are the source of this transfer. There are three types of mechanisms as illustrated Figure 2, in which the species of the gas mixture can lose their momentum in the movement [7].

Knudsen diffusion

The direct mass transfer at the level of capillary wall is as a result of the molecule-wall collisions. Gas diffusion in porous media is a major step in many chemical processes. It is therefore important to have an estimate of the quantity of gas diffused through a membrane. However, this release depends not only on the parameters of the gas but also on the porous structure. In fact, in the Knudsen diffusion, the gas transfer is controlled by the successive particle-wall collisions in the flow channel.
coefficient) of the Knudsen and Fick’s flow, which are in parallel and in series with the viscous flow (Poiseuille). This model says KMPT (Knudsen Molecular Poiseuille flow transition) considers that the diffusion coefficients of molecular Knuden and are in parallel and in series with the Poiseuille.

KMT model

The KMT model (Knudsen flow Molecular Transition) does not take into account the diffusion of Poiseuille, and that Knudsen and molecular flows are in parallel (Figure 6).

Mathematical Formulation

The flow is supposed to be laminar, permanent and bidimensional. The steam is considered to be incompressible and the cross effects of Dufour/Soret are neglected. Otherwise, there are no thermal convection of air in the space and no phase change of the membrane.

Modeling Knudsen flow’s

The transfer of gas under a pressure gradient can be made by the first Fick law. In the specific case in porous media flow transfer due to Knudsen diffusion is formulated mathematically by

$$ J_K = \frac{\epsilon D_K}{\tau_m} \delta_m (\rho_{hm} - \rho_{mg}) $$

where the difference of the densities is determined by the pressure difference across the membrane,

$$ \rho_{hm} - \rho_{mg} = \frac{M}{RT_m} (p_{hm} - p_{mg}) $$

The Knudsen diffusion coefficient is given by the relationship [8]:

$$ D_K = \frac{4}{3} \frac{\nabla K_o}{V} $$

$$ V = \left( \frac{8RT_m}{\pi M_v} \right)^{1/2} = \left( \frac{8 \pi m}{\tau m_i} \right)^{1/2} $$

The characteristic parameter of the environment wherein the gas is transferred is the morphological effect of the membrane. In the case of a capillary tube of small diameter compared to the mean free path length and when a pure substance is present in the capillary [4]. But the study of the diffusion of gases in porous media is not easy for two reasons. First, the movement of the particles is random and also the porous structure is very complex. During transport, the three mechanisms coexist. While, there are cases where one or more modes combined predominate. The challenge is to find the predominant modes. However, all three situations are taken into account in our work. That brings us to study each of these transfer mechanisms individually, and then, their coupling in a configuration in order to determine the balance of phenomena.

Modes Combination of Three Flows

DGM model

The model “Dusty Gas” (DGM) shown in Figure 3, consists of two separate contributions. Each of these is sufficient to balance the transfer by momentary wall collisions and collisions with each other species in the mixture. The problem is how to account for the different modes, individually, and then combine to describe a better transfer simultaneously. At a total pressure gradient existing, the viscous flow and diffuse one are added, according to the kinetic theory. There is no limit in the viscous diffusion equations and no diffusion limitation in the viscous flow equations. In this model, the coefficients of permeability of the membrane due to molecular diffusion of Knudsen and are combined as resistance in series, wherein the potential drops (pressure difference) are additive. The resultant stream is then combined with the viscous flow in parallel as resistors, wherein the streams (flows) are additive Figure 3. Ding et al. proposed several schemes to assess different transmembrane flux [3].

Model schofield

In this model, the coefficients of diffusion of Knudsen and Poiseuille are parallel and in series with the Fick’s flow Figure 4.

KMPT model

Figure 5 shows a similar pattern to three resistors (diffusion coefficient) of the Knudsen and Fick’s flow, which are in parallel and in series with the viscous flow (Poiseuille). This model says KMPT (Knudsen Molecular Poiseuille flow transition) considers that the diffusion coefficients of molecular Knuden and are in parallel and in series with the Poiseuille.
\[ K_s = \frac{r_e \varepsilon}{2 \tau} \left( 1 - \frac{3r_e}{2H_m} \right) \]  
(5)

\[ D_k = \frac{2 \varepsilon}{3 \tau} r_e \sqrt{\frac{8RT_m}{\pi M_v}} \]  
(6)

Combining these equations the flow becomes

\[ J_K = \frac{2 \varepsilon}{3 \tau} r_e \sqrt{\frac{8M_v}{\pi RT_m}} \left( \frac{p_{lm} - p_{mg}}{\delta_m} \right) \]  
(7)

where \( T_m \) is average temperature between the two sides of the membrane.

The permeability of the membrane due to Knudsen diffusion can be given, according to El-Bourawi et al. by the following expression [9]:

\[ K_{ex} = \frac{2 \varepsilon}{3 \tau} r_e \sqrt{\frac{8M_v}{\pi RT_m}} \]  
(8)

**Fick’s Flow or molecular diffusion**

In the specific case in porous media flow transfer due to FICK’s flow is formulated mathematically by:

\[ J_M = \rho_a V_a - \rho_v D_v \frac{dw_v}{dr} \]  
(9)

The velocity \( (V_{v,a}) \) can be derived from the relationship:

\[ \rho_a V_a = \rho_v V_v - \rho_v D_v \frac{dw_v}{dr} \]  
(10)

When the fluid treated (vapour) is assumed airtight we obtain:

\[ \rho_a V_a = 0 \]  
(11)

Equation (10) becomes:

\[ V_a = \frac{\rho_v D_v}{\rho_a} \frac{dw_a}{dr} = \frac{D_v}{w_a} \frac{dw_a}{dr} \]  
(12)

And finally we get

\[ J_M = \rho_a \frac{D_v}{\rho_a} \frac{dw_a}{dr} - \rho_v \frac{D_v}{w_a} \frac{dw_v}{dr} \]  
(13)

The mass fraction of air is a function of the fraction of water vapor by:

\[ w_a = 1 - w_v \]  
(14)

Substituting equation (11) into equation (13), we obtain:

\[ J_M = -\rho_v \frac{D_v}{w_a} \frac{dw_v}{dr} \]  
(15)

The density of an ideal gas may be given by the equation:

\[ \rho_v = \frac{PM_v}{RT} \]  
(16)

Thus equation (15) can be written like:

\[ J_M = \frac{D_v M_v}{RT_m} \frac{P}{p_a} \frac{dp_a}{dr} = -\frac{D_v M_v}{RT_m} \frac{p}{p_a} \frac{dp_a}{dr} \]  
(17)

The vapour transport through the membrane by molecular diffusion can be modeled by Stephan law integrating equation (17). This is only possible when the pore size of the membrane is in the range of micrometer. This size is much larger than the mean free molecular path of the steam.

From Stefan’s law and in any location (z) along the membrane, the flow of vapour diffusion can be written as [8]:

\[ J_{M,s} = K_{ex} \Delta p \]  
(18)

The permeability of the membrane due to molecular diffusion is defined by:

\[ K_{m,M} = \frac{\varepsilon PD_v M_v}{\tau \delta_m R p_a T_m} \]  
(19)

\[ D_v = \frac{k}{\rho_v C_v} \]  : Coefficient of vapour diffusion in the air

The total pressure is given by:

\[ P = p_a + P \]  
(20)

The average temperature of the membrane is given by the following equation:

\[ \bar{T} = \frac{T_m + T_{na}}{2} \]  
(21)

Furthermore Qtaishat et al. proposed the expression amount of the steam/air: \( PD_{va} \ (Pa.m^2.s^{-1}) \) depending on the temperature [10]:

\[ PD_{va} = 1.985 \times 10^{-3} T^{0.72} \]  
(22)

The difference in partial pressure of the saturated vapor of both sides of the membrane may be calculated from the law of Antoine [2] using the following equation:

\[ P_v = \exp \left( \frac{23,328 - \frac{3841}{T - 45}}{T} \right) \]  
(23)

By substituting the equation (19), the equation (18) becomes.

\[ J_{M,s} = \frac{\varepsilon PD_v M_v}{\tau \delta_m R p_a T_m} \left( p_{lm} - p_{mg} \right) \frac{p_a}{p_s} \]  
(24)

Note: In order to explain the reduction of vapor pressure caused by the dissolved species, Raoul’s law [4] may be used.

\[ p_{lm} = (1 - C_{ma}) p_s \]  
(25)

where \( C_{ma} \) is the mole fraction of solute or salinity

For a binary mixture (air and steam), the relationship of the diffuse flux through the membrane is obtained as follows.

**Poiseuille’s flow**

This model is based on the Poiseuille viscous flow of the steam and is given by the generalized equation:

\[ J_p = m_p \eta P \]  
(26)

Considering the circular tubes as pores and uniform balance of viscous shear forces acting over the surface produced. The velocity
distribution over the cross section of a pore is given by:

\[
\nu_p(r) = \frac{r^2 - r_p^2}{4 \mu_g} dp \frac{dr}{dr} \tag{27}
\]

Integrating this equation and multiplying by gives the flow of the liquid mass rate through the pores.

\[
\dot{m}_p = \frac{\pi}{8} \frac{r_p^4 \rho_g}{\tau \delta_{\mu}} \Delta p \tag{28}
\]

The density of an ideal gas is given by:

\[
\rho_g = \frac{M_g \rho P}{RT} \tag{29}
\]

The coefficient \( n_p \) is a function of the porosity and the pore radius and is given by:

\[
n_p = \frac{\varepsilon}{\pi r_p^2} \tag{30}
\]

By replacing in the equation (26), we obtain the equation of the flux,

\[
J_p = \frac{1}{8 \mu_g} \frac{r_p^2 \rho_g M_g \Delta p}{\tau R_T \delta_{\mu}} \tag{31}
\]

Otherwise

\[
J_p = K_p \Delta p \tag{32}
\]

With as permeability due to viscous flow:

\[
K_p = \frac{1}{8 \mu_g} \frac{\varepsilon r_p^2 M_g \bar{P}_g}{\tau R_T} \frac{\delta_{\mu}}{\varepsilon} \tag{33}
\]

The three terms of the permeability coefficient \( K \) show that this is not only affected by the characteristics of the membrane and the type of the transfer mechanism but also by the temperature of the membrane.

**Results and Discussion**

Several simulations are obtained in the following terms:

PTFE membrane

\[
\gamma_{LV} = 30.3 \times 10^{-3} \text{ N/m} : \text{surface tension}
\]

\( \delta = 8 \text{ mm} : \text{air gap thickness} \)

The quantities used in simulations and their values are given in Table 1. A validation of the theoretical model was performed by comparing our results with the experimental results reported by Banat et al. on a membrane Figure 7 [8]. This figure shows a good agreement with experiment.

By setting the input data, we simulated the three streams (Knudsen, Poiseuille and Fick) for observing the ones, which are closer to experimental values of the Banat model, taken as a reality. So, it was easily observed among the three main flows, molecular diffusion is

| Porosity \( \varepsilon \) | Tortuosity \( \tau \) | Cooling temperature \( T_c \) | Polarization index \( l_1 \) | Thickness \( \delta_{\mu} \) | Radius \( r_p \) | Temperature of the solution \( T_e \) |
|--------------------------|----------------------|-----------------------------|-----------------------------|------------------|--------------|-----------------------------|
| -                        | -                    | °C                          | -                           | \( \mu \)m        | \( \mu \)m  | °C                          |
| 0.75                     | 1.5                  | 20                          | 0.93                        | 6                | 0.11         | 40-80                        |

**Table 1:** Input Data for simulation.
closer to reality. Then we plotted the other flows to determine their evolution compared with the diffusion stream (model studied), which was taken as a reference. Figure 8 illustrated the results. In this figure it has been found the fluxes of Knudsen and Poiseuille to be lower than the molecular diffusion. Figure 9 shows the evolution of Knudsen and Poiseuille flows.

In this figure, and in the temperature range (40-80)°C, Poiseuille flow has been found to be lower. In this temperature range, the use of the solar thermal energy can be considered.

It is common to find in the literature diffusion models of a transmembrane flux. Transport models found in the membrane separation techniques, and which are related to the processes of distillation, are often based on the models “Dusty Gas” (Figure 10), “Schofield” (Figure 11), “KMT” (Figure 12), “KMPT” (Figure 13), model “series” (Figure 14) and model “parallel” (Figure 15). But predictions of these models are limited to specific cases, in which only molecular diffusion, Knudsen and/or viscous flow contributes to the process of vapour transport.

Figures 10-15 show therefore the variation of the vapour stream generated as function of the inlet temperature of the saline water. The mass flow through the membrane was found to increase with the inlet temperature of brackish water for the various models considered.

The vapour quantity has been shown to be higher for our model than for the others in Figures 10, 12, 13 and 15 while the tow fluxes were in good agreement in Figures 11 and 14.

Figure 16 exhibits the results of the comparisons of flows generated different transfer mechanisms versus the inlet temperature.
Note that the Knudsen diffusion and molecular diffusion is dominant with respect to the distribution in the case of Poiseuille, for pore radius of about 25 nm.

Conclusion

The different types of mass transfer modes through the membrane have been carried out and compared with one another.

The different results show that only configuration based on the model of “Schofield” gives similar values as the molecular model. The KMT and parallel models are more responsive for large diameter pores. Thus, the model series is not adequate in such a case.

For relatively low pore size the Knudsen and Poiseuille models were shown to underestimate the generated fluxes.

Indeed, the molecular flow is dominant, but a series combination of the three transfer modes is most appropriate for a better estimation of the vapour stream generated. This observation was found to be in good agreement with the experimental works previously reported. As the developed models work in the temperature range (40-80)°C, the use of the solar energy could be considered.

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