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Membrane Distillation Process Modeling: Dynamical Approach

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Abstract—This paper presents a complete dynamic modeling of a membrane distillation process. The model contains two consistent dynamic models. A 2D advection-diffusion equation for modeling the whole process and a modified heat equation for modeling the membrane itself. The complete model describes the temperature diffusion phenomenon across the feed, membrane, permeate containers and boundary layers of the membrane. It gives an online and complete temperature profile for each point in the domain. It explains heat conduction and convection mechanisms that take place inside the process in terms of mathematical parameters, and justify process behavior during transient and steady state phases. The process is monitored for any sudden change in the performance at any instance of time. In addition, it assists maintaining production rates as desired, and gives recommendations during membrane fabrication stages. System performance and parameters can be optimized and controlled using this complete dynamic model. Evolution of membrane boundary temperature with time, vapor mass transfer along the process, and temperature difference between membrane boundary layers are depicted and included. Simulations were performed over the complete model with real membrane specifications. The plots show consistency between 2D advection-diffusion model and the expected behavior of the systems as well as literature. Evolution of heat inside the membrane starting from transient response till reaching steady state response for fixed and varying times is illustrated.

Keywords— Membrane distillation, Dynamical modeling, Advection-diffusion equation, Thermal equilibrium, Heat equation.

I. INTRODUCTION

WORLD'S next challenge is having clean water, it was shown that shortage of fresh water kills people more a war does. Despite over than 70% of earth surface is covered by water, but that does not mean that we can use it for domestic appliances. Studies show that 97% of the available water is salty and needs treatments, where the rest 3% is not enough to cover the worlds demand [1]. Water desalination is a term that is used to describe the process of removing salt and other impurities from water to get fresh and clean water. Desalination plants turns salty water (brackish or seawater) into fresh clean water (potable or distillate water)[2][3].

Water desalination has been developed over time; starting by early sailors and their evaporation of seawater passing through the industrial revolution, and reaching our time of having many types and schools for purifying water [1]. The abundant availability of energy resources comes after the industrial revolution pushed strongly in the development of water desalination types.

Multi-stage Flash (MSF) desalination type was among the first methods that had been studied and applied. Basically, it distills sea water by flashing (converting) a small amount of the water into steam in multiple stages of counter current heat exchangers. This method succeeded to provide the world with fresh water, till it was obvious that energy resources can not stand the high consumption for such plants, in addition to thermal discharge problems [4][5]. Technology of membranes helped too much in creating another school for desalination, in mid 60's reverse osmosis (RO) emerged and commercialized in early 70's. RO was introduced as a membrane separation process in which the water from a pressurized saline solution is separated from the solutes (the dissolved material) by flowing through a membrane. No heating or phase change is necessary for this separation. The major energy required for desalting is for pressurizing the feed water [6]. RO has many advantages over the thermal methods in terms of energy consumption. However, it suffers from maintenance problems and a highly dependence on sufficient pretreatment [7]. This paper considers other type of water desalination methods that has the advantages of both MSF and RO called Membrane distillation (MD). MD is an emerging, thermally driven membrane separation process that utilizes a low-grade heat source (i.e., waste heat) to transport of only water vapor or other volatile molecules and facilitate mass transport through a hydrophobic, micro-porous non-wetted membrane [8]. MD ensures the quality of the fresh water twice with low temperature and hydrostatic pressure.

Most of the literature models were not able to describe a full dynamic behavior of the process from the moment of operation and go on, since they did not include a time component in their models. Although they have a good approximation in steady state response, but they are unable to describe a sudden change or variation at specific time instance. This work provides a full dynamical modeling that is capable of describing the behavior of the process, relate physical quantities to mathematical parameters and better understanding to the key parameters that help increasing the production of the process. Involving a dynamic model in membrane distillation process opens for control theory techniques and optimization methods to play significant role in enhancing the performance and save much energy consumption, because MD encountered over its development a serious challenge of energy inefficiency that poses a serious drawback to its commercialization in the industry [9], [10]. Next sections present description of MD

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process and a complete model for its mechanisms.

II. MD PROCESS DESCRIPTION

Process of distilling water by MD has some requirements for the deployed membranes. They should be porous and not wetted (hydrophobic) by the liquids of the process. The pores should be reasonably of a large size and narrow distribution, limited by the minimum Liquid Entry Pressure (LEP), and no capillary condensation should take place inside the pores of the membrane [11].

A. *Principle of operation*

The principle of membrane distillation (MD) process is described as if a salt solution and a fresh water are divided by a hydrophobic micro porous membrane and the temperature difference is created, while the temperature of the salt solution is higher than the temperature of the solvent, the salt concentrates in a warm solution, and the vapor of the salt solution goes to the cold one. According to the MD mechanism, when there is a temperature difference on the membrane, the solvent evaporates from its warm surface and diffuses through membrane pores to a colder surface, on which it condenses. The solution cannot transfer through membrane pores because of its hydrophobic property. The driving force of this process is the pressure difference of saturated vapors of the solvent and the solution caused by the difference of temperatures [12]. Fig. 1 describes the principle of operation of MD process.

MD provides wide range of sentiment benefits in desalination field; such as it needs low temperature and hydrostatic pressure to operate, and its productivity is independent of salt concentration, beside its efficiency and performance are independent of osmotic pressure and concentration polarization, in addition to rejection of all non-volatile solute [14].

B. *MD configurations*

Four common configurations for MD are in the literature, they share the same concept of operations but differ on how they condensate fresh water in permeate side. Direct contact membrane distillation (DCMD) is the simplest type and it ensures the quality of the fresh water through the phase change and then through the use of a membrane, and it is considered for study in this paper. Air gap membrane distillation (AGMD) is other configuration where the air gap is usually the controlling factor for the mass and heat transfers, because of its greater thermal and mass transfer resistances which imposes more heat energy to be used for water evaporation than that of DCMD. In Sweeping gas membrane distillation (SGMD) the vapor is stripped from the hot feed by a gas stream, and then condensed in an external condenser. This makes it has higher mass transfer rates than AGMD, due to the greater driving force originating from the reduced vapor pressure on the permeate side of the membrane, and has less heat loss through the membrane. The fourth configuration is the vacuum membrane distillation (VMD) in which the vapor permeate is removed continuously from the vacuum chamber to form a vapor pressure difference across the membrane. Theoretically, this configuration can provide the greatest driving force at the same feed temperature, because the vapor pressure at the cold side can be reduced to almost zero [11], [15]. Fig. 2 illustrates the 4 configurations of the membrane distillation process.

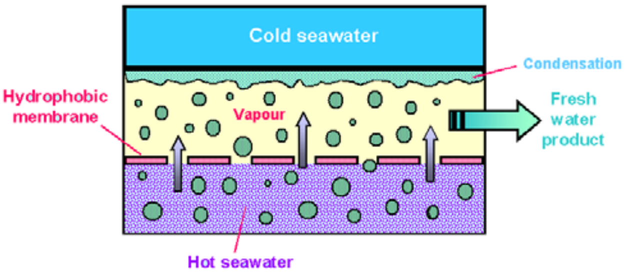

Fig. 1 MD principle of operation [13]

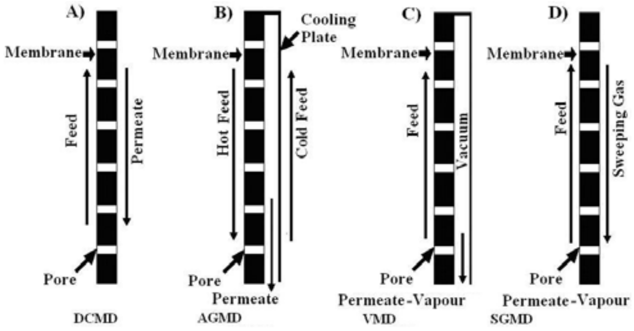

Fig. 2 MD types: A) DCMD. B) AGMD. C) VMD. D) SGMD[11]

III. MEMBRANE DISTILLATION MODELING

Although MD is widely described in literature, but all the proposed models were steady state models, in sense they do not show the internal dynamic of the process. Studying a dynamic model for such process enables to record the variation of the key parameters that are involved with time. The evolution of these key parameters such as salt concentration, flow injection velocity, temperatures across the feed/permeate containers helps a lot to fully understand the process and thus better operate it. Besides, employing a dynamic model enables to monitor those key parameters and record any sudden or unexpected change in their desired values. These changes are subject then to a control system that is responsible of adjusting back to the normal conditions of operation [8].

MD is a thermally driven process, where varying feed and permeate water temperatures imposes heat conduction and convection in the process that creates the adequate vapor gradient pressure for vapor mass transfer across the membrane. In the other hand, understanding heat transfer inside the membrane is highly important to maintain the desired production rates and for better selection of membrane materials in fabrication stages.

A. *Heat and mass transfer principles*

In membrane distillation process heat transfers in two directions; the first is a conduction from feed to permeate side in a form of sensible and latent heat, and secondly as a convection that transfers from the bulk flow of the feed/permeate to the boundary layer of the membrane via heat convection. Fig. 3 shows the conduction flow direction toward the cold side through membrane pores [11], [16], [17].

It is noticeable that temperatures adjacent to the boundary layer of the membranes from the feed side are less than the bulk, whereas membrane boundary temperatures in the permeate case are more than the bulk in that container. In literature, heat transfer was mostly modeled through heat balance equations using steady state models that offer a good approximation in steady state response with no information about the transient response or sudden changes, such models are like (1):

$$\begin{aligned} Q_f &= \alpha_f\,(T_f - T_1), \\ Q_p &= \alpha_p\,(T_2 - T_p), \\ Q_m &= \frac{k_m}{\delta_m} A(T_1 - T_2) + JH_{lat}. \end{aligned} \tag{1}$$

Vapor molecules transfer in membrane distillation process from feed side to permeate side through the hydrophobic pores of the membrane. The transfer begins when the water in the feed container starts to vaporize by heating, then the vapor passes through membrane pores based on the vapor pressure gradient. Passing vapor molecules are forced to condense by the cold injected stream in the permeate container. The amount of vapor mass transferred across the membrane is a key parameter that controls the production rate of fresh water. It is directly proportional to the rate of production and vapor gradient pressure through (2) [18]

$$J = C(P_1 - P_0). \tag{2}$$

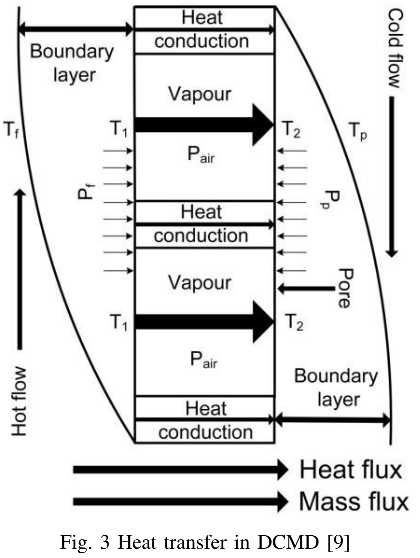

Fig. 3 Heat transfer in DCMD [9]

where C is the membrane mass transfer coefficient of the system. Knudsen diffusion model describes the mass transfer mechanism in membrane distillation process, considering that the membrane pore size is less than the mean free molecular path of the gaseous water molecules. Knudsen model is illustrated in (3):

$$J_{knudsen} = 1.064 \frac{r\epsilon}{\chi^{\delta_m}} \left(\frac{M}{RT_{mean}}\right)^{0.5} (P_1 - P_0). \tag{3}$$

B. *Dynamical model for heat and mass mechanisms*

Steady state models offered acceptable information for the MD process in the long steady state run, but the information has uncertainties as they were built over approximation and empirical relations from experiments. In addition, they were useful only on the adjacent layers of the membrane but no elsewhere, and unable to describe the transient behavior of the process and any changes that could take place suddenly in the process.

The use of 2D advection-diffusion equation is capable to describe the heat and mass transfer mechanisms across the membrane. Equation (4) shows the model for feed side and permeate side [8]:

$$\frac{\partial T_f(x,z,t)}{\partial t} + v_f \frac{\partial T_f(x,z,t)}{\partial z} = \alpha_f \frac{\partial^2 T_f(x,z,t)}{\partial x^2}, \tag{4}$$

$$\frac{\partial T_p(x,z,t)}{\partial t} + v_p \frac{\partial T_p(x,z,t)}{\partial z} = \alpha_p \frac{\partial^2 T_p(x,z,t)}{\partial x^2}, \tag{5}$$

$$0 < x < X, 0 < z < Z, 0 < t < T.$$

Constants α_f and α_p depend on thermal conductivity (k), specific heat (cp) and the density of the seawater (ρ) in such a formula $\alpha = \dfrac{k}{(cp * \rho)}$. Initial profile (6) and boundary conditions (7) for the temperature:

$$\begin{aligned} T_f(x,z,0) &= 60, \\ T_p(x,z,0) &= 20, \end{aligned} \tag{6}$$

$$\begin{aligned} \frac{\partial T_f(0,z,t)}{\partial x} &= 0, \\ \frac{\partial T_p(0,z,t)}{\partial x} &= 0, \\ \frac{\partial T_f(X,z,t)}{\partial x} &= [JH_{lat} - \frac{k_m}{\delta_m}(T_f(X,z,t) - T_p(X))]/k_f, \\ \frac{\partial T_p(X,z,t)}{\partial x} &= [JH_{lat} - \frac{k_m}{\delta_m}(T_f(X,z,t) - T_p(X))]/k_p, \\ T_f(x,0,t) &= 60, \\ T_p(x,0,t) &= 20. \end{aligned} \tag{7}$$

The interesting properties of 2D advection-diffusion equation can describe the heat diffusion that takes place during the membrane distillation process. Heat flow is divided to conduction flow through the membrane and a convection flow from the source to the rest of the container. Transport term (first derivative) in the equation represents the convection heat flow from the input source toward all the molecules of water along the membrane module length, where the conduction

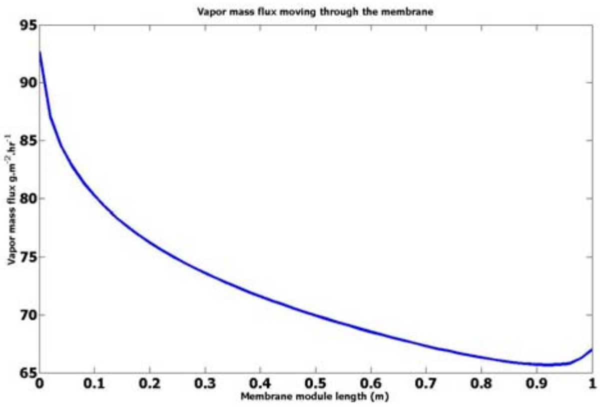

Fig. 4 Vapor mass transfer across the membrane module length

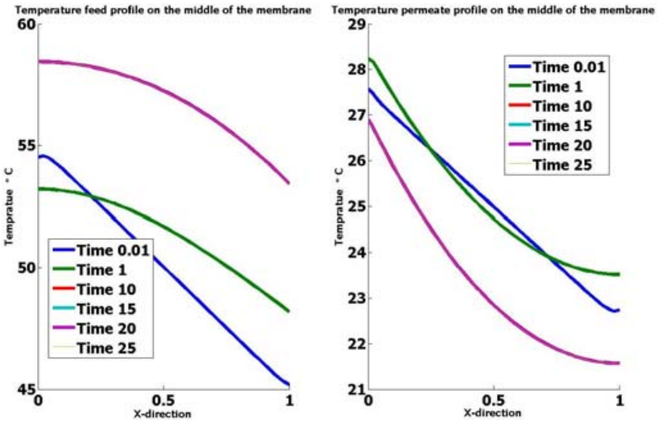

Fig. 6 Variation of the temperatue at a certain membrane length

mechanism is explained by the second derivative term flows through membrane pores. Both heat transfer forms are going to reach a phase of steady state at specific time, in which the process should run in normal conditions. At that time, the dynamic model will monitor any deviation in the system parameters and the response.

The equation was solved numerically, since it is a differential equation to multiple variables. Fig. 4 shows the vapor mass transferred along the membrane module length. The model was validated with an experimental data that was done by Hwang *et* al. in [19], the validation is acceptable with an error of percentage less than 5%.

The amount of the transferred mass is high at the top of the membrane and decreases at the bottom end, because the temperature difference across the membrane decreases at the bottom. Temperature difference between the adjacent boundary layers of the membrane can be measured as well, Fig. 5 shows the difference of the temperature along the membrane module.

Variation of temperature in certain point in the container grid can show the transition period clearly. As the process is modeled by diffusion model, then the temperature will accumulate till reaching a steady state stage. Fig. 6 shows the variation of the temperature at a certain point in the domain.

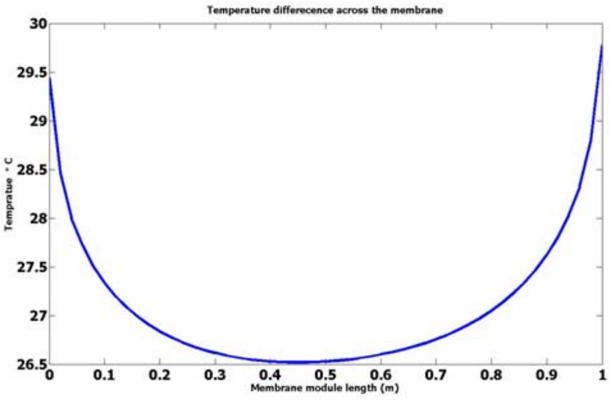

Fig. 5 Temperature difference across membrane module

Based on the dynamic 2D advection diffusion model, an online and complete temperature profile for all the points along the domain are available all the time. This means an online temperature profile for the adjacent layers of the membrane and both containers. Therefore, more precise vapor mass flux calculations and production rates can be implemented at instance.

C. Membrane modeling

The need of developing an internal model for the membrane itself in a MD process is insistent. In order to better understand the process of MD, a complete model that includes feed, permeate and membrane helps in fabrication of the membrane and material selection, which serves delivering more fresh water.

Modeling the membrane is based on thermal equilibrium equation and conservation of energy, in which the model is a modified version of the heat equation but for porous media. considering that both vapor and membrane material share same temperature. Only a conduction heat flow is considered along the membrane width. The model is dynamic and able to track the transient response of heat evolution. Equation (8) shows the modified version of the heat equation inside the membrane [20].

$$[\epsilon\,(\rho Cp)_f + (1-\epsilon)\,(\rho Cp)_s]\frac{\partial T}{\partial t} = \nabla.\,(k_e.\nabla T). \tag{8}$$

Fig. 7 depicts the evolution of heat flow from the feed side to the permeate side through the membrane with time. Amount of transferred heat increases with time. For an instance of time, a heat flow is generated between boundary points across the membrane. Fig. 8 shows heat flow inside the membrane at steady state.

IV. DISCUSSION AND CONCLUSION

Membrane distillation combines the use of membranes with all their advantages in properties, modifications and fabrications with the phase change techniques. Depending on vapor partial pressure difference created by temperature gradient that is imposed between the water phases, fresh water

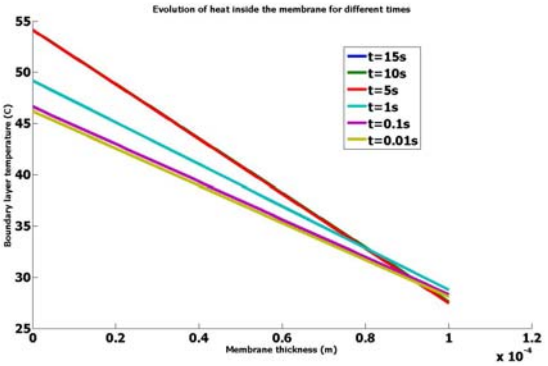

Fig. 7 Heat transfer inside the membrane for different times

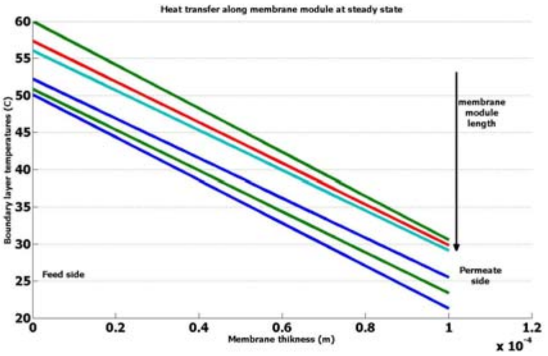

Fig. 8 Heat transfer inside the membrane for fixed time

can be obtained with less requirements of pre-treatment in the feed side and chemically free. DCMD is the most popular type for MD laboratory research. However, AGMD is more popular in commercial applications, because of its high energy efficiency and capability for latent heat recovery [11].

Modeling the MD process requires deep understanding of the main factors in the process, such as: flow rate, water density, thermal conductivity and others. In addition to this, understanding the mechanisms of heat transfer is important specially in determining the production rate of fresh water. Modeling using 2D advection-diffusion equation enabled to relate a mathematical model to physical quantities and explain behaviors in the process, such as conduction mechanism with the vapor mass flux that pass through membrane pores and convection mechanism within water containers.

The presence of the time components in the analysis was important, as now it is possible to track the response of the system even before reaching steady state phase, and feedback the operator with a complete monitoring on the process response with any changes and variations that take place. By such model, it is possible to have an online status for the temperature along the proposed domain. Control theory techniques from controllers to observers can be developed over the dynamic model to adjust the process parameters as needed. Developing an internal modeling for the membrane was consistent with the process model, since the boundary conditions that affect the process are affecting the membrane as well. Adding a model of the internal membrane helps in giving a complete vision of the process, determines the key factors to maintain production rates, and get optimum performance.

Further studies can be conducted on the validation of the complete model with real experimental data. In addition, an optimization techniques can be imposed for better system performance implementation.

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NOMENCLATURE

Constants

A	Membrane area m^2
Cp	Specific heat $kJ/(kg.C)$
D	Diffusion coefficient
h_c	Heat transfer coefficient $W/(m^2.K)$
k	Thermal conductivity coefficient $W/(m.K)$
k_e	Effective thermal conductivity of membrane and vapor $W/(m.K)$
M	Molecular weight g/mol
R	Gas universal constant $J/(mol.K)$
Y_{ln}	Mole fraction of air

Greek symbols

α	Convective heat transfer coefficient $W/(m^2.K)$
ρ	Density kg/m^3
χ	Tortuosity factor
δ_m	Membrane thickness m
ϵ	Porosity
η	Gas viscosity $kg/(s.m)$

Subscript

c	Conduction
f	Feed
m	Membrane
p	Permeate
v_a	Vapor

Variables

H_{lat}	Latent heat of vaporization kJ/kg
J	Mass flux density $kg/(m^2.s)$
Q	Heat flux W
r	membrane pore radius m
T	Temperature ^oC
v	Flow velocity m/s

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