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Simulation of transport phenomena in porous membrane evaporators using computational fluid dynamics

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Abstract. A numerical simulation of membrane evaporation process was carried out in this work. The aim of simulation is to describe transport of water through porous membranes applicable to the concentration of aqueous solutions. A three-dimensional mathematical model was developed which considers transport phenomena including mass, heat, and momentum transfer in membrane evaporation process. The equations of model were then solved numerically using finite element method. The results of simulation in terms of evaporation flux were compared with experimental data, and confirmed the accuracy of model. Moreover, profile of pressure, concentration, and heat flux were obtained and analyzed. The results revealed that developed 3D model is capable of predicting performance of membrane evaporators in concentration of aqueous solutions.

Keywords: membrane; mass transfer; membrane contactor; simulation; modeling

1. Introduction

At the moment, concentration of aqueous solutions is carried out via conventional evaporators in which water extent of an aqueous solution is reduced by application of heat. Conventional evaporators suffer from some drawbacks including consumption of much energy and not applicable to heat-sensitive compounds. Evaporators have important applications at chemical industries specially in food industry (Shahid and Pashley 2014). Finding an alternative process for concentration of aqueous solutions is a subject of greater interest for research community.

Membrane separation processes can be used for removal of water from aqueous solutions. Various membrane processes can be utilized as evaporator including membrane distillation, osmotic evaporation, and membrane evaporation (Drioli *et al*. 2006). Separation in membrane distillation is based on temperature difference between two aqueous solutions in a membrane contactor. In membrane distillation, water in transferred from high-temperature solution (feed) to the low-temperature solution. Although membrane distillation has advantages of membrane processes, it cannot be utilized for concentration of heat-sensitive solutions due to application of

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high-temperature at feed solution. However, various membrane distillation processes have been developed such as vacuum membrane distillation which can overcome the problems of membrane distillation.

In osmotic evaporation, two aqueous solutions including feed solution and a brine solution are contacted in a membrane contactor. Water is transferred from feed solution to the brine solution due to gradient of water activity across the membrane. The latter process has a major drawback, i.e., corrosion problem aroused from the use of brine solution (Nii *et al*. 2002, Jevons and Awe 2010).

Membrane evaporation is a novel membrane process that can be used for concentration of aqueous solutions. Separation in membrane evaporation is based on creation of vapor pressure gradient between two sides of membrane. In one side, a feed solution is flown while at the other side of membrane module, dry air is circulated. Difference of water vapor pressure at the interface of feed solution and bulk of air is the driving force of process (Kunz *et al*. 1996, Hengl *et al*. 2007). Membrane evaporation is appropriate for concentration of heat-sensitive solutions because it operates at ambient pressure and temperature. Moreover, the corrosion problem which is encountered in osmotic evaporation is not occurred in membrane evaporation. A few experimental and theoretical studies can be found on membrane evaporation process (Lawson and Lloyd 1997, Romero *et al*. 2006, Hengl *et al*. 2007, 2010, Mourgues *et al*. 2010).

Hengl *et al*. (2007) used a metallic flat-sheet membrane contactor as membrane evaporator for concentration of aqueous solutions. The aim of their work was to assess the applicability of membrane evaporation in separation processes. Hengl *et al*. (2007) developed a mass transfer model for simulation of membrane evaporation process. Mass transfer of water in membrane contactor was estimated using resistance-in-series model in which two mass transfer resistances corresponding to the membrane and the gas phase were considered in simulations.

Mourgues *et al*. (2010) also developed a mathematical model for simulation of water transport in membrane evaporation. Both heat and mass transfers were taken into account in their model.

There are other studies on modeling and simulation of heat transfer in porous media. Kiwan (Kiwan 2007) investigated solution of natural heat transfer equation using a simple method. He considered natural convection in a fin based on energy balance and Darcy's model. The results were satisfactory for three types of porous fins. Postelnicu (2007) studied the effect of chemical reaction on heat and mass transfer characteristics of natural convection. The considered system was a vertical surface embedded in a porous medium with a chemical reaction. The effect of diffusion-thermo and thermal-diffusion phenomena were taken into account. They developed a two dimensional model for prediction of system. There are other reported works on simulation of heat transfer in porous media (Das and Ooi 2013, Das 2014) and also mass transfer in porous media (Marjani *et al*. 2011, Marjani and Shirazian 2011a, b, c, d, e, Moghadassi *et al*. 2011, Sohrabi *et al*. 2011a, b, c, d).

However, there is a definite for a comprehensive mathematical model which can predict the performance of membrane processes involving both heat and mass transfer. Development of a comprehensive mathematical model which can provide a general simulation of membrane evaporation process is of great importance. Computational fluid dynamics (CFD) is a powerful and efficient tool for simulation of transport phenomena in membrane separation processes which can be used for simulation of water transport in this novel process (Shirazian *et al*. 2009, Fadaei *et al*. 2011a, b, Marjani and Shirazian 2011a, b, c, d, e, Rezakazemi *et al*. 2011a, b, Shirazian *et al*. 2011a, Sohrabi *et al*. 2011a, b, c, d, Fadaei *et al*. 2012, Fasihi *et al*. 2012, Rezakazemi *et al*. 2012, Shirazian *et al*. 2012, Ghadiri *et al*. 2013, Ghadiri and Shirazian 2013, Razavi *et al*. 2013).

The main aim of this work is to develop and solve a comprehensive three-dimensional

mathematical model for the simulation of water transport in membrane evaporation process. The simulations were based on computational fluid dynamics of mass, momentum and heat transfer in all phases. The governing equations are then solved via numerical method based on finite element method (FEM). The model findings are then validated through comparing with experimental data reported in literature. Moreover, profile of pressure, concentration, and heat flux in the membrane evaporator are obtained and discussed.

2. Modeling of process

As it was stated earlier, in membrane evaporation process an aqueous solution is concentrated by removal of water. This is accomplished by utilization of an extracting phase, i.e., dry air. A macroporous membrane acts as a contactor in the process. Therefore, three subdomains or compartments can be considered for simulation of process as shown in Fig. 1. As it is seen, aqueous solution (pure water) is flown in the feed side, and dry air passes counter-currently in the gas side. The membrane is hydrophobic and it is not wetted by aqueous phase. It should be pointed out that the model is considered in Cartesian coordinate and three dimensional (Mohammadi *et al*. 2015).

The assumptions for development of 3D model include:

(1) Steady state conditions
(2) Laminar flow regime for water and air
(3) The membrane is not wetted by water
(4) Thermodynamic equilibrium is established at air-water interface.

Transport of water vapor through membrane, and in the gas phase is modeled using continuity equation (Cussler 1997)

$$\frac{\partial C_w}{\partial t} + \nabla \cdot (-D_w \nabla C_w + C_w V) = 0 \tag{1}$$

where C_w refers to the concentration of water vapor in either membrane or gas phase (mol/m^3), D_w denotes diffusion coefficient of water (m^2/s), and V denotes the velocity (m/s).

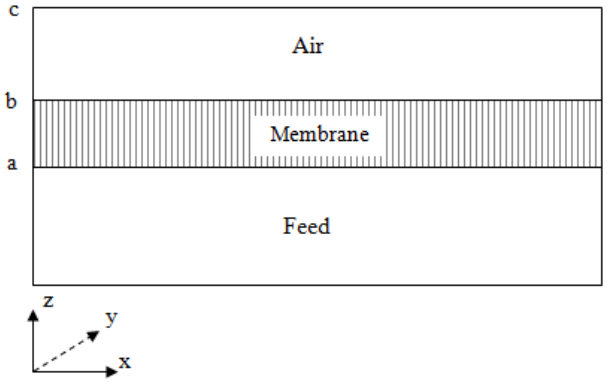

Fig. 1 Three subdomains considered in simulation of membrane evaporation process

Velocity distribution in the feed and gas phase is obtained by solving the Navier-Stokes equation (Cussler 1997)

$$\rho\frac{\partial V}{\partial t}-\nabla\cdot\eta(\nabla V+(\nabla V)^{T})+\rho(V.\nabla)V+\nabla p=F$$
$$\nabla.V=0 \tag{2}$$

where η is dynamic viscosity of fluid (kg/m.s), ρ density of the fluid (kg/m^3), p pressure (Pa), and F is external force (N).

Temperature distribution in the feed and membrane is obtained using energy equation (Cussler 1997)

$$\rho C_p\frac{\partial T}{\partial t}+\nabla\cdot(-k\nabla T+\rho C_p TV)=0 \tag{3}$$

where C_p is specific heat capacity (J mol^{-1} K^{-1}), and k thermal conductivity (W m^{-1} K^{-1}).

2.1 Boundary conditions

2.1.1 Gas phase

In the gas phase, continuity equation as well as the Navier-Stokes equations are solved to obtain concentration distribution of water vapor and pressure in the gas phase. The boundary conditions for mass transfer in the gas phase include

$$@x=0;\quad C_g=C_{g0} \tag{4}$$

$$@x=L;\quad \text{Convective flux} \tag{5}$$

$$@z=b;\quad C_g=C_{membrane} \tag{6}$$

$$@z=c;\quad \frac{\partial C_g}{\partial z}=0 \tag{7}$$

$$@y=0\ \&\ y=w;\quad \frac{\partial C_g}{\partial y}=0 \tag{8}$$

Boundary conditions for the Navier-Stokes equations in the gas phase include

$$@x=0;\quad V_g=V_{g0} \tag{9}$$

$$@x=L;\quad p_g=p_{atm} \tag{10}$$

$$@z=b;\quad V_g=0 \tag{11}$$

$$@z=c;\quad V_g=0 \tag{12}$$

$$@\, y = 0 \,\&\, y = w; \quad V_g = 0 \tag{13}$$

2.1.2 Membrane

In the membrane, continuity and energy equations are solved. The aim is to obtain concentration and temperature distribution inside the membrane. The boundary conditions for the mass transfer equation within the membrane pores include

$$@\, x = 0 \,\&\, x = L; \quad \frac{\partial C_{membrane}}{\partial x} = 0 \tag{14}$$

$$@\, z = b; \quad C_{membrane} = C_g \tag{15}$$

$$@\, z = a; \quad C_{membrane} = \frac{P_w^{sat}}{RT} \tag{16}$$

$$@\, y = 0 \,\&\, y = w; \quad \frac{\partial C_{membrane}}{\partial y} = 0 \tag{17}$$

where L refers to length of membrane (m), and P_w^{sat} denotes the vapor pressure of saturated water at the membrane-water interface (Pa). Heat transfer through the membrane is considered as conduction. The boundary conditions include

$$@\, x = 0 \,\&\, x = L; \quad \frac{\partial T_m}{\partial x} = 0 \tag{18}$$

$$@\, y = 0 \,\&\, y = w; \quad \frac{\partial T_m}{\partial y} = 0 \tag{19}$$

$$@\, z = a; \quad T_m = T_f \tag{20}$$

$$@\, z = b; \quad T_m = T_g \tag{21}$$

2.1.3 Feed phase

At the feed side, energy equation as well as the Navier-Stokes equations are solved. The boundary conditions for the energy equation in the feed side include

$$@\, x = L; \quad T_f = T_{f0} \tag{22}$$

$$@\, x = 0; \quad \text{convective flux} \tag{23}$$

$$@\, z = 0; \quad \frac{\partial T_f}{\partial z} = 0 \tag{24}$$

$$@\, z = a; \quad q = N_w \Delta H_w \tag{25}$$

$$@\, y = 0 \,\&\, y = w; \quad \frac{\partial T_f}{\partial y} = 0 \tag{26}$$

where N_w is the flux of evaporation at the membrane-water interface and ΔH_w is the evaporation enthalpy (J/kg). The boundary conditions for the Navier-Stokes equations in the feed side include

$$@\, x = 0; \quad p_w = p_{atm} \tag{27}$$

$$@\, x = L; \quad V_f = V_{f0} \tag{28}$$

$$@\, z = 0; \quad V_f = 0 \tag{29}$$

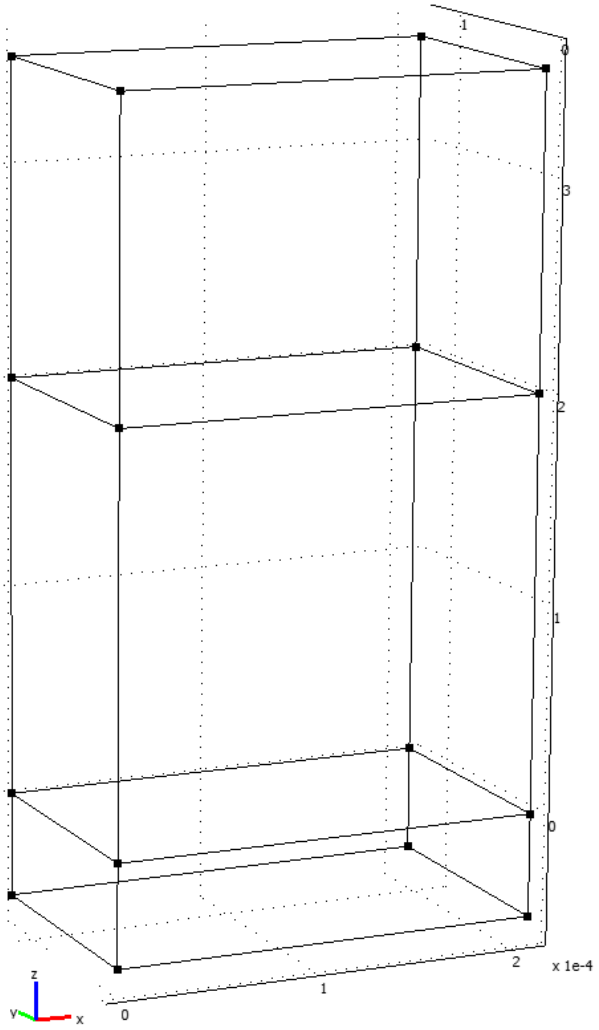

Fig. 2 Drawn geometry of membrane evaporation for simulation of process

$$@z = a; \quad V_f = 0 \tag{30}$$

$$@y = 0 \,\&\, y = w; \quad V_f = 0 \tag{31}$$

2.2 Numerical solution

The governing equations with boundary conditions derived in previous sections were solved numerically using COMSOL Multiphysics 3.5 software. The latter is a CFD based package which is appropriate for simulation of 2D and 3D models. A 3D model of membrane evaporation process was drawn in software which is shown in Fig. 2. The geometry of model was scaled to increase the accuracy and decrease the time of solution.

Finite element method (FEM) was applied for numerical solution of governing equations. The applicability and validity of this numerical method has been proved in previous publications

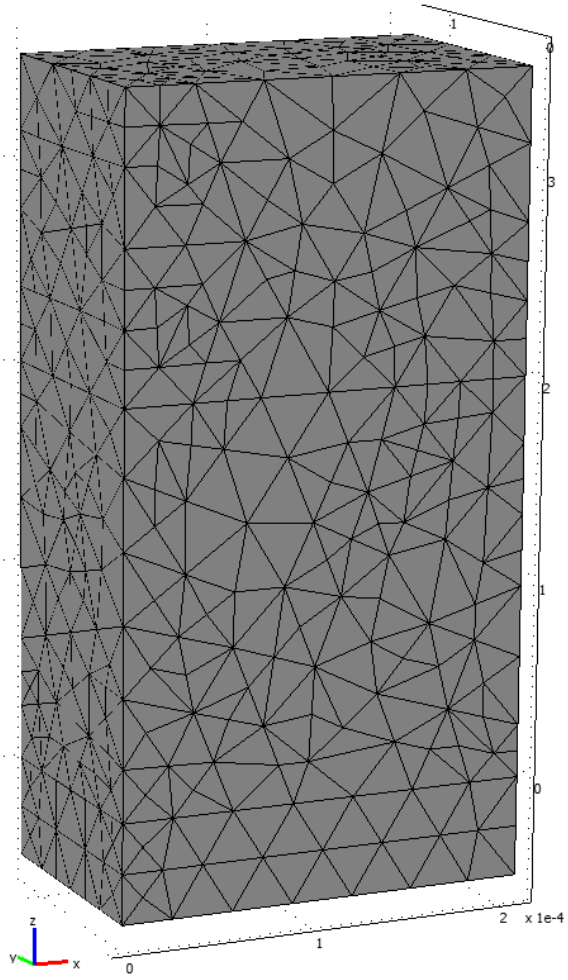

Fig. 3 Meshed geometry used in numerical simulations

(Abdullah *et al*. 2006, Ye *et al*. 2006, Abdullah and Das 2007, Al-Marzouqi *et al*. 2008, Shirazian *et al*. 2009, Shirazian and Ashrafizadeh 2010a, b, Kohnehshahri *et al*. 2011, Marjani and Shirazian 2011a, b, c, d, e, Shirazian *et al*. 2011b, Marjani and Shirazian 2012a, b, c, d, e, Marjani *et al*. 2012, Pishnamazi *et al*. 2012). UMFPACK was also used as the numerical solver in the calculations which has shown great ability in numerical simulation of membrane processes (Al-Marzouqi *et al*. 2008). The simulations were performed in an IBM-PC-Pentium5 (CPU speed of 2600 MHz and 2 GB of RAM) within 5 minutes. COMSOL creates triangular meshes for numerical solution of differential equations which are isotropic in size. About 10064 meshes were generated using software which are shown in Fig. 3. Adaptive mesh refinement in COMSOL which generates the best and minimal meshes was used to mesh the geometry of membrane evaporator (Fadaei *et al*. 2011a, b, Fasihi *et al*. 2012, Ghadiri *et al*. 2013, Shirazian and Ashrafizadeh 2013). The membrane parameters used in the simulations are the same as those reported by Hengl *et al*. (2007).

3. Results and discussions

3.1 Model validation

The model findings were validated through comparing with the experimental data reported by Hengl *et al*. (2007). They reported experimental data for evaporation of pure water in a membrane contactor in which dry air was used as stripping phase. They conducted a preliminary research on a prototype membrane evaporator developed by them. In their study, the membrane which was porous and metallic was placed in a flat module and it was divided into two distinct parts. In one part of the membrane module, pure water was recirculated whereas in the other part, a continuous flow of dry air at low pressure was applied. Since the used membrane was hydrophobic, water could not penetrate into the membrane pores and a liquid–vapor interface was formed at each pore entrance. Due to the partial pressure gradient between water-air interface and the bulk of gas phase

Table 1 Comparisons between experimental data and simulation results

Velocity of air (m/s)	Experimental evaporation flux (kg/m^2.h) (Hengl *et al*. 2007)	Simulated evaporation flux (kg/m^2.h)
0.005	0.05	0.03
0.010	0.07	0.05
0.015	0.09	0.07
0.020	0.10	0.09
0.023	0.11	0.10
0.026	0.12	0.11
0.030	0.14	0.12
0.035	0.15	0.13
0.040	0.15	0.14
0.046	0.15	0.16
0.050	0.16	0.17
0.056	0.17	0.18

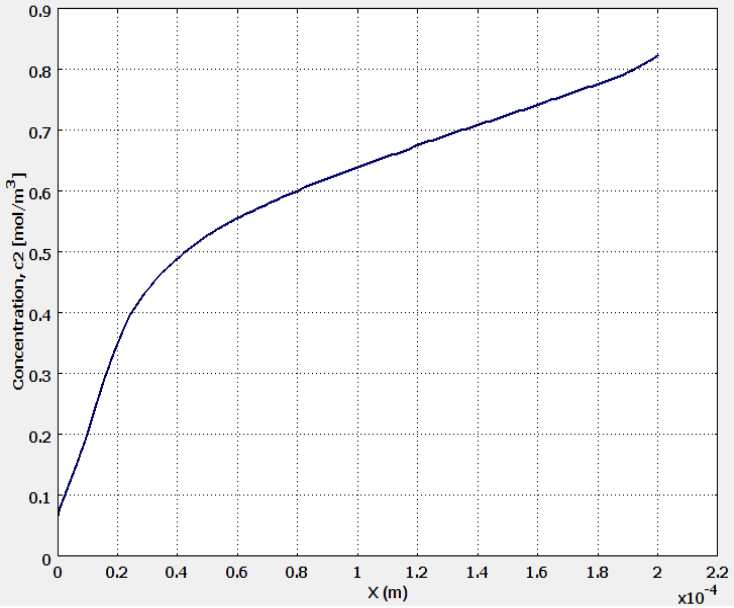

Fig. 4 Concentration profile of water vapor in the gas phase

(dry air), water evaporates and vapor diffuses through the pore and then it is carried away by the air flow. The change in the water was tracked by a balance, and the amount of water flux evaporated into the gas phase was determined experimentally (Hengl *et al*. 2007).

The results of comparisons are listed in Table 1 (Hengl *et al*. 2007). As shown in Table 1, the model findings are in good agreement with the experimental results which confirm the validity and accuracy of developed 3D mathematical model for prediction of water transport in membrane evaporation process. Moreover, Table 1 shows that the evaporation flux increases with enhancement of gas velocity in membrane module. This enhancement of evaporation flux is sharper in low gas velocities. Increasing gas velocity increases gradient of water vapor pressure at the interfaces which in turn increases water vapor flux from liquid to the gas phase.

3.2 Concentration profile of vapor in the gas phase

Concentration profile of water vapor in the gas phase and in X direction is shown in Fig. 4. It is clearly shown that the concentration of water increases in the gas phase considerably so that vapor concentration increases from zero at the inlet of gas phase to more than 80% of its saturation value at the outlet of gas phase. The latter shows the efficiency of membrane evaporation in dewatering of aqueous solutions. Moreover, Fig. 4 reveals that for enhancement of water flux, the gas phase should be taken far from saturation state. Therefore, gas phase plays crucial role in optimization of membrane evaporation.

3.3 Profile of mass transfer flux in the gas phase

Convective mass transfer flux of water vapor in the gas phase is shown in Fig. 5. The profile of mass flux was obtained in X direction. The trend of mass transfer flux in the gas phase is similar to

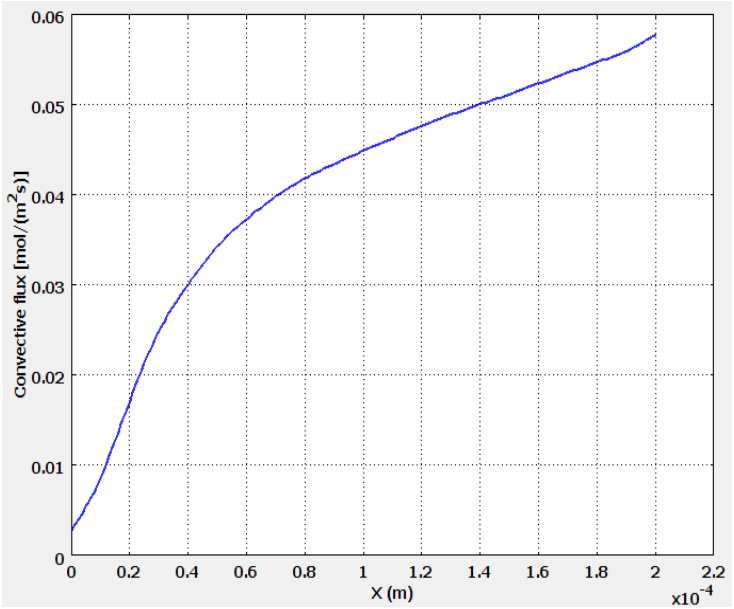

Fig. 5 Profile of convective mass transfer flux in the gas phase

concentration profile in the gas phase (see Fig. 4) in which convective mass transfer flux increases along the gas phase. Total mass transfer flux in the gas phase comprises diffusive and convective fluxes. In X direction, the contribution of convective mass transfer is high so that the diffusive mass transfer flux is negligible. The latter is due to the velocity in the gas phase which causes high convective mass transfer flux compared to diffusion.

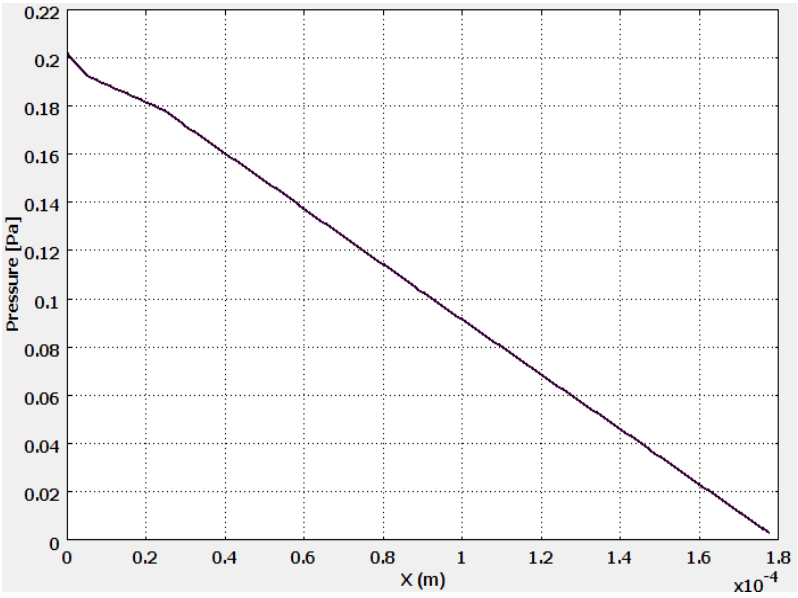

Fig. 6 Profile of pressure in the gas phase

3.4 Pressure profile

Profile of pressure of gas phase is indicated in Fig. 6. The pressure in the gas phase includes pressure of water vapor and air. A linear decrease in the total pressure of gas phase is observed in Fig. 6. However, the pressure drop is not appreciable along the gas phase which is one of advantages of membrane contactors in concentration of aqueous solutions. Although water is evaporated into the gas phase and it is predicted that the total pressure of gas phase should be increased, the effect of viscous forces is more important and predominant which results in reduction of gas phase pressure along X direction.

3.5 Heat transfer in the feed phase

Another important parameter in evaluation of membrane evaporation is heat transfer in feed phase where the aqueous solution is flown. Fig. 7 illustrates total heat flux in the feed phase of membrane evaporator. It is shown that the total heat flux increases along the feed side. The latter could be attributed to the development of velocity in this subdomain. Velocity has a profound

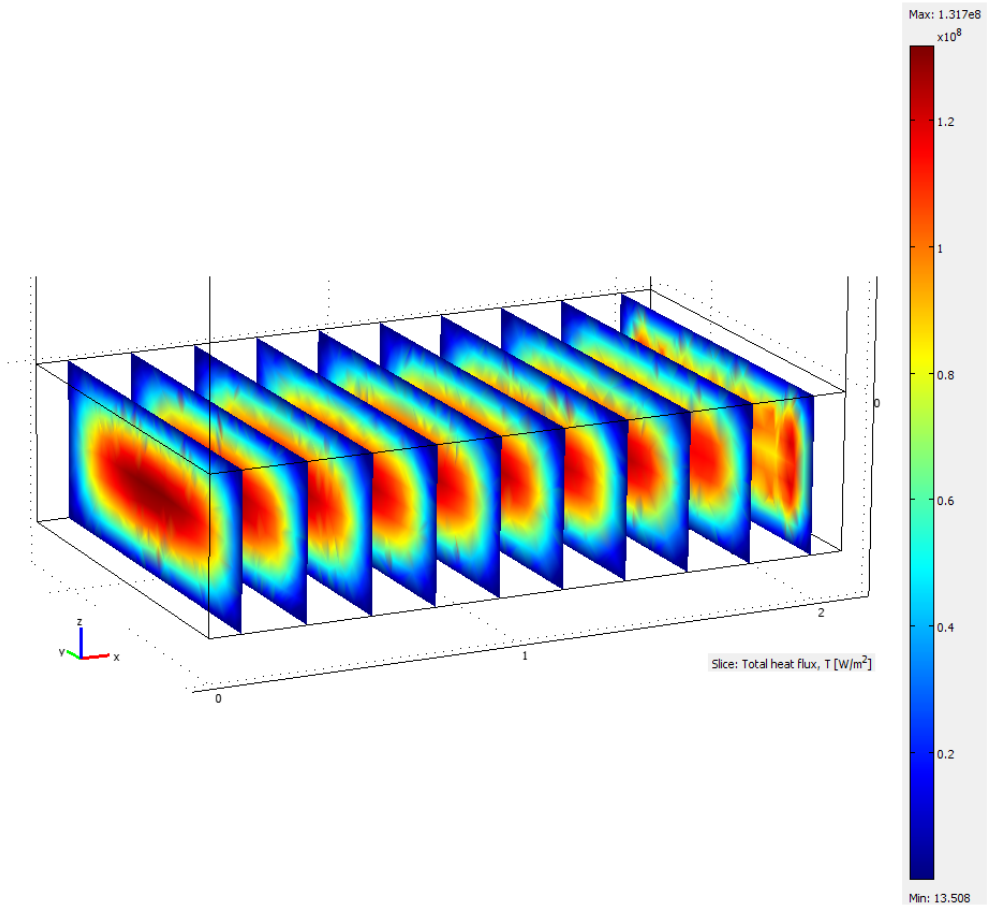

Fig. 7 Distribution of total heat flux in the feed phase

effect on total heat flux in the feed phase and enhancement of velocity along the feed phase, increases heat transfer flux accordingly. Fig. 7 also shows that the total heat flux is the highest at the center of feed side because the maximum of velocity is obtained at the center.

4. Conclusions

Concentration of aqueous solutions in membrane evaporators was simulated in this work. A three-dimensional mathematical model was developed to describe the transport of water in the membrane evaporator. Basic equations of transport phenomena were solved numerically for simulation of process. Finite element method was employed to solve the governing equations of model. The model findings were compared with the experimental data for the evaporation of pure water in a flat-sheet membrane contactor. Comparisons showed good agreement among the simulation and experimental results. The results showed that pressure loss is not appreciable in the membrane evaporators, and the optimum conditions can be obtained by adjusting mass transfer resistance in the gas phase.

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