# Mechanistic Modeling of Organic Compounds Separation from Water *via* Polymeric Membranes

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**ABSTRACT:** *A mathematical model considering mass and momentum transfer was developed for simulation of ethanol dewatering via pervaporation process. The process involves removal of water from a water/ethanol liquid mixture using a dense polymeric membrane. The model domain was divided into two compartments including feed and membrane. For a description of water transport in the feed solution, Maxwell-Stefan approach was used, while for mass transfer inside the membrane the molecular diffusion mechanism was assumed. The governing equations were solved numerically using finite element method. The concentration profile inside the membrane showed a linear decrease and a parabolic fully developed velocity profile was obtained on the feed side. The results also confirmed that formation of concentration layer can be easily predicted using Maxwell-Stefan approach in dewatering of organic compounds using pervaporation process.*

**KEYWORDS:** *Mass transfer; Membranes; Modeling; Pervaporation; Maxwell-Stefan model.*

## INTRODUCTION

Dehydration of organic solvents is an important unit operation in the production of solvents at industrial scale. The operation can be conducted using typical separation units such as distillation, adsorption, etc. These processes involve removal of water from the solvent by application of energy as heat or by application of another phase like in adsorption. The major problem with conventional dehydration processes is the consumption of much energy in these processes especially for those processes that use heat for the creation of vapor phase [1]. Moreover, the conventional separation processes suffer from other difficulties such as difficult scale up, design, high capital and maintenance costs, and huge equipment.

Researchers are trying to find alternative separation processes for dehydration of chemical solvents. The main criteria for alternative separation processes are efficiency, consumption of low energy, low cost, and easy design and operation. Recently membrane separation technology has attracted much attention in separation processes due to its superior properties compared to other processes [2-33]. Membrane processes can provide a great medium for separation of close-boiling point materials such as water-alcohol. Moreover, membrane technology is also capable of separation of liquid mixtures that form an azeotrope at specific concentration [34-37]. Additionally, design and scale-up of membrane processes is easy and linear which can make the process fascinating for industrial applications. Research on membrane separation processes mostly focuses on synthesis and fabrication of novel and composite material for the purpose of separation [15]. However, development of mathematical models for simulation of membrane processes is of great importance.

Development of a mechanistic model which can relate process parameters to product properties is of great interests for design and optimization of separation processes [38-46].

Some researchers have developed mechanistic models for simulation of polymeric and inorganic membranes to predict the performance of process [47-58]. Recently, data-driven models have shown great capability if process modeling and simulation [59-64]. However, these models are a black box and cannot capture the process.

Various models have been developed for prediction and description of membrane processes. *Shirazian et al.* [38-44, 49, 65] developed a mathematical model for prediction of transport phenomena in porous membranes. They developed a 2D comprehensive model for prediction of $CO_2$ & $SO_2$ concentration in hollow-fiber membrane contactors. The model considers both diffusional and convective mass transfer in the membrane module. Their results revealed that 2D mathematical model based on Computational Fluid Dynamics (CFD) can provide a powerful tool for design and optimization of membrane processes. *Rezakazemi et al.* [66] developed a mathematical model for prediction of water transport through dense membranes in a pervaporation process. The model considers mass transfer flux in the membrane and the feed solution. The mass transfer equations were coupled with the momentum equation to completely model the process. CFD technique was used for simulation of the process. The results showed satisfactory agreement with the experimental data. Shirazian and *Ashrafizadeh* [67] developed a 3D mass transfer model for simulation of water transport in membrane evaporation process. The authors considered Fick's law of diffusion for prediction of mass transfer in feed solution and membrane pores. In the developed models for modeling and simulations of membrane processes, the authors used Fick's law of diffusion for estimation of diffusional mass transfer. The latter could produce satisfactory results at low concentration and also for binary systems. For concentrated systems, the model would deviate from experimental data.

Therefore, there is a definite need for a comprehensive mathematical model for simulation of separation in membrane systems. The model should be capable of predicting mass transfer flux as well as hydrodynamics of process at various feed concentrations. Application of multicomponent mass transfer theory, i.e.

Maxwell-Stefan model for simulation of membrane processes can provide a better understanding of the separation mechanism in membrane processes. The main objective of the present work is to develop a 2D mathematical model based on Maxwell-Stefan theory for simulation of membrane separation processes. The model is developed for dehydration of ethanol using pervaporation.

**THEORETICAL SECTION**

In this work, a 2D comprehensive model is developed for simulation of membrane process. The considered process here is a pervaporation process for removal of water from ethanol (ethanol dehydration). For modeling of the process, a model domain is considered and model equations are then derived. Fig. 1 shows model domain used for modeling. The feed solution involving a mixture of 10 % wt. water and 90% wt. ethanol flows through the feed side of the membrane module (at y = 0). The feed solution exits from the upper side and recirculates inside the module. The membrane module at x = 0 is assumed to be insulated. Therefore, the model domain consists of two subdomains called membrane and feed sides. The governing equations are derived and solved for these two regions separately.

*Model development*

In order to develop the mechanistic model for prediction of the process, the following assumptions are made:

(1) Steady state and isothermal conditions for both feed and membrane sides

(2) The feed flow is in the laminar regime

(3) Thermodynamic equilibrium is established the feed - membrane interface

(4) Water is the only penetrant.

The next step is to derive the governing equations for description of water transport in the feed and membrane side. It should be pointed out that the permeate side is neglected in the simulation because the considered process here is pervaporation and the permeate pressure is very low. Therefore the concentration at the permeate side is assumed to be zero.

The main equation that describes the transfer of water from the feed phase to permeate side is continuity equation. The continuity equation is used to obtain
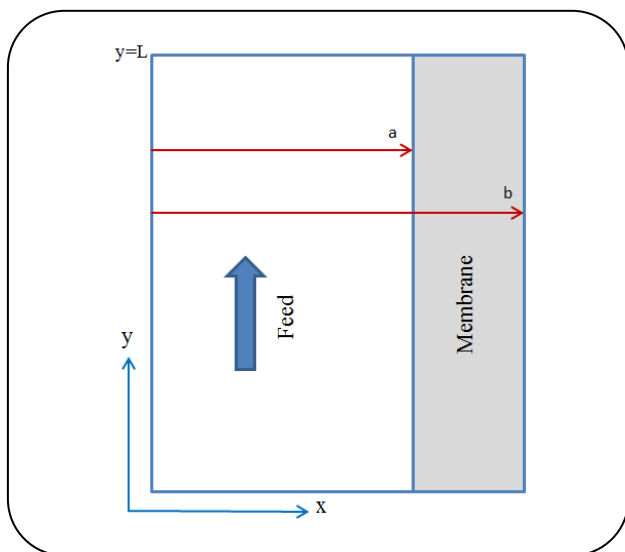
***Fig. 1: Model domain.***

concentration and mass transfer flux of water in the membrane module. The basic form of continuity equation is as follows [68]:

$$\frac{\partial C_w}{\partial t} + \nabla \cdot (J_w + C_w V) = R_w \qquad (1)$$

Where $C_w$ denotes the concentration of water (mol/m$^3$), $J_w$ refers to diffusive mass transfer flux of water (mol/m$^2$.s), $V$ stands for the velocity vector (m/s), $t$ the time (s), and $R_w$ refers to the chemical reaction (mol/m$^3$.s) which is zero in this case. Now the equations are derived for each subdomain, i.e. feed and membrane.

*Feed phase equations*

Equation (1) is the main equation of mass transfer which should be solved numerically to obtain the concentration and mass flux distribution of water in the membrane module. In order to solve this equation, velocity distribution is required to be coupled to the continuity equation. Velocity distribution can be calculated by solving the Navier-Stokes equations. Therefore, the Navier-Stokes, as well as continuity equation, should be solved simultaneously to specify the concentration distribution of water on the feed side. It is worth mentioning that the Navier-Stokes equations describe flow in viscous fluids through momentum balances for each of the components of the momentum vector in all spatial dimensions. In laminar flow regime, Navier-Stokes equations are given as [68]:

$$-\nabla \cdot \eta (\nabla V_y + (\nabla V_y)^T) + \rho (V_y . \nabla) V_y + \nabla p = F \qquad (2)$$
$$\nabla . V_y = 0$$

where $\eta$ denotes the dynamic viscosity (kg/m.s) of feed solution, $V_y$ refers to the velocity of feed in y-direction (m/s), $\rho$ is the density of the feed solution (kg/m$^3$), $p$ is the pressure (Pa) and $F$ refers to a body force term (N) which is zero in this case.

Another important issue in deriving feed equation is estimation of diffusive mass transfer flux, i.e. $J_w$ in equation (1). $J_w$ stands for the amount of mass (water) transferred to the tube side of membrane module by a diffusion mechanism. The latter can be estimated by either Fick approach or Maxwell-Stefan approach. Fick approach is useful for dilute and binary systems, whereas Maxwell-Stefan (MS) approach is capable of prediction of diffusion in multicomponent systems. MS approach is used for estimation of diffusional mass transfer. In the steady state condition, Maxwell-Stefan can be expressed as [68]:

$$d_i = -\sum_{j \neq i}^{n} \frac{x_j J_i - x_i J_j}{c D_{ij}} \qquad (3)$$

Where $d$ is diffusion driving force, $x$ is mole fraction, $c$ is a total concentration of the solution (mol/m$^3$), $n$ is a number of components and $D$ is MS coefficient (m$^2$/s). The assumptions for Equation (3) are constant pressure and ideal mixture. Therefore, Equations 1-3 should solve to obtain the concentration and velocity distribution in the feed side of the membrane module. It should be noted that the convective mass transfer in the x-direction is neglected due to its negligible contribution to the total mass transfer flux.

The boundary conditions for the continuity equation are:

$$y = 0, \ C_{w\text{-feed}} = C_0 \text{ (Inlet concentration)} \qquad (4)$$

$$y = L, \text{ convective flux} \qquad (5)$$

$$x = 0, \ \frac{\partial C_{w-feed}}{\partial y} = 0 \qquad \text{(Insulation boundary)} \qquad (6)$$

The convective flux boundary condition imposed on the boundary at y=L (Equation (5)) assumes that all mass transfer through this boundary is convection.

$$x = a, \ C_{w\text{-feed}} = C_{w\text{-feed}}/m \qquad (7)$$
(thermodynamic equilibrium)

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where m refers to partition coefficient for water between the feed and the membrane wall.

The boundary conditions for Navier-stokes equations are as follow:

$$y = 0, \ V_y = V_0 \ \text{(Inlet velocity)} \tag{8}$$

$$y = L, \ p = p_{atm} \tag{9}$$

$$x = 0, \ V = 0 \ \text{(no slip condition)} \tag{10}$$

$$x = a, \ V = 0 \ \text{(no slip condition)} \tag{11}$$

*Membrane equation*

Inside the membrane, diffusion is the predominant phenomenon; therefore a diffusion mass transfer equation is derived and solved. For prediction of diffusion inside the membrane, Fick's law of diffusion is applied which has shown great results in the literature [22, 41, 44, 67, 69]. The steady-state continuity equation for transport of water through the membrane is as following [66]:

$$D_{w-membrane}\left[\frac{\partial^2 C_{w-membrane}}{\partial x^2}+\frac{\partial^2 C_{w-membrane}}{\partial y^2}\right]=0 \tag{12}$$

The boundary conditions for the continuity equation in the membrane are:

$$x = a, \ C_{w-membrane}=C_{w-feed}\times m \tag{13}$$

$$x = b, \ C_{w-membrane}=0 \tag{14}$$

$$y = 0 \ \& \ y = L, \ \frac{\partial C_{w-membrane}}{\partial y}=0 \tag{15}$$

The boundary condition (14) states that the concentration of water is zero at membrane/permeate interface. Since the membrane is kept at vacuum condition at permeate side (at x=b), the water concentration at this boundary is assumed to be negligible. The latter means that when the water reaches this boundary, it evaporates instantaneously.

*Numerical simulation of the process*

The model equations including continuity, Maxwell-Stefan, and Navier-Stokes equations for the feed and the membrane with the boundary conditions were solved numerically using COMSOL Multiphysics software version 3.5. The continuity equation is used to obtain a concentration In order to simulate the process, the
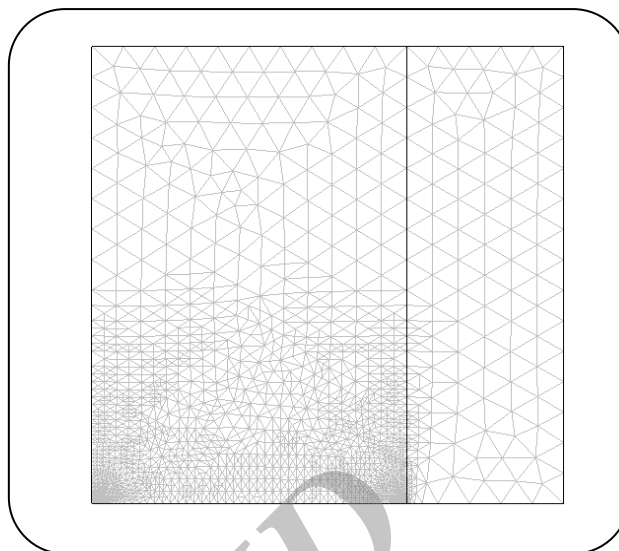


*Fig. 2: Magnified segments of the mesh used in the numerical simulation.*

software utilizes finite element technique for discretization of equations and numerical solution. The latter method has shown great capability in the simulation of transport phenomena in membrane separation processes [7-11, 22-26, 30, 32, 70-78]. The numerical solver of UMFPACK was set entire the simulation for the numerical solution of the governing equations. An IBM-PC-Pentium 5 (CPU speed was 2600 MHz and 4 GB of RAM) was used to solve the set of equations within a short time. It should be pointed out that the COMSOL mesh generator creates triangular meshes that are isotropic in size. Adaptive mesh refinement in COMSOL, which generates the best and minimal meshes, was used to mesh the domain of process. Fig. 2 indicates the nodes generated by software for the process simulation [66]. The membrane and process parameters used in the simulations are listed in Table 1.

**RESULTS AND DISCUSSION**
*Concentration distribution in the feed*

The concentration distribution of water on the feed side is illustrated in Fig. 3. The water concentration is shown in terms of mass fraction. Moreover, concentration profiles of water in x and y directions are shown in Figs. 4 and 5 respectively. As it is clearly seen, concentration change is very sharp near the membrane wall whereas at the zones far from the membrane, the concentration does not change considerably. This is also clearly seen in Fig. 4

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*Tab. 1: Parameters used in numerical simulations [12, 68].*

| Parameter | value | unit |
|---|---|---|
| Feed side width | 2e-5 | m |
| Feed side length | 3e-5 | m |
| Membrane thickness | 1e-5 | m |
| Feed temperature | 300 | K |
| MS diffusivity | 1e-10 | $m^2/s$ |
| Membrane diffusivity | 1e-12 | $m^2/s$ |
| Inlet water mass fraction | 0.1 | - |
| Inlet feed velocity | 0.001 | m/s |
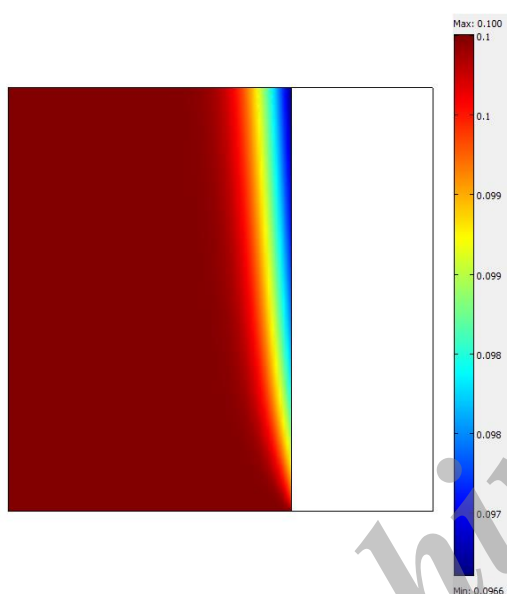


*Fig. 3: Concentration distribution of water on the feed side.*

where the concentration of water is almost constant at the bulk of feed while a sharp decrease in water concentration is observed in the vicinity of membrane wall. The latter could be an evidence for the formation of mass transfer boundary layer. Therefore, the developed model is capable of predicting concentration boundary layer in the feed side.

### Concentration distribution inside the membrane

The concentration distribution of water inside the membrane is shown in Fig. 6. Moreover, the concentration profile of water inside the membrane in the x-direction is depicted in Fig. 7. Since the only diffusional mass transfer

is assumed for transport of water through the membrane, a uniform and linear concentration profile in the x-direction is observed. Moreover, two upper and bottom sides of membranes (at y=0 & y=L) are assumed Insulation boundary. However, a sharp decrease in water concentration is observed whereas the concentration reaches zero at the feed/permeate interface. The latter is due to the implementation of zero concentration for water in the boundary.

### Velocity profile

Velocity distribution of feed solution in 2 dimensions is represented in Fig. 8. As mentioned before, velocity field of the feed solution is obtained by numerical solution of the Navier-Stokes equations. Analysis of velocity field reveals that the maximum of velocity occurs at the middle of feed side, whereas the velocity decreases sharply in the vicinity of membrane wall and also feed wall. The latter is also an evidence for the formation of velocity boundary layer which is well predicted by the developed model. The reduction in the velocity near the membrane wall could be attributed to the effect of viscous forces exerted on the layer of fluid.

### Distribution of mass transfer flux

Fig. 9 shows the distribution of mass transfer flux along with arrows of flux in the feed side of the membrane module. The only diffusional mass transfer is depicted in Fig. 9, because it has a major effect on the transport of water from feed phase to the membrane phase. As it is clearly seen, the diffusion in the bulk of feed solution is almost zero,
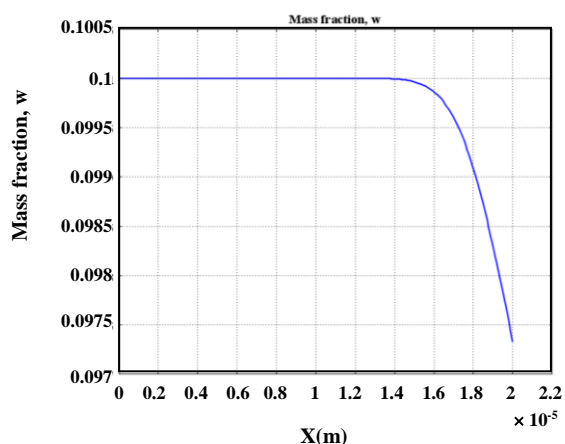
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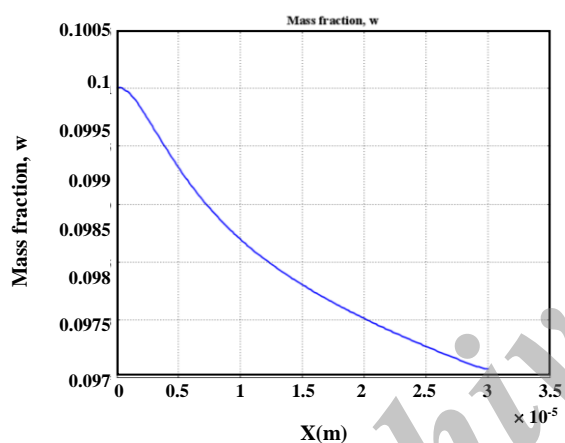*Fig. 4: Concentration profile of water in the feed side (x-direction).*



*Fig.6: Concentration distribution of water inside the membrane.*



*Fig. 5: Concentration profile of water on the feed side (y-direction).*



*Fig. 7: Concentration profile of water inside the membrane.*

whereas in the area near the membrane wall, a significant increase in diffusion is observed. Basically, mechanism of mass transfer for water in the feed side is diffusion and convection. Convection is controlled by the velocity of the fluid, whereas diffusion is mainly controlled by the concentration gradient of species. Since the velocity in the bulk of feed solution is high (see Fig. 8), convection contribution in the bulk is high and diffusion is negligible. On the other hand, diffusion is significant near the membrane wall due to the reduction of velocity in this zone. This can also be from the arrows of mass transfer flux in Fig. 9 which is high near the membrane wall.
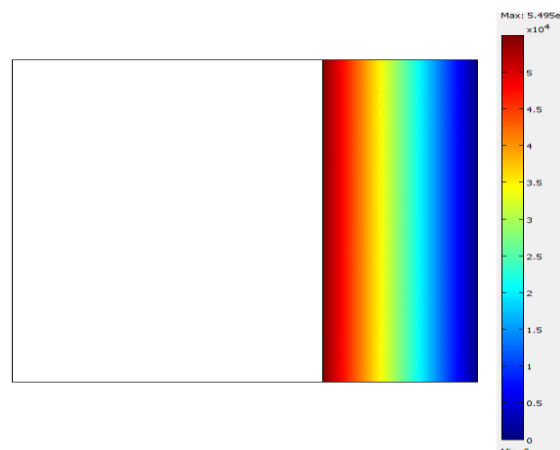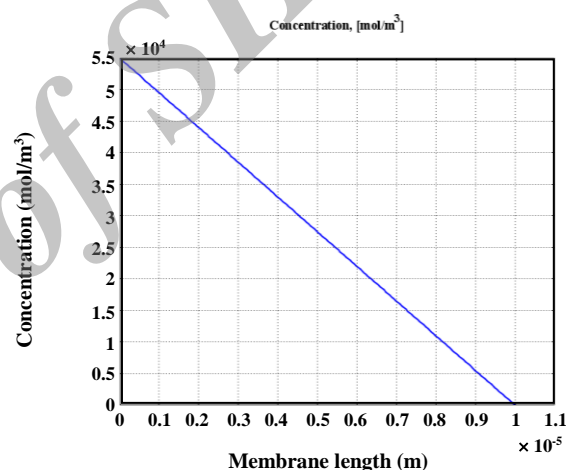
**CONCLUSIONS**

A two-dimensional mathematical model was developed in this work considering mass transfer as well as momentum transfer. The process studied in this work involved removal of water from alcohol/water solution by means of a dense polymeric membrane. Evaporation is considered to be the separation method in which the separation is achieved by applying a vacuum pressure at the permeate side. Therefore, vapor pressure gradient is the main driving force of the process. Maxwell-Stefan approach was used for estimation of diffusional mass transfer in the model, and the velocity of fluid was modeled using the Navier-Stokes equation. Finite element
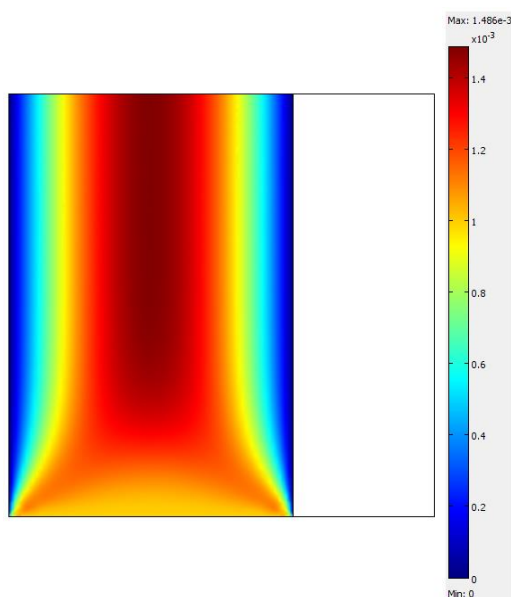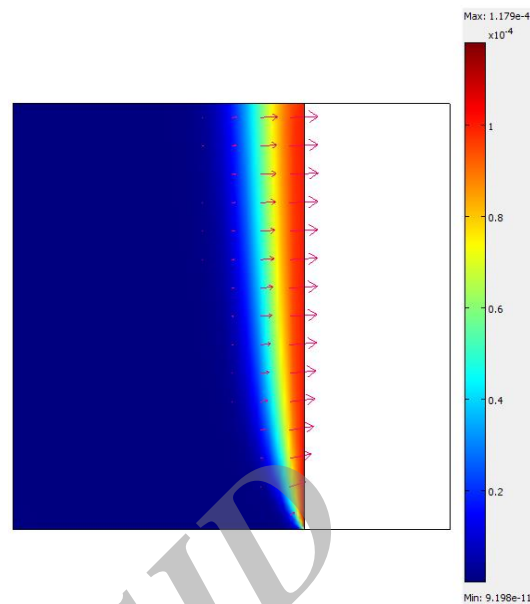
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***Fig. 8: Velocity profile of feed.***



***Fig. 9: Diffusive mass transfer flux of water in the feed.***

the method was used for numerical solution of the model equation and the results indicated that increasing feed velocity decreases the removal of water due to a reduction in residence time of feed solution in the membrane module.

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