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CFD Simulation of Mass Transfer in Membrane Evaporators for Concentration of Aqueous Solutions

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ABSTRACT

Osmotic evaporation (OE) process is usually suggested to concentrate aqueous solutions. OE is a concentration technique based on the use of mesoporous or macroporous and hydrophobic membranes. The difference between the activity of solutions results in a pressure difference between the upstream diluted solution and the downstream (usually concentrated brine) solution. The latter generates a water flow. Osmotic evaporation can be used to selectively extract water from aqueous solutions under atmospheric pressure and at ambient temperature; thus avoiding thermal degradation of the solutions. In spite of the obvious advantages of OE, this technique presents some shortcomings linked to the use of brine such as corrosion and regeneration.

In order to develop an alternative and complementary membrane process, the brine was replaced by a sweep flow of a low pressure gas, i.e. generally air. In that case, the flow of water vapor is not condensed but it is taken away by the extracting phase. This new process is named membrane evaporation (ME). Similar to OE, membrane evaporation occurs at room temperature and the driving force of the process is not the thermal gradient but the difference of the partial pressure of the water vapor between the water surface and the dry air. Membrane evaporation presents interesting working conditions including low operating temperature; the latter makes this process attractive for heat-sensitive solutions.

Performance of a ME contactor is studied in this work. A two-dimensional mass transfer model was developed to predict the flux of water evaporation in the membrane contactor. The model was based on solving the continuity and momentum equations for water in the membrane contactor. Both axial and radial diffusions were considered in the mass transfer equations. The model equations were numerically solved using finite element method to obtain the concentration distribution of water in the contactor. By obtaining the concentration distribution, the flux of evaporation was determined and compared with the experimental data. The findings of the model were in good agreement with the experimental data. It was also indicated that the proposed model is appropriate for the prediction of membrane evaporator performance.

Keywords: Membrane Evaporator; Mass Transfer; Simulation; Hydrophobic; Membrane.

INTRODUCTION

During the past few decades, membrane technology for concentration of aqueous solutions has emerged as a viable alternative to conventional technologies such as distillation and evaporation. Among the membranes processes, membrane contactors are expected to play a major role in

separation processes. The key concept is to use a solid, microporous, hydrophobic (or hydrophilic) polymeric matrix in order to create an interface for mass transfer and/or reaction between two phases. Large mass transfer area and independent fluid dynamics allow an easily controlled operation. Membrane contactors are membrane systems that are employed to "keep in contact" two phases. On the contrary of the traditional idea of membranes as media for performing separations thanks to their selectivity, membrane contactors do not offer any selectivity for a particular species with respect to another, but act as a barrier between the phases involved, by allowing their contact in correspondence of a well defined interfacial area. Being the two phases separate by the membrane, there is no mix of them and dispersion phenomena do not occur[1].

At present, two main membrane contactor processes are suggested to carry out aqueous solutions concentration: osmotic evaporation and membrane distillation.

Osmotic evaporation (OE) is a concentration process based on the use of macroporous and hydrophobic membranes which separates two circulating aqueous liquid phases: a solution to be concentrated and a hypertonic solution, typically concentrated brine. Due to hydrophobic nature of membrane used in the OE, the membrane cannot be wetted by the liquids thus creating vapor-liquid interfaces at each pore entrance. The difference of activity of solutions results in a water vapor pressure difference between the upstream diluted solution and the downstream concentrated brine which generates the water flow to the gas phase[2,3].

The second membrane contactor, membrane distillation, is also a concentration technique in which a porous hydrophobic membrane is used as physical barrier between the feed and the distillate[4]. A temperature difference between both phases which are contacted in the membrane causes a vapor pressure difference. This vapor pressure difference is the driving force of the membrane distillation. This vapor pressure gradient causes a mass-transfer across the membrane.

In spite of the obvious advantages of these membrane processes for concentration of aqueous solutions, they present also some drawbacks linked to the use of brine (corrosion and regeneration) in the case of osmotic evaporation and relatively high temperature in the membrane distillation. The problems of these two membrane processes limit their applications for the concentration of aqueous solutions and hence, there is a need to develop alternative and complementary membrane contactor processes[3].

Hengl *et al.,*[3] developed a new membrane process for concentration of aqueous solutions. This membrane concentration process, named membrane evaporation, which is halfway between osmotic evaporation and membrane distillation, presents the advantages of both techniques. It is based on the use of a hydrophobic macroporous membrane which separates an aqueous solution to be concentrated and an extracting phase: a sweep flow of low pressure gas, which is generally air (Fig. 1)[3].

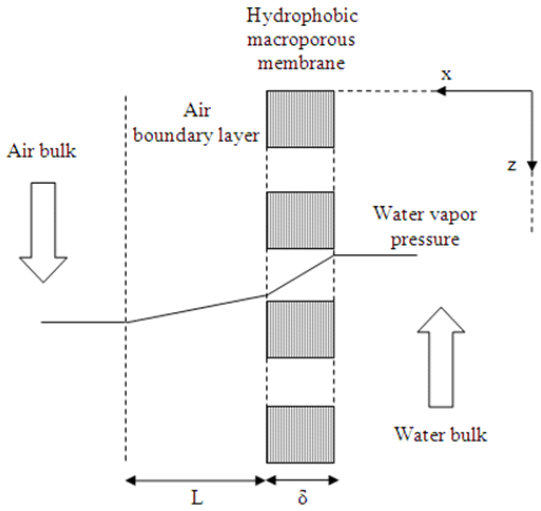

Fig. 1: Basic Principle of membrane evaporation [3]

On the contrary of membrane distillation and OE, the flow of water vapor is not condensed but it is taken away by the extracting phase (air), because the objective of the process is to concentrate the aqueous solution. Membrane evaporation (ME) operates at room temperature and

the driving force of the process is not the thermal gradient but the difference of the water vapor partial pressure between the water surface and the dry air. Membrane evaporation presents interesting working conditions, like low operating temperature, which makes this process attractive for heat-sensitive solutions[3-5].

The main purpose of this study is to develop and solve a mass transfer model for simulation of membrane evaporation process. The simulations are based on computational fluid dynamics of mass and momentum transfer in the membrane and gas phases. The model equations are solved by a numerical procedure based on finite element method (FEM). The modeling findings are then validated with the experimental data for evaporation of water in a hydrophobic metallic membrane reported by Hengl *et al.,*[3].

Model development

The continuity equation for each species can be expressed as [6]:

$$\frac{\partial C_i}{\partial t} = -(\nabla \cdot C_i V) - (\nabla \cdot J_i) + R_i \quad ...(1)$$

where C_i, J_i, R_i, V and t are the concentration, diffusive flux, reaction rate of species *i*, velocity and time, respectively. Either Fick's law of diffusion or Maxwell–Stefan theory can be used for the calculation of diffusive fluxes of species *i*.

2.1. Gas phase equations

The continuity equation for steady state for transport of water in the gas phase (air) of membrane contactor is obtained using Fick's law of diffusion for estimation of diffusive flux [7-9]:

$$D_{w-air}\left[\frac{\partial^2 C_{w-gas}}{\partial x^2} + \frac{\partial^2 C_{w-gas}}{\partial z^2}\right] = V_z \frac{\partial C_{w-gas}}{\partial z} \quad ...(2)$$

In a laminar flow, a fully developed velocity profile can be described as [6]:

$$V_z = 6\overline{V}\left[\left(\frac{x}{L}\right) - \left(\frac{x}{L}\right)^2\right] \quad ...(3)$$

where $\overline{V}$ is the average velocity of air in the membrane contactor.

The boundary conditions for mass transfer equations are:

at z = 0, $C_{w\text{-}gas}$ = 0 (Inlet dry air) ...(4)

at x = δ, $C_{w-gas} = C_{w-membrane}$ (macroporous membrane) ...(5)

at x = L, $\frac{\partial C_{w-gas}}{\partial x} = 0$ (Insulation boundary) ...(6)

Membrane equations

The continuity equation for steady state for transport of water through membrane pores filled by the gas phase (air) is as following [10]:

$$D_{w-membrane}\left[\frac{\partial^2 C_{w-membrane}}{\partial x^2} + \frac{\partial^2 C_{w-membrane}}{\partial z^2}\right] = 0 \quad ...(7)$$

The boundary conditions for mass transfer equation in the membrane are:

at x = 0, $C_{w-membrane} = \frac{P_w^{sat}}{RT}$ ...(8)

at x = δ, $C_{w-membrane} = C_{w-gas}$ (macroporous membrane) ...(9)

at z = 0, $\frac{\partial C_{w-membrane}}{\partial z} = 0$ (Insulation boundary) ...(10)

Numerical solution

The model equations with appropriate boundary conditions were solved numerically using COMSOL software. This software employs finite element method (FEM) for numerical solutions of

differential equations. The use of FEM allows mass conservation in the domain; therefore 'numerical loss' of mass in the computational domain is not a major concern. The applicability, validity and robustness of the FEM for the type of domain encountered in the present work have been demonstrated by a number of previous authors[7-10]. The finite element analysis is combined with adaptive meshing and error control using numerical solver of UMFPACK. This solver is an implicit time-stepping scheme, which is well suited for solving stiff and non-stiff non-linear boundary value problems [10]. An IBM-PC-Pentium5 (CPU speed of 2600 MHz and 2 GB of RAM) was used to solve the set of equations. The computational time for solving the set of equations was about 5 minutes. It should be pointed out that the COMSOL mesh generator creates triangular meshes which are isotropic in size. A large number of elements are then created with scaling. Different scaling factors have been employed in all directions due to large differences among dimensions. COMSOL software automatically scales back the geometry after meshing. This would generate an anisotropic mesh around 1098 elements. Adaptive mesh refinement in COMSOL, which generates the best and minimal meshes, was used to mesh the contactor geometry. Grid independence test showed that the optimum numbers of meshes were 1098 for numerical simulation.

Table 1 indicates the membrane parameters which are used in the simulations. The membrane parameters used in the simulations are the same as those reported by Hengl *et al.,*[3].

Table 1: Membrane parameters of Hengl et al.'s experiments [3]

Membrane type	Flat metallic stainless steel
Membrane length (mm)	210
Membrane width (mm)	127
Membrane thickness (mm)	0.2
Membrane porosity	0.3
Mean pore diameter (mm)	2.6
Water side height (mm)	5
Gas side height (mm)	15
Water temperature (K)	298.15
Air temperature (K)	293.15

RESULTS AND DISCUSSION

Model validation

In order to verify the mass transfer model used for simulation, the simulation results were compared with the experimental values reported by Hengl *et al.,*[3]. They reported experimental results for evaporation of pure water by a hydrophobic metallic membrane module. In this section the evaporation flux of water calculated by simulation is compared with the experimental values of Hengl *et al.,*[3] to verify the simulation results. Figure 2 shows the comparison between experimental and simulated values for water evaporation flux.

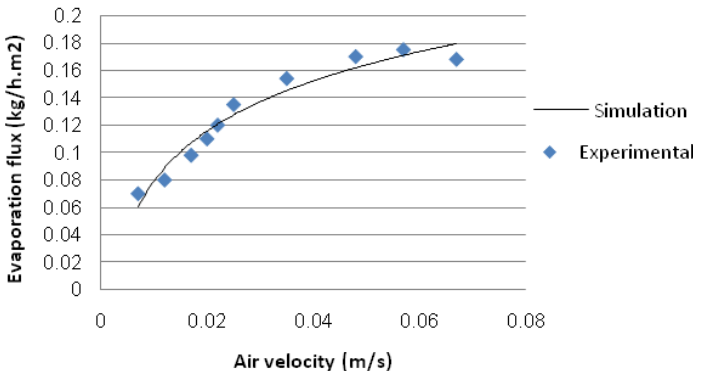

Fig. 2: Comparison between experimental [3] and calculated values of water evaporation flux

As shown in the figure 2, the results of the simulation match quite well with the experimental data. In the low regime of air velocity (< 0.04 m/s), the flux of water increases with the air velocity. As it is shown, by increasing the air velocity, the mass transfer rate of water into the gas phase is increased. The latter is due to the increase in concentration gradients of water in the liquid phase. Therefore, the water concentration in the gas phase outlet stream increases; i.e. the evaporation of water increases (Fig. 2).

CONCLUSIONS

Performance of a membrane evaporator was studied theoretically in this work. A mass transfer model was developed to describe the transport of water through the membrane contactor. The model was based on the conservation equations for two sections of the contactor, i.e. membrane and gas phase. Finite element method (FEM) was employed to solve the model equations. Effect of contactor operating parameter including gas velocity on the removal of water was investigated. The simulation results were compared with the experimental data from literature obtained for pure water evaporation. Comparison revealed a good agreement among the model predictions and the experimental data for flux of water evaporation at different air velocities. The simulation results indicated that the evaporation of water is increased with increasing the air velocity in the contactor.

REFERENCES

1. Drioli, E., Criscuoli, A., Curcio, E., Membrane Contactors: Fundamentals, Applications and Potentialities, Membrane Science and Technology Series 11, Elsevier (2006).
2. Kunz, W., Benhabiles, A., Ben-Aim, R., Osmotic evaporation through macroporous hydrophobic membranes: a survey of current research and applications, *J. Membrane Sci.* **121**: 25 (1996).
3. Hengl, N., Mourgues, A., Pomier, E., Belleville, M.P., Paolucci-Jeanjean, D., Sanchez, J., Rios, G., Study of a new membrane evaporator with a hydrophobic metallic membrane, *J. Membrane Sci.* **289**: 169-177 (2007).
4. Lawson, K.W., Lloyd, D.R., Membrane distillation, *J. Membrane Sci.* **124**: 1 (1997).
5. Romero, J., Draga, H., Belleville, M.P., Sanchez, J., Combe-James, C., Dornier, M., Rios, G.M., New hydrophobic membranes for contactor processes – Applications to isothermal concentration of solutions, *Desalination* **193**: 280-285 (2006).
6. Bird R.B., Stewart W.E., Lightfoot, E.N. Transport Phenomena. New York: John Wiley & Sons (1960).
7. Azam Marjani, Saeed Shirazian, Simulation of heavy metal extraction in membrane contactors using computational fluid dynamics, *Desalination,* **281**: 422-428 (2011).
8. Saeed Shirazian, Azam Marjani, Fatemeh Azizmohammadi, Prediction of SO_2 Transport Across Ceramic Membranes Using Finite Element Method (FEM), *Oriental journal of Chemistry* **27**(2): Page No. 485-490.
9. Shirazian, S., A. Moghadassi, and S. Moradi, Numerical simulation of mass transfer in gas-liquid hollow fiber membrane contactors for laminar flow conditions. *Simulation Modelling Practice and Theory,* **17**(4): p. 708-718 (2009).
10. Saeed Shirazian, Azam Marjani, Farzad Fadaei, Supercritical extraction of organic solutes from aqueous solutions by means of membrane contactors: CFD simulation, *Desalination,* **277**(1-3): Pages 135-140 (2011).