Analysis of Heat Transfer Coefficients in Direct Contact Membrane Distillation Modules Using CFD Simulation

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Abstract

Membrane distillation (MD) is an emerging separation technology for desalination, solution concentration and waste water treatment. As a thermal driven device, heat transfer coefficients are critical to the MD performance. In this study, the transmembrane heat and mass transfers are rigorously accounted for in the computational fluid dynamics (CFD) simulation. Flat plate direct contact membrane distillation (DCMD) modules with smooth-surface and rough-surface channels as well as in co-flow and counter-flow configurations are analyzed for the desalination application. For different rough-surface channels, flow configurations and operation conditions, the simulated permeation fluxes are fairly close to the experimental results. The local distributions of heat transfer coefficients show very high values at fluid inlets. For the simulated flat plate modules, the local heat transfer coefficients fall between conventional correlations of heat exchangers with circular channels and parallel plates and the module average heat transfer coefficients are much higher than the conventional correlations. This study reveals the values and distribution characteristics of the heat transfer coefficients in DCMD modules, which is important for the design of DCMD modules.

Key Words: Computational Fluid Dynamics, Membrane Distillation, Mass Transfer, Heat Transfer, Rough Surface

1. Introduction

Membrane distillation (MD) is a separation process which only volatile species permeate through a porous hydrophobic membrane. MD can be carried out at low temperature by waste heat or solar heat and shows great potential to replace conventional energy intensive separation technologies. Direct contact membrane distillation (DCMD), in which the membrane is in direct contact with a hot liquid and a cold liquid, is the simplest MD configuration capable of producing reasonably high flux. It is best suited for applications such as desalination and concentration of aqueous solutions (e.g., juice concentrates) [1].

Membrane distillation operation is a non-isothermal process, which involves both heat transfer and mass transfer from the hot side to the cold side of the membrane. In a DCMD, the permeable species are vaporized and condensed at the membrane-liquid interfaces of the hot feed side and the cold permeate side, respectively. The transmembrane temperature difference induces the vapor pressure difference, which is the driving force of the transmembrane mass transfer. The temperatures at the membrane surface are different from the bulk fluid temperatures due to the boundary layer heat transfer resistances. The heat transfer through the boundary layers is recognized as the key factor deciding the MD performance.

Eddy promoting methods, such as filling fluid chan-
nels with spacers or using rough-surface channels, can be applied on MD modules to minimize the heat transfer resistances of the boundary layers. Ho et al. [2] used rough-surface channels with different roughness levels in a plate type DCMD module for desalination. The experimental study demonstrated up to 37% enhancement in the transmembrane mass flux.

Many researchers have conducted the analysis of MD processes using empirical correlations of heat transfer coefficients and resistance-in-series model [3–7]. Because of the integrated heat and mass transfer in the MD modules, the use of the conventional correlations developed for heat exchangers with non-porous walls has been questioned [8].

Most of the simulation analysis of MD modules are zero dimensional or simplified one dimensional. The former treats the module as a whole and the latter considers the variation of the temperature distribution along the module length [8]. To improve the model applicability and accuracy, computational fluid dynamics (CFD) simulation studies of MD modules have been reported. Charfi et al. [9] developed a 2D CFD model which considers the heat, mass and momentum transport through the feed channel, membrane and permeate channel of a plate-and-frame type sweeping gas MD module. The conservation and constitutive equations of the thin membrane layer were included in the model. The model is comprehensive but is highly complicated and difficult to use. Yu et al. [10] conducted a 2D CFD simulation of a single-tube hollow fiber DCMD module using the commercial code Fluent. The simulation employed a simplified heat transfer model by ignoring the influence of the transmembrane mass flux in the conservation equation but combining the latent heat incurred by evaporation/condensation into the heat transfer process. The transmembrane mass flux was determined using the transmembrane temperature difference and a specified fixed permeability of the membrane.

CFD simulations of DCMD modules employing some eddy promoting techniques have been reported. For the spacer-filled DCMD modules, Shakaib et al. [11] conducted 2D CFD simulations of a representative length of the module to study the effects of spacer orientation and filament spacing on the shear stress distribution and temperature polarization in the modules. Yu et al. [12–14] used 2D and 3D CFD simulations to obtain the hydrodynamics and the temperature polarization coefficient of the single hollow fiber DCMD modules which employed baffles in the shell side, wavy shape fiber or fiber with gear-shaped cross section. For the DCMD modules using rough-surface channels [2], the transfer characteristics inside the MD modules have not been analyzed.

This paper presents the CFD simulation of the DCMD modules using smooth-surface and rough-surface channels for desalination with the emphasis on the heat transfer coefficients in the modules. The comprehensive 3D simulation covers the entire length of the module and takes in the transmembrane heat and mass transfer. The two major techniques for the simulation developed in this study including the simulation of rough surface using cubic blocks with checkerboard arrangement and the approach to incorporating transmembrane fluxes into the commercial code Fluent are presented. The local distribution as well as the module average heat transfer coefficients are compared with the conventional correlations.

2. Modeling

The simulated DCMD modules are the plate-type experimental modules reported in Ho et al. [2]. The length, width and height of both the hot and cold channels are 0.21 m, 0.29 m and 2 mm. The membrane is a composite PTFE (poly-tetrafluoroethylene) membrane (ADVANTEC) with a nominal pore size of 0.1 μm, a porosity of 0.72 and a thickness of 130 μm. As shown in Figure 1, the non-membrane plate on the bottom of the hot fluid channel has a smooth surface or a rough surface. The rough surface was fabricated using siphonic-blasting with aluminum oxide (Al₂O₃) sand grains and arc spraying for Ni film coating [2]. Three rough surfaces were used. The relative roughness, which is the ratio of surface roughness (ε) and hydraulic diameter of the channel (dₜ), of these surfaces are 0.0035, 0.0686 and 0.1413, respectively. The channels with these surfaces are identified as R0, R24 and R44 channels in this paper. R0 channel is the smooth-surface channel.

2.1 Computational Domain and Grids

The roughness elements are simulated using cubic blocks of the dimension of the roughness with a checker-
board arrangement shown in Figure 1. Because the roughness of R0 channel is very small, it is simulated using smooth surface, i.e. without cubic blocks. The simulation domain, also shown in Figure 1, covers the entire length and height but only two-cubic-block width of the module. At the entrance and exit of the module, a small extra length of 0.005 m was added to simulate the actual module and to avoid the convergence difficulty in simulation. In these extra zones, the interface between the top and bottom channels is a non-porous solid wall.

The laminar flow model of FLUENT 6.3 [15] and the grid generation preprocessor GAMBIT were used for this simulation work. For the simulation domain, structured hexahedral grids were used. Grids of smaller sizes were used in the regions near all the boundary faces. The membrane layer was defined as a non-permeable wall and the transmembrane heat and mass transfers were incorporated into the simulation using user-defined functions.

2.2 Governing Equations

2.2.1 Fluid Channels

For the laminar-flow hot and cold fluids in the channels, the mass, momentum and energy conservation equations to be solved are described in this section.

The total mass conservation equation with a source term \( S_m \) is:

\[
\nabla \cdot (\rho \vec{v}) = S_m
\]

(1)

For a non-reacting system, the mass conservation equation of species \( i \) with a source term \( S_i \) is:

\[
\nabla \cdot (\rho_i \vec{v}_i) = - \nabla \cdot J_i + S_i
\]

(2)

where the diffusion flux of species \( i \), which arises due to concentration gradients, in laminar flow is:

\[
\vec{J}_i = -D_{x,ij} \nabla y_i
\]

(3)

The momentum conservation equation for a system when neglecting the gravitational and external body forces is:

\[
\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot \vec{\tau}
\]

(4)

where \( \vec{\tau} \) is the stress tensor:

\[
\vec{\tau} = \mu ((\nabla \vec{v} + \nabla \vec{v}^T) - \frac{2}{3} \nabla \cdot \vec{v})
\]

(5)

The energy conservation equation with a source term \( S_h \) is:

\[
\nabla \cdot (\rho (\vec{v}E + \vec{v}P)) = \nabla \cdot (k \nabla T - \sum_{i} h_i J_i + (\vec{\tau} \cdot \vec{v})) + S_h
\]

(6)

where \( E \) is energy of the flow streams, including the enthalpy, flow work and kinetic energy:

\[
E = \left( \sum_{i} y_i h_i - \frac{\vec{v}^2}{2} \right)
\]

(7)

2.2.2 Membrane Layer

In DCMD, the volatile species in the hot liquid will vaporize at the hot-side membrane surface, transfer across the membrane and condense at the cold-side membrane surface. Vapor-liquid equilibrium is normally assumed at the membrane surfaces. The transmembrane mass flux
can be determined using the saturation vapor pressures corresponding to the membrane surface temperatures and the membrane mass transfer coefficient.

\[ N_i = \frac{k_{m,i}}{RT_m} (P_{sat,i} - P_{sat,m}) \]  

(8)

The mass transfer in the membrane layer can be described by Dusty-Gas Model [16]. Based on the value of Knudsen number \( Kn = \lambda / d_p \), the Knudsen diffusion and molecular diffusion are significant for this study [17]. The membrane mass transfer coefficient can be estimated using the resistance-in-series relationship:

\[ k_{m,i} = \frac{\varepsilon \delta_m}{\tau \delta_m} \left( \frac{1}{D_{k,i}} + \frac{1}{D_{m,i}} \right) \]  

(9)

The heat flux across the membrane is contributed by the conductive heat transfer across the membrane and the latent heat flow associated with the transmembrane mass transfer. For the case where only water vapor is the permeating species, the transmembrane heat flux is:

\[ Q = NH_{amp} + \frac{k_{c,m} \delta_m}{\delta_m} (T_j - T_p, n) \]  

(10)

The thermal conductivity of the membrane layer can be determined by the isostrain model [18] using the thermal conductivities of the vapor and the membrane material:

\[ k_{c,m} = \varepsilon k_{c,v} + (1 - \varepsilon) k_{c,m} \]  

(11)

The approach to incorporating the transmembrane heat and mass transfers into Fluent is depicted in Figures 2 and 3. For each location on the membrane surface, a set of membrane adjacent cells, one on hot fluid side and the other one on cold fluid side, can be located as shown in Figure 2. The states of these cells are used to determine the transmembrane mass flux and heat flux using Eqs. (8) and (10). User-defined functions were developed to perform these calculations. The calculation flow diagram is illustrated in Figure 3. The steps include the determination of properties for the vapor inside the membrane, heat transfer coefficient and mass transfer coefficient inside the membrane, transmembrane mass flux and heat flux, and the assignment of mass and energy source terms to the membrane adjacent cells.

2.3 Boundary Conditions and Solution Algorithms

The boundaries of the simulation domain as shown in Figure 1 must be defined. The top and bottom walls of the module are adiabatic. The two vertical sides of the module are symmetric boundaries. The hot and cold feed streams are co-current or counter-current flow. The outlet faces of both streams are set as pressure-outlet boundaries.

The governing equations were solved using finite...
volume method and the second-order upwind scheme. SIMPLE algorithm (Semi-Implicit Method for Pressure-Linked Equation) [15] was used to solve the pressure-velocity coupling. The simulation was assumed to have achieved an iterative convergence when the residuals of the mass, momentum and energy conservation equations are less than $1 \times 10^{-5}$ and the transmembrane mass flux does not vary more than 1% for every 1000 times of iteration.

3. Results and Discussion

3.1 Grid Independence

Grid independence analysis was conducted for each simulated module. The pressure drops of the tested grid systems were compared to determine the appropriate grid sizes. The grid edges fall between 40 to 120 μm and the total grid numbers for R0, R24 and R44 modules are 0.72, 1.25 and 1.4 million, respectively.

3.2 Model Verification

The model verification uses the experimental results reported in Ho et al. [2]. The simulated and experimental results, in terms of the module average transmembrane mass flux, are compared in Figure 4. The average deviation of simulation predictions from experimental results is less than 10%.

In Figure 4 as well as all the other figures, the legend with and without ‘Co’ represents counter-flow and co-flow, respectively. The experimental data shown in Figure 4 include experimental cases operated in both co-flow and counter-flow configurations using R0, R24 and R44 channels. The operation conditions include the hot fluid inlet temperatures of 60 °C (T1), 50 °C (T2) and 40 °C (T3) and the flow rates of 0.026 m/s (V1), 0.02 m/s (V2) and 0.0144 m/s (V3). The hot and cold fluids are controlled at the same flow rate. For all the cases, the cold fluid inlet temperature is fixed at 25 °C.

3.3 Effects of Modules, Flow Configurations and Operation Conditions

The simulation results of the module average mass flux for different modules (surface roughness), flow configurations (co-flow and counter-flow) and operation conditions (temperature and flow rate) are summarized in Figure 5.

The average mass flux increases with hot fluid inlet temperature, flow rate and surface roughness of channel. For the same module, under the same operation conditions, the counter-flow configuration gives higher mass flux than the co-flow configuration. All these effects are more significant when the hot fluid inlet temperature is higher.

3.4 Mass Flux and Heat Transfer Coefficient Distributions

The CFD simulation allows the prediction of local
distributions of the bulk fluid and membrane surface temperatures as well as the transmembrane heat and mass fluxes for the DCMD modules. For the purpose of this study, which is to analyze the heat transfer coefficients in DCMD modules, only the local distributions of mass flux and heat transfer coefficient for the T1 and V1 operation condition case are presented in Figure 6. Using transmembrane heat flux, bulk fluid temperature and membrane surface temperature, the local heat transfer coefficient can be calculated by:

$$h = \frac{Q}{(T_{\text{bulk}} - T_{\text{m}})} \quad (12)$$

The mass flux and heat transfer coefficient distributions shown in Figures 6(a) and 6(b) reveal much higher mass flux and heat transfer coefficient at the inlets for both co-flow and counter-flow configuration. According to these distributions, it is not realistic to assume uniform flux or heat transfer coefficient in MD modules.

For both mass flux and heat transfer coefficient, the values are higher for channels with greater surface roughness. The values are higher in counter-flow than in co-flow.

### 3.5 Comparison of Heat Transfer Coefficients with Correlations

In order to examine the applicability of conventional correlations of heat transfer coefficient, which are commonly applied for the design of heat exchangers, the heat transfer coefficients obtained from CFD simulation are compared to the well-known correlations. For direct comparison, local and average Nusselt numbers are used.

The local Nusselt number can be calculated from local heat transfer coefficient via its definition:

$$Nu = \frac{hD_t}{k_c} \quad (13)$$

The average Nusselt number ($Nu_{\text{avg}}$) of the module is the arithmetic mean of the local Nusselt number.

The conventional correlations adopted for comparison are listed in Table 1. These correlations are applicable to heat transfer devices of different shapes, i.e. circular tubes or parallel plates, with different boundary conditions, i.e. uniform heat flux or uniform temperature, as well as under various developing conditions, i.e. fully developed, hydrodynamic developing or thermal developing. Correlations [1–3] are for the prediction of local Nusselt number and correlations [4–6] are for the prediction of average Nusselt number.

The comparisons of the local Nusselt number for the R44 module under T1 and V1 operation condition in co-flow and counter-flow are shown in Figures 7(a) and 7(b), respectively. For the R44 module, because only the hot side channel employs rough surface, the hot side $Nu$ is higher than the cold side. In Figure 7(a), all the local distributions have similar shapes, i.e. much higher values in the inlet followed by a lower value asymptotic curve. In Figure 7(b), the distributions of R44 from CFD simulation show higher values in both inlets. The distributions of correlations based on the cold side fluid conditions are shown in Figure 7(b). The comparisons reveal
that although the distributions are in similar shapes, the values of Nu from CFD simulation and correlations are not close.

The comparisons of average Nusselt number for co-flow and counter-flow are shown in Figures 8(a) and 8(b), respectively. The predicted values from all correlations are much lower than the CFD simulation results. This outcome could be explained by the enhanced heat transfer from the latent heat effect associated with the transmembrane mass transfer. Regarding to the CFD simulation results, the average Nusselt number increases with the surface roughness of the channel and the flow rate. The average Nusselt numbers are higher for counter-flow than co-flow.

4. Conclusions

The 3D CFD simulation results of the internal transfer characteristics of DCMD modules using rough-surface channels for desalination have been presented and compared to the conventional correlations of heat transfer coefficients.
This simulation study has clarified and confirmed the following points:

(i) The simulation of rough-surface channels using cubic blocks with a checkerboard arrangement gives fairly close predictions of mass flux to the experimental results.

(ii) The approach of using information of membrane-adjacent cells with transfer mechanisms in the membrane allows the incorporation of transmembrane heat and mass fluxes into commercial CFD code for the simulation of membrane separation systems.

(iii) Both transmembrane mass flux and heat transfer coefficients show distributions with very high values in the inlets.

(iv) For the heat transfer coefficients, significant differences between the predictions from conventional correlations developed for non-porous heat exchangers and the CFD simulation results of the DCMD modules are found from this study.

Acknowledgements

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### List of Symbols

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<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>C₀</td>
<td>counter-flow</td>
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<tr>
<td>Dₘ</td>
<td>hydraulic diameter (m)</td>
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<td>D₅</td>
<td>Knudsen diffusivity (m²/s)</td>
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<td>Dₘₕ</td>
<td>molecular diffusivity (m²/s)</td>
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<td>dₚ</td>
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<td>energy (J)</td>
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<td>G₂</td>
<td>Graetz number, RePrDₘ/L</td>
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<tr>
<td>h</td>
<td>heat transfer coefficient (W/m² K)</td>
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<tr>
<td>I</td>
<td>unit matrix</td>
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<tr>
<td>jᵢ</td>
<td>diffusion flux of species i (kg/m² s)</td>
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<td>kₘ</td>
<td>mass transfer coefficient in the membrane (m/s)</td>
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<td>Kn</td>
<td>Knudsen number</td>
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<td>L</td>
<td>length of module (m)</td>
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<td>N</td>
<td>mass flux (kg/m²s)</td>
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<td>Nu</td>
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<td>Re</td>
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<td>Sᵢ</td>
<td>mass source term of species i (kg/m³ s)</td>
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<td>yᵢ</td>
<td>mass fraction of species i</td>
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<td>z*</td>
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### Greek Symbols

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<td>τ</td>
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### Subscript

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### References


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