Coupled Modelling of Membrane Desalination

Isam Janajreh*, Dana Suwwan , Raed Hashaikeh

Mechanical and Materials Engineering Department, Masdar Institute of Science and Technology
P.O. Box 54224, Masdar city, Abu Dhabi, UAE

Abstract—**Direct Contact Membrane Distillation has received much attention due to its total salt rejections and low operational energy demand. There are however many parameters influencing the process demanding a tedious effort to study each parameter individually. High fidelity numerical simulation is the applicable answer particularly when utilizing the advantages of the multiphasic and algorithm in the field of CFD and the advancements in computer speed, memory and storage. In this work, a numerical simulation of the conjugated heat transfer of the feed-membrane-permeate system is developed. Following the initial evaluation of the temperature, pressure and mass flux, the associated latent heat are coupled to compensate for the variability in heat addition or reduction at the feed and permeate membrane surfaces. An updated temperature profile is produced, which endures a slight change from the uncoupled profile. Results suggest the accuracy of conjugated heat model and its reliability in carrying further parametrical studies.**
Keywords: Membrane; Desalination; Permeability; Conjugate-heat.

I.   INTRODUCTION

There are several methods to simulate the process of Direct Contact Membrane (DCMD) separation is applied for desalination, juice concentration, or pharmaceutical applications [1]. Being governed by several parameters ranging from geometrical configurations, operating conditions, and thermal properties of the system, the integration of the system is challenging therefore coupled modelling is implemented in this paper.

Computational fluid dynamics (CFD) observed a leapfrog advancement in the last few decades with the application of algorithms and solvers that possess better stability, consistency and accuracy. Furthermore, advancement memory storage made it possible to target larger system at one's multiple physics system of [2]. Using CFD in the analysis of DCMD system appears in several work [3]. Earlier work included semi empirical correlation of a single sided membrane flow or thermal resistance analogy to evaluate the membrane surface temperature which is responsible for the mass flux [4]. Zhang et al [5] attempted to capture the true essence of the DCMD in their conjugate heat transfer model. Their model also viewed the effectiveness of the counter over parallel flow configurations.

On a micro level, Murad et all and others have tackled Molecular Dynamic (MD) simulation of the water molecules-materials interaction [6] considering thermal molecular transport of materials. MD is used in the field of solid fluid interaction as in the case of membrane of porous media for small domain of few tens of nano-meters size as it became computationally demanding and impractical in large system. It is a non-continuum approach based on statistical and quantum mechanics along with kinetic theory as the fluid is represented by discrete atoms with specific Van der Walls and electrostatic or Coulomb interaction forces [7]. The outcome aided with thermodynamic properties, velocities, special energies and stresses additional to the diffusion coefficients. Combined molecule dynamics and CFD also appears in the work of Ko et al [8]. A combined of Knudson-Poiseuille models as was presented by Chen et al [9]:

$$c_m = c_k + c_p = 1.064 \; \alpha(T) \frac{\varepsilon \, r}{\tau \, \delta_m} \sqrt{\frac{M_w}{R \, T_{mt}}} + 0.125 \; \beta(T) \, \frac{\varepsilon \, r^2}{\tau \, \delta_m} \quad (1)$$

This work not only conducts a conjugate heat transfer analysis, but also re-evaluates the temperature by accounting for the transported latent heat of evaporation at the two membrane surfaces. The successive temperatures, mass flux, and polarization temperature factor were computed.

II.   SYSTEM SET UP AND GOVERNING EQUATIONS

The model setup is retrieved from the author's previous work (see fig. 1). Consisting of short segment (14mm) of thin (0.13mm) porous membrane in counter flow configuration subjected to a Laminar (Re=10) and steady state conjugated-heat transfer flow.
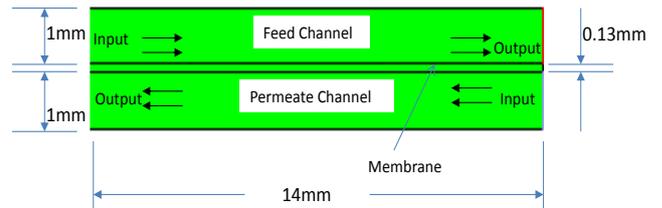
Fig.1 Schematic diagram of counter-flow DCMD [10]

The governing system of equations comprises conservation of mass, momentum and continuity and is written as and the material and solution specifications were retrieved from [10]

$$Continuity: \quad \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \overline{\rho u_i}}{\partial x_i} = S_c \qquad (2)$$

$$Momentum: \quad \frac{\partial \overline{\rho u_i}}{\partial t} + \frac{\partial \overline{\rho u_i u_j}}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \overline{\rho} g_i + S_i \qquad (3)$$

$$Energy: \quad \frac{\partial}{\partial x_i}[u_i(\rho e + p)] = \frac{\partial}{\partial x_i}[(K + \frac{c_p \mu_t}{Pr_t})\frac{\partial T}{\partial x_i} - \sum_j h_j J_j] + S_h \qquad (4)$$

III.   RESULTS

Fig. 2 represents the computational algorithms applied to the modelling process. On the other hand, Fig. 3. Depicts colored contours of the evaluated flow velocity field, and temperature fields include the membrane

Fig.2. Algorithmic process flow chart for modelling the DCMD
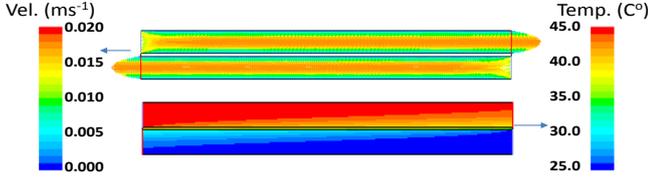
Fig. 3. Velocity and temperature fields of the system

Mass flux (see Fig. 4) is evaluated based on the calculated saturation pressure, which is found using Antoine equation (eq. 5) from the membrane surface temperature. It also accounts for the purity/activity of each fluid side, such as:

$$P_{pure}^{sat} = \exp\left(23.238 - \frac{3841}{T_m - 45}\right), i \in \{f, p\} \quad (5)$$

$$J'' = c_m \left(P_{mf}^{sat} - P_{mp}^{sat}\right) \quad (6)$$

$$\theta = \frac{T_{m,f} - T_{m,p}}{T_{b,f} - T_{b,p}} \quad (7)$$

The temperature is re-evaluated (see Fig. 4) by accounting for the associated mass flux as a latent heat of evaporation across the membrane surfaces. Temperature polarization have decreased slightly influencing the mass flux. Fig. 5 shows the real mass flux, which is overestimated prior to the coupling.
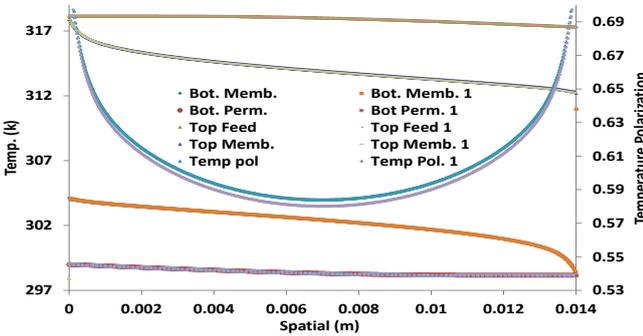
Fig.4. Temperature distribution w/without accounting for latent heat of evaporation and condensation
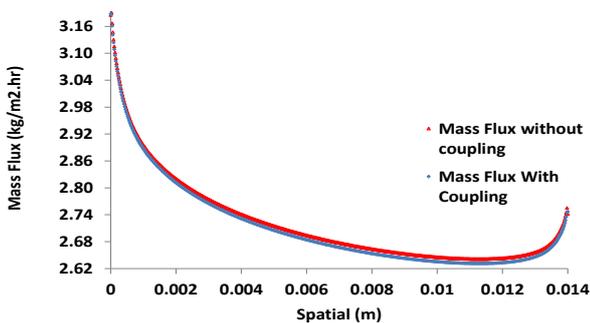
Fig. 5. The evaluated mass flux with and without coupling

IV. CONCLUSIONS

Coupled flow modelling was implemented and the latent heat of vaporization was accounted for with the aid of external loop algorithms. It was found that a slight temperature change is evident, that does not alter the mass flux significantly, which indeed justifies the applicability and sufficiency of the non-coupled model and its usage for further sensitivity studies.

NOMENCLATURE

ρ	Density of the fluid (kg/m^3)
u, v	Fluid velocity in the x & y-direction (m/s)
μ	Dynamic viscosity of the flow $(pa.s)$
c_m	Intrinsic mass membrane coefficient
K_m, K_b	Bulk and vapor conductivity K_v(W/mK)
P_{mf}^{sat}	Saturated pressure of water on the feed (Pa)
M_w	Molar mass of the water in (kg/mol)
T_{mt}	Mean membrane temperature (K)
δ_m	Thickness of the membrane (μm)
r	Pores radius (nm)
$\alpha(T), \beta(T)$	Knudsen and Poiseuille coefficients
ε	Porosity of the membrane (%)
τ	Tortuosity factor (%)
θ	Temperature Polarization (%)

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