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Direct Contact Membrane Distillation Module Scale-Up Calculations: Choosing Between Convective and Conjugate Approaches

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ABSTRACT

Membrane distillation (MD) process technology is swiftly moving to industrial prototyping where efficient scale-up calculations are crucial to shorten product development cycle. The aim of this numerical investigation is to suggest the best modeling strategy that will enable to innovate; modify or check new direct contact MD (DCMD) module designs or operation in a timely manner. Two main modeling strategies are presented, namely convective and conjugate approaches. For a given flat module, it is shown that replacing the permeate side by a modified convection boundary condition that accounts for every known resistance to heat transfer gives similar results in the feed side as a coupled conjugate approach where the membrane, with a modified thermal conductivity, is part of the computational domain. The two methods are compared for different module lengths in terms of permeate flux and temperature distribution. Simulation time reports show the important gain in CPU time when using the convective approach while retaining desired calculation accuracy during scale-up. Furthermore, investigations were carried out to assess the effect of 3D inlet and outlet effects. Results for a laboratory scale module suggest that the convective approach can be safely used during early design stages and scale-up of single modules in the range of high permeate fluxes, while the conjugate approach has to be used for an accurate prediction of permeate temperatures needed in heat recovery strategy and equipment design.

Keywords: DCMD, CFD, Conjugate approach, Convective approach, Large scale module

1 INTRODUCTION

Membrane distillation (MD) stands among the most viable emerging technologies for water treatment and desalination. MD easy process design, relatively low energy consumption, and low investment cost compared to thermally-driven processes are the most attractive advantages [1]. Indeed, the intrinsic nature of the process differs from classical membrane processes such as reverse osmosis (RO) where high fluid pressures are required. MD relies on a thermal non-equilibrium state between the feed side and the permeate side as a driving force for species transfer across the membrane [2]. Specifically, the surface of the membrane is hydrophobic which prevents liquid feed to flow through. Therefore, species are transferred in a vapor state with a rate set by membrane properties and thermodynamic conditions. The MD process, currently at the prototyping and scale-up stage [3-10], will be swiftly moving towards industrial implementation. Module unit design and optimization is therefore central to successful process scale-up. However, complex phenomena occur in MD modules involving simultaneous momentum, heat and mass transport in both continuum and porous media making scale-up calculations only possible using powerful computational fluid dynamics (CFD) software. Numerical modeling is now very well established to support engineering development and minimize trial and error expensive procedures. CFD has been used extensively to investigate transport phenomena in DCMD modules and abundant literature is now available using 2D and 3D approaches with different coupling levels between feed and permeate sides [11-25].

Two state of the art CFD approaches are available in the literature. The first one considers only the feed side of the module while the second is a conjugate approach that includes both the feed and the permeate sides. Regarding the first approach, models evolved from simple boundary conditions setting constant values for the permeate flux [26], or the heat flux [16, 27], or the membrane mass transfer coefficient [28, 29] to more complex formulations coupling to the module scale both heat and species transport across the membrane [30]. The second approach has often been used to circumvent the complexity of the strongly non-linear boundary condition at the membrane permeate interface, leaving to the CFD code the calculation of the temperature at the permeate side of the membrane surface. However, the adaptation of commercial CFD codes to coupled mass and heat transfer across the membrane in a conjugate approach is not straightforward. Likewise, the conjugate approach evolved from sole contribution of conduction to heat transfer across the membrane [18, 24, 31] to a higher extent of coupling [22, 32] and

eventually full account of the contribution of both conduction and species evaporation to heat transfer [11, 12, 15, 19].

CFD modeling of DCMD processes necessitates the use of relatively fine meshes to resolve both temperature and concentration polarization phenomena [30, 33]. Resulting mesh size is generally large leading to significant computational burden. In order for modeling to be efficient and replace experimental trial and error procedures, it has to be performed in a timely manner. In the current article, a thorough comparison is carried out between the two main approaches. It is demonstrated that for practical module lengths, replacing the permeate side of the DCMD module by an appropriate boundary condition leads to similar results as a conjugate approach where both feed and permeate sides are considered. The first modeling approach, denoted in the present article as “convective approach” has been used successfully to predict flow evolution in DCMD module and emphasize its effect on the distribution of permeate fluxes over the membrane surface [30]. The permeate side is replaced by an appropriate boundary condition and the steady state temperature at the permeate side of the membrane is solved through an iterative process. The second approach, denoted in this article as “conjugate approach”, includes both the feed and the permeate side in the CFD calculations. The mass transfer contribution to heat transfer is taken into account by setting an equivalent thermal conductivity to the membrane [15].

The two modeling strategies use ANSYS fluent V16 to solve coupled turbulent momentum, heat and mass transfer in the module channel, although an in-house non-linear solver is called for each node subject to the convection boundary condition in the convective approach [30]. Two-dimensional calculations are carried out for different module lengths and different operating conditions. It is shown that scale-up design can be performed without considering the permeate side thus leading to a significant reduction of mesh size and computational burden. Results are verified for a large span of flat module sizes and should be considered in scale-up calculations to accelerate product development. The convective approach is shown as reliable in the design stage of moderate size single module calculations even though inlet and outlet effects have a more significant impact in the prototype range size, while the conjugate approach remains necessary for an accurate prediction of permeate temperature, crucial in the design of system heat recovery and module integration.

2 CONVECTIVE APPROACH

The convective approach consists of discarding the membrane and the permeate sides from the computational domain, as depicted in figure 1. All heat transfer modes, namely conduction and evaporation through the membrane as well as convection and condensation in permeate compartment are naturally taken into account by setting an appropriate boundary condition.

Figure 1 – Convective approach

In the “convective approach”, solution of turbulent transport of momentum heat and mass is sought only in the feed side of the channel. Governing equations are summarized as:

2.1 The continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

2.2 Momentum transport

The Reynolds averaged momentum equations are expressed as:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right\} + \frac{\partial}{\partial x_j}(-\rho \overline{u'_i u'_j}) \quad (2)$$

where Reynolds stresses are given by;

$$-\rho \overline{u'_i u'_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left(\rho k + \mu_t \frac{\partial u_l}{\partial x_l} \right) \delta_{ij} \quad (3)$$

The standard k, ε model of ANSYS-fluent is used for all simulations, in which the turbulent viscosity is expressed as:

$$\mu_t = \rho c_\mu \frac{k^2}{\varepsilon} \quad (4)$$

where c_μ is a constant, $k = \frac{1}{2}(\overline{u_1^2} + \overline{u_2^2} + \overline{u_3^2})$ represents the average turbulent kinetic energy and

$\varepsilon = \frac{\mu}{\rho} \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right)$ the turbulent kinetic energy dissipation rate.

The transport equations for k and ε are given by:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left\{ \left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right\} + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (5)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left\{ \left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right\} + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \quad (6)$$

Where G_k and G_b represent the generation of turbulent kinetic energy due to mean velocity gradients and buoyancy, respectively, σ_k and σ_ε are turbulent Prandtl numbers for k and ε , respectively, Y_M is the contribution of dilatation to the dissipation rate, $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are constants, S_k and S_ε are source terms [34].

In the case of incompressible flow with no buoyancy and no source term ($Y_M = 0$, $G_b = 0$, $S_k = 0$ and $S_\varepsilon = 0$), Eqs (5) and (6) simplify into:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left\{ \left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right\} + G_k - \rho \varepsilon \quad (7)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left\{ \left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right\} + C_{1\varepsilon} \frac{\varepsilon}{k} G_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (8)$$

where G_k is given by:

$$G_k = \mu_t S^2 \quad (9)$$

where S is the magnitude of the mean rate of the strain tensor, viz.

$$S = \sqrt{2 S_{ij} S_{ij}} \quad (10)$$

with,

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \quad (11)$$

2.2.1 Boundary conditions

Feed channel inlet: a fixed velocity is assigned, normal to the inlet boundary, viz.

$$u_n = u_{fin} \quad (12)$$

Channel walls and membrane surface: no slip boundary condition:

$$u_w = 0 \quad (13)$$

2.3 Heat transfer

The turbulent heat transfer balance is expressed as [34]:

$$\frac{\partial(\rho H)}{\partial t} + \frac{\partial}{\partial x_i} [u_i (\rho H)] = \frac{\partial}{\partial x_j} \left[\left(\lambda + \frac{c_p \mu_t}{Pr_t} \right) \frac{\partial T}{\partial x_j} - \sum_k H^{(k)} J^{(k)} \right] \quad (14)$$

where c_p is the fluid specific heat, Pr_t is the turbulent Prandtl number, and $H = \sum_k w^{(k)} H^{(k)}$ is

the total enthalpy calculated using the species enthalpy and specific heat $H^{(k)} = \int_{298.15}^T c_p^{(k)} dT$.

2.3.1 Boundary conditions

Feed channel inlet: a constant temperature is set at the inlet:

$$T = T_{fin} \quad (15)$$

Channel walls: an adiabatic boundary condition is set at the feed channel walls.

$$\frac{\partial T}{\partial n} = 0 \quad (16)$$

Membrane surface: in the convective approach, the permeate side is replaced by an appropriate convection boundary condition using a modified heat transfer coefficient that includes both the membrane and the permeate side resistances to heat flow. Heat flow in series across the membrane to the permeate side is depicted in Figure 1.

There is parallel contribution, to heat transfer, of conduction and vapor transfer across the membrane. Likewise, there is parallel contribution of convective transfer and heat release by condensation in the permeate side. The modified heat transfer coefficient can be written as [30]:

$$h_{ext} = \left(\frac{1}{R_m} + \frac{1}{R_p} \right)^{-1} = \left(\frac{1}{\frac{\lambda_m}{\delta_m} + \frac{J_p H_v}{T_{mf} - T_{mp}}} + \frac{1}{h + \frac{J_p H_L}{T_{mp} - T_p}} \right)^{-1} \quad (17)$$

where R_m is the total resistance to heat transfer across the membrane, R_p is the total resistance to heat transfer through the permeate, λ_m is the membrane-air composite conductivity, δ_m is the membrane thickness, J_p the permeate flux, T_{mf} is the membrane temperature at the feed side, T_{mp} is the membrane temperature at the permeate side, H_v the vapor enthalpy, and H_L is the permeate enthalpy.

The convection heat transfer coefficient h is given by:

$$h = \frac{\text{Nu } \lambda}{l} \quad (18)$$

with the Nusselt number calculated using the following correlation previously used for turbulent flow conditions in DCMD [35]:

$$\text{Nu} = 0.036 \text{Re}^{0.8} \text{Pr}^{1/3} \left(\frac{d_h}{l} \right)^{0.055} \quad (19)$$

The calculation of the modified heat transfer coefficient h_{ext} using Eq. (17) is subject to the knowledge of the permeate flux J_p as well as the temperature at both sides of the membrane. The permeate flux is commonly estimated in MD calculations using:

$$J_p = C (P_{mf} - P_{mp}) \quad (20)$$

where C represents the membrane mass transfer coefficient, and P_{mf} the vapor pressure at the meniscus and P_{mp} the vapor pressure at the permeate side.

The thermal non-equilibrium state between both sides of the membrane leads to a pressure difference. For pure chemical species, the vapor pressure is related to the local temperature by Antoine's equation, viz.

$$P = \exp \left(a - \frac{b}{T - c} \right) \quad (21)$$

where $a = 23.1964$, $b = 3816.44$ and $c = 46.13$ for pure water. Eq. (21) is corrected in the case of seawater to account for the effect of salinity “ s ” as:

$$P_{sw} = \frac{P}{1 + 0.57357 \left(\frac{s}{1000 - s} \right)} \quad (22)$$

In DCMD mass transport across the membrane is considered as a contribution of both Knudsen diffusion and ordinary diffusion. The mass transfer coefficient is consequently expressed as:

$$C = \left(\frac{3\xi\delta_m}{2\varepsilon_m r} \sqrt{\frac{\pi RT_{av}}{8M}} + \frac{\xi\delta_m}{\varepsilon_m} \frac{P_a}{PD_s} \frac{RT_{av}}{M} \right)^{-1} \quad (23)$$

where the average temperature T_{av} is computed using the temperature at both sides of the membrane, while the product PD_s of the pressure by the species diffusion coefficient inside the membrane pores is given by:

$$PD_s = 1.8958 \cdot 10^{-5} T_{av}^{2.072} \quad (24)$$

At steady state, the permeate side temperature of the membrane is the solution of the following nonlinear equation:

$$T_{mp} - T_{mf} \exp\left(\frac{J_p c_{pv} \delta_m}{\lambda_m}\right) + \left(\exp\left(\frac{J_p c_{pv} \delta_m}{\lambda_m}\right) - 1\right) \frac{[h(T_{mp} - T_p) + J_p H_L - J_p (H_v - c_{pv} T_{ref})]}{c_{pv} J_p} = 0 \quad (25)$$

An in-house non-linear solver is called for each boundary node to solve Eq. (25) though an iterative process. Details on the derivation of the equations and algorithm flowchart can be found in a previous investigation by Soukane et al. [30].

2.4 Mass transfer

Seawater is considered as a mixture of water and NaCl species. With no Soret effect, species (k) mass balance is written as:

$$\frac{\partial(\rho w^{(k)})}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i w^{(k)}) = -\frac{\partial J_i^{(k)}}{\partial x_i} \quad (26)$$

where $w^{(k)}$ represents the mass fraction of species (k) and $J_i^{(k)}$ the diffusion flux given in turbulent flow by:

$$J_i^{(k)} = -\left(\rho D^{(k)} + \frac{\mu_t}{Sc_t}\right) \frac{\partial w^{(k)}}{\partial x_i} \quad (27)$$

where the turbulent Schmidt number Sc_t is set to the default value of 0.7 . The diffusion coefficient of salt species $D^{(NaCl)} = 1.62 \cdot 10^{-9} \text{ m}^2 \cdot \text{s}^{-1}$ is calculated from the diffusion coefficients of its ions Na^+ and Cl^- [36].

2.4.1 Boundary conditions

Feed channel inlet: species mass fraction is set following the salinity of the incoming seawater:

$$w^{(H_2O)} = 1 - 10^{-3} s \quad (28)$$

$$w^{(NaCl)} = 1 - w^{(H_2O)} \quad (29)$$

Channel walls: at the channel walls, no species transfer is assumed and therefore:

$$\frac{\partial w^{(k)}}{\partial n} = 0 \quad (30)$$

Membrane surface: at the membrane surface, species are transferred from the feed side to the permeate side of the membrane. In ANSYS fluent, this is taken into account by setting a consumption rate for water at the feed side of the membrane, viz.

$$\rho D^{(k)} \frac{\partial w^{(k)}}{\partial n} = J_p \quad (31)$$

where J_p is estimated using Eq. (20).

3 CONJUGATE APPROACH

The conjugate approach consists of including the permeate side in the computational domain. Therefore, the membrane is represented as a solid phase between the feed and permeate channels (see Figure 2). Consequently, convection is part of the CFD solution while conduction, evaporation and condensation are ensured by a modified membrane thermal conductivity. Analogously to the convective approach, ANSYS fluent V16 is used to solve momentum, heat and mass transport in both the feed and the permeate sides.

Figure 2 – Conjugate approach

3.1 Continuity equation and momentum transport

Governing equations and boundary conditions for momentum are the same as those enumerated in the convective approach. The standard k, ε model is therefore used in both module compartments. A constant velocity is assigned at the both the feed and permeate inlets, while a no-slip boundary condition is set at all walls as well as membrane surface.

3.2 Heat transfer

Heat transfer constitutive equations in the bulk are identical to those enumerated in the convective approach. Regarding the boundary conditions, an adiabatic condition is assigned to all inner walls. It is recalled that heat transfer through the membrane is now part of the solution and heat transfer caused by vapor transfer through the membrane is included via a modified thermal conductivity of the membrane as explained in the sequel.

4 EXPERIMENTAL CONDITIONS

4.1. Membrane properties

The properties of the membrane are those of a composite membrane with a poly-tetra-fluoro-ethylene (PTFE) active layer and a nonwoven polyester support layer. Membrane characteristics are reported in Table 1.

Table 1 - Membranes characteristics [4, 37].

Property	M1
Thickness, δ_m (μm)	170 $\pm$ 4
Porosity, ε_m	0.73
Mean flow pore size, r (μm)	0.26

The tortuosity of the membrane, needed in the computation of the mass transfer coefficient (see Eq. (23)), is calculated using the porosity [30, 38] to give $\xi = 1.25$. The thermal conductivity is that of the composite membrane-air. It is calculated using the isostress model [35] to give 0.031 W/m/K.

Regarding the conjugate approach, the thermal conductivity of the membrane is modified to account for the contribution of mass transfer to heat transfer. The membrane is therefore considered as a solid phase, in which heat transfer is numerically ensured via sole conduction with a thermal conductivity λ' given by [15]:

$$\lambda' = \frac{J_p (H_v - H_L) + \lambda_m (T_{mf} - T_{mp}) / \delta_m}{(T_{mf} - T_{mp})} \Delta \quad (32)$$

where Δ represents the thickness of the membrane mesh.

4.2. Fluid properties

Seawater with salinity of 4.2 wt% is used as feed in all simulations for both modeling strategies. Seawater properties including, viscosity, specific heat, thermal conductivity are taken from Sharqawy et al. [39].

4.3. Simulation set up

In order to compare the two CFD strategies, calculations are carried for different module lengths, namely; 0.1 m, 0.5 m, 1.0 m, 2.5 m and 5.0 m. This length range is assumed to cover DCMD module dimensions from laboratory scale and prototypes to industrial scale.

Figure 3 – Computational domains with identical nodes distribution for convective and conjugate approaches

Simulations are performed for different feed inlet temperatures and inlet flow rates. Inlet temperatures used are 50°C, 60°C, 70°C and 80°C and the inlet flow rates considered are 1 LPM, 1.5 LPM, 2 LPM and 2.5 LPM. The flow rate range is selected such as turbulent conditions prevail in all cases. In the case of the conjugate approach, a counter current mode is considered with the same inlet permeate temperature of 20°C used in all cases while the permeate flow rate is kept identical to the feed inlet flow rate. Module width is the same for all models and is set to 0.05 m, while the channel height for both feed and permeate sides is set to 2 mm. The inlet velocity is calculated using the channel cross section and the assigned flow rate. Mesh generation is carefully performed in both approaches. Structured meshes are used in order to create identical mesh distribution of the computational nodes along the membrane surface in order to carry out a one-to-one node comparison of simulation results (see Figure 3). The mesh is carefully refined to ensure dimensionless height y^+ below 1 along the domain boundaries [30].

5 RESULTS AND DISCUSSIONS

5.1 Average permeate fluxes

The first variable of interest is the average permeate flux, which is obtained by summing up all local flux values weighted by the corresponding computational element size, divided by the membrane total area. In all cases the relative error between the convective and the conjugate (reference value) approach does not exceed 2%. Therefore, results in terms of average permeate flux are reported only for module lengths of 0.1 m and 5.0 m as depicted in Figures 4 and 5, respectively.

Figure 4 - Comparison of the average permeate flux for a module length of 0.1 m at different inlet temperatures and different flow rates. (CJG) conjugate approach. (CV) convective approach

Both approaches give the expected trend with an increase of the average permeate flux when the inlet temperature is increased. However, as the module length increases from 0.1 m to 5.0 m, a fall of the average permeate flux is observed which is in accordance with recent results carried out for long modules by Lee et al. [40].

It is interesting to note that for all module lengths that were investigated, the inlet flow rate has a negligible effect when inlet temperatures of 50°C and 60°C are used, as observed elsewhere [40]. This is related to the relatively low permeate fluxes obtained using these temperatures at which the lowest flow rates are able to sustain the moderate permeation rate. However, more sensitivity is observed when using a feed inlet temperature of 80°C, as the average permeate flux

increases from $70 \text{ kg.m}^{-2}.\text{hr}^{-1}$ to $78 \text{ kg.m}^{-2}.\text{hr}^{-1}$ for module length of 0.1 m and from $50 \text{ kg.m}^{-2}.\text{hr}^{-1}$ to $65 \text{ kg.m}^{-2}.\text{hr}^{-1}$ for module length of 0.5 m when the inlet flow rate is increased from 1 LPM to 2.5 LPM.

Figure 5 - Comparison of the average permeate flux for a module length of 5 m at different inlet temperatures and different flow rates. (CJG) conjugate approach. (CV) convective approach

5.2 Local permeate flux

A one-to-one node comparison of permeate fluxes along the membrane surface shows near equal values for all simulations for module lengths of 0.1 m and 0.5 m. In this short module range, the percentage difference of local flux remains below 2% for all feed inlet temperatures and inlet flow rates (see Figure 6). The difference in local flux by the two approaches for a given module length seems not to be sensitive to the inlet temperature while the gap increases when increasing the module length. However, the rate of increase varies with the inlet flow rate. The lower the latter the higher the discrepancy between the two approaches, which occurs for a module length of 5 m and an inlet flow rate of 1 LPM with a value of approximately 8 %.

Figure 6 – Maximum percentage difference in local permeate flux as a function of module length for different feed inlet temperatures and different inlet flow rates

Nevertheless, all simulation cases (excluding the above-mentioned case) exhibit a percentage difference in local permeate flux below 6% and as low as 3% for the highest input flow rate of 2.5 LPM. It is also worth noting that the longest module considered in this investigation is believed to lie beyond a practical industrial size of a single module and both convective and conjugate approaches lead to similar results in terms of local permeate flux along the module.

Figure 7 – Permeate flux distribution along the membrane surface for a single module of 5.0 m length at different feed inlet temperatures and different inlet flow rates. Symbols (o) represent selected values along the module obtained by the conjugate approach. Lines represent results of the convective approach

In order to identify the location of the zones of highest discrepancy, the flux distribution along the membrane surface for a module length of 5 m is represented as a function of distance along the module (see Figure 7). It is important to emphasize that for the sake of clarity only few symbols are used to represent the results of the conjugate approach. The relative difference is nearly identical for all temperatures, although it is best noticeable for the highest values of the local permeate flux. Indeed, the permeate flux distribution for an inlet temperature of 80°C shows

that the two approaches depart from each other close to the boundaries while exhibiting very close results in the central region of the module. This is very likely due to the essence of the conjugate approach which forces the temperature at the inlet of the permeate side with a Dirichlet condition leading to a distinctive distribution of the temperature along the permeate side surface of the membrane as described in the sequel.

5.3 *Membrane surface temperature*

5.3.1 *Feed side*

Node-to-node comparison of the membrane surface temperature at the feed side reveals similar results with both convective and conjugate approaches. The maximum percentage difference in absolute scale temperature remains below 1% for all simulated cases. Since negligible difference is observed between the two approaches, the temperature distribution at the feed side surface of the membrane is only reported for a module length of 5 m (see Figure 8, for the sake of clarity symbols represent only selected values obtained by the conjugate approach along the module). The feed side temperature decreases from inlet to outlet in both approaches due to heat losses caused by conduction and evaporation. In all cases, the temperatures near the inlet are nearly identical since the inlet feed temperature is set in both conjugate and convective approaches to the same fixed value. For the lowest flow rates of 1 LPM and 1.5 LPM the temperature obtained by the convective approach departs from the conjugate profile while reaching the outlet of the feed channel due to the forced inlet conditions that prevails in the permeate side in the conjugate approach. However, overall results for the surface temperature at the feed side of the membrane show that both convective and conjugate approaches lead to similar results.

Figure 8 – Distribution of feed side membrane temperature for module length of 5 m at different feed inlet temperatures and different inlet flow rates. Symbols (o) represent selected values along the module obtained by the conjugate approach. Lines represent results of the convective approach

5.3.2 Permeate side

The difference in membrane permeate side temperature for all module lengths, inlet feed temperatures and inlet flow rates is reported in Figure 9. The gap between the two numerical approaches increases with module length and inlet feed temperature while a decrease is observed when the inlet flow rate is increased. Taking the conjugate case as the reference, these observations suggest that the convective approach underestimates the permeate side polarization phenomena. Indeed, as the feed inlet temperature increases, the distillation rate increases thus the

increase in polarization, which coincides with a higher discrepancy between the two approaches. Similarly, a higher inlet flow rate transfers more heat along the module and reduces polarization, which is reflected by smaller discrepancies between the two methodologies.

Figure 9 - Maximum difference in membrane permeate side temperature (°C) as a function of module length for different feed inlet temperatures and different inlet flow rates

Simulations for a module length up to 1 m exhibit less than 5°C difference in permeate side temperature except for the highest inlet feed temperature of 80°C at the lowest flow rate of

1 LPM. For longer modules, the temperature difference grows severely to exceed 10°C for lowest flow rates and long modules.

Since the largest differences observed correspond to the lowest flow rate of 1 LPM, the permeate side temperature profile is represented in Figure 10 for an inlet flow rate of 1 LPM and different inlet temperature and module length. The permeate side temperature resulting from the convective approach remains nearly constant along the module in all simulations cases except for the longest module where few degrees difference is observed. This is mostly due to the high value of the convection heat transfer coefficient as obtained from turbulent correlations of Nusselt number. Indeed, for high fluxes, the permeate side temperature of the membrane tends to the permeate bulk temperature. The resulting variations of the permeate side temperature of the membrane along the module, although effective, remain negligible. However, the conjugate approach shows an increase of the temperature from the permeate inlet to the outlet for all simulations. The imposed temperature at the feed inlet in the conjugate approach has a drastic effect on the temperature distribution at the neighboring cells (in the permeate side) which results in a stiff increase of the permeate side temperature while approaching the permeate side outlet. Consequently, the profile evolution of the permeate side temperature of the membrane in the conjugate approach ranges between the imposed temperature at the permeate inlet and a relatively high temperature at the outlet while the convective approach computes the surface temperature as a result of a flux boundary condition leading to an evened out temperature profile.

Figure 10 - Distribution of permeate side membrane temperature for different module lengths and different feed inlet temperatures and an inlet flow rate of 1 LPM. Symbols (o) represent selected values along the module obtained by the conjugate approach. Lines represent results of the convective approach

Unexpectedly, permeate temperature differences between the two approaches reach values as high as 15°C close to the inlet for a 5 m length module. A clear discrepancy exists in the distribution of permeate temperature as module length is increased due to the limitation of the convective approach. However, this temperature difference seem not to effect much the value of the permeate flux as well as the feed side temperature of the membrane as reported in Figures 7 and 8, respectively. In order to understand the weak effect of the membrane permeate side temperature on the permeate fluxes in both approaches, a global view of the permeate flux distribution as a function of the feed side and permeate side membrane temperature is given in Figure 11, where the permeate flux is computed using Eqs. (20) to (24). The white inclined lines represent isovalues of the difference between the feed and the permeate sides temperatures of the membrane. Point P₁ (see Figure 11) corresponds to conditions similar to those observed in the convective approach with a permeate side temperature of 25°C, while point P₂ (see Figure 11) corresponds to conditions close to those obtained with the conjugate approach with a permeate side temperature of 40°C.

Figure 11 – Permeate flux as a function of feed side (T_{mf}) and permeate side (T_{mp}) membrane surface temperature. White parallel lines represent isovalues of ($T_{mf} - T_{mp}$)

The feed side temperature is 80°C in both cases. The permeate temperature differs by 15 degrees between the two cases, yet the resulting permeate fluxes are 9% apart. This is because in the high feed temperature region, the permeate flux isovalues flatten to become less sensitive to the values of the permeate side temperature (top left corner of Figure 11). Consequently, the discrepancy in the calculation of the permeate side temperature between the convective and the conjugate approaches, which actually occurs for long modules and the highest feed side temperatures has a relatively weak effect on the predicted values of the permeate flux. Nevertheless, the permeate side temperature remains critical during MD module integration stage where calculations have to be carried out using a conjugate approach; since the heated permeate solution can be used as a heat source for intake seawater as part of a heat recovery strategy.

5.4 *Prototype inlet and outlet effects*

The inlet and outlet effect have a greater impact on reduced size prototypes due to the relatively high inlet velocities that prevail over a significant part of module feed and permeate channels. Therefore, three-dimensional simulations are carried out on a laboratory reduced size prototype to assess the ability of the convective approach to safely predict permeate fluxes distribution over the membrane surface. Calculations are compared in terms of average permeate fluxes to experimental results from the DCMD laboratory prototype shown in Figure 12.

Figure 12 – Sketch of the DCMD laboratory prototype module

The module is made of poly-methyl-methacrylate. The dimensions of the feed and permeate channels are 0.1 m x 0.05 m x 0.002 m. The membrane, of which characteristics are reported in Table 1, is a composite membrane with a poly-tetra-fluoroethylene active layer supported by nonwoven polyester. A detailed description of the experimental set-up can be found elsewhere [4, 30].

A single experimental base case is considered to illustrate the effect of the inlet and outlet boundary conditions in the convective and the conjugate modeling strategies. In a counter-current mode, yet asymmetric locations, the feed and permeate inlet flow rates are both set to 1.5 LPM, the feed inlet temperature to 60°C and the permeate inlet temperature to 20°C. For the above-mentioned conditions, the average experimental permeate flux is 23 Kg.m⁻².hr⁻¹.

The boundary conditions for the 3D model are similar to those presented for the 2D model. They can be summarized as follows:

1. Momentum:
 - a. Imposed velocity at the inlet as given by Eq. (12).
 - b. No slip boundary condition at module walls and membrane surface as expressed by Eq. (13).
2. Heat transfer:
 - a. Imposed temperature at the inlet as given by Eq. (15).
 - b. Adiabatic conditions at module walls represented by Eq. (16).
 - c. In the case of the convective approach, the membrane is part of the boundary. The overall heat transfer coefficient is modified consequently using Eq. (17).
3. Mass transfer:
 - a. Species mass fractions are set at the inlet using Eq. (28) and Eq. (29).
 - b. No species transfer across module sidewalls as well as top and bottom surface as expressed by Eq. (30).
 - c. Species are transferred across the membrane surface at a rate given by Eq. (31)

Figure 13 – Streamlines in the feed compartment (color by velocity magnitude). Black arrows indicate inlet and outlet locations

The prototype module geometry is carefully meshed while keeping the same node distribution for the feed and permeate channels (see Numerical set-up section). The relatively high inlet velocity (due to the small inlet cross section) results in a large recirculation loop inside the prototype module (see Figure 13). The inlet jet impinges on the sidewalls to evolve towards the module outlet. The large recirculation exhibits relatively low velocity magnitude which is very likely to affect the permeate flux distribution [30] and consequently the choice of the computational approach.

Figure 14 – Distribution of permeate fluxes ($\text{Kg}/\text{m}^2/\text{hr}$) over the membrane for both conjugate (top) and convective (bottom) approaches. Black arrows show inlet and outlet locations

The average permeate flux obtained using the convective approach is equal to $21.8 \text{ Kg} \cdot \text{m}^{-2} \cdot \text{hr}^{-1}$ while the one obtained using the conjugate approach is equal to $22.0 \text{ Kg} \cdot \text{m}^{-2} \cdot \text{hr}^{-1}$. Therefore, both methodologies are able to predict the average permeate flux within 5% accuracy. The permeate flux distribution over the membrane surface, as shown in Figure 14, remains similar with both approaches with a clear effect of the inlet jet on the fluxes spatial variations. Indeed, fluxes remain high where the tangential velocities are the most significant while a drop is observed in the central region of the prototype where the large recirculation zone prevails.

The distribution of the membrane feed side temperature is represented in Figure 15 for both convective and conjugate approaches. Analogously to the permeate fluxes, the feed side temperature follows closely the flow pattern in a similar fashion for both modeling strategies with the highest differences observed in the central regions. Although these differences occur in small portion of the membrane total area, thus not affecting the resulting average permeate flux values.

Figure 15 – Distribution of the membrane feed side temperature for both conjugate (top) and convective (bottom) approaches. Black arrows show inlet and outlet locations

Figure 16 - Distribution of the membrane permeate side temperature for both conjugate (top) and convective (bottom) approaches. Black arrows show inlet and outlet locations

The distribution of the membrane permeate side temperature as shown in Figure 16 exhibits a significant discrepancy. The effect of the asymmetry of the feed and permeate inlets affects the permeate temperature as clearly seen with the cold stream entering the permeate channel from the lower left corner in the conjugate approach. The stream creates a central recirculation loop where the permeate temperature sees an increase that is not observed in the convective approach where the permeate domain is omitted. However, the membrane permeate temperature has a relatively negligible effect on the resulting permeate fluxes. Therefore, inlet and outlet effect do not nullify convective approach results as long as process parameters lie within a given range of operating conditions as described in the sequel.

5.5 Convective approach constraints

Although the gap between the convective and the conjugate approaches remains low in terms of permeate flux and feed side temperature, it increases with feed temperature and decreases when flow rate is increased. Based on these observations, constraints are drawn as depicted in Figure 17 following Reynolds number in the range of simulated flow rates. For instance, if a Reynolds number of 10,000 is used, then distillation cases with operating conditions located in the zone below the horizontal line of $Re \leq 10,000$ of Figure 17 can be equivalently modeled using the convective approach even for very long modules. Moreover, as emphasized in the analysis of Figure 11, there are operating conditions where the permeate temperature distribution has a weak effect on the permeate flux. In view of this observation, a validity zone is delimited with “curve C” where the convective approach can be safely used for initial calculations even though the predictions of the permeate temperature might exhibit a significant discrepancy. For a given feed temperature, increasing horizontally the permeate temperature from 25°C to the limit set by “curve C” will result in no more than 10% change in the permeate flux. Consequently, the convective approach can be used for feed and permeate temperature distributions that lie in the zone labeled “ T_{mp} weak effect zone”, to lead to permeate fluxes and feed side temperatures with practical accuracy regardless of the flow rate. Nevertheless, as MD modules are versatile and processing conditions wide, it is recommended that 3D models be initially assessed with both approaches regardless of design and operating conditions. Results comparison should lead designers to the appropriate choice to accelerate their scale-up calculations.

Figure 17 –Constraints on the convective approach

6 MESH SIZE VS CPU TIME

The effect of mesh size on CPU time has been investigated by carrying out calculations on different meshes with increasing resolution. Simulations were performed for dimensional flat module of 100 mm length. The channel height is set to 2 mm for the feed side (convective) and both feed and permeate sides (conjugate). The meshes are structured and are represented by square sized cells. The feed side mesh is identical in both convective and conjugate approaches. Moreover, the feed side and the permeate side are identically meshed in the conjugate approach. Seven structured meshes were used with different refinement levels. The number of cells used for the channel height as well as the number of cells along the modules lengths are reported in Table 2.

The total number of elements in the conjugate approach is nearly double the one required for the convective approach, since feed and permeate sides have the same resolution and only a single layer of elements is needed to represent the membrane in the conjugate approach.

Simulations were carried out for a inlet flow rate of 2.5 LPM and a feed inlet temperature of 80°C on an Intel® Core™ i5 with a clock speed of 2,394 MHz.

Table 2 - Summary of mesh information used for CPU time investigation

Approach	Zone	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Mesh 5	Mesh 6	Mesh 7
Convective	Feed	6x300	9x450	12x600	20x1000	30x1500	40x2000	50x2500
	Total	1,800	4,050	7,200	20,000	45,000	80,000	125,000
Conjugate	Feed	6x300	9x450	12x600	20x1000	30x1500	40x2000	50x2500
	Membrane	1x300	1x450	1x600	1x1000	1x1500	1x2000	1x2500
	Permeate	6x300	9x450	12x600	20x1000	30x1500	40x2000	50x2500
	Total	3,900	8,550	15,000	41,000	91,500	162,000	252,500
Cell size (mm)	All zones	$3.33 \cdot 10^{-1}$	$2.22 \cdot 10^{-1}$	$1.67 \cdot 10^{-1}$	$1.00 \cdot 10^{-1}$	$0.67 \cdot 10^{-1}$	$0.50 \cdot 10^{-1}$	$0.40 \cdot 10^{-1}$

Figure 18 – Evolution of CPU time as a function of mesh cell size for both conjugate and convective approaches

CPU time evolution as a function of mesh unit cell size for both the conjugate and the convective approach is represented in Figure 18. The horizontal axis is inverted in order to better visualize the evolution of the computation burden with mesh refinement. For all meshes, the time required by the conjugate approach is higher than the one needed for the convective approach. For relatively coarse meshes, down to a cell size of 0.1 mm which actually represents the 1/20 of the channel height, the evolution of the CPU time with mesh size remains slow. However, for smaller cell size (0.05 and below), the CPU time exhibits a stiff increase. For a unit cell size of 0.04 mm, 1,106 sec are required to run a convective case of 125,000 elements (Mesh 7) while the corresponding conjugate case of 252,500 elements runs in 2,075 sec to reach the same accuracy, even though the convective approach needs more iterations to converge due to the strong non-linearity of the convective boundary condition. The computational burden is expected to increase drastically with finer meshes therefore impacting the pace of product development. Therefore, there is a clear advantage of using the convective approach during scale-up design iterations, particularly that average and local values of permeate flux remain very close over a large span of module lengths and practical range of operating conditions.

7 CONCLUSION

State of the art CFD strategies, used in the modeling of DCMD modules have been implemented and compared. The two approaches, namely the convective approach and the conjugate approach differ the way the permeate side of the DCMD module is handled. The conjugate approach takes into account the whole module geometry including the membrane while the convective approach considers only the feed side of the module and replaces the membrane and the permeate side by an appropriate boundary condition. Simulations were performed for different operating conditions and several module lengths ranging from laboratory scale to prototype and industrial scale. It was shown that both methods lead to very close results in terms of average permeate fluxes for all simulated cases. Post-processing results in a node-to-node fashion revealed that the distribution of the local average fluxes and the feed side temperature of the membrane along the module is nearly identical for the two strategies. Calculations were extended to a three-dimensional model to assess the effect of inlet and outlet locations on the performance of both methodologies. Simulations revealed that both the convective and the conjugate approaches are able to predict an average permeate flux within 5% of the experimental values. The effect of the

inlet and outlet, although significant on the distribution of the permeate side temperature, do not discredit the convective approach results in terms of permeate fluxes as long as these lies within the drawn constraints. Furthermore, the analysis of the CPU evolution shows a clear advantage of the convective approach despite the non-linear boundary condition that requires more solver iterations for convergence. Indeed, the nearly half size of the mesh has a greater impact and suggests, in view of all similar results obtained in the feed side, that the convective approach saves a significant computational burden while providing practical answers at early stages of DCMD single module design and scale-up calculations. However, the distribution of the permeate side temperature at the membrane surface along the module exhibits a significant discrepancy that increases with module length, suggesting the use of a conjugate approach to finalize module design and integration with a heat recovery system and subsequent optimization procedures.

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NOMENCLATURE

- a coefficient in Antoine's equation
- b coefficient in Antoine's equation
- c coefficient in Antoine's equation
- c_p fluid specific heat
- $c_p^{(k)}$ species (k) specific heat
- h convective heat transfer coefficient
- h_{ext} modified external heat transfer coefficient
- k turbulent kinetic energy
- l characteristic length
- p fluid pressure
- r pore mean radius

s salinity

u fluid velocity

$\bar{u}$ mean fluid velocity

u' fluid fluctuating velocity

u_{fin} feed inlet velocity

u_{pin} permeate inlet velocity

u_w velocity at module walls

$w^{(k)}$ species (k) mass fraction

y^+ dimensionless height

C membrane mass transfer coefficient

$C_{1\varepsilon}$ constant in k - ε turbulence model

$C_{2\varepsilon}$ constant in k - ε turbulence model

$C_{3\varepsilon}$ constant in k - ε turbulence model

C_μ constant in k - ε turbulence model

$D^{(k)}$ species (k) diffusion coefficient

D_s species diffusion coefficient in pores

G_b generation of turbulent kinetic energy due to buoyancy

G_k generation of turbulent kinetic energy due to mean velocity gradients

H fluid enthalpy

$H^{(k)}$ species (k) enthalpy

H_L enthalpy of the permeate solution

H_v vapor enthalpy

$J^{(k)}$ species (k) flux density

J_p permeate flux

M molecular weight

Nu Nusselt number

P vapor pressure

P_a air pressure inside pores

P_{mf} vapor pressure at the feed side of the membrane

P_{mp} vapor pressure at the permeate side of the membrane

P_{sw} seawater vapor pressure

Pr_t turbulent Prandtl number

R ideal gas constant

R_m membrane total resistance to heat transfer

R_p permeate side resistance to heat transfer

S modulus of mean rate of stress tensor

Sc_t turbulent Schmidt number

S_{ij} mean strain rate

S_k source term for k equation

S_ε source term for ε equation

T temperature

T_{av} average temperature inside the pore

T_{fin} feed inlet temperature

T_{mf} temperature at the membrane surface on the feed side

T_{mp} temperature at the membrane surface on the permeate side

T_p permeate temperature

T_{pin} permeate inlet temperature

T_{ref} reference temperature

Y_M contribution of fluctuating dissipation to overall dissipation rate

Greek letters

δ_m membrane thickness

δ_{ij} Kronecker delta

ε turbulent kinetic energy dissipation

ε_m membrane porosity

ξ pore tortuosity

λ_m membrane-air composite thermal conductivity

λ fluid thermal conductivity

λ' modified membrane thermal conductivity

ρ fluid density

μ fluid viscosity

μ_t fluid turbulent viscosity

σ_ε turbulent Prandtl number for ε

σ_k turbulent Prandtl number for k

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Highlights

- Conjugate vs convective CFD modeling is implemented and compared for DCMD
- Temperature and permeate flux distribution for several module lengths is studied
- The convective approach is less CPU demanding
- The convective approach can be used safely for early DCMD module design
- The conjugate approach need to be used for overall DCMD module operation