

Supplementary Materials

S1. The hollow fiber DCMD module

The heat transferred through the boundary of the tube feed side (Q_f) is

$$Q_f = h_f A_f \alpha (T_f - T_{fm}) \quad (S1)$$

where A_f is the membrane area for heat transfer through the feed side to the membrane. α is membrane surface area coefficient based on fiber inside diameter d_i per unit length per fiber layer N_f , which is defined as

$$\alpha = \pi N_f d_i \quad (S2)$$

h_f is the heat transfer coefficient in the tube side. It can be divided into the laminar flow and turbulent flow:

$$h_f = \begin{cases} 1.62 k_f \left(Re_f Pr_f \frac{1}{d_i^2 L} \right)^{0.33}, & Re_f < 2100 \\ 0.023 k_f \frac{(Re_f)^{0.8} (Pr_f)^{0.33}}{d_i}, & Re_f > 2100 \end{cases} \quad (S3)$$

Re and Pr are Reynolds number and Prandtl number defined as

$$Re_f = \frac{d_i v_h \rho_f}{\mu_f} \quad (S4)$$

$$Pr_f = \frac{C_{ph} \mu_f}{k_f} \quad (S5)$$

The heat transferred across the membrane (Q_m) can be divided into latent heat of vaporization and sensible conduction heat.

$$Q_m = A_m \alpha [J \Delta H + h_m (T_{fm} - T_{pm})] \quad (S6)$$

where A_m is the membrane area for heat transfer, J is the transmembrane mass flux. ΔH is the enthalpy of evaporation at the average temperatures of the feed side and the permeate side of the membrane. h_m is the convective heat transfer coefficient

of the membrane determined by thermal conductivity (k_m) and membrane thickness (δ_m). A_m , ΔH , and h_m are defined as

$$A_m = \frac{\frac{d_o - d_i}{\ln(d_o/d_i)}}{d_i} \quad (S7)$$

$$\Delta H = 2489.7 - 2.412 \left(\frac{T_{fm} - T_{pm}}{2} - 278.15 \right) \quad (S8)$$

$$h_m = \frac{k_m}{\delta_m} \quad (S9)$$

where k_m refers to the conductive coefficients of vapor within the membrane pore (air and steam, k_{mg}) and the solid membrane (polymer, k_{ms}) and the membrane porosity (ϵ) by Alkhudhiri et al. [2]. It is defined as

$$k_m = \epsilon k_{mg} + (1 - \epsilon) k_{ms} \quad (S10)$$

The heat transferred through the boundary of the shell cold side (Q_p) is

$$Q_p = h_p A_p \alpha (T_{pm} - T_p) \quad (S11)$$

where A_p is the membrane area for heat transfer through the membrane to permeate side and h_p is the heat transfer coefficient in the shell side. According to Mengual et al. [33], the heat transfer mechanism of fluid flow at the tube side is different from the inside the tube. They are defined as

$$A_p = \frac{d_o}{d_i} \quad (S12)$$

$$h_p = \frac{0.206 k_p (Pr_p)^{0.36}}{d_h} \quad (S13)$$

Where d_h is the heat transfer at the shell side refers to the hydraulic diameter of shell. It is a function of the packing density (ϕ) of the module and is defined as

$$d_h = d_o \left(\frac{1 - \phi}{\phi} \right) \quad (S14)$$

At the steady state, the heat transferred through the boundaries of both fluids

is equal to that across the membrane. Thus, equations (S1), (S6), and (S11) satisfy

$$Q_f = Q_m = Q_p \quad (S15)$$

The transmembrane mass flux (J) is determined by the vapor pressure difference across the membrane is defined as

$$J = C(P_{fm} - P_{pm}) \quad (S16)$$

where P_{fm} and P_{pm} are the water vapor pressures on the feed and the permeate sides of the membrane, respectively. There is dissolved substances with the molar concentration (X_{fs}) at the feed side, and the vapor pressure drop can be described according to Raoult's law:

$$P_{fm} = P_{w,m}(1 - X_{fs}) \quad (S17)$$

where $P_{w,m}$ refers to the vapor pressure when there are no dissolved substances in the water. It uses the temperatures of the feed side or the permeate side of the membrane (T_i) to calculate $P_{w,m}$, which can be described according to Antoine equation:

$$\log_{10}(133.3P_{w,m}) = 8.07131 - \frac{1730.63}{T_i + 233.426} \quad (S18)$$

In equation (S16) C is the membrane distillation coefficient. According to the mass transfer theory established by Ding et al. [34], the gas transport behavior is considered in the porous medium. It is defined by Knudsen-diffusion, Molecular-diffusion and Poiseuille-flow all three modes.

$$C = (R_k + R_m)^{-1} + R_p^{-1} \quad (S19)$$

$$R_k^{-1} = C_k \left(\frac{M_w}{RT_m} \right)^{0.5} \quad (S20)$$

$$R_m^{-1} = C_m \left(\frac{DM_w}{P_{am}RT_m} \right) \quad (S21)$$

$$R_p^{-1} = C_p \left(\frac{M_w P_m}{\mu_w R T_m} \right) \quad (S22)$$

where T_m is the mean temperature across the membrane. P_m is the mean water vapor pressure inside the membrane. D is the diffusion coefficient. P_{am} is the log-mean air pressure at both sides of the membrane. They can be calculated as:

$$T_m = \frac{T_{fm} + T_{pm}}{2} \quad (S23)$$

$$P_m = \frac{P_{fm} + P_{pm}}{2} \quad (S24)$$

$$D = 1.19 \times 10^{-4} \left(\frac{T_m^{1.75}}{P_m} \right) \quad (S25)$$

$$P_{am} = \frac{P_{fm} - P_{pm}}{\ln \left(\frac{P_{fm}}{P_{pm}} \right)} \quad (S26)$$

Note that J depends on not only the feed side but also the permeate side conditions. The following equations in terms of velocity (v_f), compositions (X_{fs}), pressure (P_f), and temperature (T_f) are derived for the retentate as well as for the permeate side of the module. Accordingly, the transport behavior of this module is described based on the momentum, mass and energy balances for the feed side in the tube.

$$\frac{dP_f}{dz} = - \frac{32\mu_f}{d_i^2} v_f \quad (S27)$$

$$\frac{1}{V_f} \frac{dv_f}{dz} - \frac{v_f}{V_f^2} \left(\frac{M_s}{\rho_s} - \frac{M_w}{\rho_w} \right) \frac{dX_{fs}}{dz} = - \frac{4Jd_o}{M_f(d_i^2)} \quad (S28)$$

$$\frac{X_{fs}}{V_f} \frac{dv_f}{dz} + \frac{v_f M_w}{\rho_w (V_f^2)} \frac{dX_{fs}}{dz} = 0 \quad (S29)$$

$$\frac{d\rho_f v_f C_{ph} T_f}{dz} = - \frac{4Q_f}{N_f \pi (d_i^2)} \quad (S30)$$

On the permeate side, the momentum, mass, and energy balances are in the

form of coupled differential equations in terms of velocity (v_p), pressure (P_p), and temperature (T_p) in equations (S31)-(S33). The composition term is neglected due to the near 100% rejection of non-volatile ionic solutes in the cold fluid of the shell side.

$$\frac{dP_p}{dz} = \frac{32\mu_p}{d_h^2} v_p \quad (S31)$$

$$\frac{dv_p}{dz} = -\frac{4 N_f V_p J d_o}{M_p(d_s^2 - N_f d_o^2)} \quad (S32)$$

$$\frac{d\rho_p v_p C_{pf} T_p}{dz} = -\frac{4Q_p}{\pi(d_s^2 - N_f d_o^2)} \quad (S33)$$

The local flux ($J(z)$) is estimated for the non-isothermal process DCMD module. This includes both the mean permeate flux (J_m) and the local thermal efficiency (η) as shown in equations (S34) -(S35). η refers to the ratio of heat for evaporation of water to the heat transferred across the membrane. TDP_h is the water production per hour, which is calculated by J_m , and some parameters of DCMD are defined as:

$$J_m = \frac{1}{L} \int_0^L J(z) dz \quad (S34)$$

$$\eta = \frac{J(z) \Delta H(T_m)}{J(z) \Delta H(T_m) + h_m [T_{fm}(z) - T_{pm}(z)]} \quad (S35)$$

$$TDP_h = J_m N_f \pi d_o L \quad (S36)$$

The set of coupled ordinary differential equations (equations (S27)-(S33)) are numerically solved, and the changes of velocity, composition, pressure, and temperature are subject to the boundary conditions in equations (S37)-(S38). The DCMD parameters are shown in Table 1.

(1) For the feed side:

$$v_f(0) = v_{f,in}, X_{fs}(0) = X_{fs,in}, P_f(L) = P_o, T_f(0) = T_{f,in} \quad (S37)$$

P_o is equal to the ambient atmospheric pressure (101.325 kPa) at both outlets of the fluids.

(2) For the permeate side:

$$v_p(L) = v_{p,in}, P_p(0) = P_o, T_p(L) = T_{p,in} \quad (S38)$$

The temperatures of both sides of the membrane (T_{fm} , T_{pm}) can not be measured with experiment or calculated directly. Hence, the equation (S15) is organized into equations (S39)-(S40) before solving the overall mathematical model. The numerical iterative method by Martínez [35] estimates T_{fm} , T_{pm} , and other parameters in the equations.

$$T_{fm} = \frac{h_m A_m \left(T_p + T_f \frac{h_f A_f}{h_p A_p} \right) + h_f A_f T_f - J A_m \Delta H}{h_m A_m + h_f A_f \left(1 + \frac{h_m A_m}{h_p A_p} \right)} \quad (S39)$$

$$T_{pm} = \frac{h_m A_m \left(T_f + T_p \frac{h_p A_p}{h_f A_f} \right) + h_p A_p T_p + J A_m \Delta H}{h_m A_m + h_p A_p \left(1 + \frac{h_m A_m}{h_f A_f} \right)} \quad (S40)$$

However, to solve the ordinary differential equations with splitting boundary values, the fiber length of the membrane is divided into n segments. It is solved by the Shooting Method [3]. First, the boundary conditions of the unknown initial values are set with the assumed values. Then, the velocity, concentration, pressure, and temperature distribution in each segment are calculated by successive iteration methods. The difference between two subsequent iterations is less than 0.1% until the fiber length ends at the boundary L . The simulated is repeated until the boundary condition is satisfied.

S2. The PEMFC module

The energy balance of PEMFC is defined as:

$$M_{st} C_{pst} \frac{dT_{st}}{dt} = Q_{tot} + Q_{in} - Q_{out} - Q_{cl} - Q_{amb} - P_{st} \quad (S41)$$

where Q_{tot} is the total power from the electrochemical reaction. Q_{in} is the heat flow rate of the input reactant (gas). Q_{out} is the heat flow rate of the output product (liquid water). Q_{cl} is the heat removal rate by the coolant. Q_{amb} is the rate of heat loss to the atmosphere, and P_{st} is the power consumed by the electrical load. Next, the energy balance of the PEMFC for thermal and electrochemical models is listed.

Q_{tot} is defined by the enthalpy of combustion for hydrogen (ΔH_{H_2}) and the reacted hydrogen molar flow rate (N_{an, H_2}^{re}):

$$Q_{tot} = \Delta H_{H_2} \times N_{an, H_2}^{re} \quad (S42)$$

$$N_{an, H_2}^{re} = \frac{N_{fc} I_{st}}{2F} \quad (S43)$$

$$I_{st} = j_{fc} A_{fc} \quad (S44)$$

Q_{in} is defined by the anode and cathode inputs vapor molar flow rate, and the input gases are humidified:

$$Q_{in} = (N_{an, H_2}^{in} C_{p, H_2} + N_{an, H_2 O}^{in} C_{pg, H_2 O}) (T_{an}^{in} - T_0) \\ + (N_{ca, air}^{in} C_{p, air} + N_{ca, H_2 O}^{in} C_{pg, H_2 O}) (T_{ca}^{in} - T_0) \quad (S45)$$

where N_{an, H_2}^{in} is the anode input hydrogen molar flow rate. $N_{ca, air}^{in}$ is the cathode input air molar flow rate. The input gases can change proportionally based on consumption. Therefore, they are defined by the input gases flow rate factor (λ_{H_2} , λ_{O_2}) and the reacted gases molar flow rate (N_{an, H_2}^{re} , N_{ca, O_2}^{re}) in equations (S46)-(S47). $N_{ca, H_2 O}^{in}$ and $N_{an, H_2 O}^{in}$ are the input gases which are humidified to

saturation. The anode and cathode input vapor molar flow rate is described in equations (S49)-(S50):

$$N_{an, H_2}^{in} = \lambda_{H_2} N_{an, H_2}^{re} \quad (S46)$$

$$N_{ca, air}^{in} = \lambda_{O_2} N_{ca, O_2}^{re} / 21\% \quad (S47)$$

$$N_{ca, O_2}^{re} = \frac{N_{fc} I_{st}}{4F} \quad (S48)$$

$$N_{an, H_2O}^{in} = \frac{P_{sat}(T_{an}^{in})}{P_{an} - P_{sat}(T_{an}^{in})} N_{an, H_2}^{in} \quad (S49)$$

$$N_{ca, H_2O}^{in} = \frac{P_{sat}(T_{ca}^{in})}{P_{ca} - P_{sat}(T_{ca}^{in})} N_{ca, air}^{in} \quad (S50)$$

Q_{out} is defined by the unreacted gases of the anode and cathode, the remaining of the input gases are humidified to saturation, and the generated water is in a liquid state:

$$Q_{out} = \left(N_{an, H_2}^{out} C_{p, H_2} + N_{an, H_2O}^{out} C_{pg, H_2O} + N_{ca, O_2}^{out} C_{p, O_2} + N_{ca, N_2}^{out} C_{p, N_2} + N_{ca, H_2O}^{out} C_{pg, H_2O} + N_{ca, H_2O}^{gen} C_{pl, H_2O} \right) (T_{st} - T_0) \quad (S51)$$

where N_{an, H_2}^{out} is the anode output unreacted hydrogen molar flow rate. N_{ca, O_2}^{out} and N_{ca, N_2}^{out} are the cathode output unreacted oxygen and nitrogen molar flow rate. N_{ca, H_2O}^{out} and N_{an, H_2O}^{out} are the cathode and anode remaining of the output gases which are humidified to saturation. N_{ca, H_2O}^{gen} is the cathode output generated water in liquid state. They can be calculated as:

$$N_{an, H_2}^{out} = N_{an, H_2}^{in} - N_{an, H_2}^{re} \quad (S52)$$

$$N_{ca, O_2}^{out} = N_{ca, O_2}^{in} - N_{ca, O_2}^{re} \quad (S53)$$

$$N_{ca, O_2}^{in} = \lambda_{O_2} N_{ca, O_2}^{re} \quad (S54)$$

$$N_{ca, N_2}^{out} = 0.79 N_{ca, air}^{in} \quad (S55)$$

$$N_{an, H_2O}^{out} = N_{an, H_2O}^{in} - \frac{P_{sat}(T_{st})}{P_{an} - P_{sat}(T_{st})} N_{an, H_2}^{re} \quad (S56)$$

$$N_{ca, H_2O}^{out} = N_{ca, H_2O}^{in} - \frac{P_{sat}(T_{st})}{P_{ca} - P_{sat}(T_{st})} N_{ca, O_2}^{re} \quad (S57)$$

$$N_{ca, H_2O}^{gen} = \frac{N_{fc} I_{st}}{2F} \quad (S58)$$

Q_{cl} is defined as:

$$Q_{cl} = m_{cl} C_{ph} (T_{st} - T_{stin}) \quad (S58)$$

Q_{amb} is defined as:

$$Q_{amb} = \frac{(T_{st} - T_a)}{R_t} \quad (S59)$$

The electrochemical model is applied to predict the PEMFC output electrical power (P_{st}) as the PEMFC delivers electrical power to the load. The open-circuit cell voltage (E_{Nernst}) is reduced by the activation overpotential (V_{act}) and the ohmic overpotential (V_{ohm}). Thus, the PEMFC output voltage is defined as:

$$V_{fc} = E_{Nernst} + V_{act} + V_{ohm} \quad (S60)$$

In equation (S60), E_{Nernst} is defined by Nernst equation:

$$E_{Nernst} = 1.229 - 0.85 \times 10^{-3} (T_{st} - 298.15) + \left(\frac{RT_{st}}{2F} \right) \times \ln [P_{H_2} (P_{O_2})^{0.5}] \quad (S61)$$

where P_{H_2} and P_{O_2} are the partial pressure of the anode hydrogen and the cathode oxygen.

$$P_{H_2} = \left[\frac{P_{an}}{\exp(1.635 j_{fc} / T_{st}^{1.334}) \times P_{sat}(T_{st})} - 1 \right] \times P_{sat}(T_{st}) \quad (S62)$$

$$P_{O_2} = \left[\frac{P_{ca} - P_{sat}(T_{st})}{1 + 3.762 \exp(0.291 j_{fc} / T_{st}^{0.832})} \right] \quad (S63)$$

$P_{sat}(T)$ is the saturation vapor pressure according to vapor temperature (T) is calculated as:

$$P_{\text{sat}}(T)=10^{(-20.92+0.143T-3.39\times10^{-4}T^2+3.85\times10^{-7}T^3-1.69\times10^{-10}T^4)} \quad (\text{S64})$$

In equation (S60), V_{act} is in terms of the electric field created at the electrode-electrolyte interface due to the charge transfer and is analyzed by Tafel's equations.

$$V_{\text{act}} = -0.948 + \xi \times T_{\text{st}} + 7.6 \times 10^{-5} T_{\text{st}} \times \ln(C_{\text{O}_2}) - 1.93 \times 10^{-4} T_{\text{st}} \times \ln(I_{\text{st}}) \quad (\text{S65})$$

$$\xi = 2.86 \times 10^{-3} + 2 \times 10^{-4} \times \ln(A_{\text{fc}}) + 4.3 \times 10^{-5} \times \ln(C_{\text{H}_2}) \quad (\text{S66})$$

where C_{O_2} and C_{H_2} are the oxygen and hydrogen concentrations that are defined by Henry's law:

$$C_{\text{O}_2} = 1.97 \times 10^{-7} \times P_{\text{O}_2} \times \exp\left(\frac{498}{T_{\text{st}}}\right) \quad (\text{S67})$$

$$C_{\text{H}_2} = 9.174 \times 10^{-7} \times P_{\text{H}_2} \times \exp\left(\frac{-77}{T_{\text{st}}}\right) \quad (\text{S68})$$

In equation (S60), V_{ohm} is defined by Ohm's law:

$$V_{\text{ohm}} = -j_{\text{fc}} R_{\text{int}} \quad (\text{S69})$$

where R_{int} is the resistance, that is attributed to the electrolyte membrane and can be expressed by the membrane thickness (t_m) and the membrane water content (λ_m):

$$R_{\text{int}} = \frac{t_m}{(0.005139\lambda_m - 0.00326) \times \exp\left(350\left(\frac{1}{303} - \frac{1}{T_{\text{st}}}\right)\right)} \quad (\text{S70})$$

Since n cells are packaged in series, the PEMFC output voltage (P_{st}) is defined as:

$$P_{\text{st}} = N_{\text{fc}} I_{\text{st}} V_{\text{fc}} \quad (\text{S71})$$

S3 DCMD Module verification

A verification procedure is carried out to confirm the correctness of the established hollow fiber DCMD mathematical module on the MATLAB platform. This work uses the experimental data provided in the literature by Al-Obaidani et

al. [3] to compare different temperatures and feed flow velocity. The specification of the membrane physical properties and parameters are shown in Table S1. The simulation flux data is consistent with the experimental results, as shown in Fig. S1(a) for different feed temperatures. Although the error between the simulation flux data and the experimental results increased with increased velocity when the feed temperature is 40 or 60 °C, the two trends are consistent, as shown in Fig. S1(b).

Table S1. Specification of the membrane physical properties and parameters

Parameter Description	Symbol	Value	Unit
The fiber inside diameter	d_i	1.5	mm
The fiber outside diameter	d_o	2.8	mm
The fibers length	L	0.45	m
The fibers number	N_f	40	-
Membrane thickness	δ_m	0.65	mm
Porosity	ε	70	%
Packing density	φ	70	%
feed side inlet salt concentration	X_{fs}	0.035	kg salt/kg water

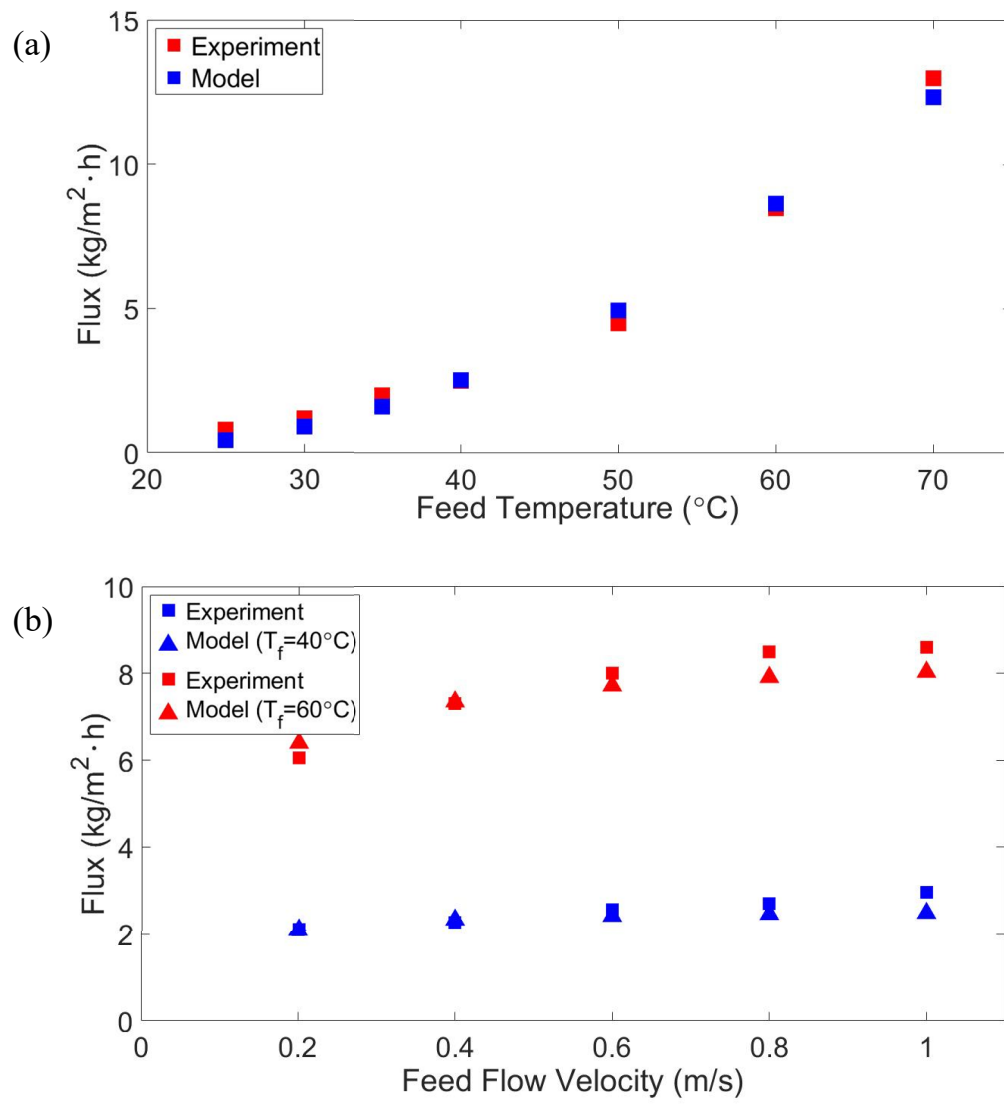


Figure S1. The verification flux result for (a). different temperature; (b). different velocity at two temperatures ($v_p=0.28 \text{ m/s}$, $T_{p, \text{in}}=15^{\circ}\text{C}$, $X_{fs}=0.035$) and literature data [3]