

Assessment of Pilot Direct Contact Membrane Distillation Regeneration of Lithium Chloride Solution in Liquid Desiccant Air-conditioning Systems Using Computer Simulation

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22 **Abstract:** Membrane distillation (MD) has been increasingly explored for treatment of various
23 hyper saline waters, including lithium chloride (LiCl) solutions used in liquid desiccant air-
24 conditioning (LDAC) systems. In this study, the regeneration of liquid desiccant LiCl solution by
25 a pilot direct contact membrane distillation (DCMD) process is assessed using computer
26 simulation. Unlike previous experimental investigations, the simulation allows to incorporate both
27 temperature and concentration polarisation effects in the analysis of heat and mass transfer through
28 the membrane, thus enabling the systematic assessment of the pilot DCMD regeneration of the
29 LiCl solution. The simulation results demonstrate distinctive profiles of water flux, thermal
30 efficiency, and LiCl concentration along the membrane under co-current and counter-current flow
31 modes, and the pilot DCMD process under counter-current flow is superior to that under co-current
32 flow regarding the process thermal efficiency and LiCl concentration enrichment. Moreover, for
33 the pilot DCMD regeneration of LiCl solution under the counter-current flow, the feed inlet
34 temperature, LiCl concentration, and especially the membrane leaf length exert profound impacts
35 on the process performance: the process water flux halves from 12 to 6 L/(m²·h) while thermal
36 efficiency decreases by 20% from 0.46 to 0.37 when the membrane leaf length increases from 0.5
37 to 1.5 m.

38 **Keywords:** membrane distillation (MD); direct contact membrane distillation (DCMD);
39 polarisation effects; heat and mass transfer, liquid desiccant air-conditioning (LDAC); liquid
40 desiccant regeneration.

41

42 **Declarations**

43 **Ethics approval and consent to participate**

44 Not applicable

45 **Consent for publication**

46 Not applicable

47 **Availability of data and materials**

48 The datasets generated and/or analysed during the current study are not publicly available due
49 to regulations of the funding but are available from the corresponding author on reasonable request.

50 **Competing interests**

51 The authors declare the following financial interests/personal relationships which may be
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58 **Authors' contributions**

59 HCD: Conceptualisation, Methodology, Software, Formal Analysis, Resources, Writing-
60 Original Draft;

61 LDN: Conceptualisation, Methodology, Review & Editing

62 AJA: Methodology, Validation, Formal Analysis

63 TDV: Validation, Writing, Review & Editing

64 KMN: Methodology, Validation, Formal Analysis, Review & Editing

65

66

67 **1. Introduction**

68 Membrane distillation (MD), a hybrid thermal-driven separation process, has been increasingly
69 explored for treatment of various hyper saline waters due to its distinguishing attributes (Nguyen
70 et al. 2018; Abdelkader et al. 2019; Duong et al. 2019). In the MD process, a hydrophobic
71 microporous membrane is used to separate a saline water feed from a fresh distillate stream. Given
72 its hydrophobic nature, the membrane retains liquid water on the feed side, but allows the transfer
73 of water vapour through its pores to the other side, hence concentrating the feed water. The driving
74 force for the transfer of water in the MD process is not the hydraulic and/or osmotic pressure
75 difference but the water vapour pressure gradient induced by a temperature difference across the
76 membrane. As a result, unlike pressure-driven membrane processes, MD is less subject to the salt
77 concentration of the feed water, and hence it is workable with various hyper saline waters including
78 concentrated brine from reverse osmosis (RO) desalination (Yan et al. 2017; Bindels et al. 2020),
79 diluted draw solution from forward osmosis (FO) (Nguyen et al. 2018), and liquid desiccant
80 solutions used in air-conditioning industry (Duong et al. 2019; Zhou et al. 2020; Liu et al. 2021).
81 Because only water vapour and volatile compounds are allowed to permeate through its membrane,
82 the MD process can achieve theoretically complete salt rejections, enabling the regeneration and/or
83 recovery of valuable dissolved salts in saline waters. More importantly, as a thermal-driven
84 separation technology, the MD process can be powered by low-grade waste heat or renewable solar
85 thermal energy to reduce the process energy cost. Given these notable attributes, MD has emerged
86 as an ideal candidate to be integrated into other process for treatment of hyper saline waters with
87 improved energy efficiency. One notable example can be the integration of MD into the liquid
88 desiccant air-conditioning (LDAC) process (Duong et al. 2017; Duong et al. 2018; Lefers et al.
89 2018; Zhou et al. 2020; Zhou et al. 2020).

90 LDAC is a potential game changer in advancing the air-conditioning industry to become
91 greener and more energy-efficient (Gurubalan et al. 2019; Chen et al. 2020; Salikandi et al. 2021).
92 Currently, most conventional air-conditioning systems are based on the vapour compression
93 process, whereby the air is first dehumidified by deep cooling to dew point temperature to condense
94 moisture and then reheated to achieve a desired temperature. The deep cooling and the subsequent
95 reheating of the air waste energy, rendering the conventional air-conditioning systems energy-
96 inefficient (Modi and Shukla 2018; Duong et al. 2019). On the other hand, LDAC systems

97 dehumidify and cool the air via the direct absorption of moisture into a liquid desiccant solution
98 (i.e. lithium chloride (LiCl) solution). The hygroscopic nature of the liquid desiccant solution drives
99 the moisture removal without the need for deep cooling and reheating the air; therefore, the energy
100 consumption of the LDAC systems is markedly reduced compared to that of the conventional
101 vapour-compression based air-conditioners (Gurubalan et al. 2019; Chen et al. 2020; Salikandi et
102 al. 2021).

103 Regeneration of liquid desiccant solution is a key step of the LDAC process (Duong et al. 2018;
104 Lefers et al. 2018; Zhou et al. 2020). The moisture holding capacity (i.e. hygroscopicity) of the
105 liquid desiccant solution depends on concentration and temperature. During the air
106 dehumidification of the LDAC process, moisture absorption dilutes and warms the liquid desiccant
107 solution, hence gradually reducing its hygroscopicity. To restore the liquid desiccant solution's
108 hygroscopicity and hence the LDAC process's air dehumidification efficiency, the diluted (i.e.
109 weak) liquid desiccant solution needs to be regenerated (i.e. reconcentrated and cooled) in a
110 regenerator. Most current LDAC systems rely on thermal evaporation for the regeneration of liquid
111 desiccant solutions (Cheng and Zhang 2013; Duong et al. 2019). This regeneration method involves
112 heating the diluted liquid desiccant solution to a high temperature prior to spraying it in counter-
113 current flow with a hot air stream in a packed bed media (Lowenstein 2008; Cheng and Zhang
114 2013; Salikandi et al. 2021). The direct contact between the hot liquid desiccant solution and the
115 air stream inevitably leads to the carry-over of desiccant droplets in the air stream, which is
116 regarded as a vexing technical issue of the thermal evaporation regeneration method (Duong et al.
117 2019; Gurubalan et al. 2019; Chen et al. 2020; Salikandi et al. 2021). Moreover, high-temperature
118 heating required for the regeneration of liquid desiccant solution in the evaporation regenerator
119 primarily contributes to the energy consumption of the LDAC process. As a result, novel
120 regeneration methods that are resistant to desiccant carry-over and workable at mild temperature
121 are urgently needed for the realisation of LDAC systems. In this context, the MD process can be
122 tapped into given its complete salt rejection and workability with hyper saline waters at mild
123 temperature.

124 Previous experimental works have been conducted to prove the technical feasibility of MD for
125 the regeneration of liquid desiccant solutions used in the LDAC process (Duong et al. 2017; Duong
126 et al. 2018; Lefers et al. 2018; Zhou et al. 2019; Zhou et al. 2020; Zhou et al. 2020; Liu et al. 2021).
127 Most notably, Duong et al. (2017) experimentally investigated the direct contact membrane

128 distillation (DCMD) regeneration of liquid desiccant LiCl solutions and proved that the DCMD
129 process could regenerate the liquid desiccant LiCl solution of 29% without any issue of desiccant
130 carry-over at the feed temperature of 65 °C. Zhou et al. (2020) systematically examined the
131 performance of vacuum membrane distillation (VMD) during the regeneration of LiCl solution.
132 Despite using short hollow fibre membranes (i.e. 0.52 m in length), the lab-scale VMD process
133 could increase the concentration of the LiCl 20% solution by 0.2% when operating in the single-
134 pass mode at the feed temperature of 65 °C (Zhou et al. 2020). Particularly, the experimental results
135 demonstrated the profound impacts of LiCl solution temperature and membrane length on the
136 regeneration performance of the VMD process.

137 Previous lab-scale experimental works have demonstrated the viability of MD regeneration of
138 liquid desiccant LiCl solutions. It is, however, necessary to underline that there have been no
139 experimental investigations or simulation studies on pilot or large-scale MD regeneration of liquid
140 desiccant solutions, despite a great number of pilot MD processes experimentally demonstrated
141 and simulated for seawater desalination applications (Hitsov et al. 2015; Dong et al. 2017; Duong
142 et al. 2017; Andrés-Mañas et al. 2018; Andrés-Mañas et al. 2020). To facilitate the realisation of
143 MD regeneration of liquid desiccant solutions, pilot or large-scale studies are of vital importance.
144 Therefore, this study aims to assess a pilot MD process for regeneration of liquid desiccant LiCl
145 solution with the aid of computer simulation. Unlike previous simulations of pilot seawater MD
146 desalination, the pilot DCMD simulation reported in this study incorporates the influences of the
147 LiCl solution hyper salinity and the negative effects of polarisation phenomena, particularly the
148 concentration polarisation, on the process mass and heat transfer. Given its flexibility and high
149 accuracy, the simulation package offers useful means to elucidate the mass and heat transfer inside
150 the pilot DCMD membrane module, thus allowing to elaborate the impacts of process operating
151 conditions and membrane module specifications on the process performance during the
152 regeneration of liquid desiccant LiCl solution.

153 **2. Heat and mass transfer calculations and simulation approaches**

154 **2.1. Heat and mass transfer calculations**

155 During the DCMD regeneration of LiCl solution, the transfer of water (i.e. mass transfer) occurs
156 simultaneously with the heat flux through the membrane. While the mass transfer directly controls

157 the moisture desorption and hence the regeneration of the LiCl solution, the heat flux through the
 158 membrane is undesirable as it reduces the driving force of the regeneration process. The mass
 159 transfer through the membrane is proportional to the water vapour pressure difference between the
 160 two sides of the membrane, and is expressed as (Alkhudhiri et al. 2012):

$$161 \quad J = C_m \times (P_{m.f} - P_{m.d}) \quad (1)$$

162 where J is water flux (kg/(m²·h)); C_m is the membrane mass transfer coefficient (kg/(m²·h·Pa)); and
 163 $P_{m.f}$ and $P_{m.d}$ are the water vapour pressures (Pa) at the feed and distillate membrane surfaces,
 164 respectively. C_m , a function of membrane characteristics and process operating conditions, is
 165 calculated as below (Alkhudhiri et al. 2012):

$$166 \quad C_m = \left[\frac{3}{2} \frac{\tau \delta}{\varepsilon r} \left(\frac{\pi RT}{8M} \right)^{1/2} + \frac{\tau \delta}{\varepsilon} \frac{P_a}{PD} \frac{RT}{M} \right]^{-1} \quad (2)$$

167 where δ , ε , τ , and r are the membrane thickness (m), porosity (dimensionless), pore tortuosity
 168 (dimensionless), and pore radius (m), respectively; M is the molecular weight of water (kg/mol); R
 169 is the gas constant (i.e. 8.314 J/(mol·K)); T is the mean water vapour temperature (K) inside the
 170 membrane pore; P and P_a are the total pressure and the air partial pressure (Pa) inside the membrane
 171 pore; and D is the water diffusion coefficient (m²/s). The distillate water vapour pressure at the
 172 membrane surface (i.e. $P_{m.d}$) can be calculated using the Antoine equation (Alkhudhiri et al. 2012):

$$173 \quad P_{m.d} = \exp\left(23.1964 - \frac{3816.44}{T_{m.d} - 46.13}\right) \quad (3)$$

174 where $T_{m.d}$ is the distillate temperature (K) at the membrane surface. On the other hand, the
 175 calculation of water vapour pressure at the feed membrane surface (i.e. $P_{m.f}$) involves complex
 176 functions of LiCl solution concentration and temperature at the feed membrane surface (e.g. $S_{m.f}$
 177 and $T_{m.f}$). More details of the water vapour pressure calculation of the LiCl solution at high
 178 concentrations are provided elsewhere (Conde 2004; Duong et al. 2020).

179 During the DCMD process of the LiCl solution, in tandem with water vapour flux, heat is
 180 transferred from the feed to the distillate via conduction through the membrane matrix and the

181 latent heat associated with the transferred water vapour. The heat flux (Q) through the membrane
182 is described as (Alkhudhiri et al. 2012):

$$183 \quad Q = \frac{k_m}{\delta} (T_{m,f} - T_{m,d}) + J\Delta H_v \quad (4)$$

184 where Q is in $\text{kJ}/(\text{m}^2 \cdot \text{h})$; k_m is the membrane thermal conductivity ($\text{W}/(\text{m} \cdot \text{K})$); and ΔH_v is the latent
185 heat of evaporation of water (kJ/kg). The membrane thermal conductivity is a function of polymer
186 thermal conductivity (k_s) and gas thermal conductivity (k_g), expressed as (Alkhudhiri et al. 2012):

$$187 \quad k_m = \left[\frac{\varepsilon}{k_g} + \frac{1-\varepsilon}{k_s} \right]^{-1} \quad (5)$$

188 The latent heat of water evaporation (i.e. ΔH_v) is a function of the mean water vapour temperature
189 inside the membrane pore, and is calculated as (Alkhudhiri et al. 2012):

$$190 \quad \Delta H_v = 1.7535T + 2024.3 \quad (6)$$

191 Water flux calculation using the membrane mass transfer coefficient (C_m) in equation (1)
192 involves temperature and salt concentration at the membrane surfaces (e.g. $T_{m,f}$, $T_{m,d}$, and $S_{m,f}$).
193 During the DCMD process of LiCl solutions, polarisation effects cause the temperature and salt
194 concentration at the membrane surfaces different to those in the bulk feed and distillate streams
195 (e.g. $T_{b,f}$, $T_{b,d}$, and $S_{b,f}$) (Kuang et al. 2019; Anvari et al. 2020). While the bulk temperature and salt
196 concentration of the feed and distillate streams can be experimentally measured, the measurements
197 of these parameters at the membrane surfaces require complex instruments and impractical
198 membrane module designs (Kuang et al. 2019; Lokare et al. 2019). In this context, several studies
199 have utilised the process mass transfer coefficient (i.e. K_m) together with the bulk feed and distillate
200 temperature and salt concentration for water flux calculation. This water flux calculation is more
201 practical when involving the measurable thermodynamic properties of the bulk feed and distillate;
202 however, it fails to incorporate polarisation effects, particularly concentration polarisation,
203 resulting in considerable deviations between the calculated and experimentally measured water
204 flux (Duong et al. 2017; Duong et al. 2018). The computer model developed for the simulation of
205 the pilot DCMD process of seawater reported by Duong et al. (2017) includes the temperature

206 polarisation effect in water flux calculation, but deliberately neglects the concentration polarisation
 207 effect given the negligible impacts of seawater salinity on water flux. For the pilot DCMD
 208 regeneration of liquid desiccant LiCl solutions, the hyper salinity of the feed exerts profound
 209 influences on water flux; therefore, the concentration polarisation effect must be incorporated in
 210 water flux calculation together with the temperature polarisation effect.

211 The simulation model built for this study incorporates both temperature and concentration
 212 polarisation effects in water flux calculation and heat transfer analysis. Initially, water flux (J) is
 213 calculated using the bulk thermodynamic properties of the feed and distillate, then the temperature
 214 and LiCl concentration at the feed and distillate membrane surfaces (i.e. $T_{m,f}$, $S_{m,f}$, and $T_{m,d}$) are
 215 calculated as below (Khayet et al. 2004; Hitsov et al. 2015):

$$216 \quad T_{m,f} = \frac{T_{b,f}h_f + h_m\left(T_{b,d} + T_{b,f}\frac{h_f}{h_d}\right) - J\Delta H_v}{h_f\left(1 + \frac{h_m}{h_d}\right) + h_m} \quad (7)$$

$$217 \quad T_{m,d} = \frac{T_{b,d}h_d + h_m\left(T_{b,f} + T_{b,d}\frac{h_d}{h_f}\right) + J\Delta H_v}{h_d\left(1 + \frac{h_m}{h_f}\right) + h_m} \quad (8)$$

$$218 \quad S_{m,f} = S_{b,f} \times \exp\left(\frac{J}{\rho \times k}\right) \quad (9)$$

219 where h_m , h_f , and h_d are respectively the heat transfer coefficient across the membrane and in the
 220 feed and distillate thermal boundary layers; ρ and k are the density and the water transfer coefficient
 221 of the LiCl solution feed. The heat transfer coefficient across the membrane (h_m) is dependent on
 222 the membrane thermal conductivity (k_m) and the membrane thickness (δ), while the calculations of
 223 the heat transfer coefficients in the feed and distillate boundary layers (h_f and h_d) involve Nusselt
 224 number (Nu), Reynolds number (Re), and Prandtl number (Pr) using the fluid thermodynamic
 225 properties (e.g. density, dynamic viscosity, specific heat capacity, and cross flow velocity) and the
 226 hydraulic diameter of the feed and distillate channels. Empirical equations for the calculations of

227 the thermodynamic properties of the LiCl solution feed and the distillate are provided in (Conde
 228 2004). The calculated $T_{m,f}$, $T_{m,d}$, and $S_{m,f}$ are then used for the calculation of J in equation (1). The
 229 new calculated value is now assigned to J in the calculation of new $T_{m,f}$, $T_{m,d}$, and $S_{m,f}$ in the
 230 equations (7-9). This calculation process is iterated until the difference between the two
 231 consecutive values of J is negligible.

232 Thermal efficiency is an important aspect of the DCMD process of LiCl solutions as the
 233 regeneration step contributes over three quarters of the energy consumption of LDAC systems, and
 234 the energy consumption of the DCMD process is primarily attributed to thermal energy required
 235 for heating the feed stream. The thermal efficiency (Π) of the DCMD process is evaluated using
 236 the following equation (Alkhudhiri et al. 2012):

$$237 \quad \Pi = \frac{J \Delta H_v}{J \Delta H_v + \frac{k_m}{\delta} (T_{m,f} - T_{m,d})} \quad (10)$$

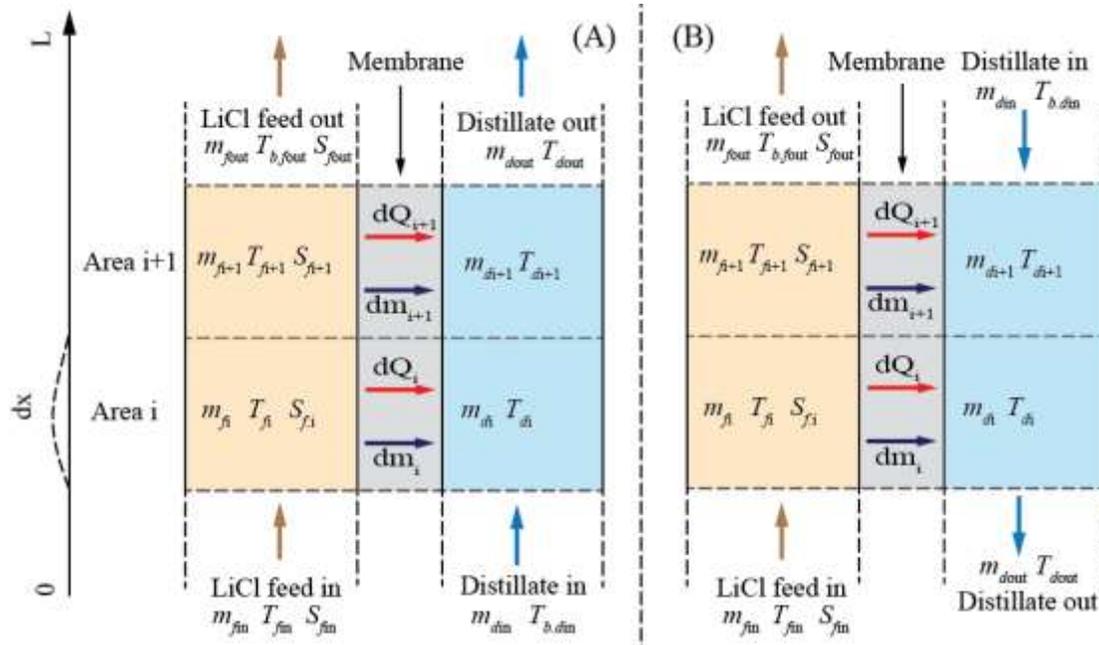
238 Besides thermal efficiency, the specific thermal energy consumption (i.e. $STEC$) of the DCMD
 239 process of the LiCl solution is also assessed. $STEC$ is the heating required to increase the weight
 240 concentration of one volume unit of LiCl solution feed by 1%, and can be calculated as:

$$241 \quad STEC = \frac{m_{f.in} \times C_p \times (T_{f.in} - 25)}{3.6 \times 10^3 \times \Delta S \times V_{f.in}} \quad (11)$$

242 where $STEC$ is in kWh/(%·m³); m_{fin} is the feed inlet mass flow rate (kg/h); C_p is the specific heat
 243 capacity of the LiCl solution feed (kJ/(kg·°C)); $T_{f.in}$ is the feed inlet temperature of the DCMD
 244 process; ΔS is the LiCl concentration enrichment (i.e. the difference between the LiCl concentration
 245 at the outlet and the inlet of the feed channel) (%); and $V_{f.in}$ is the feed inlet volume flow rate (m³/h).
 246 It is necessary to note that while $STEC$ offers a practical indicator for the DCMD process energy
 247 efficiency, Π demonstrates the proportion of the useful heat (i.e. that is associated with the transfer
 248 of water) to the total heat transfer from the feed to the distillate along the membrane leaf inside the
 249 DCMD membrane module. Moreover, the calculation of $STEC$ for the DCMD process in this study
 250 differs from that normally reported for seawater MD desalination applications because the main
 251 product of the DCMD process in this study is the concentrated LiCl solution but not fresh water as
 252 for seawater desalination.

253 **2.2. Simulation approach**

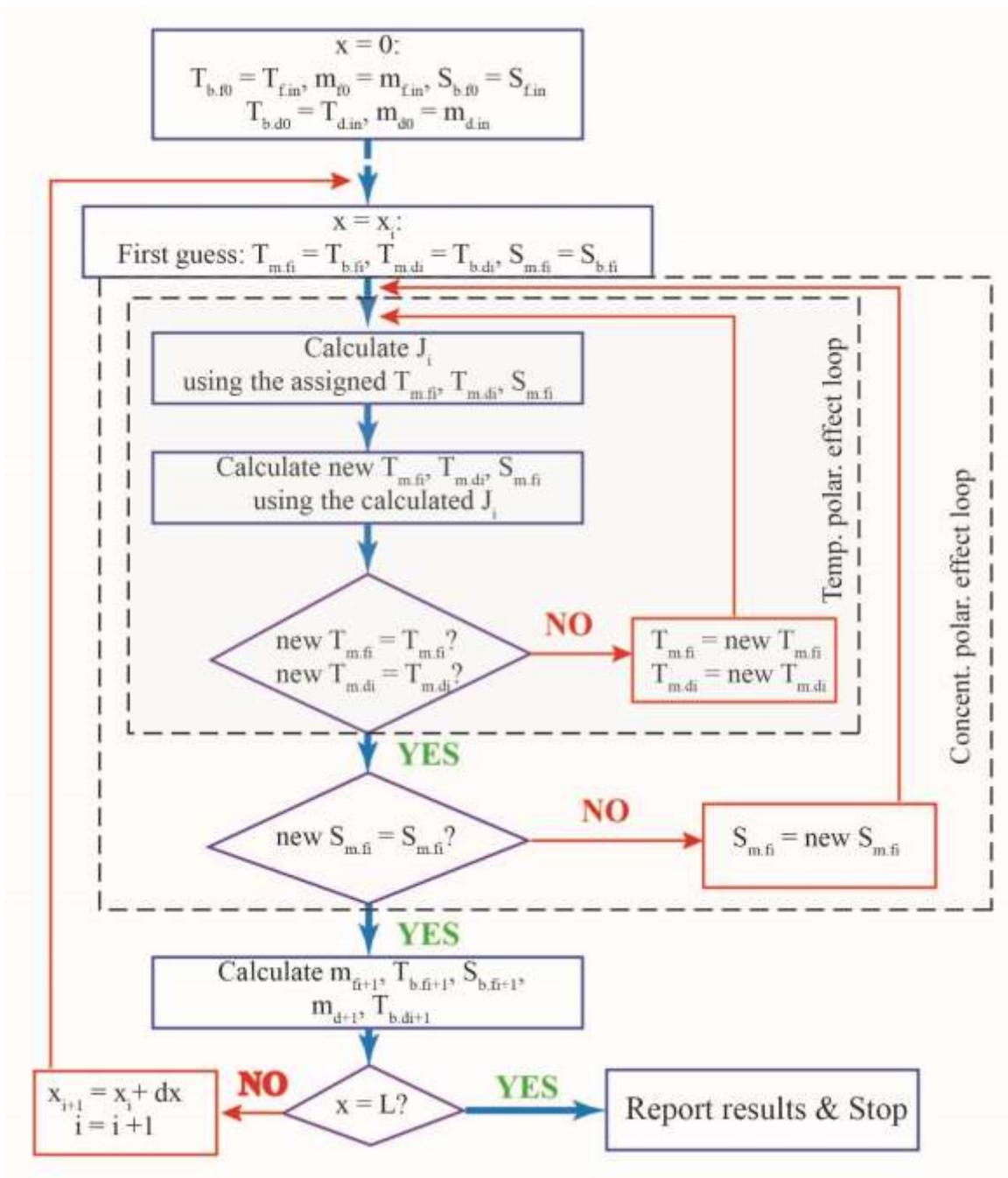
254 The simulation package used in this study is developed based on the descriptive mass and heat
 255 transfer (DMHT) model that has been validated and reported in a previous study by Duong et al.
 256 (2020). One notable feature of this simulation package is the inclusion of both temperature and
 257 concentration polarisation effects in the mass and heat transfer analyses, and it allows for the
 258 simulation of the DCMD process of the LiCl solution under two flow modes: co-current and
 259 counter-current flow (Fig. 1). Details about the DMHT model and the calculation of heat and mass
 260 flux through each membrane area under the two flow modes can be found in the previous study by
 261 Duong et al. (2020).



262
 263 **Fig. 1.** Schematic diagram of two incremental membrane areas along the DCMD module under
 264 the (A) co-current and (B) counter-current flow mode.

265 The calculation algorithms of the DCMD process with the LiCl solution feed are illustrated in
 266 Fig. 2 and Fig. 3 for co-current and counter-current flow mode, respectively. The inputs of the
 267 calculation algorithms are the temperature, concentration, and mass flow rate of the LiCl solution
 268 feed and distillate respectively at the feed and distillate inlets (e.g. $T_{f.in}$, $S_{f.in}$, $m_{f.in}$, $T_{d.in}$, and $m_{d.in}$).
 269 The calculation starts from the feed inlet end (i.e. $x_0 = 0$) and finishes at the feed outlet end (i.e. x_n
 270 $= L$) of the DCMD module. For co-current flow, the initial parameters of the feed and distillate

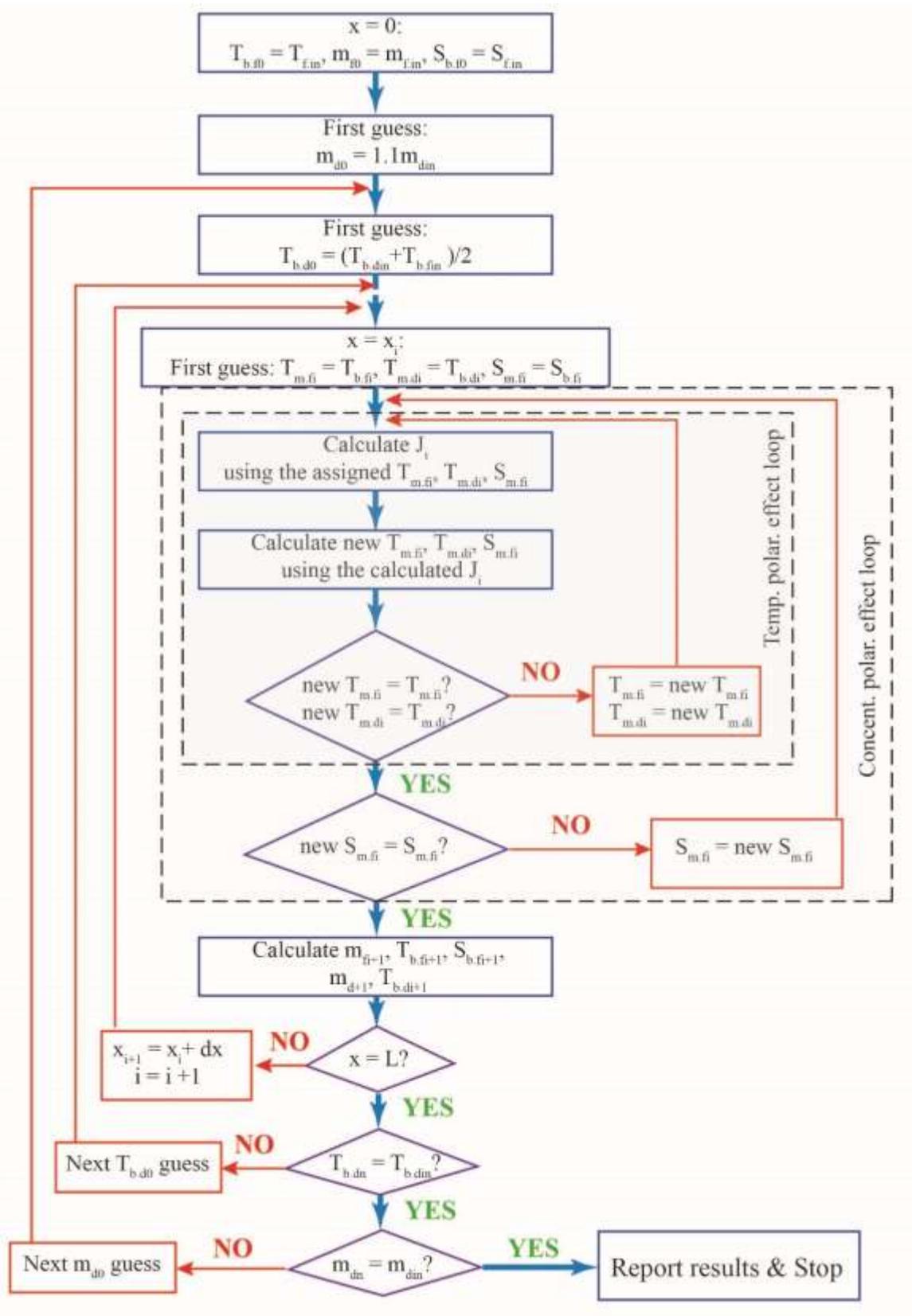
271 streams are readily available. On the other hand, for counter-current flow, initial guesses of the
 272 mass flow and temperature of the distillate at the outlet (i.e. $m_{d,out}$ and $T_{d,out}$) are required (Fig. 3).



273

274

Fig. 2. Calculation algorithm of the DCMD simulation for co-current flow.



275

276

Fig. 3. Calculation algorithm of the DCMD simulation for counter-current flow.

277 The specifications of the membrane leaf and feed and distillate channels of the pilot DCMD
 278 membrane module provided by AquaStill (Sittard, The Netherlands) (Hitsov et al. 2017) were used
 279 for the simulation in this study. These specifications include membrane pore radius, membrane
 280 porosity, membrane thickness, feed and distillate channel width and depth, and the membrane leaf
 281 length. Unless otherwise stated, their default values are provided in Table 1. The pilot DCMD
 282 membrane module used in (Hitsov et al. 2017) had six feed and six distillate channels, but they
 283 were parallel. Thus, for simplicity the pilot DCMD membrane module simulated in this study is
 284 composed of one feed and one distillate channels with the same specifications.

285 **Table 1.** Specifications of the membrane leaf and flow channels of the pilot DCMD membrane
 286 module

<i>Membrane specifications</i>	
Pore radius (μm)	0.15
Membrane porosity (–)	0.76
Membrane thickness (μm)	92
<i>Feed and distillate channels</i>	
Channel width (m)	0.4
Channel depth (m)	0.002
Channel length (m)	1.5

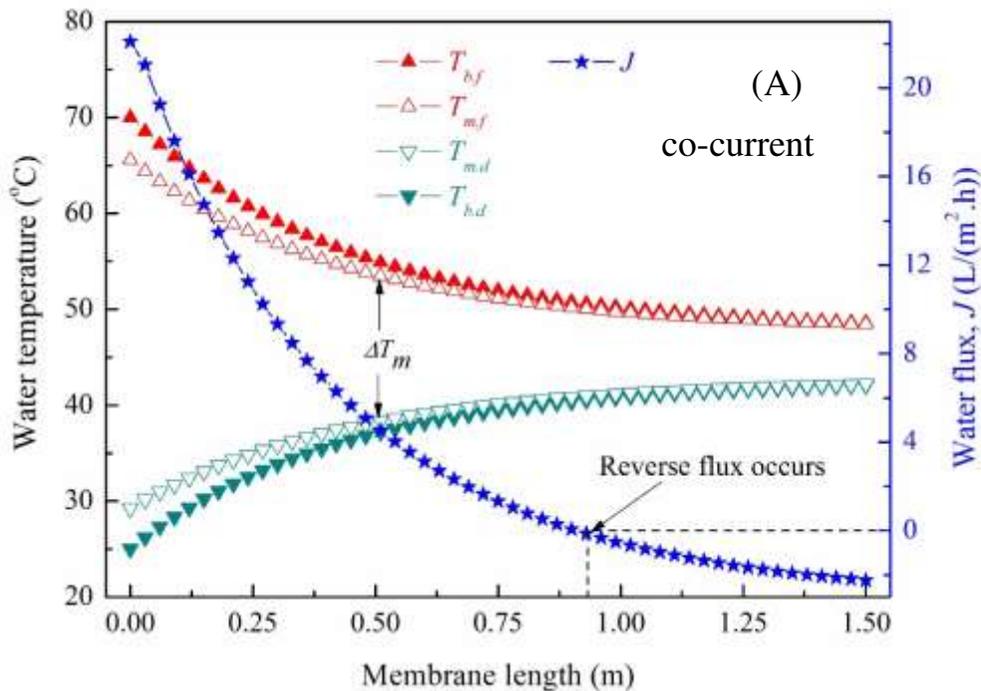
287 3. Results and discussions

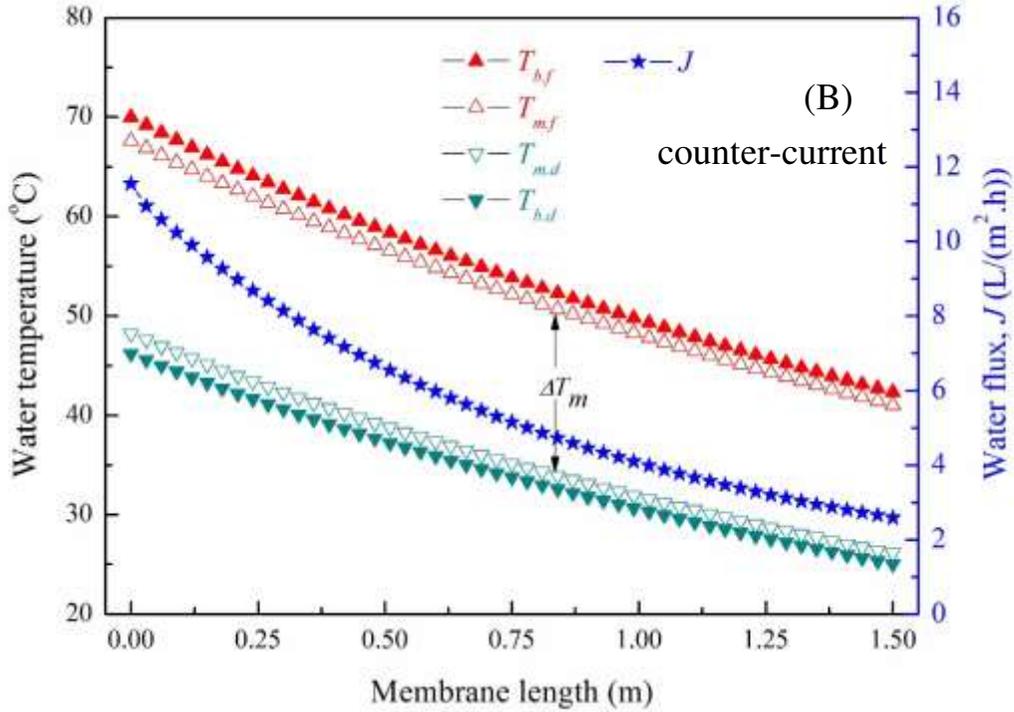
288 3.1. Mass and heat transfer through the membrane inside the module

289 In the pilot DCMD regeneration of liquid desiccant LiCl solution, the flow mode exerts decisive
 290 influence on the heat and mass transfer through the membrane. As demonstrated in Fig. 4, co-
 291 current and counter-current modes result in two different feed and distillate temperatures and water
 292 flux profiles inside the membrane module. Under the co-current flow mode, from the inlet to the
 293 outlet of the membrane module the membrane surface feed temperature ($T_{m,f}$) declines while the
 294 membrane surface distillate temperature ($T_{m,d}$) increases due to heat transferred from the feed to
 295 the distillate, leading to a decrease in the transmembrane water temperature difference (i.e. ΔT_m)
 296 (Fig. 4A). This decreased ΔT_m together with the increase in the LiCl concentration along the
 297 membrane results in a rapid decline in local water flux (J) inside the membrane module from the
 298 inlet to the outlet. Moreover, it is noteworthy that after the membrane length of 0.9 m, negative
 299 water flux is observed despite the positive ΔT_m (>10 °C) (Fig. 4A). This finding confirms that the

300 actual driving force for water transfer through the membrane in MD is the transmembrane water
 301 vapour pressure (i.e. ΔP_m), not the transmembrane water temperature difference (ΔT_m). After the
 302 membrane length of 0.9 m, $T_{m,f}$ remains markedly higher than $T_{m,d}$; however, the water vapour
 303 pressure at the feed membrane surface is lower than that at the distillate membrane surface due to
 304 the hyper salinity of the LiCl solution. As a result, reverse water flux from the distillate to the LiCl
 305 solution feed occurs after the membrane length of 0.9 m (Fig. 4A).

306 On the other hand, the feed and distillate temperatures at the membrane surfaces and in the bulk
 307 streams linearly decrease from the feed inlet to the feed outlet of the membrane module under the
 308 counter-current mode (Fig. 4B). Although the temperature difference between the feed and
 309 distillate membrane surfaces (ΔT_m) remains largely constant along the membrane leaf, the local
 310 water flux markedly declines from the feed inlet to the feed outlet. The declining water flux along
 311 the membrane module under counter-current mode has been elucidated in the previous study by
 312 Duong et al. (2020) using a lab-scale membrane module. It is noteworthy that the local water flux
 313 declines at a higher rate near the feed inlet than toward the feed outlet due to the exponential
 314 relation between the water vapour pressure and the temperature of solutions (Fig. 4B).





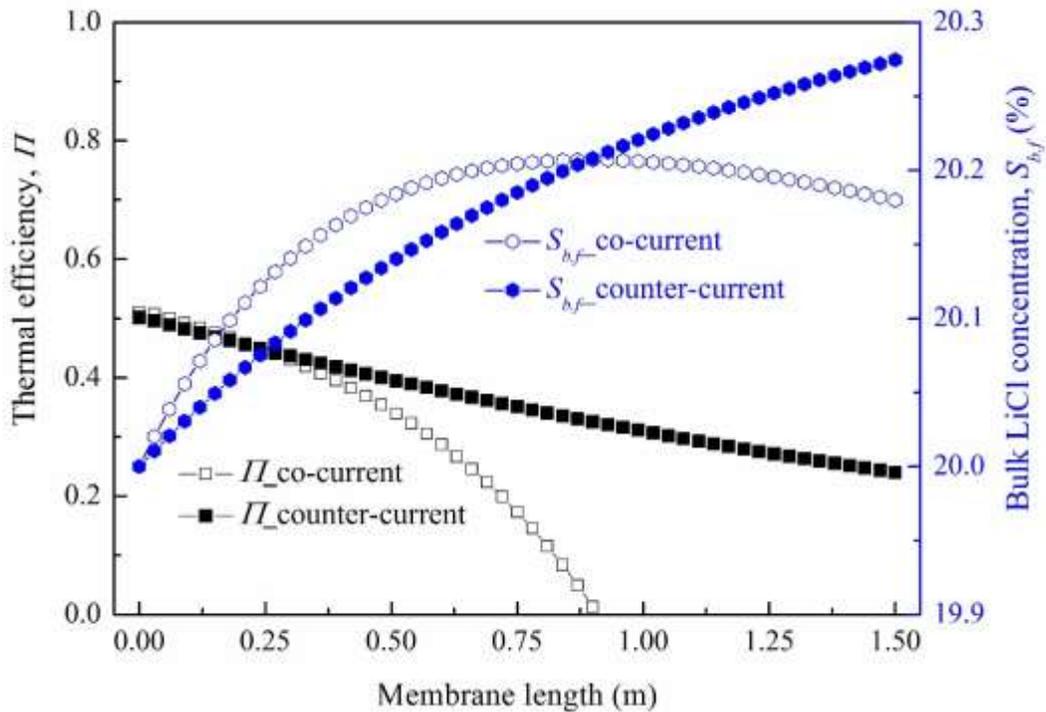
315 **Fig. 4.** Feed and distillate temperature at the membrane surfaces and in the bulk streams and
 316 water flux along the membrane inside the module during the DCMD regeneration of the LiCl
 317 20% solution under (A) co-current and (B) counter-current flow. Operating conditions: feed inlet
 318 temperature ($T_{f.in}$) = 70 °C, distillate inlet temperature $T_{d.in}$ = 25 °C, feed and distillate inlet
 319 circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

320 The discrepancy in local water flux inside the membrane module under the two operation modes
 321 results in noticeably different profiles of thermal efficiency and the LiCl solution concentration
 322 (Fig. 5). The thermal efficiency of the DCMD process with the LiCl 20% solution feed under both
 323 operation modes is mostly below 0.5. This means that during the DCMD regeneration of the LiCl
 324 20% solution feed using the pilot system, more than half of the heat transfer from the feed to the
 325 distillate is due to the heat conduction through the membrane and is deemed the heat loss.
 326 Furthermore, thermal efficiency under co-current mode is discernibly lower than that under the
 327 counter-current mode, demonstrating that the counter-current operation is more beneficial to the
 328 pilot DCMD regeneration of LiCl solution with respect to thermal efficiency. It is important to
 329 stress that previous experimental studies on lab-scale DCMD regeneration of liquid desiccant LiCl
 330 solutions have not investigated the process thermal efficiency.

331 The bulk LiCl concentration (i.e. $S_{b,f}$) profiles along the membrane leaf under the two flow
 332 modes also clearly differ (Fig. 5). Under the co-current flow, from the feed inlet the LiCl
 333 concentration steadily increases and maximizes at the membrane length of 0.9 m before gradually

334 decreasing toward the feed outlet (i.e. 1.5 m). On the other hand, the LiCl concentration under the
 335 counter-current mode progressively rises from the feed inlet to the feed outlet (Fig. 5). Indeed,
 336 these LiCl concentration profiles are consistent with the water flux profiles shown in Fig. 4. The
 337 decreased LiCl concentration under the co-current flow after the membrane length of 0.9 m is due
 338 to the negative water flux (Fig. 4A). Moreover, the LiCl concentration at the feed outlet under the
 339 counter-current flow is noticeably higher than that under the co-current mode. This also manifests
 340 the advantage of the counter-current operation over the co-current one for the pilot DCMD
 341 regeneration of LiCl solutions.

342 The analysis of heat and mass transfer through the membrane inside the module has revealed
 343 the superiority of the counter-current to the co-current mode during the pilot DCMD regeneration
 344 of the liquid desiccant LiCl solution. Thus, the counter-current mode is selected for further
 345 investigations on the influences of the operating conditions and membrane length on the pilot
 346 DCMD process performance discussed in the next section.

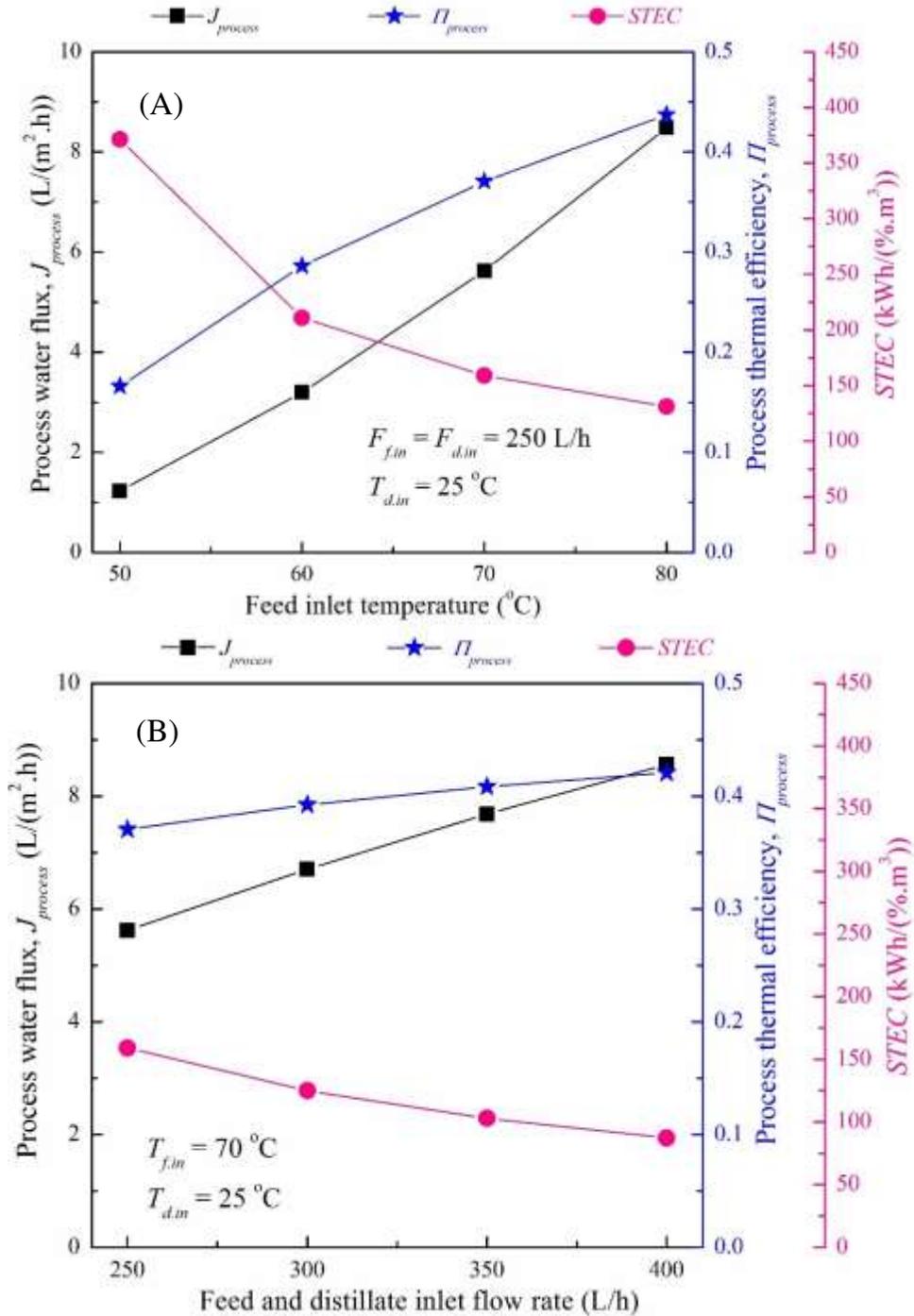


347
 348 **Fig. 5.** Thermal efficiency and the bulk LiCl concentration along the membrane inside the
 349 module during the DCMD regeneration of the LiCl 20% solution under co-current and counter-
 350 current flow. Operating conditions: feed inlet temperature ($T_{f.in}$) = 70 °C, distillate inlet
 351 temperature $T_{d.in}$ = 25 °C, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

352 3.2. Influences of operating conditions on the DCMD process performance

353 The key operating conditions of the pilot DCMD regeneration of LiCl solutions include the
354 feed inlet temperature, the feed and distillate circulation rate, and the inlet LiCl concentration. The
355 distillate inlet temperature has less influence on the DCMD process performance; thus, it is fixed
356 at 25 °C in all simulations. The performance of the DCMD regeneration of LiCl solutions is
357 assessed using the process water flux ($J_{process}$), thermal efficiency ($\Pi_{process}$), specific thermal energy
358 consumption ($STEC$), and the increase in the LiCl concentration from the inlet to the outlet (i.e.
359 ΔS). While $STEC$ is calculated using equation (11), $J_{process}$ and $\Pi_{process}$ are the average values of
360 local water flux (J) and thermal efficiency (Π) along the membrane leaf.

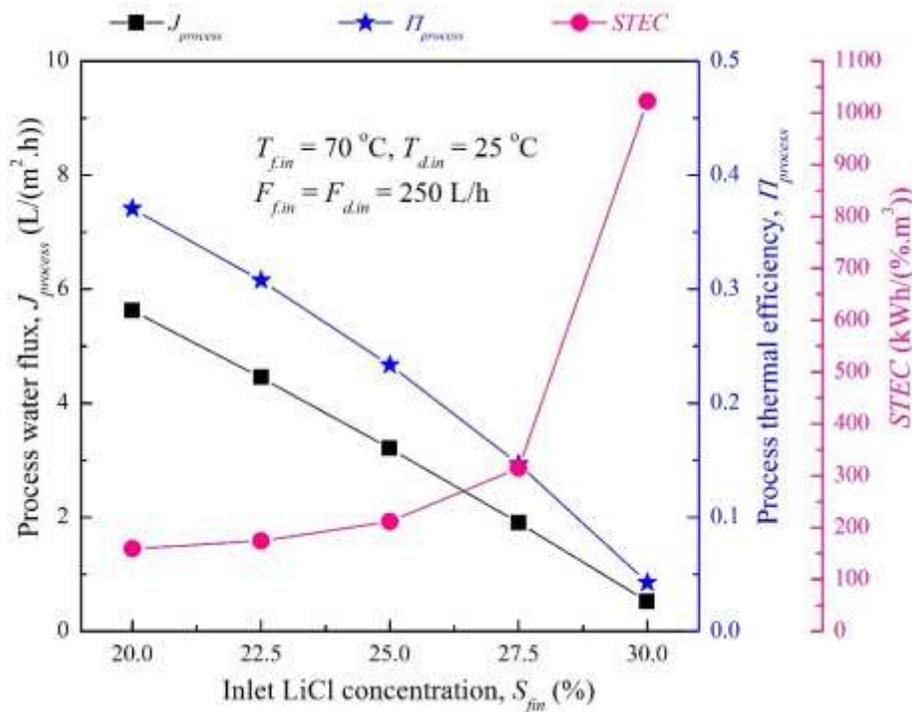
361 The simulation results reveal that it is beneficial to operate the pilot DCMD process of LiCl
362 solutions at higher feed inlet temperature and higher water circulation rates. As demonstrated in
363 Fig. 6A, elevating the feed inlet temperature boosts both $J_{process}$ and $\Pi_{process}$ while substantially
364 reducing $STEC$ of the DCMD process. Increasing feed and distillate circulation rates also favours
365 the improvement of the $J_{process}$ and $\Pi_{process}$ and the reduction in $STEC$ (Fig. 6B), but at a lower
366 extent compared to elevating the feed inlet temperature. Indeed, the benefits of operating the
367 DCMD process of LiCl solution at high feed inlet temperature and water circulation rates have
368 been proven in experimental works using lab-scale units (Duong et al. 2017; Duong et al. 2018).
369 The results reported here, however, highlight that even under the optimal feed inlet temperature
370 and water circulation rates, the pilot DCMD regeneration of LiCl solutions exhibits limited thermal
371 efficiency (i.e. $\Pi_{process} < 0.5$) and discernibly high $STEC$ (i.e. ~ 100 kWh/(%.m³)). The poor thermal
372 efficiency of the DCMD process with the LiCl solution can be attributed to the hyper salinity of
373 the LiCl solution feed.



374 **Fig. 6.** The process water flux ($J_{process}$), process thermal efficiency ($\Pi_{process}$), and specific thermal
 375 energy consumption (STEC) of the DCMD regeneration of the LiCl 20% solution at (A) different
 376 feed inlet temperature and (B) different feed and distillate flow rate under counter-current flow.
 377 Other operating conditions: distillate inlet temperature $T_{d.in} = 25$ °C.

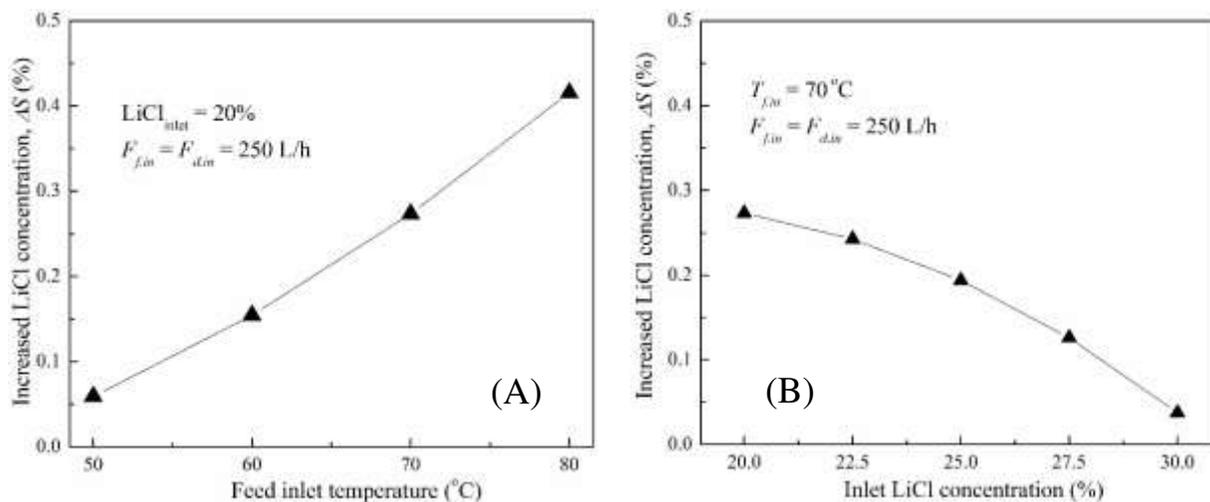
378 The inlet LiCl concentration profoundly affects the performance of the DCMD process (Fig.
 379 7). When the inlet LiCl concentration is elevated from 20% to 30%, $J_{process}$ reduces by 91% from

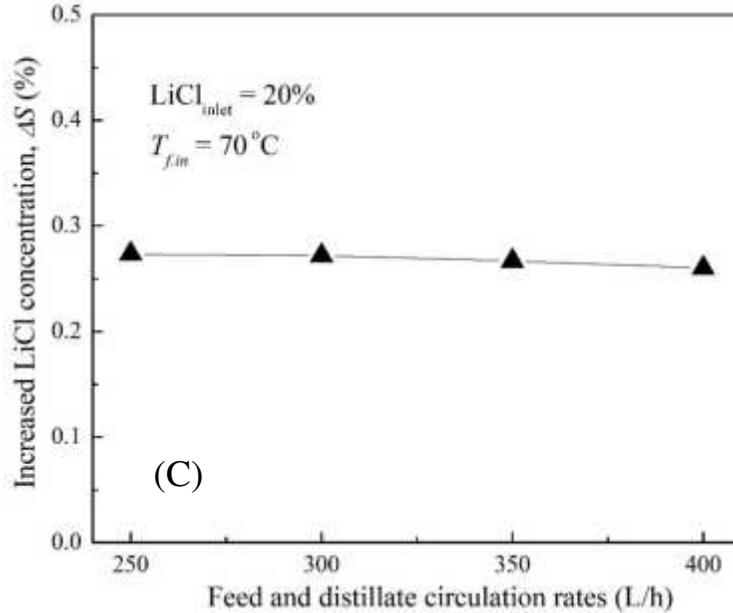
380 5.6 to 0.5 L/(m²·h), coinciding with a reduction in the $\Pi_{process}$ by 89% (i.e. from 0.37 to 0.04). The
 381 LiCl concentration regulates not only the water vapour pressure but also the thermodynamic
 382 properties (i.e. particularly the viscosity) of the feed solution, thus restraining the mass transfer
 383 coefficient and water vapour flux through the membrane. Indeed, the simulation results reveal that
 384 the dynamic viscosity of the LiCl solution doubles when the LiCl concentration is increased from
 385 20% to 30%. Previous experimental lab-scale works have demonstrated the strong impacts of the
 386 feed concentration on water flux during the DCMD regeneration of LiCl solutions (Duong et al.
 387 2017; Duong et al. 2018). These impacts are even more profound for the pilot DCMD process of
 388 LiCl solutions given its much longer membrane leaf compared to that used in the lab-scale units.
 389 The effects of membrane leaf length on the water flux and hence the thermal efficiency of the pilot
 390 DCMD process with LiCl solution will be further elucidated in section 3.3. The limited water flux
 391 and poor thermal efficiency inevitably leads to the discernibly high values of $STEC$ at higher inlet
 392 LiCl concentration (Fig. 7).



393
 394 **Fig. 7.** The process water flux ($J_{process}$), thermal efficiency ($\Pi_{process}$), and specific thermal energy
 395 consumption ($STEC$) of the DCMD process of the LiCl solution at different concentration. Other
 396 operating conditions: feed inlet temperature ($T_{f.in}$) = 70 °C, distillate inlet temperature $T_{d.in}$ = 25
 397 °C, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

398 Another important indicator for the performance of the DCMD regeneration of LiCl solutions
399 is the enrichment of LiCl in the feed (i.e. ΔS). The three key operating conditions (e.g. feed inlet
400 temperature, water circulation rate, and the inlet LiCl concentration) exhibit different effects on ΔS
401 (Fig. 8). The feed inlet temperature is proportional with ΔS while elevating the LiCl solution
402 concentration noticeably reduces ΔS (Fig. 8A&B). The impacts of feed inlet temperature and the
403 LiCl concentration on ΔS appear similarly to their effects on water flux shown in Fig. 6A and Fig.
404 7. On the other hand, the feed and distillate circulation rates exert negligible impacts on ΔS despite
405 having a linear relationship with water flux (Fig. 6B). Unlike the feed inlet temperature and the
406 LiCl concentration, the feed and distillate circulation rates determine the retention time of the LiCl
407 solution inside the membrane module. Increasing the water circulation rates enhances water flux
408 but also shortens the retention time of the LiCl solution feed. As a result, the impacts of the feed
409 and distillate circulation rates on ΔS seem to be neutralized (Fig. 8C).





410 **Fig. 8.** The LiCl concentration enrichment achieved during the DCMD regeneration of the LiCl
 411 solution at various (A) feed inlet temperature, (B) inlet LiCl concentration, and (C) feed and
 412 distillate water circulation rates under counter-current flow. Other operating conditions: distillate
 413 inlet temperature $T_{d.in} = 25$ °C.

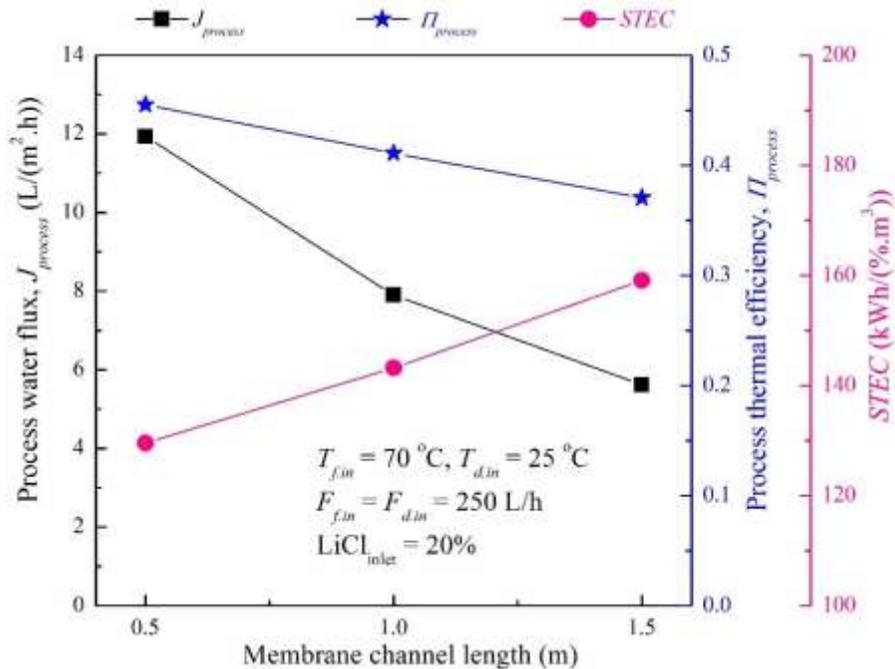
414 3.3. Influences of the membrane length on the DCMD process performance

415 Unlike experimental works using lab-scale units with fix membrane module specifications, the
 416 simulation in this study allows for systematically assessing the influences of membrane module
 417 specifications on the performance of the pilot DCMD regeneration of LiCl solutions. One of the
 418 most critical membrane module specifications for the pilot DCMD process is the membrane leaf
 419 length.

420 The simulation results reveal that the pilot DCMD process with LiCl solutions is more efficient
 421 when using a shorter membrane leaf (Fig. 9). The process with the shorter membrane leaf achieves
 422 higher water flux and thermal efficiency but lower *STEC* under the same operating conditions (e.g.
 423 feed inlet temperature, feed and distillate circulation rate, and inlet LiCl concentration). The
 424 enhanced process performance with the shortened membrane leaf can be attributed to the increased
 425 transmembrane temperature difference (i.e. ΔT_m). For example, at the feed inlet and the distillate
 426 inlet temperatures of 70 °C and 25 °C, feed and distillate circulation rate of 250 L/h, and the inlet
 427 LiCl concentration of 20%, the average ΔT_m of the process with the membrane length of 0.5 m and
 428 1.5 m is 25.5 °C and 17.1 °C, respectively. Given the exponential relation between the water vapour

429 pressure and the temperature, the reduction in ΔT_m when increasing the membrane leaf length
 430 inevitably leads to the decline in water flux (Fig. 9). This decreasing water flux in turn negatively
 431 affects thermal efficiency ($\Pi_{process}$) and hence raises the $STEC$ of the process.

432 The results reported here have important implications to the design of the membrane modules
 433 destined for liquid desiccant air-conditioning applications. Membrane modules with longer
 434 membrane leaves offer larger membrane areas for water evaporation and hence achieve a higher
 435 LiCl concentration at the outlet of the membrane modules. However, the process using longer
 436 membrane exhibits lower water flux and thermal efficiency as discussed above. Therefore, for the
 437 pilot DCMD regeneration of liquid desiccant solutions, it is more beneficial to deploy membrane
 438 modules with short membrane leaves. The process can be operated in batch mode or brine recycling
 439 mode (i.e. whereby the brine leaving the membrane modules is returned to the feed tank for further
 440 treatment cycles) (Duong et al. 2015; Duong et al. 2017). Operating under these modes, the LiCl
 441 concentration can be achieved without compromising the water flux and thermal efficiency of the
 442 pilot DCMD process.



443
 444 **Fig. 9.** The process water flux ($J_{process}$), thermal efficiency ($\Pi_{process}$), and specific thermal energy
 445 consumption ($STEC$) of the pilot DCMD regeneration of the LiCl 20% solution using the
 446 membrane module with different membrane length. Other operating conditions: feed inlet
 447 temperature ($T_{f.in}$) = 70 °C, distillate inlet temperature $T_{d.in}$ = 25 °C, feed and distillate inlet
 448 circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

449 **4. Conclusions**

450 This study assesses the pilot DCMD regeneration of liquid desiccant LiCl solution in LDAC
451 systems using computer simulation. In contrast to experimental investigations, the simulation
452 allows for the insightful evaluation of the heat and mass transfer through the membrane inside the
453 DCMD membrane module as it can incorporate both temperature and concentration polarisation
454 effects in the calculation of heat and water flux. The simulation results demonstrate that the flow
455 mode of the pilot DCMD process strongly affects the heat and mass transfer across the membrane,
456 and the counter-current flow mode is more beneficial than co-current one regarding the process
457 water flux, thermal efficiency, and LiCl concentration enrichment. Moreover, when operating the
458 pilot DCMD process of LiCl solution under the counter-current flow, the feed inlet temperature,
459 the feed LiCl concentration, and particularly the membrane leaf length are significant factors
460 governing the process performance. When increasing the membrane leaf length from 0.5 to 1.5 m,
461 the process water flux decreases by a half from 12 to 6 L/(m²·h) and thermal efficiency decreases
462 by 20%. These simulation results have important implications to the design of the pilot DCMD
463 membrane modules, particularly the membrane leaf length.

464 **Acknowledgements**

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Figures

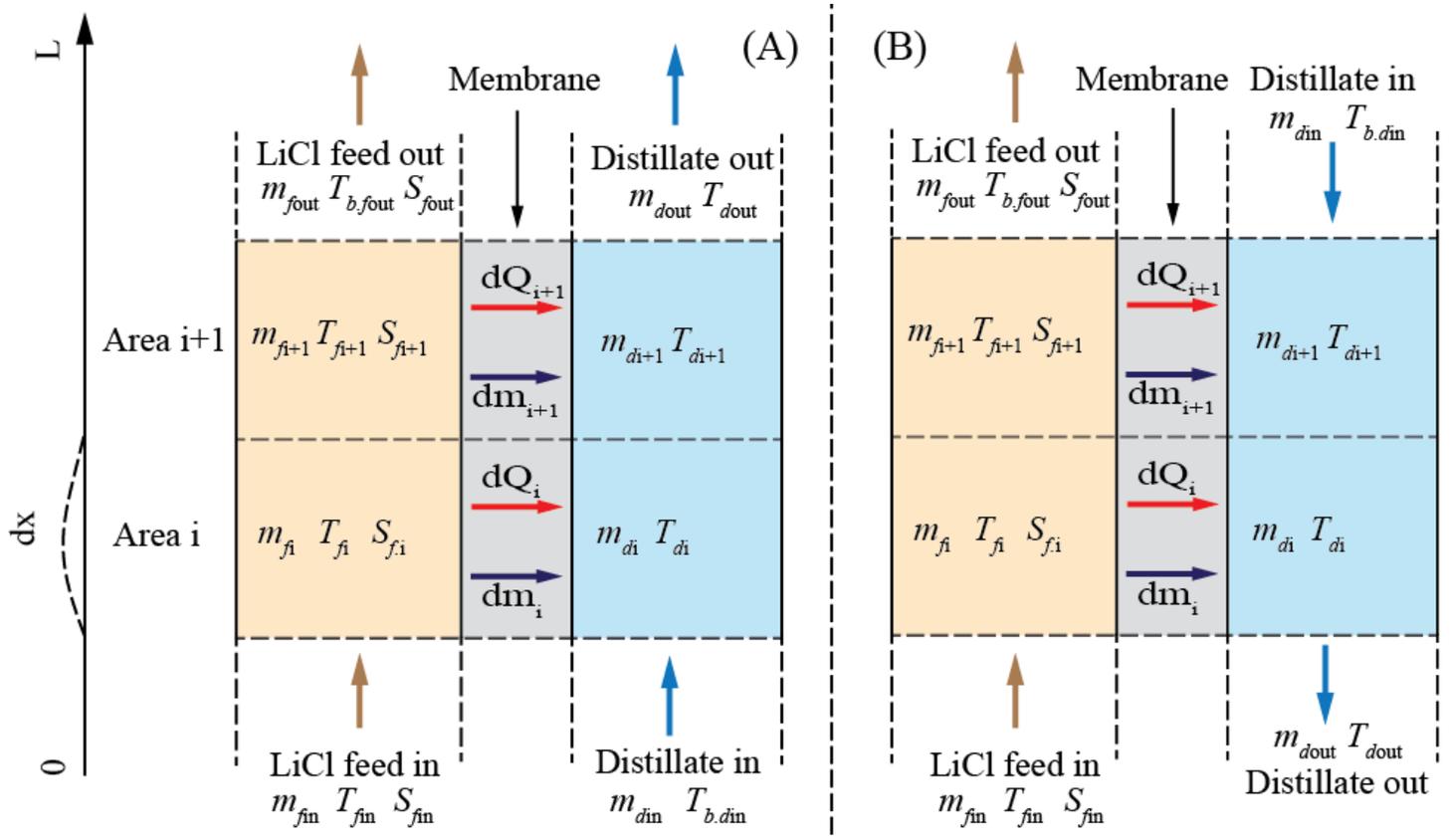


Figure 1

Schematic diagram of two incremental membrane areas along the DCMD module under the (A) co-current and (B) counter-current flow mode.

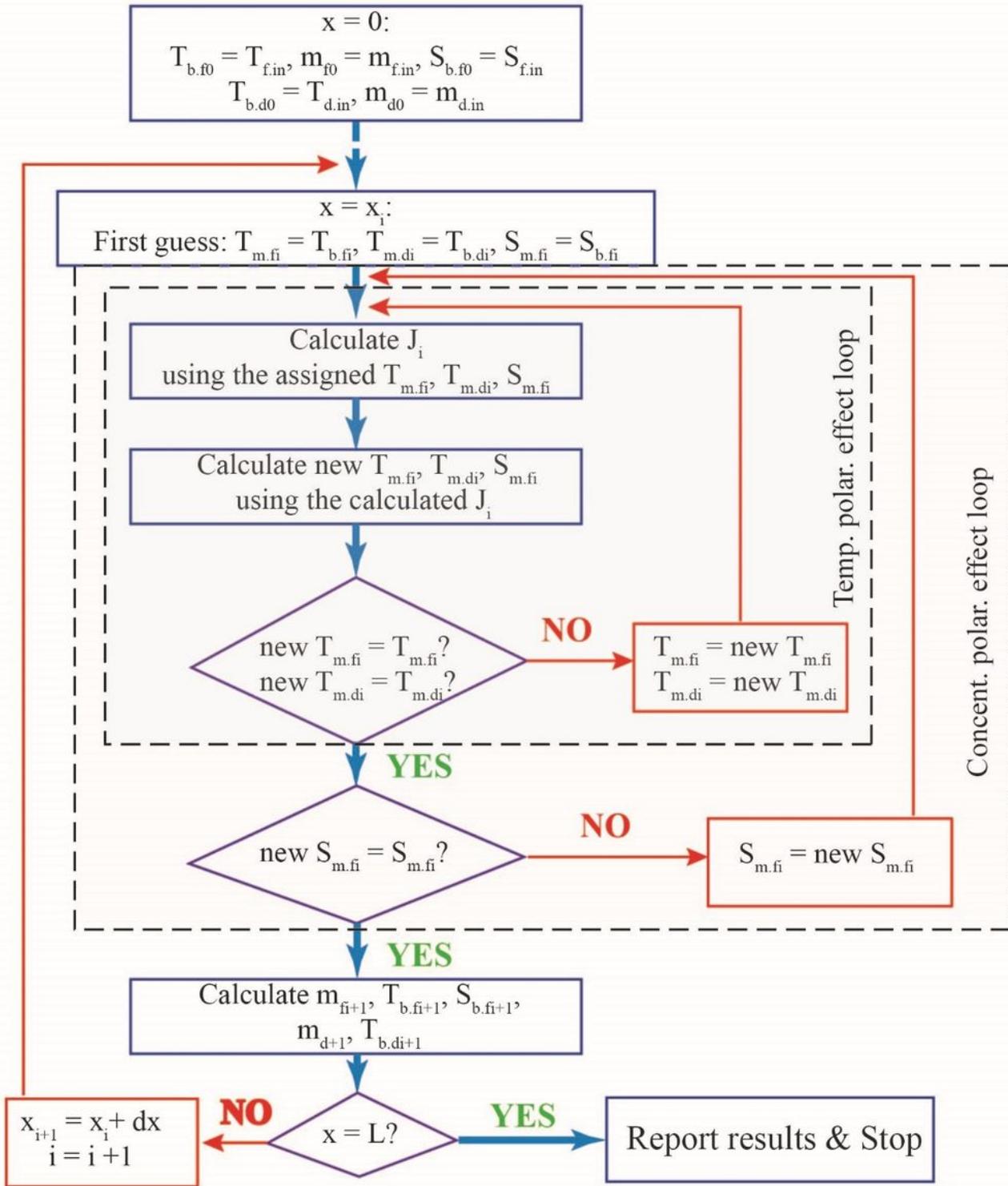


Figure 2

Calculation algorithm of the DCMD simulation for co-current flow.

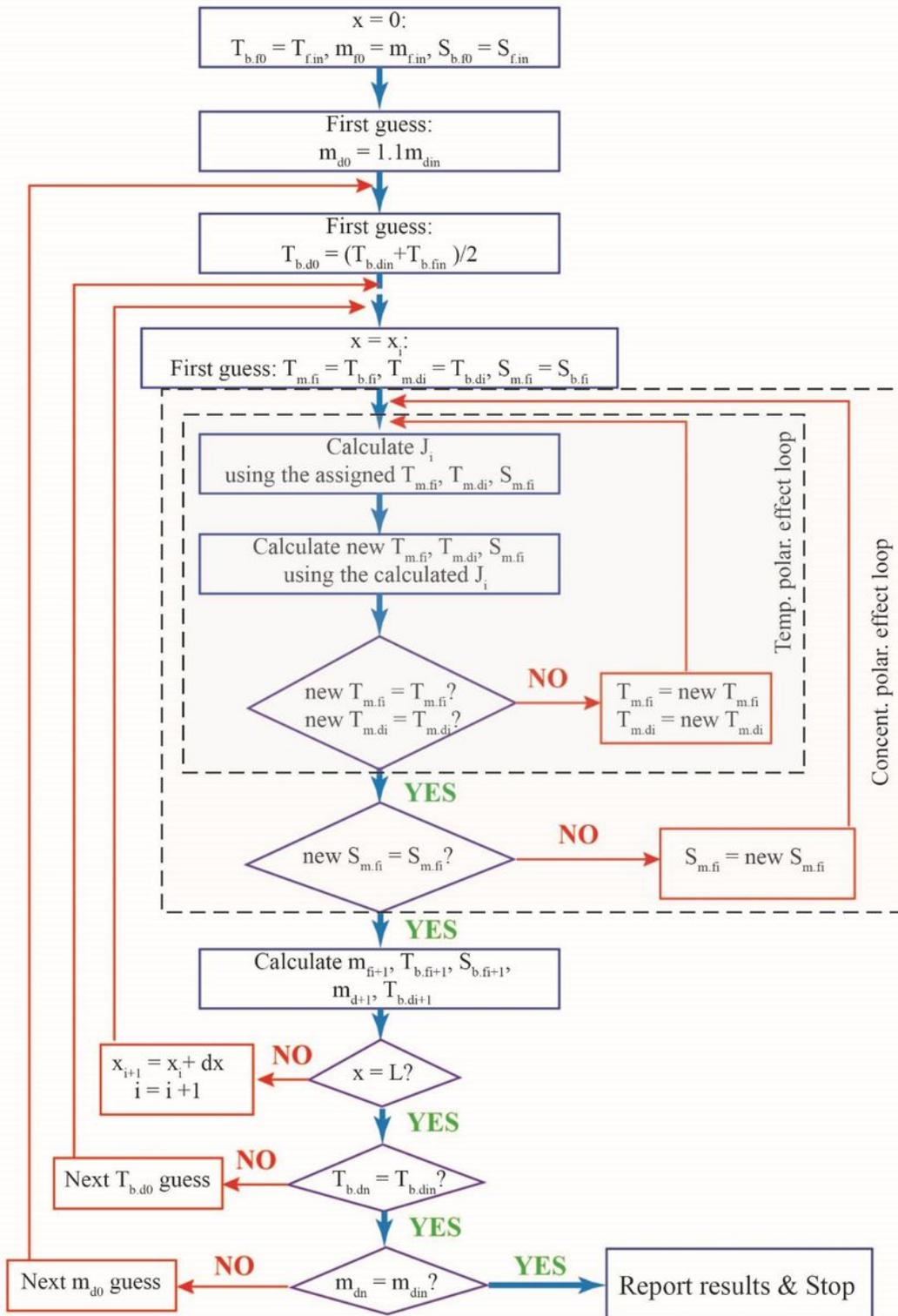


Figure 3

Calculation algorithm of the DCMD simulation for counter-current flow.

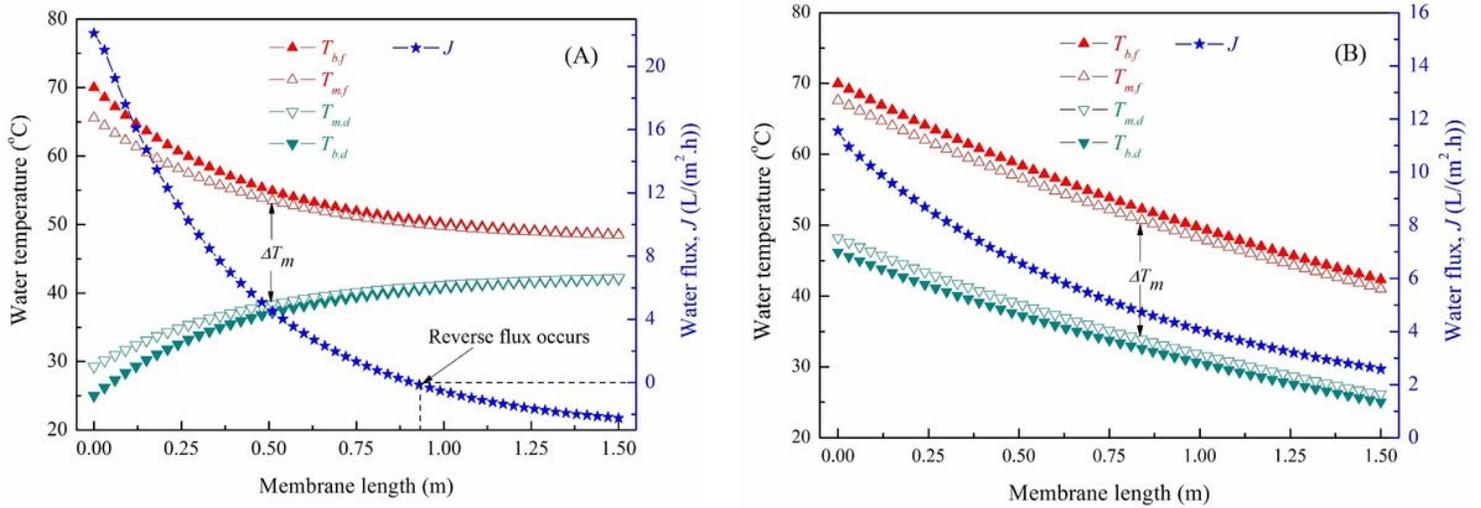


Figure 4

Feed and distillate temperature at the membrane surfaces and in the bulk streams and water flux along the membrane inside the module during the DCMD regeneration of the LiCl 20% solution under (A) co-current and (B) counter-current flow. Operating conditions: feed inlet temperature ($T_{f.in}$) = 70 oC, distillate inlet temperature $T_{d.in}$ = 25 oC, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

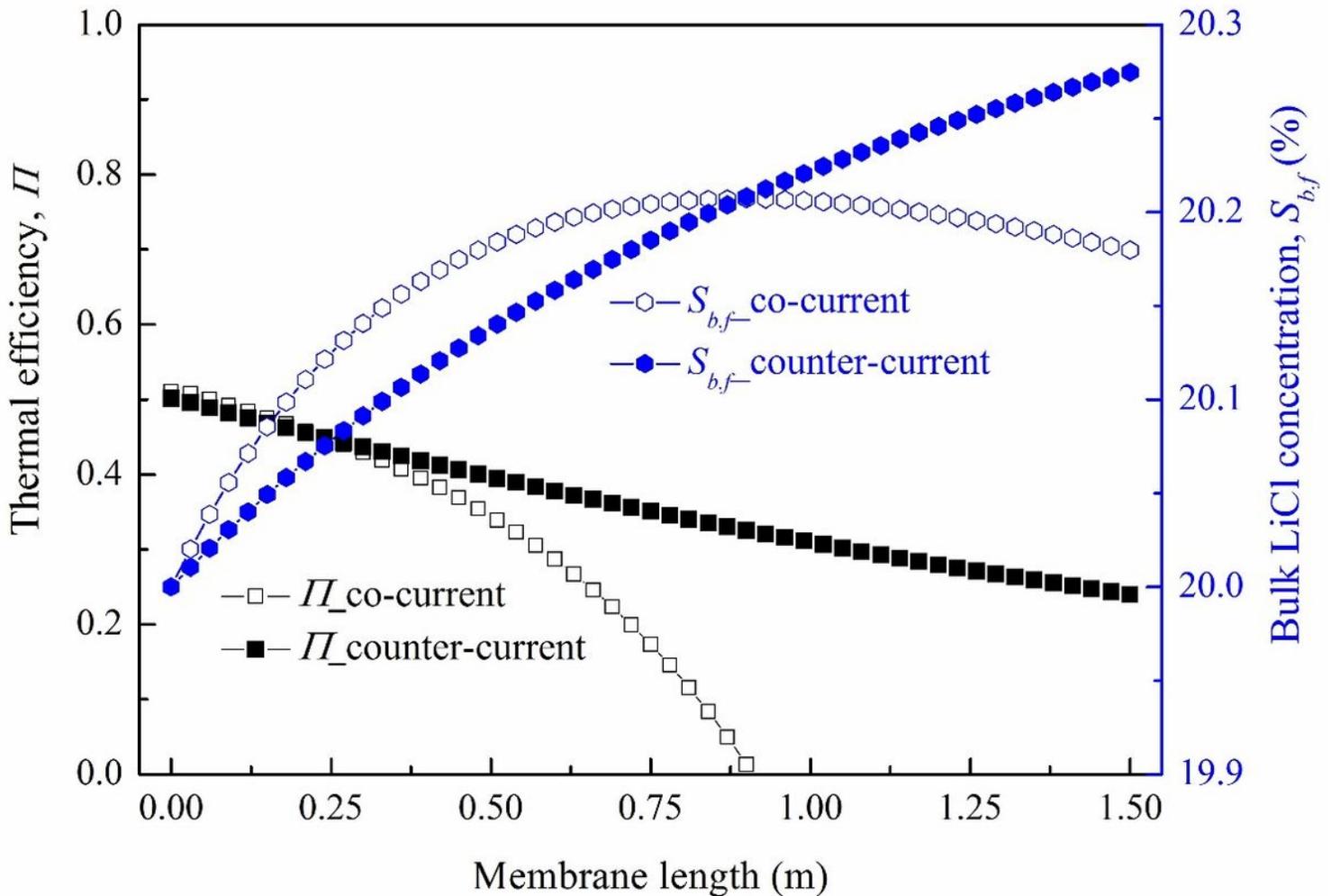


Figure 5

Thermal efficiency and the bulk LiCl concentration along the membrane inside the module during the DCMD regeneration of the LiCl 20% solution under co-current and counter-current flow. Operating conditions: feed inlet temperature ($T_{f.in}$) = 70 °C, distillate inlet temperature $T_{d.in}$ = 25 °C, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.

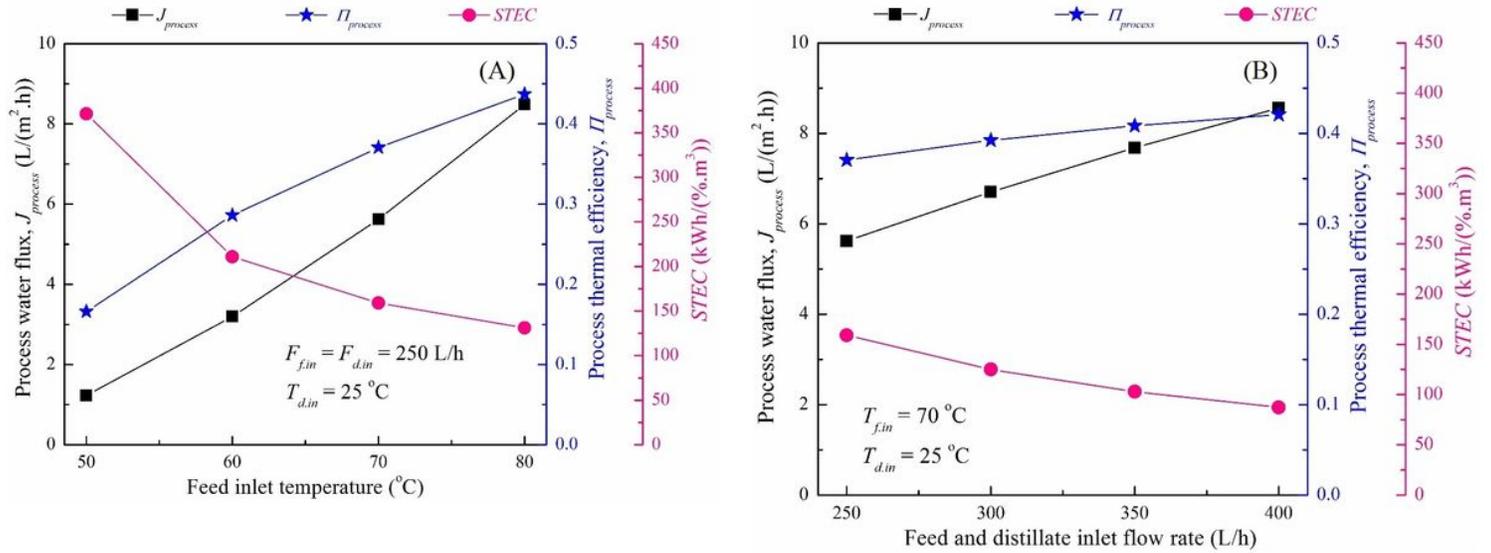


Figure 6

The process water flux ($J_{process}$), process thermal efficiency ($\Pi_{process}$), and specific thermal energy consumption (STEC) of the DCMD regeneration of the LiCl 20% solution at (A) different feed inlet temperature and (B) different feed and distillate flow rate under counter-current flow. Other operating conditions: distillate inlet temperature $T_{d.in} = 25$ °C.

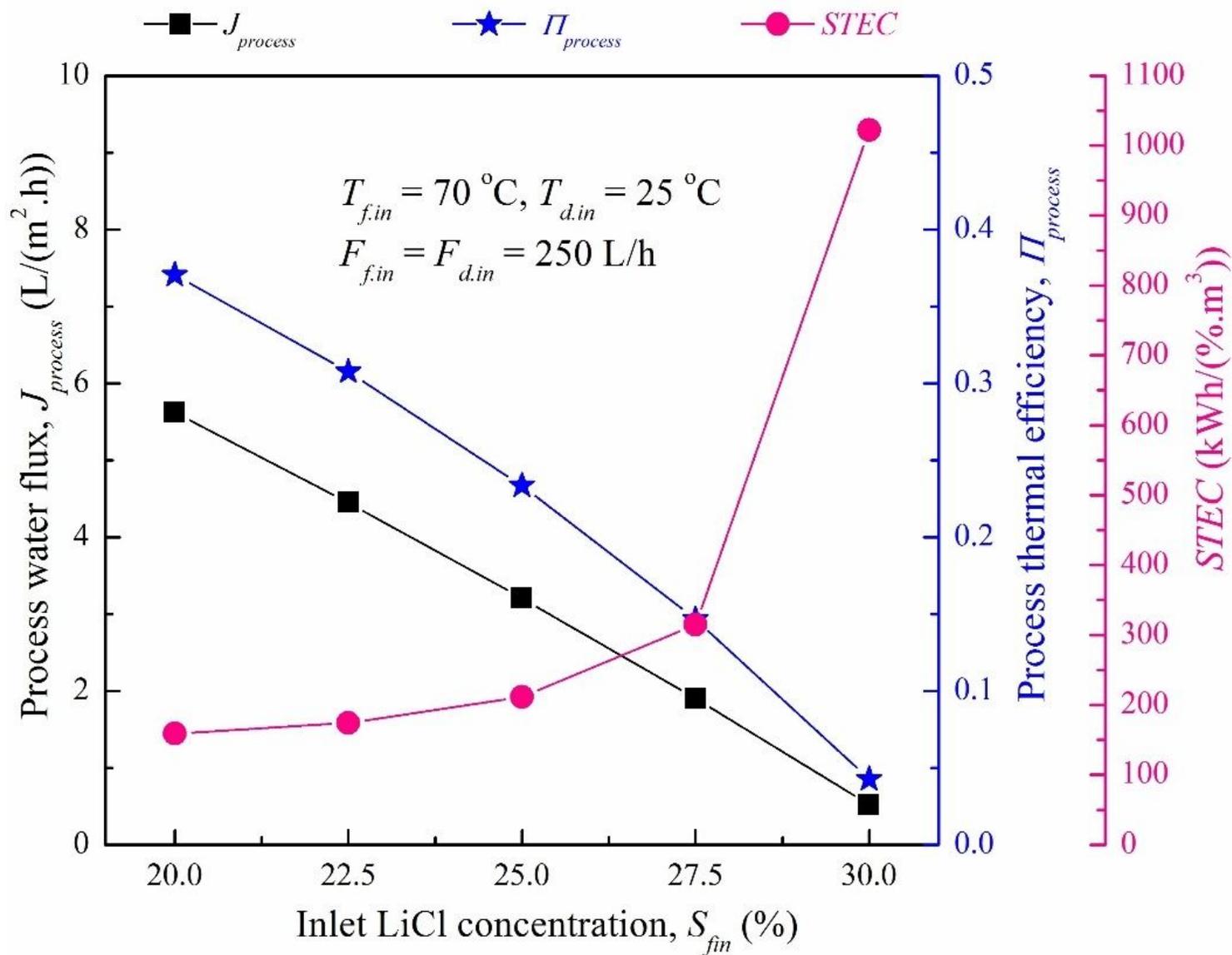


Figure 7

The process water flux ($J_{process}$), thermal efficiency ($\Pi_{process}$), and specific thermal energy consumption (STEC) of the DCMD process of the LiCl solution at different concentration. Other operating conditions: feed inlet temperature ($T_{f.in}$) = 70oC, distillate inlet temperature $T_{d.in}$ = 25oC, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250\text{ L/h}$.

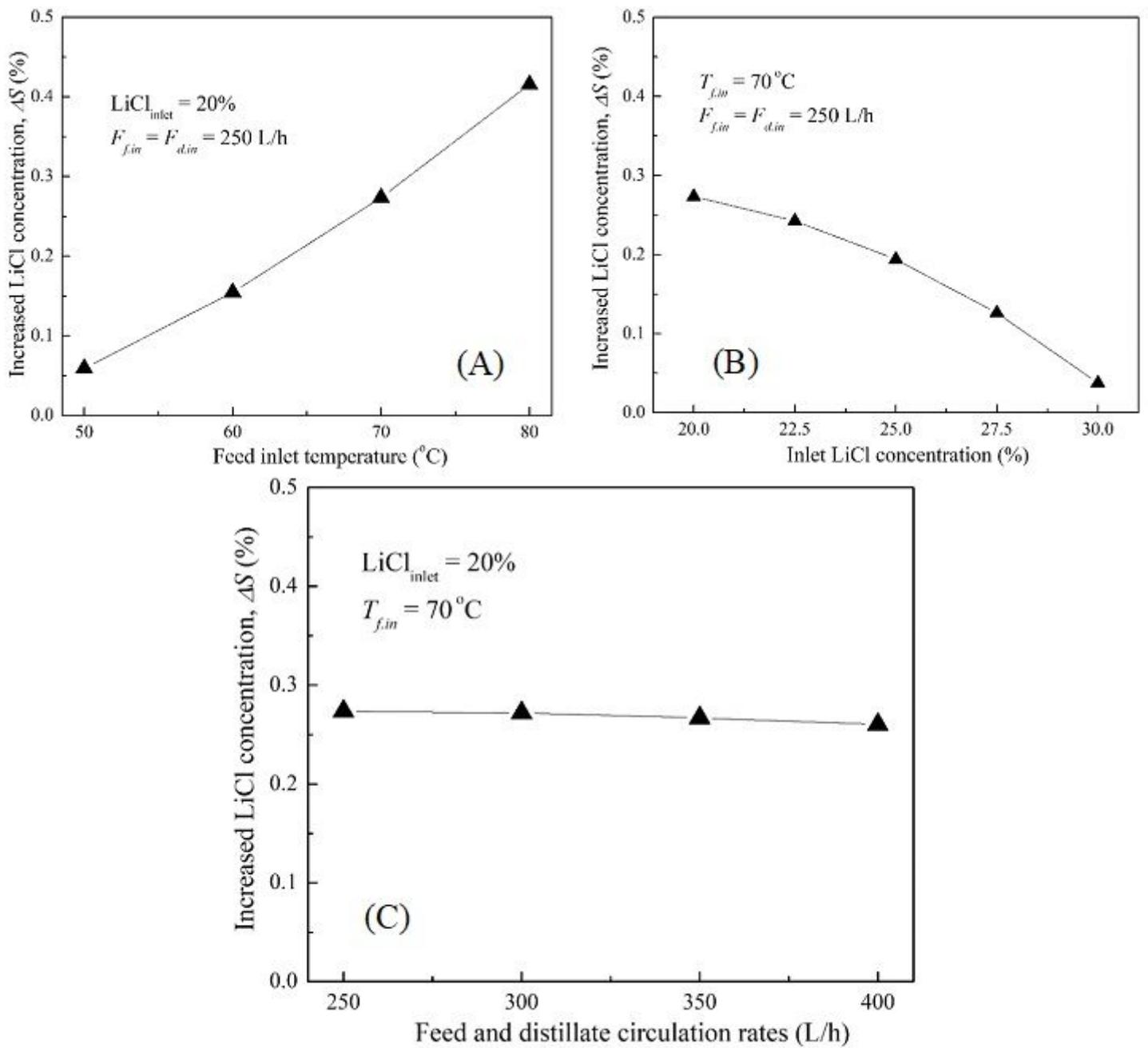


Figure 8

The LiCl concentration enrichment achieved during the DCMD regeneration of the LiCl solution at various (A) feed inlet temperature, (B) inlet LiCl concentration, and (C) feed and distillate water circulation rates under counter-current flow. Other operating conditions: distillate inlet temperature $T_{d,\text{in}} = 25 \text{ }^{\circ}\text{C}$.

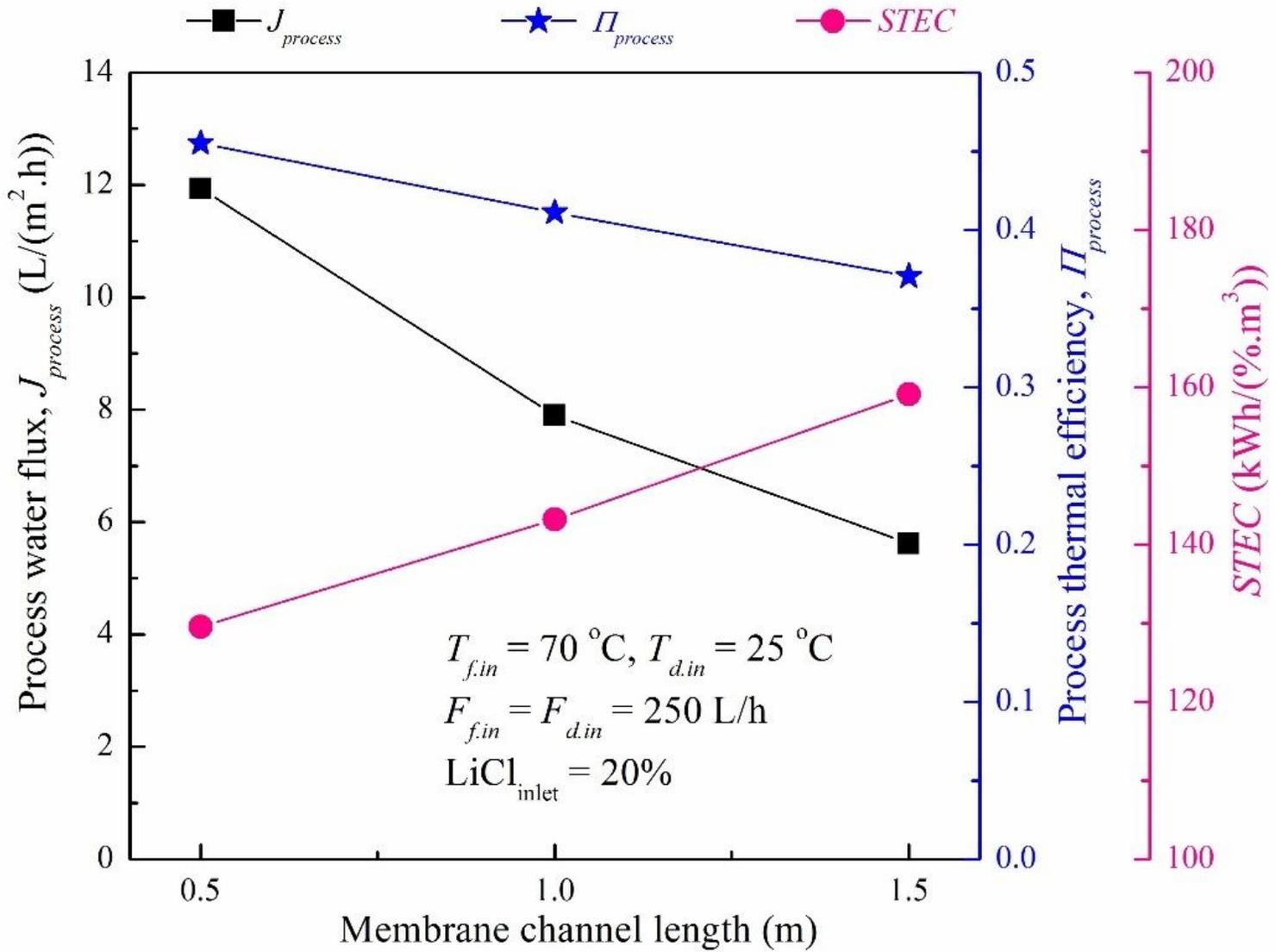


Figure 9

The process water flux ($J_{process}$), thermal efficiency ($\Pi_{process}$), and specific thermal energy consumption (STEC) of the pilot DCMD regeneration of the LiCl 20% solution using the membrane module with different membrane length. Other operating conditions: feed inlet temperature ($T_{f.in}$) = 70 oC, distillate inlet temperature $T_{d.in}$ = 25 oC, feed and distillate inlet circulation rate $F_{f.in} = F_{d.in} = 250$ L/h.