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1 **Simulation and optimisation of spiral-wound reverse osmosis process for the removal of**  
2 **N-nitrosamine from wastewater**

3  
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10  
11 **Abstract**

12 N-nitrosamine in wastewater treatment processes can contribute to several public health  
13 impacts including human carcinogens even at very low concentration. In this work, spiral-  
14 wound reverse osmosis (SWRO) process is used to remove N-nitrosamine compounds from  
15 wastewater. Effects of operating parameters of the SWRO process on the removal of N-  
16 nitrosamine, total water recovery, and specific energy consumption for a SWRO  
17 configurations are evaluated via simulation and optimisation. For this purpose, the one-  
18 dimensional distributed model developed earlier by the authors is modified by including  
19 different mass transfer coefficient correlation, temperature dependent water and solute  
20 permeability correlations and energy equations. The model is first validated by estimating a  
21 new set of model parameters using eight set of experimental data from the literature and is  
22 then used to simulate the process with and without energy recovery device to facilitate deeper  
23 insight of the effect of operating conditions on the process performance. The model is then  
24 embedded within an optimisation framework and optimisation problems to maximise N-  
25 nitrosamine rejections and to minimise specific energy consumption are formulated and  
26 solved while the operating conditions are optimized simultaneously.

27 **Keywords:** Reverse Osmosis; Spiral-wound Module; One-dimensional Modelling;  
28 Optimisation; N-nitrosamine Removal; Energy Consumption.

29 **1. Introduction**

30 N-nitrosamine is considered as one of the by-products of disinfection process of secondary-  
31 treated wastewater effluent with chloramines, chlorines and ozone (Bond et al., 2011). Also,  
32 the International Agency for Research on Cancer has classified N-nitrosamine as possible  
33 human carcinogen where a cancer risk level is exhibited at 0.7 ng/l concentration (US EPA,  
34 2009a). N-nitrosamine (especially NDMA, N-nitrosodimethylamine-D6) has been detected  
35 above established limits in treated water supply systems including drinking water and

36 wastewater facilities. Therefore, many water authorities around the globe have been regulated  
37 against an allowable N-nitrosamine concentration level in drinking water and recycled water  
38 intended for potable consumption (US EPA, 2009b). The removal of N-nitrosamine from  
39 water and wastewater has been achieved using several approaches such as UV/H<sub>2</sub>O<sub>2</sub>  
40 oxidation, photolytic degradation, photocatalytic oxidation, chemical oxidation, adsorption on  
41 resin and zeolites and membrane technology (Sharma, 2012). Sharma (2012) has reviewed  
42 many N-nitrosamine treatment processes and illustrated the specification of each one. It is  
43 concluded that resin and zeolites adsorption, activated carbon adsorption, sand filtration and  
44 ozonation have a little effect in removing NDMA (Krauss et al., 2010). Also, the possibility  
45 of formation of undesirable compounds as by-products including NDMA is valid after  
46 chlorinating the ultraviolet-treated water (Miyashita et al., 2009). Moreover, all the advanced  
47 technologies require high energy and are therefore expensive (Steinle-Darling et al., 2007;  
48 Sharma, 2012; Fujioka, 2014).

49 However, Reverse Osmosis is not only a significantly cheaper solution in terms of energy  
50 consumption in water desalination and wastewater treatment process, but also can achieve the  
51 stringent limits of undesirable particles and pollutants, which are likely to increase in the  
52 future (Marcovecchio et al., 2005; Akin and Temelli, 2011; Reverberi et al., 2014).  
53 Furthermore, spiral-wound RO modules are less susceptible to membrane fouling (compared  
54 to hollow fiber module) and are easier to clean and the cost of filtration has decreased  
55 significantly due to the improvements made in membrane manufacturing materials in recent  
56 years (Butt et al., 1997; Wagner, 2001). However, the energy consumption contributes most  
57 to the operating cost of the RO filtration process despite the promotion of efficient and  
58 reliable high-pressure pumps and power recovery turbines. This is due to the requirement of  
59 operating the process at high pressure to overcome the osmotic pressure (Song et al., 2002;  
60 Geraldès et al., 2005; Qi et al., 2012).

61 The performance of the RO process is quite sensitive to many design and operating  
62 conditions as demonstrated in several RO simulation and optimisation studies (Villafafila and  
63 Mujtaba, 2003; Abbas, 2005; Sassi and Mujtaba, 2013). Turbines and pressure exchangers  
64 options are used in the optimisation solution of Villafafila and Mujtaba (2003), who have  
65 reduced energy consumption by up to 50%.

66 In wastewater treatment, Madaeni et al. (2006) studied the operating parameters of trans-  
67 membrane pressure, temperature, and concentration, which influence the total flux and  
68 rejection of a solution containing nitrate, nitrite, sulfite and phosphate using SWRO pilot-  
69 plant. The optimisation results showed that trans-membrane pressure and temperature cause

70 the highest impact on water flux in comparison to the feed concentration while the solute  
71 rejection is extremely affected by the feed concentration with a minor contribution for both  
72 the feed pressure and temperature. [Sannino et al. \(2013\)](#) identified the critical feed operating  
73 pressure, which keeps a constant permeate flow rate. This yields a short-term inhibit fouling  
74 in the batch process of a pilot-scale plant of two spiral-wound nano-filtration and reverse  
75 osmosis membranes supplied by Osmonics. Most recently [Al-Obaidi et al. \(2017a\)](#) studied  
76 Genetic Algorithm based optimisation in RO process for the removal of chlorophenol from  
77 wastewater.

78 To the best of the authors' knowledge, the development of a spiral-wound RO model based  
79 on the Spiegler and Kedem concepts and its validation for N-nitrosamine compounds have  
80 only been explored by [Fujioka et al. \(2014\)](#). A maximum rejection of eight N-nitrosamine  
81 compounds between 62% and 99% has been obtained by the experiments at 10.1 atm  
82 pressure,  $2.43E-3$  m<sup>3</sup>/s of feed flow rate and 20 °C temperature. However, no previous studies  
83 focussed on the analysis of the energy consumption of RO process for the removal of N-  
84 nitrosamine from wastewater. Also, the optimisation of the RO process for the removal of N-  
85 nitrosamine has not been considered yet.

86 Therefore, in this work, first we provide the full analysis of the energy consumption of the  
87 RO process via simulation. For this purpose, a modified model developed earlier by [Al-  
88 Obaidi et al. \(2017b\)](#) will be used. The modified model considers the impact of temperature  
89 on the transport parameters and incorporates additional equations specific to energy  
90 consumption of high-pressure pump, boiler, and energy recovery devices. The new model  
91 will be validated using the published experimental data of eight N-nitrosamine solutes of  
92 [Fujioka et al. \(2014\)](#). The impacts of operating parameters on N-nitrosamine rejection, water  
93 recovery, and energy consumption for two RO process configurations are presented in detail  
94 which have facilitated optimisation problem formulation with feasible bounds on constraints  
95 within gPROMS. Finally, two optimisation problems are formulated and solved, one to  
96 maximise the N-nitrosamine rejection and the other to minimise the energy consumption of  
97 the process.

98

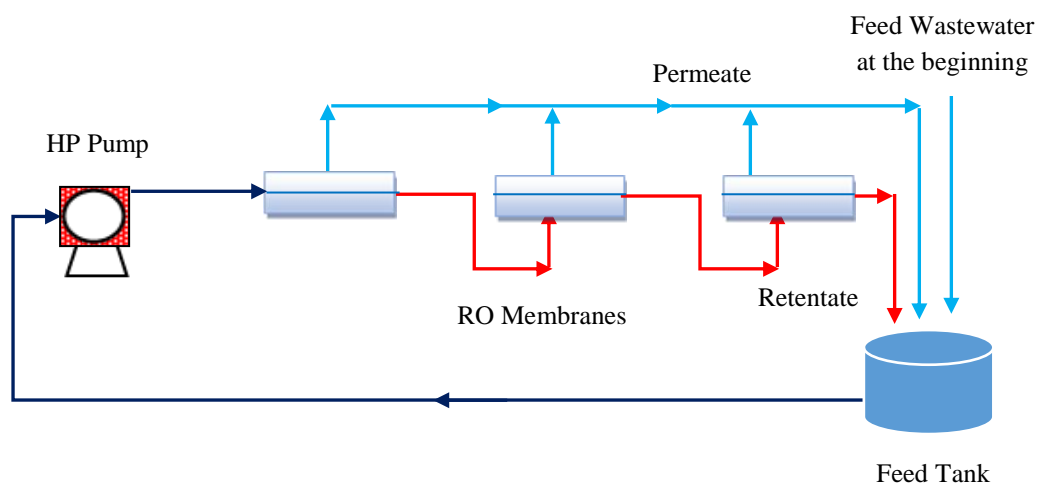
## 99 **2. Previous experimental work of [Fujioka et al. \(2014\)](#)**

100 A pilot-scale cross-flow RO filtration system of three 4" glass-fiber pressure vessels ([Fig. 1](#))  
101 used by [Fujioka et al. \(2014\)](#) consists eight N-nitrosamine solutes with a molecular weight in  
102 the range of (74 – 158 g/mol) as summarised in [Table 1](#). The N-nitrosamine stock solution  
103 containing 10 mg/L of each N-nitrosamine solutes [N-nitrosodimethylamine-D6 (NDMA), N-

104 nitrosomethylethylamine-D3 (NMEA), N-nitrosopyrrolidine-D8 (NPYR), N-  
 105 nitrosodiethylamine-D10 (NDEA), N-nitrosopiperidine-D10 (NPIP), N-nitrosomorpholine-  
 106 D8 (NMOR), N-nitrosodipropylamine-D14 (NDPA) and N-nitrosodi-n-butylamine-D9  
 107 (NDBA)] were prepared in pure methanol. Also, aqueous feed stock solutions of NaCl,  
 108 CaCl<sub>2</sub> and NaHCO<sub>3</sub> were prepared in Milli-Q water at 2M (NaCl) and 0.1 M (CaCl<sub>2</sub> and  
 109 NaHCO<sub>3</sub>) concentrations to mimic the background electrolyte composition typically found in  
 110 the secondary or tertiary treated wastewater. The stock solution of N-nitrosamine compounds  
 111 is mixed with the aqueous feed stock solution to obtain approximately 250 ng/L of each  
 112 target Nitrosamine compound in the feed to the RO process (Fujioka, 2014). The inlet  
 113 concentrations of all N-nitrosamine solutes are given in Table 1.

114 The feed tank (0.3 m<sup>3</sup>) in Fig. 1 was filled in with the model wastewater (as described above)  
 115 at the beginning of the process. After the process being started the concentrate and permeate  
 116 streams are collected back in the feed tank to maintain a constant feed concentration. The  
 117 experimental work of Fujioka et al. (2014) has considered a very low concentration of N-  
 118 nitrosamine. Therefore, the physical properties of diffusivity, density and viscosity have been  
 119 assumed identical to water equations and are calculated using Eqs. (14 - 17) (Appendix A in  
 120 Table A.1). Each pressure vessel holds only one spiral-wound element and are linked in  
 121 series.

122 The feed was pumped using a pump type (CRN 3-25, Grundfos, Bjerringbro, Denmark) at  
 123 constant volumetric flow rate of 2.43x10<sup>-3</sup> m<sup>3</sup>/s, while the average permeate flux was adjusted  
 124 at 2.78x10<sup>-6</sup>, 5.56x10<sup>-6</sup> and 8.33x10<sup>-6</sup> m/s during the experiments by increasing the operating  
 125 feed pressure from 4, 6.5 and 10.1 atm respectively. The feed temperature was controlled at  
 126 20±0.1 °C along the experiments (Fujioka, 2014).



137 Fig.1. Schematic diagram of the pilot-scale plant used by Fujioka et al. (2014)

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**Table 1.** Physical and transport parameters of the eight N-nitrosamines (Fujioka et al., 2014)

Name	Molecular weight (g/mol)	Inlet feed concentration, $C_{s(0)} \times 10^9$ (kmol/m <sup>3</sup> )	Solute permeability coefficient, $B_s$ (m/s) at 20 °C	Reflection coefficient, $\sigma$ (dimensionless)
NDMA	74.05	3.3761	$5.35 \times 10^{-6}$	0.953
NMEA	88.06	2.8389	$1.14 \times 10^{-6}$	0.958
NPYR	100.06	2.4985	$5.12 \times 10^{-7}$	0.973
NDEA	102.08	2.4490	$2.26 \times 10^{-7}$	0.985
NPIP	114.08	2.1914	$9.25 \times 10^{-8}$	0.993
NMOR	116.06	2.1540	$2.06 \times 10^{-7}$	0.991
NDPA	130.11	1.9214	$6.02 \times 10^{-8}$	0.992
NDBA	158.14	1.5808	$4.33 \times 10^{-8}$	0.990

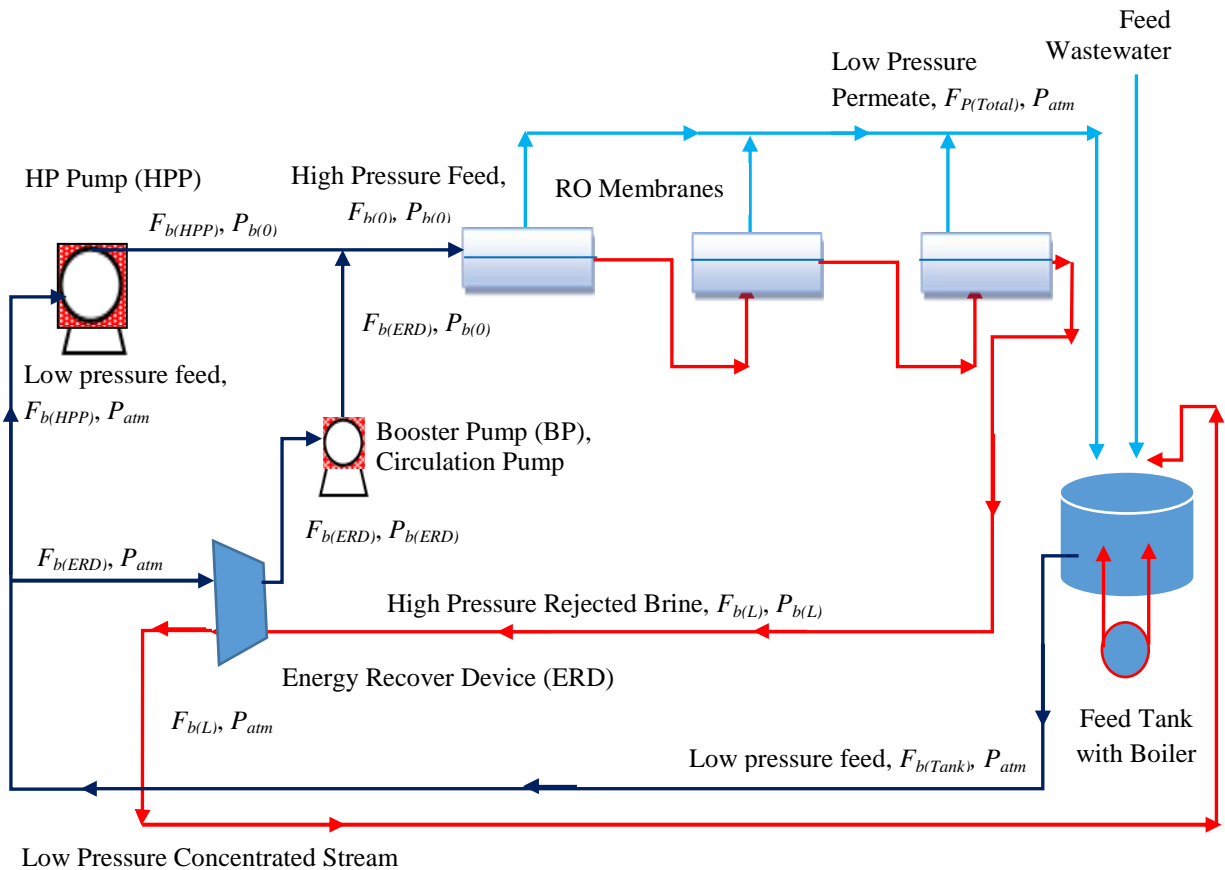
143

### 144 3. Proposed Spiral Wound RO configuration

145 Fig. 2 shows the proposed configuration of RO configuration of this study. The main addition  
146 to this configuration compared to the configuration of Fig. 1 are the existence of the high-  
147 pressure pump HPP, booster pump BP, energy recovery device ERD, and the feed tank boiler  
148 (electric) as we wanted to study the impact of feed temperature on the solute rejection. The  
149 feed tank is filled with wastewater (with the same specification as considered by Fujioka et  
150 al. (2014)). The first run is carried out at a reference temperature  $T_{Ref}$  of 20 °C followed by  
151 boiling the feed tank from 20 to 22 °C in one hour. Then, another treatment is carried out at  
152 the new temperature (22 °C). This is followed by a series of several runs which are carried  
153 out in a step change of 2 °C for each run till 44 °C. Note that the maximum operating  
154 temperature of the membrane selected is 45 °C (Table 4).

155 The tank feed flow rate  $F_{b(Tank)}$  is split into two fractions towards ERD ( $F_{b(ERD)}$ ) and HPP  
156 ( $F_{b(HPP)}$ ) at atmospheric pressure  $P_{atm}$ . While, the total permeate  $F_{P(Total)}$  at atmospheric  
157 pressure and the retentate are collected in the feed tank as in Fig. 1 to maintain a constant  
158 feed concentration. The total rejected brine  $F_{b(L)}$  discharged from the last module is 100%  
159 recycled to ERD with high pressure  $P_{b(L)}$  to pressurise the feed entering ERD. More  
160 specifically, the importance of ERD is to transfer the energy from the high-pressure brine  
161 stream by recovering the surplus pressure and delivering it directly to the incoming feed  
162 stream, which reduces the energy consumption of the RO process by recycling the brine  
163 energy (Anderson et al., 2009). The pressure losses in the membrane module will be  
164 compensated by BP (Greenlee et al., 2009). Then, the feed flow rate of HPP ( $F_{b(HPP)}$ ) and BP

165 ( $F_{b(ERD)}$ ) are collected to form the inlet feed flow rate of reverse osmosis unit  $F_{b(0)}$  with the  
 166 inlet feed pressure  $P_{b(0)}$ . The performance of process rejection and recovery will be estimated  
 167 by specifying the total permeate concentration and flow rate of the plant permeate stream.  
 168 Moreover, the calculations of the specific energy consumption will be carried out for both  
 169 configurations of the RO pilot-plant with and without ERD (Figs. 1 and 2).  
 170



171  
 172 **Fig. 2.** Schematic diagram of a conventional RO pilot-scale plant

173  
 174 **4. Process Model**  
 175 **4.1. Assumptions**

176 The mathematical model is based on the following assumptions.

- 177 1. The membrane is made up of flat channels and spacers with neglecting the curvature  
 178 of the channel.
- 179 2. Validity of the Spiegler-Kedem model for the transport of water and solute through  
 180 the membrane (Spiegler and Kedem, 1966).
- 181 3. Validity of Darcy's law concerning the pressure drop in porous media where the  
 182 friction parameter is used to characterise the pressure drop.

- 183 4. The film theory quantifies the concentration polarisation.  
 184 5. The permeate pressure is constant and equal to 1 atm.  
 185 6. A constant solute concentration is assumed in the permeate channel and the average  
 186 value will be calculated from the inlet and outlet permeate solute concentrations.  
 187 7. The model is investigated for simply one-dimensional transport (x- coordinate).  
 188 8. The underlying process is assumed to be isothermal. Therefore, the temperatures of  
 189 the feed, brine, and permeate are equal.  
 190 9. Constant pump and energy recovery device efficiencies. This is to quantify the  
 191 efficiency of HPP and ERD.

192

## 193 4.2. Model Equations

194 Based on the above assumptions (1-8) Al-Obaidi et al. (2017b) described the transport  
 195 phenomena of water and solute through the membrane module and to simulate the  
 196 performance of N-nitrosamine compounds rejection using a spiral-wound RO membrane  
 197 module. Their model equations are given in Appendix A, Table A.1. In this work, following  
 198 equations required are added to the original model thus giving the modified model.

199 The mass transfer coefficient along the x-axis  $k_{(x)}$  was estimated using the empirical  
 200 correlation of Senthilmurugan et al. (2005) of Eq. (1).

$$201 \quad k_{(x)} = 0.753 \left( \frac{K}{2-K} \right)^{0.5} \left( \frac{D_{b(x)}}{t_f} \right) \left( \frac{\mu_{b(x)} \rho_{b(x)}}{D_{b(x)}} \right)^{0.1666} \left( \frac{2 t_f^2 U_{b(x)}}{D_{b(x)} \Delta L} \right)^{0.5} \quad (1)$$

202 Furthermore, the effects of temperature variation on both water permeability  $L_p$  and solute  
 203 permeability  $B_s$  coefficients are described in Eqs. (2) and (3) respectively as used by Sarkar et  
 204 al. (2008).

$$205 \quad L_{p(T_b+273.15)} = L_{p(T_0+273.15)} \frac{\mu_{b(T_0+273.15)}}{\mu_{b(T_b+273.15)}} \quad (2)$$

$$206 \quad B_{s(T_b+273.15)} = B_{s(T_0+273.15)} \frac{T_b+273.15}{T_0+273.15} \frac{\mu_{b(T_0+273.15)}}{\mu_{b(T_b+273.15)}}$$

207 (3)

208 where  $T_0$  is the reference temperature of 20 °C. Moreover, the specific energy consumption  
 209  $E1$  of RO filtration system used by Fujioka et al. (2014) is calculated using Eq. (4) of Qi et  
 210 al. (2012) based on the use of only a high-pressure pump. Here,  $P_{b(0)}$  in atm and  $E1$  in  
 211 kWh/m<sup>3</sup>.



$$E1 = \frac{\left( (P_{b(0)}^{101325}) F_{b(0)} \right)}{F_{p(Total)} \varepsilon_{pump} 36 \times 10^5} \quad (4)$$

The calculation of the specific energy consumption for the conventional configuration of RO filtration system  $E2$ , which consists of a high-pressure pump (HPP), booster pump (BP) and energy recovery device (ERD) is carried out using Eq. (5). More specifically, the energy performance of the conventional pilot-plant is analysed based on the outgoing and ingoing entering energies. One of the aims of this paper is to determine the energy consumption due to its major contribution in total filtration cost, and which can reach values as high as 45% (Zhu et al., 2009).

$$E2 = \frac{\left( P_{b(0)}^{101325} F_{b(0)} \right) - \left( P_{b(L)}^{101325} F_{b(L)} \varepsilon_{ERD} \right)}{F_{p(Total)} \varepsilon_{pump} 36 \times 10^5}$$

(5)

Eq. (6) calculates the outlet pressure of ERD  $P_{b(ERD)}$  regarding the outlet pressure of membrane modules  $P_{b(L)}$ .

$$\varepsilon_{ERD} = \frac{P_{b(L)}}{P_{b(ERD)}}$$

(6)

For the case where the temperature of the feed tank is raised using a boiler, the heat supplied  $Q$  (j/s) by the boiler is calculated using Eq. (7) with  $T_{Ref} = 20$  °C. The boiler energy consumption  $E3$  (kWh/m<sup>3</sup> of permeate) is calculated using Eq. (8), while the total energy consumption  $E4$  (kWh/ m<sup>3</sup> of permeate) is calculated using Eq. (9), taking into account the energy consumption of the HPP and boiler in addition to the gain of energy using ERD.

$$\frac{d(T_{Tank} - T_{Ref})}{dt} = \frac{Q}{\rho C_p V}$$

(7)

where ( $\rho$ ,  $C_p$  and  $V$ ) are the density of water (kg/m<sup>3</sup>), specific heat capacity of water (j/kg K) and volume of feed tank (m<sup>3</sup>) respectively.

$$E3 = \frac{\left( Q / F_{p(Total)} \right)}{36 \times 10^5}$$

(8)

$$E4 = E2 + E3$$

(9)

The process model presented in Appendix A in Table A.1 and Eqs. (1 – 9) can be written in the following compact form:

241  $f(z, x(z), x'(z), u(z), v) = 0; [z_0, z_f]$   
 242 (10)

243 Where,  $z$  is the independent variable (length of membrane),  $x(z)$  is the set of all differential  
 244 and algebraic variables,  $x'(z)$  represents the derivative of  $x(z)$  with respect to length of  
 245 membrane,  $u(z)$  is the control variables and  $v$  denotes the constant parameters of the process.  
 246 The membrane length under consideration  $[z_0, z_f]$  and function  $f$  are assumed to be  
 247 continuously differentiable with respect to all their arguments.

248

## 249 **5. Determination of transport parameters**

250 Experimental data of [Fujioka et al. \(2014\)](#) is used to estimate unknown transport parameters  
 251 of the process model. The unknown parameters of the model are water permeability  
 252 coefficient  $L_p$ , solute transport parameter  $B_s$ , the reflection coefficient  $\sigma$  and friction  
 253 parameters  $b$ . The membrane transport parameters  $B_s$  and the reflection coefficients  $\sigma$  of the  
 254 eight selected N-nitrosamine solutes are assumed to be constants ([Table 1](#)) and taken from  
 255 [Fujioka et al. \(2014\)](#) who considered a constant feed flowrate. Note, [Murthy and Gupta](#)  
 256 [\(1999\)](#) proved a nearly constant solute transport parameter and reflection coefficient for the  
 257 experiments of Sodium Cyanide-water system using a commercial thin film composite  
 258 polyamide membrane at a range of feed flow rate 300 to 900 ml/min. However, [Fujioka et al.](#)  
 259 [\(2014\)](#) considered variable operating pressures in their experiments for the removal of eight  
 260 N-nitrosamine. For this purpose, the water permeability coefficient  $L_p$  and the friction  
 261 parameter  $b$  will be estimated for each run from these experiments using the gEST parameter  
 262 estimation tool available in the gPROMS ([Process System Enterprise Ltd., 2001](#)).

263 The estimation of these parameters is achieved by minimising the sum of the square errors  
 264 (SSE) between the experimental outlet flow rate  $F_{b(L)}$ , total permeated water  $F_{p(Total)}$ , outlet  
 265 feed pressure  $P_{b(L)}$  and average N-nitrosamine rejection  $Rej_{(av)}$  and the predicted values  
 266 from the model.

267 The parameter estimation problem can be therefore described as follows:

268 Given: The time invariant parameters: Inlet feed concentration, flow rate, pressure  
 269 and temperature.

270 The measured parameters: Outlet measured feed flow rate, pressure, water  
 271 flux, total permeated flow rate, and average rejection.

272 Obtain: Water permeability coefficients and friction parameters.

273 Minimise: The sum of square errors (SSE).

274 Subject to: Process model, Process constraints.

275 SSE is defined as:

$$276 \quad SSE = \sum_{i=1}^{N_{Data}} \left[ F_{b(L),i}^{Exp.} - F_{b(L),i}^{Cal.} \right]^2 \quad (11)$$

277 Where  $N_{Data}$ ,  $F_{b(L)}^{Exp.}$  and  $F_{b(L)}^{Cal.}$  are the numbers of test runs, experimental and the calculated  
278 retentate feed flow rate respectively. Also, it is important to mention that the estimation of  
279 friction factor ( $b$ ) is mainly related to both the experimental and predicted value of the  
280 retentate pressure ( $P_{b(L)}$ ) linked to the trans-membrane pressure drop along the module.

281 The parameter estimation problem can be mathematically presented as follows:

282

$$283 \quad \begin{array}{ll} \text{Min} & SSE \\ L_p, b & \end{array}$$

284

285 Subject to:

286 Equality constraints:

$$287 \quad \text{Process Model: } f(z, x(z), x^-(z), u(z), v) = 0; \quad [z_0, z_f]$$

288 Inequality constraints:

$$289 \quad L_p^L \leq L_p \leq L_p^U \\ 290 \quad b^L \leq b \leq b^U$$

291  $L$  and  $U$  are the lower and upper bounds. The results of the parameter estimation are given in  
292 [Table 2](#) which clearly show the variation of transport parameters with the inlet operating  
293 conditions for eight N-nitrosamine experiments. These results clearly establish the fact that a  
294 single model should not be blindly used under different conditions or for different pollutants  
295 but must be validated each time before it can be confidently used for simulation, design,  
296 optimisation, etc. For the convenience of the reader, few experimental and predicted values of  
297 retentate flow rate and retentate pressure are included in [Table 3](#) with the calculation of  
298 relative error and sum of the squared errors. The results of parameter estimation ([Table 2](#))  
299 show that permeability constants vary with the operating pressure enhancing (although  
300 slightly) the permeability constant of water with increasing pressure except for 10.1 atm that  
301 associated with higher values of friction.

302 The registered values of friction parameters vary between [58 to 353 atm s/m<sup>4</sup>](#) for the  
303 operating pressures [4, 6.51 and 10.1 atm](#) respectively. This in turn can confirm the relation  
304 between the operating pressure and friction factor. While, the parameter estimation method  
305 shows that the water permeability coefficients  $L_p$  for the set of used pressures varies between  
306 [1.0x10<sup>-6</sup> to 1.30x10<sup>-6</sup> m/s atm](#) for the membrane type ESPA2-4040 Hydranautics, Oceanside,

307 CA., USA at  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$  and  $20 \text{ }^\circ\text{C}$  of feed flow rate and temperature respectively. These  
 308 model parameters were used for the remainder of this work. Table 4 includes the design and  
 309 operating parameters of the spiral-wound membrane element.

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**Table 2.** Results of parameter estimation

N-nitrosamine	$C_{s(0)} \times 10^9$ (kmol/m <sup>3</sup> )	$P_{b(0)}$ (atm)	$b$ (atm s/m <sup>4</sup> )	$L_p \times 10^6$ (m/s atm)
NDMA	3.3761	4.0	58.89	1.1000
NDMA	3.3761	6.51	177.23	1.1293
NDMA	3.3761	10.1	352.74	1.1770
NMEA	2.8389	4.0	58.81	1.0878
NMEA	2.8389	6.51	177.76	1.1283
NMEA	2.8389	10.1	353.34	1.0730
NPYR	2.4985	4.0	59.46	1.0994
NPYR	2.4985	6.51	177.42	1.1349
NPYR	2.4985	10.1	351.14	1.0431
NDEA	2.4490	4.0	59.02	1.0000
NDEA	2.4490	6.51	176.24	1.3060
NDEA	2.4490	10.1	351.03	1.0053
NPIP	2.1914	4.0	58.96	1.0000
NPIP	2.1914	6.51	175.01	1.0565
NPIP	2.1914	10.1	352.53	1.0282
NMOR	2.1540	4.0	58.94	1.000
NMOR	2.1540	6.51	177.34	1.1724
NMOR	2.1540	10.1	353.15	1.0867
NDPA	1.9214	4.0	58.98	1.0000
NDPA	1.9214	6.51	177.64	1.0897
NDPA	1.9214	10.1	350.79	1.0568
NDBA	1.5808	4.0	58.96	1.0000
NDBA	1.5808	6.51	175.33	1.2104
NDBA	1.5808	10.1	351.86	1.0301

$F_{b(0)} = 2.43 \times 10^{-3} \text{ m}^3/\text{s}$  and  $T_b = 20 \text{ }^\circ\text{C}$

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 324

**Table 3.** Results of relative errors and sum of square errors

N-nitrosamine	$C_{s(0)} \times 10^9$ (kmol/m <sup>3</sup> )	$P_{b(0)}$ (atm)	$F_{b(L)}^{Exp.} \times 10^3$ (m <sup>3</sup> /s)	$F_{b(L)}^{Cal.} \times 10^3$ (m <sup>3</sup> /s)	Relative Errors	$P_{b(L)}^{Exp.}$	$P_{b(L)}^{Cal.}$	Relative Errors	Sun of square errors SSE (-) $\times 10^4$
---------------	--	---------------------	--	--	-----------------	-------------------	-------------------	-----------------	--

NDMA	3.3761	10.1	2.23	2.225	$4.31 \times 10^{-6}$	7.890	7.895	$-5.28 \times 10^{-3}$	5.16
NMEA	2.8389	10.1	2.23	2.234	$3.18 \times 10^{-5}$	7.890	7.887	$1.09 \times 10^{-2}$	9.44
NPYR	2.4985	10.1	2.23	2.233	$-3.35 \times 10^{-6}$	7.890	7.893	$-3.71 \times 10^{-3}$	3.69

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326

327

**Table 4.** Specifications of the spiral-wound membrane element

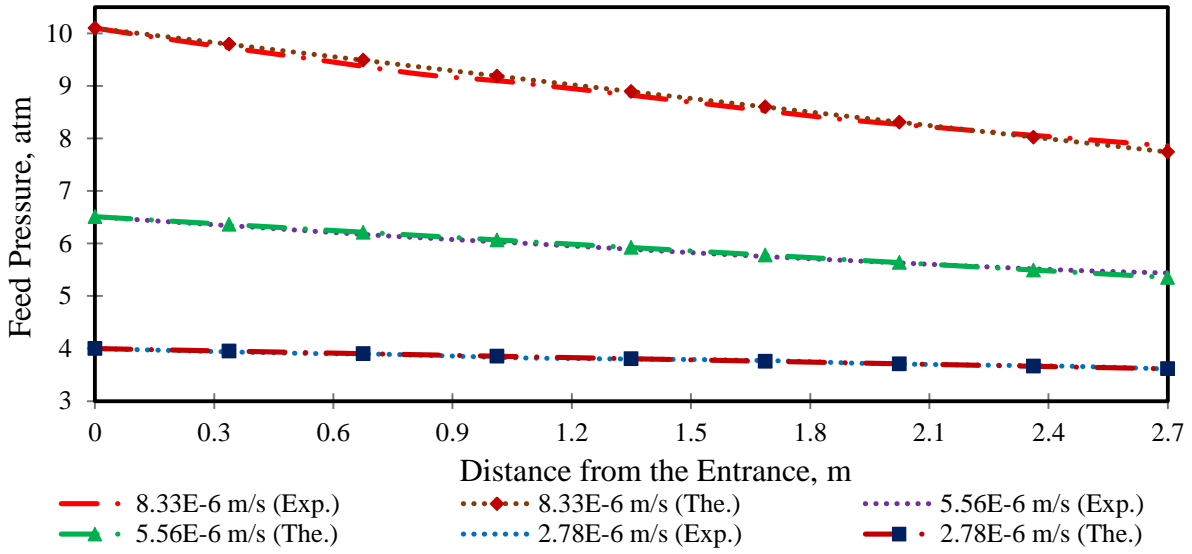
<b>Make</b>	<b>Hydranautics, Oceanside, CA., USA</b>
Membrane type	ESPA2-4040
Module configuration	Spiral-wound
Membrane polymer	Composite Polyamide
Feed spacer thickness $t_f$ (m)	$6.6 \times 10^{-4}$
Membrane sheet active area ( $m^2$ )	7.9
Membrane sheet length L (m)	0.9
Membrane sheet width W (m)	8.7778
Characteristics length of spacer $\Delta L$ (m)	0.006
Membrane diameter (in) (m)	3.95, 0.1003
Maximum applied pressure (atm)	41.056
Maximum operating temperature ( $^{\circ}C$ )	45
Salt Rejection (dimensionless)	99.6% (99.4 % minimum)

328

## 329 **6. Model validation**

330 The model data listed in [Table A.1](#) in [Appendix A](#) has been validated by comparing the  
331 model predictions results with those obtained from actual experimentation of [Fujioka et al.](#)  
332 [\(2014\)](#) for a spiral-wound RO membrane. [Fig. 3](#) compares the observed and modeled feed  
333 pressure along the x-axis of three membranes in series (2.7 m length) for three different  
334 overall permeate fluxes. [Fig. 4](#) compares the observed and modeled average permeate flux  
335 and retentate flow rate as a function to inlet feed pressure. Finally, [Fig. 5](#) compares the model  
336 rejections of eight N-nitrosamines solutes at three different overall permeate fluxes against  
337 experimental results, which shows high value of  $R^2$ . Furthermore, [Fig. 4](#) shows that the model  
338 can be used to simulate the observed data of an outlet feed flow rate at high operating  
339 pressure (high average permeate flux) albeit with a minor deviation (1%). It is expected that  
340 the inaccurate estimation of the water permeability coefficient of such pressure might causes  
341 this deviation. It is important to note that [Fujioka et al. \(2014\)](#) have experimentally measured  
342 the feed pressure of each membrane (three in series) and plotted them against the total  
343 membranes length with a fitting line. While, the model developed by [Al-Obaidi et al. \(2017b\)](#)  
344 can estimate the pressure at any dimension of x-axis (one dimensional distributed model).

345



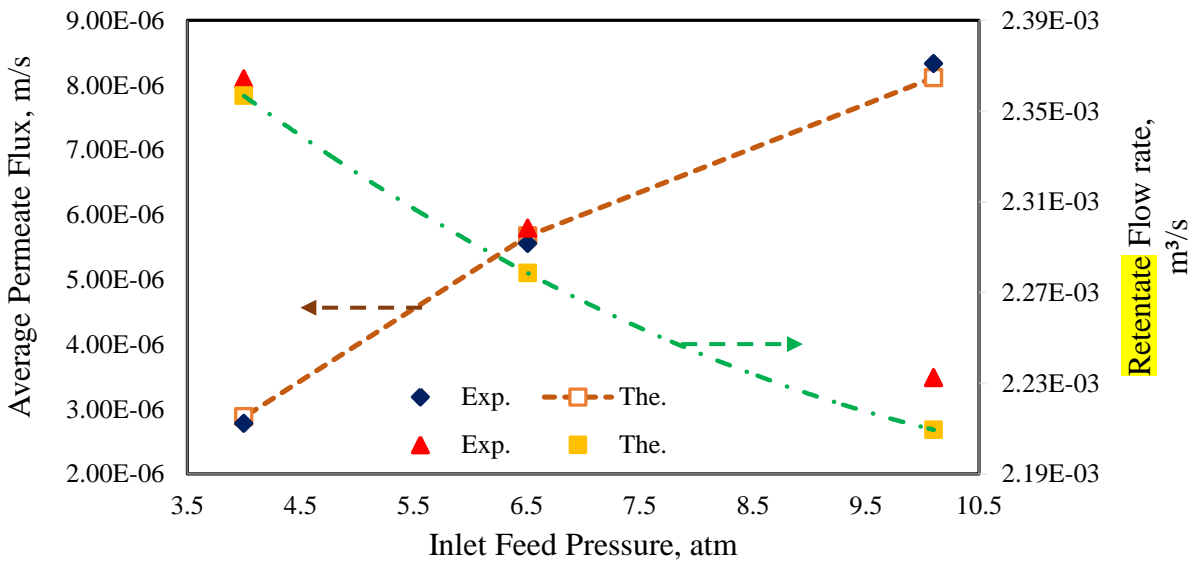
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347

**Fig. 3.** Observed and modeled feed pressure versus the membrane length for three different average permeate fluxes (initial conditions of NDMA,  $3.3761 \times 10^{-9}$  kmol/m<sup>3</sup>,  $2.43 \times 10^{-3}$  m<sup>3</sup>/s and 20 °C)

348

349



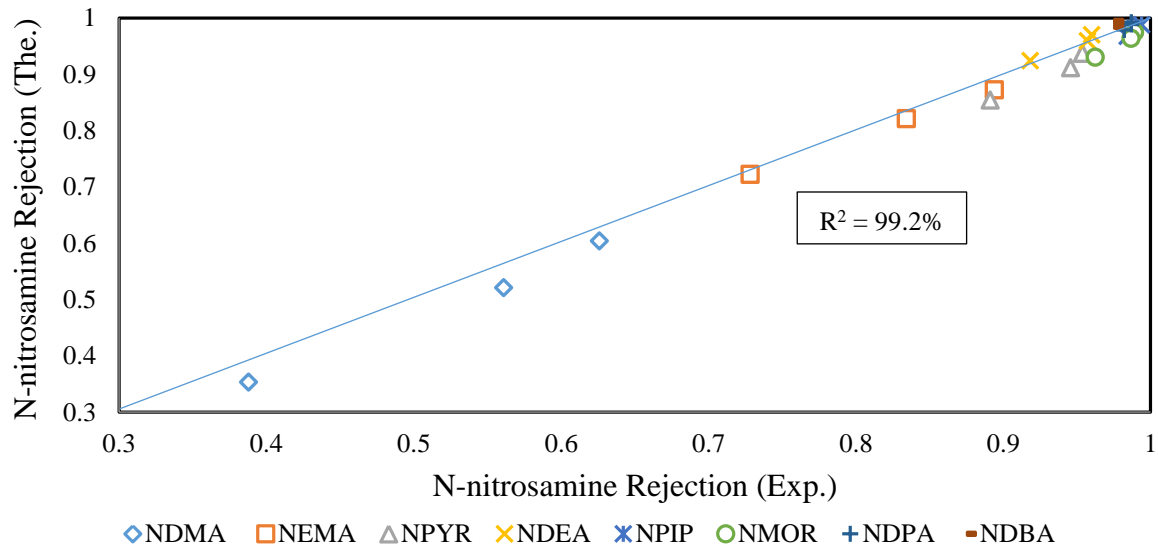
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351

**Fig. 4.** Observed and modeled average permeate flux and retentate flow rate versus inlet feed pressure (initial conditions of NDMA,  $3.3761 \times 10^{-9}$  kmol/m<sup>3</sup>,  $2.43 \times 10^{-3}$  m<sup>3</sup>/s and 20 °C)

352

353



354

355 **Fig. 5.** Experimental and modelled rejections of eight N-nitrosamine solutes at three average permeate fluxes of  
 356 ( $2.78 \times 10^{-6}$ ,  $5.56 \times 10^{-6}$  and  $8.33 \times 10^{-6}$  m/s) (initial conditions,  $2.43 \times 10^{-3}$  m<sup>3</sup>/s and 20 °C)

357

### 358 **7. Process Simulation: Effect of operating parameters**

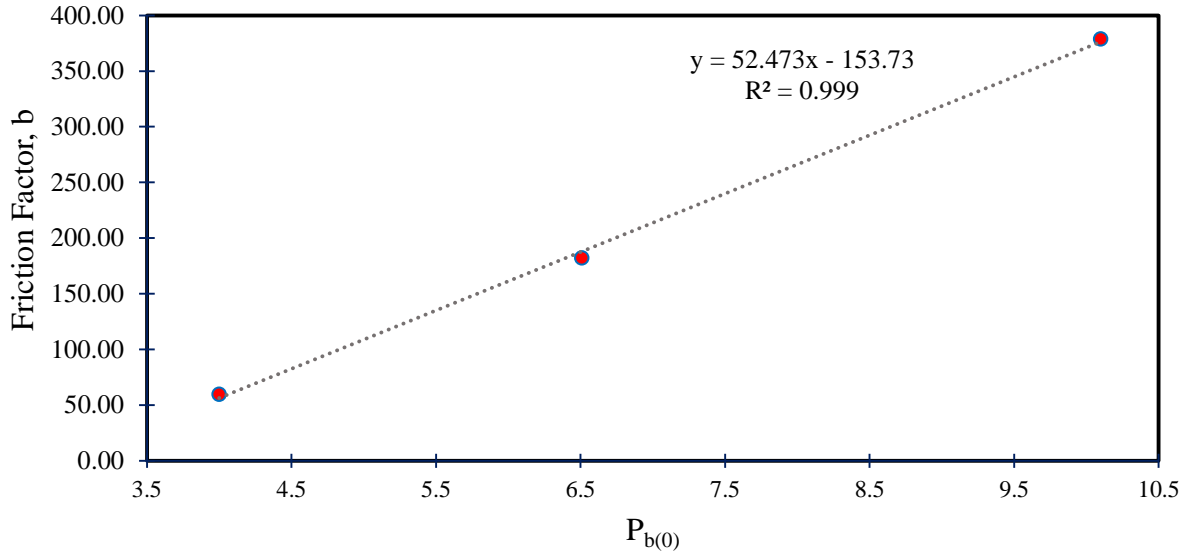
359 To have a better insight of the impact of operating parameters on several performance  
 360 measures of the process (such as N-nitrosamine rejections, specific energy consumptions,  
 361 etc.), simulations of the process configurations (Fig.1 and Fig. 2) are carried out before  
 362 optimization formulation and results are presented.

#### 363 **7.1 Effect of inlet feed pressure**

364 Table 2 shows that the friction parameter increases due to an increase in the operating feed  
 365 pressure. Fig. 6 shows a linear relationship between the applied feed pressure and friction  
 366 factor for a spiral-wound RO module type ESPA2-4040. This relation will be used to  
 367 estimate the friction parameter for each run of operating pressure.

368 The solute rejection, total recovery and specific energy consumption are directly affected by  
 369 the operating feed pressure of the RO filtration system, which directly affects the solvent and  
 370 solute fluxes through the membrane (Thomson et al., 2002). The impact of inlet feed pressure  
 371 variation at constant inlet feed flow rate and temperature of  $2.43 \times 10^{-3}$  m<sup>3</sup>/s and 20 °C  
 372 respectively on N-nitrosamine rejection, total recovery, and specific energy consumption for  
 373 the RO configurations (shown in Fig.1 and Fig. 2) is highlighted within the manufacturer's  
 374 specification of membrane area and the maximum operating pressure.

375



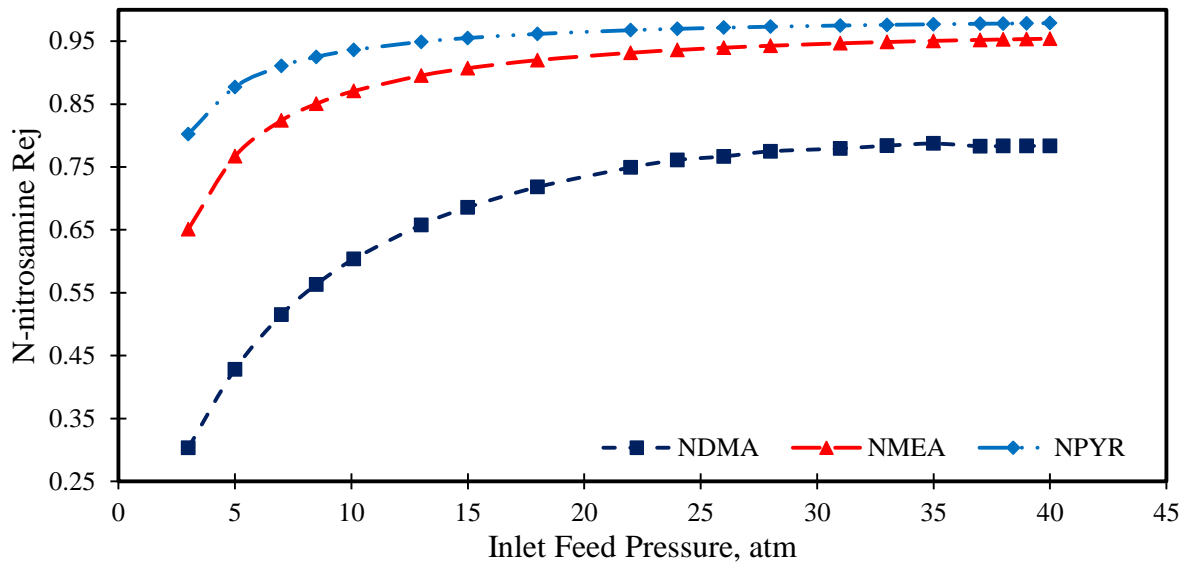
**Fig. 6.** Friction parameter versus inlet feed pressure for module type ESPA2-4040 (with initial conditions,  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$  and  $20 \text{ }^\circ\text{C}$ )

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380 **Fig. 7** displays the relationship existing between the inlet feed pressure and N-nitrosamine  
381 rejection for three different compounds using their initial concentrations as presented in **Table**  
382 **2**. It is clearly shown that increasing the feed pressure from **10.1** to **40 atm** (within the  
383 manufacturer's specification, **Table 3**) has a significant impact on N-nitrosamine rejection. It  
384 is expected that higher permeate flux increases the dilution of solute at the feed side, which  
385 passed through the membrane, and therefore results in lower permeate concentration. NDMA  
386 rejection is increased by **30%** from **0.60** to **0.78** as a response to an increase in the inlet feed  
387 pressure from **10.1** to **40 atm**. NMEA and NPYR rejections are increased simultaneously by  
388 **9.57%** and **4.55%** from **0.87** to **0.95** and from **0.936** to **0.978** respectively. These results  
389 indicate that the higher feed pressure is required to obtain higher N-nitrosamine rejection due  
390 to an increase in water flux and total water recovery.

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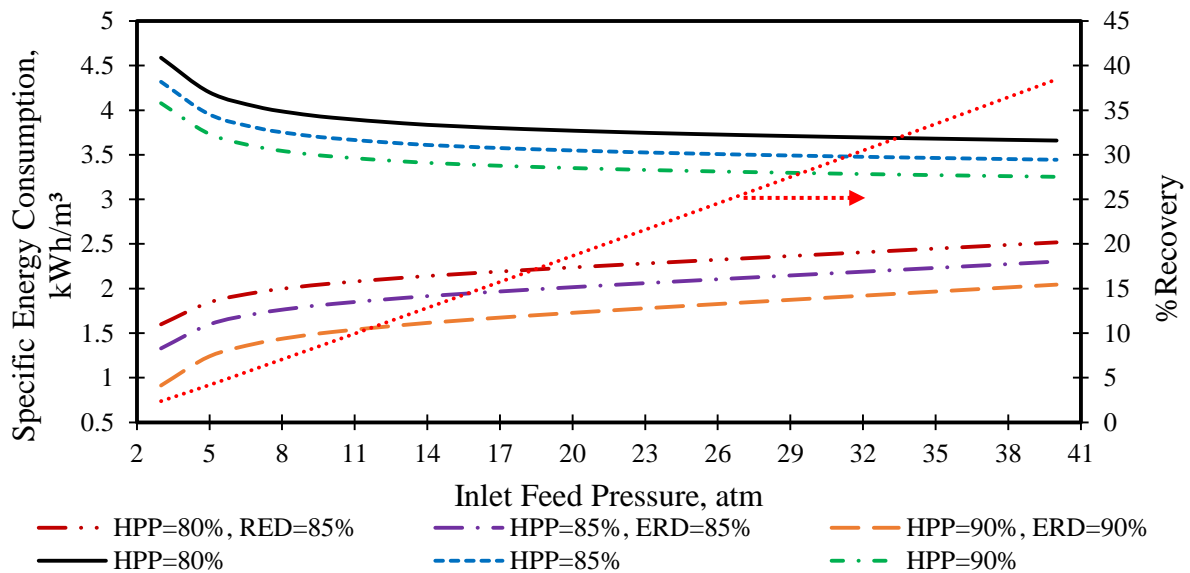


393  
 394 **Fig. 7.** Dependence of N-nitrosamine rejection on inlet feed pressure at inlet feed conditions of  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$   
 395 and  $20^\circ\text{C}$   
 396  
 397

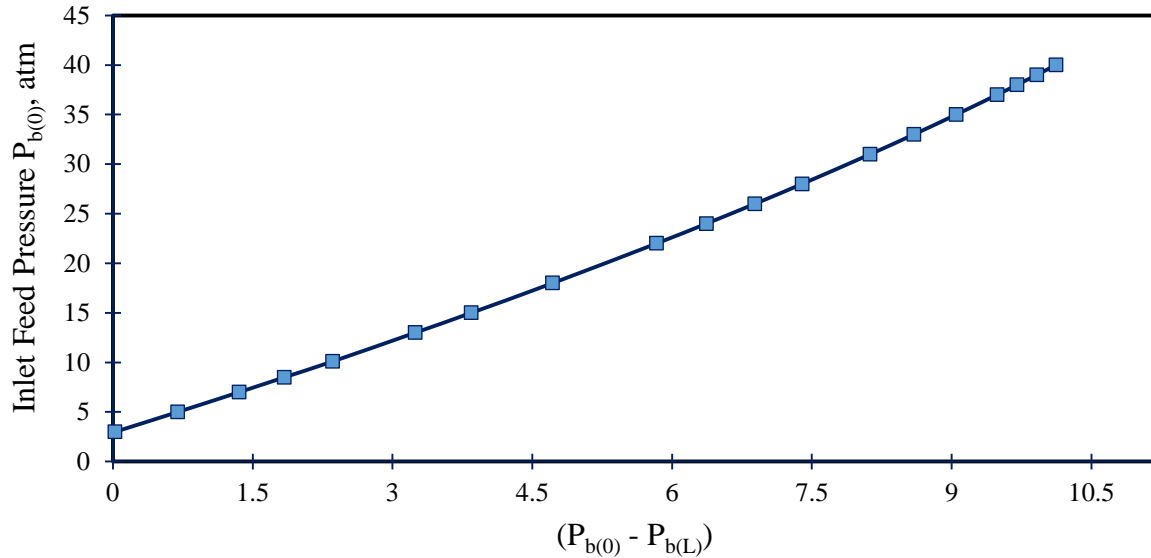
398 **Fig. 8** displays the relationship existing between the specific energy consumption and total  
 399 recovery as a function of inlet feed pressure for the RO configurations (**Figs. 1 and 2**). This  
 400 includes an investigation of the impact of both HPP and ERD efficiency for the same step  
 401 change in inlet feed pressure. It is clear that the energy consumption decreases with  
 402 increasing inlet feed pressure in case of using only HPP. This lower energy consumption is  
 403 caused by an increase in the efficiency of pump from 80% to 85% and then to 90%. More  
 404 specifically, the energy consumption is brought down by a constant value of 5.88 % for all  
 405 pressures by increasing the pump efficiency from 80% to 85%, while, a reduction of a  
 406 constant value of 5.55% for all pressures is registered by increasing the pump efficiency from  
 407 85% to 90%. Therefore, using a higher efficiency pump can significantly reduce the energy  
 408 consumption. These results concur with the findings of **Du et al. (2014)**.

409 For the RO system shown in **Fig. 2**, **Fig. 8** shows that the addition of ERD in the RO filtration  
 410 system is very important where the energy consumption can be reduced by approximately  
 411 47% at operating pressure of 10.1 atm and 31% at 40 atm than the case of only HPP mode.  
 412 The reason for this is that the rejected stream flow rate is about 61 – 97% of the inlet feed  
 413 flow rate and the outlet brine pressure is about 74 – 99% of the inlet pressure for a set of  
 414 operating pressure varied between 40 to 3 atm, which results in a high amount of hydraulic  
 415 energy in the rejected side. This is a substantial energy saving for the system. Also, these  
 416 results indicate that increasing feed pressure will increase the total water recovery as well as  
 417 an increase in the specific energy consumption. The impact of increasing the efficiency of

418 ERD is shown by reducing the consumption of energy. However, it is clearly shown that the  
 419 impact of pressure on energy consumption is more obvious at low pressures than at high  
 420 pressures. The consumption of energy is slightly increased at high recovery region in  
 421 comparison to a dramatic growth at low recovery region (low operating pressures). The  
 422 reason of this phenomenon is that at high feed pressures and recoveries, the quantity of water  
 423 to be pressurised will be less than at low recoveries and pressures. Another explanation can  
 424 be drawn from Fig. 9 which shows a steady increase of the pressure difference between the  
 425 inlet and outlet pressures due to an increase in inlet pressure. This shows that higher recovery  
 426 can be achieved at higher pressures due to a higher-pressure difference along the membrane  
 427 length, which reduces the energy consumption for HPP mode as illustrated in Eq. (5) in  
 428 comparison to lower operating pressures, which are characterised by lower values of pressure  
 429 difference and higher energy consumption. However, Fig. 8 shows that the energy  
 430 consumption increases due to an increase in water recovery for the system. This test indicates  
 431 that the beneficial effect of ERD addition becomes less significant in energy saving at high  
 432 operating pressures in comparison to low operating pressures despite achieving higher solute  
 433 rejection and lower energy consumption when compared with HPP mode.  
 434



435  
 436 **Fig. 8.** Specific energy consumption of two types RO pilot-plants with and without ERD (Figs. 1 and 2) and  
 437 total recovery versus inlet feed pressure at inlet feed conditions of  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$  and  $20 \text{ }^\circ\text{C}$  (Note: The  
 438 efficiency of booster pump is assumed same as high pressure pump)  
 439  
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**Fig. 9.** The relation between the inlet feed pressure and the pressure difference at inlet and outlet edges at inlet conditions of  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$  and  $20 \text{ }^\circ\text{C}$

445 **7.2 Effect of inlet feed flow rate**

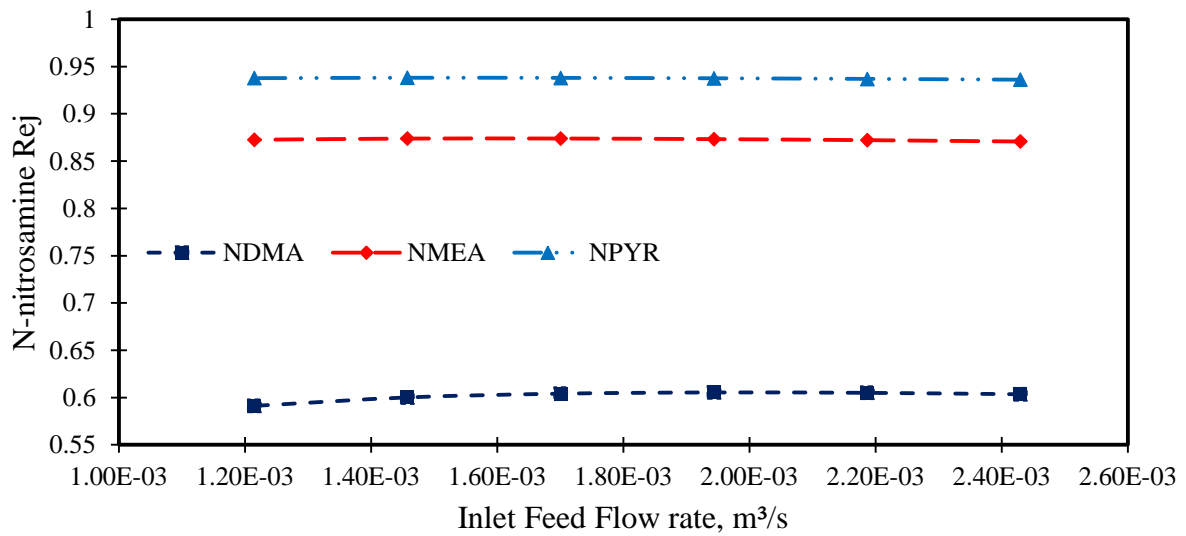
446 The influence of the inlet feed flow rate at constant values of inlet feed pressure and  
 447 temperature on N-nitrosamine rejection and energy consumption is considered in this section.

448 The inlet feed flow rate is reduced by 50% from  $2.43 \times 10^{-3} \text{ m}^3/\text{s}$  to  $1.215 \times 10^{-3} \text{ m}^3/\text{s}$  by 10%  
 449 step change for each run at constant inlet feed pressure and temperature of 10.1 atm and 20  
 450  $^\circ\text{C}$  respectively.

451 It was found that a maximum recovery can be achieved at low inlet feed flow rate. This  
 452 behaviour is due to the pressure drop in the high-pressure channel, which decreases when the  
 453 operating feed flow rate also decreases. Similarly, an increase in the feed flow rate will  
 454 increase the loss in pressure due to higher friction along the membrane length. This reduces  
 455 the advantage of having a lower average osmotic pressure and concentration polarisation; as  
 456 this in turn decreases the water flux and total permeate recovery. It can therefore be  
 457 concluded that N-nitrosamine rejection insignificantly decreases due to increase in the feed  
 458 flow rate as can be shown in Fig. 10. These results are in line with the findings of Abbas  
 459 (2005).

460 Moreover, increasing the inlet feed flow rate at constant pressure and temperature will  
 461 increase the specific energy consumption due to a lower gain in total recovery, as can be  
 462 shown in Fig. 11. Therefore, at constant operating pressure and temperature, it is  
 463 recommended to work within low feed flow rates to guarantee lower energy consumption and  
 464 higher solute rejection.

465



466

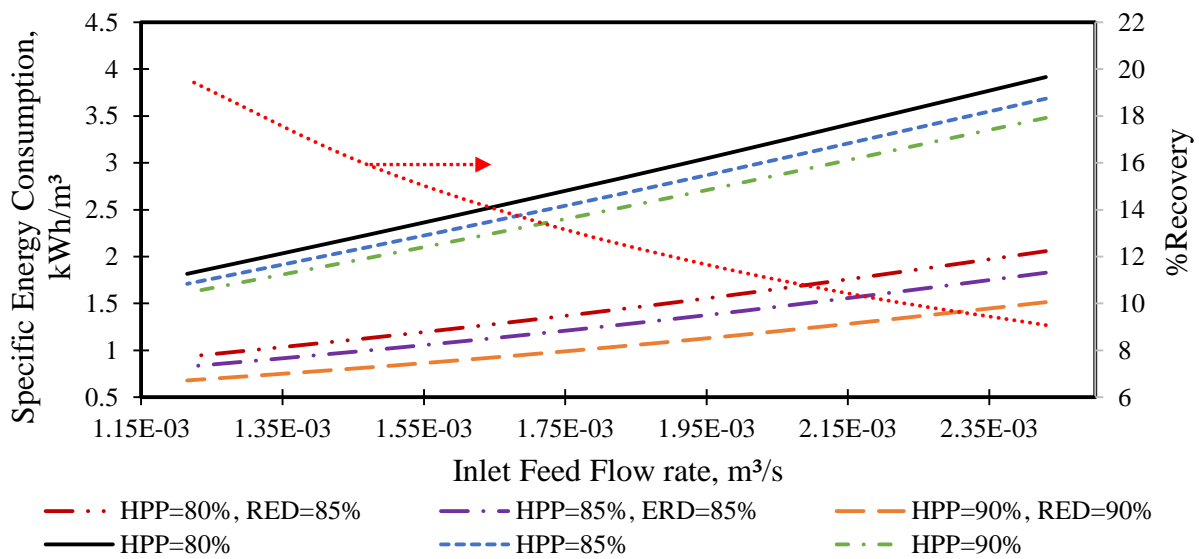
467

**Fig. 10.** Dependence of N-nitrosamine rejection on inlet feed flow rate at inlet feed conditions of 10.1 atm and 20 °C

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**Fig. 11.** Specific energy consumption of two types RO pilot-plants with and without ERD and total recovery versus inlet feed flow rate at inlet feed conditions of 10.1 atm and 20 °C

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### 475 7.3 Effect of inlet feed temperature

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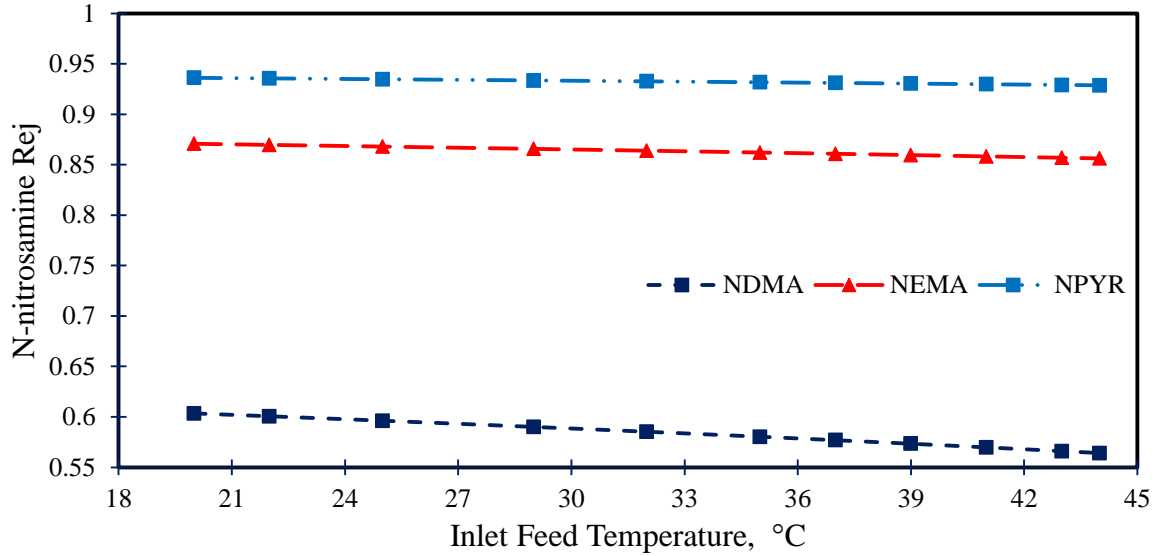
478

479

The inlet feed temperature can have a clear effect on solute rejection, water recovery and energy consumption according to Jiang et al. (2015). In this work, we evaluated and reported the performance of the RO network for every 2 °C rise in feed temperature (note the reference feed temperature is 20 °C). The total permeate recovery increase due to an increase in the

480 feed temperature at constant inlet feed flow rate and pressure (Figs. 12 and 13). This is  
481 compared to a slight decrease of N-nitrosamine compounds rejection. This same trend has  
482 been reported by Fujioka (2014) which is already attributed to increase the membrane pore  
483 size as a result to increasing operating temperature in addition to increasing the solute  
484 transport parameter. This in turn increases the solute flux and reduces the rejection parameter.  
485 The registered reduction of NDMA, NEMA and NPYR rejections are 6.5%, 1.7%, and 0.79%  
486 respectively, compared to 67% increase in total recovery rate, when the temperature  
487 gradually increases from 20 to 44 °C. More specifically, the rejections are decreased from 0.6  
488 to 0.56 for NDMA and from 0.87 to 0.85 for NEMA and from 0.936 to 0.926 for NPYR (Fig.  
489 12). Occasionally, the gain of energy consumption is around 28% and 32% for with and  
490 without ERD configurations (Fig. 13). These results show the significant role of feed  
491 temperature to capture higher recovery rate in addition to lower energy consumptions.  
492 However, the above results did not include the contribution of the boiler energy required to  
493 raise the feed temperature from 20 to 44 °C. We assumed 1 hour to raise the feed temperature  
494 to the next level and the total heat supplied, Q, in Watt, is calculated using Eq. (7) with  
495 assuming no heat loss. To be consistent with Eqs. (4) and (5), the heat supplied is divided by  
496 the volume of produced permeate in Eq. (8) to calculate the boiler energy consumption. Eq.  
497 (9) then gives the total energy consumption for the whole system.  
498 Fig. 13 also shows the cases of the total energy consumption of the system. As expected, the  
499 addition of this energy will lift the total energy consumption of the whole system. However,  
500 the interesting point here is that the consumption of energy with the boiler addition is still  
501 lower than the registered values of RO consumption without the ERD mode. Also, Fig. 13  
502 shows that the total energy consumption of the process (Fig. 2) is reasonably increased from  
503 20 to 22 °C due to the addition of consumed boiler power calculated by Eq. (8) and then  
504 continuously decreased when the tank temperature increased from 22 to 44 °C. This can be  
505 explained due to a noticeable increase of permeate flowrate as a result of increasing feed  
506 temperature. The increasing total permeate ( $F_{p(Total)}$ ) will reduce the total energy  
507 consumptions (E1, E2, E3, E4) according to Eqs. (4), (5), (8) and (9). Note that the  
508 calculation of the boiler energy consumption is carried out when the temperature increases by  
509 an increment of 2 °C assuming no heat loss. This is done by assuming that wastewater will  
510 keep its energy before supplying any further heat.

511



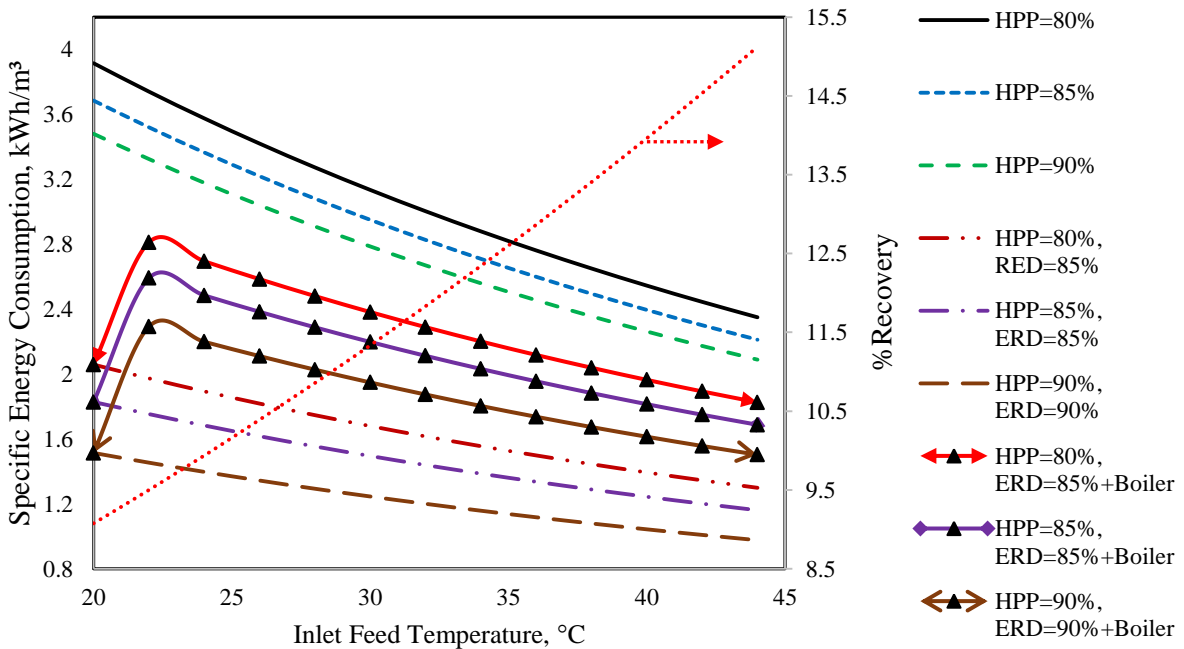
512

513 **Fig. 12.** Dependence of N-nitrosamine rejection on inlet feed temperature at inlet feed conditions of  $2.43 \times 10^{-3}$   
 514  $\text{m}^3/\text{s}$  and 10.1 atm

515

516

517



518

519 **Fig. 13.** Specific energy consumption of two types RO pilot-plants with and without ERD and ERD with Boiler  
 520 and total recovery versus inlet feed temperature at inlet conditions of  $2.43 \times 10^{-3}$   $\text{m}^3/\text{s}$  and 10.1 atm

521

522 Finally, it is easy to notice that an increase in the inlet feed pressure (at a constant feed flow  
 523 rate and temperature) has a significant impact on N-nitrosamine rejection and total recovery.  
 524 This is compared to a negative impact on N-nitrosamine rejection due to increasing the  
 525 operating temperature (at constant pressure and flow rate), and flow rate (at a constant  
 526 pressure and temperature). However, it is evident that the increment in the inlet feed flow rate

527 has a negative impact on total permeate recovery. Moreover, both an increase in the inlet feed  
528 pressure (at a constant feed flow rate and temperature) and feed flow rate (at a constant feed  
529 pressure and temperature) have an adverse impact on energy consumption of ERD and HPP  
530 configurations. Also, an increase in the inlet feed temperature (at constant feed pressure and  
531 flow rate) will increase the consumption of energy within acceptable levels despite the added  
532 consumed energy of the boiler (source of heat). Also, the combination of ERD and HPP (Fig.  
533 2) can lead to a higher reduction in energy consumption compared to the experimental RO  
534 pilot-plant used by Fujioka et al. (2014) (Fig. 1).

535

## 536 **8. Process Optimisation**

537 Having developed a deeper insight (in the earlier sections) of the impact of a number of  
538 operating parameters (by varying these parameters one at a time) on the rejection rates of N-  
539 nitrosamine contaminants and energy consumptions for two given RO configurations with  
540 and without energy recovery options (Fig. 1 and Fig. 2), we have decided to formulate two  
541 optimisation problems which will maximize the rejection rates and minimise the energy  
542 consumptions while optimizing the operating parameters. The readers are directed to the  
543 work of Evangelista et al. (1985), El-Halwagi (1992), Voros et al. (1997), Maskan et al,  
544 (2000), Marriott et al. (2003), Guria et al. (2005), Marcovecchio et al. (2005), and Lu et al.  
545 (2007) to have further exposure to different optimisation techniques applied in membrane-  
546 based separation processes including RO,

547 The first objective is to maximise the NDMA rejection of the configuration of RO pilot-plant  
548 used by Fujioka et al. (2014) (Fig. 1, without ERD) and the RO system described in Fig. 2 by  
549 allowing the system operating conditions to vary within the limits set in the manufacturer's  
550 specification. Any optimised operating conditions that maximise NDMA rejection would  
551 serve the rejections of NMEA and NPYR too.

552 The second objective is to minimise the total energy consumption of the two configurations  
553 (Fig. 1 and Fig. 2) measured in kWh per m<sup>3</sup> of the total permeate. The results of Fujioka et al.  
554 (2014) for solute rejections were taken as the minimum accepted values for the optimisation.

555

### 556 **8.1 Optimisation Problem 1 (OPI)**

557 The optimisation problem can be described as follows:

558 Given: Operating feed conditions, module specifications.

559 Optimise: Inlet feed pressure, flow rate and temperature (the optimisation variables).  
 560 Maximize: NDMA rejection.  
 561 Subject to: Equality (process model) and inequality constraints (linear bounds of optimisation  
 562 variables).

563 As the optimisation problem can be represented mathematically as:

564 OP1:

$$565 \quad \text{Max} \quad \text{Rej}$$

$$566 \quad F_{b(0)}, P_{b(0)}, T_b$$

$$567$$

568 Subject to:

569 Equality constraints:

$$570 \quad \text{Process Model:} \quad f(z, x(z), x^-(z), u(z), v) = 0; \quad [z_0, z_f]$$

571 Inequality constraints:

$$572 \quad (1 \times 10^{-3} \text{ m}^3/\text{s}) \quad F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U \quad (2.43 \times 10^{-3} \text{ m}^3/\text{s})$$

$$573 \quad (3.0 \text{ atm}) \quad P_{b(0)}^L \leq P_{b(0)} \leq P_{b(0)}^U \quad (41.0 \text{ atm})$$

$$574 \quad (20 \text{ }^\circ\text{C}) \quad T_b^L \leq T_b \leq T_b^U \quad (44 \text{ }^\circ\text{C})$$

575 The optimisation will be carried out for only NDMA, NMEA and NPYR with initial feed  
 576 concentrations shown in [Table 1](#).

577

## 578 **8.2 Optimisation Problem 2 (OP2):**

579 The optimisation problem can be described as follows:

580 Given: Operating feed conditions, module specifications.

581 Optimise: Inlet feed pressure, flow rate and temperature (the optimisation variables).

582 Minimise: The specific energy consumption defined in [Eq. \(9\)](#).

583 Subject to: Equality (process model) and inequality constraints (linear bounds of optimisation  
 584 Variables and solute rejection)

585 As the optimisation problem can be represented mathematically as:



586

587 Min  $E_4$  (defined in Eq. 9)

588  $F_{b(0)}, P_{b(0)}, T_b$

589

590 Subject to:

591 Equality constraints:

592 Process Model:  $f(z, x(z), x^-(z), u(z), v) = 0; [z_0, z_f]$

593 Inequality constraints:

594  $(1 \times 10^{-3} \text{ m}^3/\text{s}) F_{b(0)}^L \leq F_{b(0)} \leq F_{b(0)}^U (2.43 \times 10^{-3} \text{ m}^3/\text{s})$

595  $(3.0 \text{ atm}) P_{b(0)}^L \leq P_{b(0)} \leq P_{b(0)}^U (41.0 \text{ atm})$

596  $(20 \text{ }^\circ\text{C}) T_b^L \leq T_b \leq T_b^U (44 \text{ }^\circ\text{C})$

597  $Rej_{NDMA} \geq 0.6273 \quad Rej_{NMEA} \geq 0.8864 \quad Rej_{NPYR} \geq 0.9454$

598

599 Firstly, the results of [Fujioka et al. \(2014\)](#) are given in the first row of [Table 5](#) for the purpose  
600 of comparison with the optimisation results (base case). For OP1, the maximum rejections for  
601 NDMA, NMEA and NPYR are found to be [0.80](#), [0.951](#) and [0.977](#) with optimum feed  
602 flowrate of [2.43x10<sup>-3</sup> m<sup>3</sup>/s](#), pressure [35.406 atm](#) and temperature at [20 °C](#) with significant  
603 reduction ([4.48 kWh/m<sup>3</sup>](#) to [3.678 kWh/m<sup>3</sup>](#) to [2.454 kWh/m<sup>3</sup>](#)) in energy consumption (for all  
604 energy recovery options). For NDMA, NMEA and NPYR there is an increase of [27.5%](#),  
605 [7.3%](#) and [3.34%](#) in rejections respectively compared to [Fujioka et al. \(2014\)](#). Interestingly,  
606 the optimisation confirms that the RO process is not efficient for the removal of NDMA  
607 (compared to NMEA and NPYR) as reported by [Mitch et al. \(2003\)](#).

608 Increasing the operating temperature from [42 °C](#) to [44 °C](#) at the optimised conditions of OP1  
609 showed a positive impact on the reduction in energy consumptions (all options) compared to  
610 the case at [20 °C](#). However, NDMA, NMMA and NPYR rejections are decreased to [0.514](#),  
611 [0.915](#) and [0.962](#) respectively.

612 The results of OP2 show that the minimum energy consumption can be significantly reduced  
613 from [4.48 kWh/m<sup>3</sup>](#) to [1.912 kWh/m<sup>3</sup>](#) to [1.046 kWh/m<sup>3</sup>](#) with no significant gain of N-  
614 nitrosamine rejection compared to the base case. This was possible for a much lower value of  
615 feed rate ([1.30x10<sup>-3</sup> m<sup>3</sup>/s](#)), pressure ([12.98 atm](#)), and temperature at [20 °C](#) compared to  
616 [Fujioka et al. \(2014\)](#). The reduction of specific energy consumption was about [57.3%](#)  
617 compared to [Fujioka et al. \(2014\)](#).

618 Increasing the operating temperature from 42 °C to 44 °C, OP2 results in further reduction in  
619 energy consumption (1.146 and 0.73 kWh/m<sup>3</sup> for Figs. 1 and 2 respectively) with the same  
620 optimized conditions of OP2. For this case, the NDMA, NMEA and NPYR rejections are  
621 found to be 0.514, 0.866 and 0.936 respectively which are worse than those found at 20 °C.  
622 The reduction of specific energy consumption was about 74.4% compared to Fujioka et al.  
623 (2014). The results in Table 5 clearly indicate how the inlet feed pressure, temperature, and  
624 feed flow rate can potentially affect N-nitrosamine rejection and plays an important role in  
625 reducing the energy consumption.

626

627

628

**Table 5.** The optimisation results

No.	Optimisation Problem	$F_{b(0)} \times 10^3, \text{m}^3/\text{s}$	$P_{b(0)}, \text{atm}$	$T_b, \text{ }^\circ\text{C}$	$Rej$ (NDMA)	$Rej$ (NMEA)	$Rej$ (NPYR)	Energy Consumption kWh/m <sup>3</sup>				Comments
								HPP 80% (Fig. 1)	HPP 80%+ERD 85%	Boiler Consumed Power	(total energy consumption) HPP 80%+ERD 85%+Boiler (Fig. 2)	
1	Base Case	2.43	10.100	20	0.6273	0.8864	0.9454	4.48	0	0	4.48	Fujioka et al. (2014) results
2	OP1	2.43 (opt)	35.406 (opt)	20 (opt)	0.80 (max)	0.951 (max)	0.977 (max)	3.678 (calc)	2.454 (calc)	0	2.454 (calc)	Optimised rejection at 20 °C
3		2.43 (opt)	35.406 (opt)	42-44 (Selected)	0.514	0.915	0.962	2.181 (min)	1.686 (min)	0.139	1.825	Calculated energy consumption at 44 °C
4	OP2	1.30 (opt)	12.982 (opt)	20 (opt)	0.634 (calc)	0.8941 (calc)	0.949 (calc)	1.912 (min)	1.046 (min)	0	1.046	Optimised energy consumption at 20 °C
5		1.30 (opt)	12.982 (opt)	42-44 (Selected)	0.514 (calc)	0.866 (calc)	0.936 (calc)	1.146 (min)	0.730 (min)	0.374	1.104	Calculated energy consumption at 44 °C

Inlet feed concentration  $C_{b(0)}$  of each N-nitrosamine is given in Table 1. opt = optimised value; max = maximised value; min = minimised value

## 9. Conclusions

In this work, the removal of N-nitrosamine compounds from wastewater is considered using an experimental RO process considered in the literature (Fig. 1). The impact of different operating parameters such as inlet feed pressure, flow rate and temperature on the rejection of N-nitrosamine compounds is investigated in detail using modelling and simulation. The process model used for this purpose has been validated using experimental data from the literature which in turn estimated a number of model parameters. A number of energy recovery options have also been considered on the process (Fig. 2) and the impact of different operating parameters on the energy consumption is evaluated.

Having developed clear understandings of the impact of a number of operating parameters on the rejection of N-nitrosamine compounds and the energy consumption via sensitivity analysis (varying one parameter at a time), it was decided to simultaneously optimise these parameters to either maximise the rejections or minimise the energy consumption of the process. The optimisation results clearly show that rejection of some of the compounds can be improved by more than 27% and energy consumption can be minimised by more than 70%. Specifically, NDMA rejection is improved from 62.7% to 80%. Also, the energy consumption is improved from 4.48 to 1.1 kWh/m<sup>3</sup> at the optimised operating conditions.

### Symbols

$b$  : The feed channel friction parameter (atm s/m<sup>4</sup>)

$B_s$  : The solute permeability coefficient used in the Solution-diffusion model (m/s)

$C_{s(av)}$  : The average mean solute concentration in the feed channel (kmol/m<sup>3</sup>)

$C_{s(0)}$  : The inlet mean solute concentration (kmol/m<sup>3</sup>)

$C_{s(L)}$  : The outlet mean solute concentration (kmol/m<sup>3</sup>)

$C_{p(av)}$  : The average permeate solute concentration in the permeate channel (kmol/m<sup>3</sup>)

$C_p$  : The specific heat capacity of water (4181 j/kg K)

$C_{s(0)}$  : The inlet feed solute concentrations in feed channel (kmol/m<sup>3</sup>)

$C_{s(L)}$  : The outlet feed solute concentrations in feed channel (kmol/m<sup>3</sup>)

$C_{w(x)}$  : The molar solute concentration on the membrane surface at any point along the x-axis in feed channel (kmol/m<sup>3</sup>)

$D_{b(x)}$  : The solute diffusion coefficient of feed at any point along the x-axis (m<sup>2</sup>/s)

$E1$  : The specific energy consumption for high pressure pump (kW h/m<sup>3</sup>)

$E_2$  : The specific energy consumption for high pressure pump and ERD (kW h/m<sup>3</sup>)  
 $E_3$  : The specific energy consumption for the boiler (kW h/m<sup>3</sup>)  
 $E_4$  : The specific energy consumption for high pressure pump, ERD and Boiler (kW h/m<sup>3</sup>)  
 $ERD$  : Energy recovery device  
 $F_{b(x)}$  : The feed flow rate at any point along the x-axis in feed channel (m<sup>3</sup>/s)  
 $F_{b(0)}$  : The feed flow rate at x=0 in feed channel (m<sup>3</sup>/s)  
 $F_{b(L)}$  : The feed flow rate at x=L in feed channel (m<sup>3</sup>/s)  
 $F_{b(ERD)}$  : The feed flow rate of energy recovery device (m<sup>3</sup>/s)  
 $F_{b(HPP)}$  : The feed flow of the high pressure pump (m<sup>3</sup>/s)  
 $F_{b(Tank)}$  : The feed flow rate of feed tank (m<sup>3</sup>/s)  
 $F_p(x)$  : The permeate flow rate at any point along the x-axis in permeate channel (m<sup>3</sup>/s)  
 $F_{p(Total)}$  : The total permeated flow rate at the permeate channel (m<sup>3</sup>/s)  
 $F_{in(Tank)}$  : The inlet feed flow rate to the feed tank (m<sup>3</sup>/s)  
 $F_{out(Tank)}$  : The outlet feed flow rate from the feed tank (m<sup>3</sup>/s)  
HPP : High pressure pump  
 $J_s(x)$  : The solute molar flux through the membrane at any point along the x-axis (kmol/m<sup>2</sup> s)  
 $J_w(x)$  : The water flux at any point along the x-axis (m/s)  
 $K$  : The efficiency of mixing net (i.e. spacer) ( $K = 0.5$ ) (dimensionless)  
 $k(x)$  : The mass transfer coefficient at any point along the x-axis (m/s)  
 $L$  : The length of the membrane (m)  
 $L_p$  : The solvent transport coefficient (m/atm s)  
 $P_{b(x)}$  : The feed channel pressure at any point along the x-axis (atm)  
 $P_p$  : The permeate channel pressure (atm)  
 $P_{atm}$  : The pressure of feed tank (1 atm)  
 $P_{b(ERD)}$  : The outlet pressure of energy recovery device (atm)  
 $R$  : The gas law constant ( $R=0.082$  atm m<sup>3</sup>/ K kmol)  
 $Rej$  : The solute rejection coefficient (dimensionless)  
 $Q$  : The supplied heat by the boiler (j/s)  
 $T_b$  : The feed temperature (°C)  
 $T_{Ref}$  : The reference temperature (°K)  
 $T_{Tank}$  : The temperature accumulated at the tank (°K)  
 $t_f$  : The feed spacer thickness (m)

$U_{b(x)}$  : The feed velocity at any point along x-axis in feed channel (m/s)

$V$  : The volume of feed tank (m<sup>3</sup>)

$W$  : The membrane width (m)

$x$  : The specific width of the membrane (m)

$Z$  : Parameter defined in [Eq. \(2\)](#) in [Table A.1 in Appendix A](#)

### Subscript

$\rho_{b(x)}$  : The feed density at any point along the x-axis in feed channel (kg/m<sup>3</sup>)

$\sigma$  : The reflection coefficient (dimensionless)

$\rho$  : The density of water (1000 kg/m<sup>3</sup>)

$\omega$  : The solute permeability coefficients of the membrane (kmol/m<sup>2</sup> s atm)

$\Delta L$  : The characteristics length of spacer (m)

$\Delta x$  : Length of the sub-section (m)

$\Delta P_{b(x)}$  : Trans-membrane pressure at any point along the x-axis (atm)

$\Delta \pi_{s(x)}$  : The osmotic pressure difference at any point along the x-axis (atm)

$\mu_{b(x)}$  : The Feed viscosity at any point along the x-axis (kg/m s)

$\varepsilon_{pump}$  : Pump efficiency (dimensionless)

$\varepsilon_{ERD}$  : Energy recovery device efficiency (dimensionless)

$\varepsilon_{BP}$  : Booster pump efficiency (dimensionless)

$\beta$  : The leakage ration of ERD (dimensionless)

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## Appendix A

**Table A. 1.** Spiral-wound reverse osmosis modelling of Al-Obaidi et al. (2017b)

Model Equations	Eq. no.
$F_{b(x)} = \frac{F_{b(L)} \left( e^{\sqrt{\frac{L_p}{Z}} x} - e^{-\sqrt{\frac{L_p}{Z}} x} \right) + F_{b(0)} \left( e^{\sqrt{\frac{L_p}{Z}} (L-x)} - e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right)}{\left( e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)}$	1
Where, $Z = \frac{1 + \frac{\sigma C_{p(av)} L_p(T_b)}{\omega(T_b)} - \frac{C_{s(av)}^{(1-\sigma)} L_p(T_b) \sigma}{\omega(T_b)}}{W b}$	2
$\omega = \frac{B_s}{R(T_b + 273.15)}$	3
$C_{s(av)} = \frac{C_{s(0)} + C_{s(L)}}{2}$	4
Where, $C_{s(0)} = \frac{C_{s(0)} - C_{p(av)}}{\ln\left(\frac{C_{s(0)}}{C_{p(av)}}\right)}$ and $C_{s(L)} = \frac{C_{s(L)} - C_{p(av)}}{\ln\left(\frac{C_{s(L)}}{C_{p(av)}}\right)}$	5,6
$F_{b(0)} = \frac{F_{b(L)} \left( e^{\sqrt{\frac{L_p}{Z}} L} + e^{-\sqrt{\frac{L_p}{Z}} L} \right) - \Delta P_{b(0)} \sqrt{\frac{L_p}{Z}} \left( e^{\sqrt{\frac{L_p}{Z}} L} + e^{-\sqrt{\frac{L_p}{Z}} L} \right)}{2 - 2b}$	7
$U_b(x) = \frac{F_{b(x)}}{t_f W}$	8
$P_b(x) = P_{b(0)} - \frac{b}{\sqrt{\frac{L_p}{Z}} \left( e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \left\{ \left[ F_{b(L)} \left[ e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} - 2 \right] - F_{b(0)} \left[ \left( e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) - \left( e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right) \right] \right\}$	9
$\Delta P_{b(x)} = \frac{\sqrt{\frac{L_p}{Z}} Z b \left\{ \left[ F_{b(0)} \left( e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) \right] - \left[ F_{b(L)} \left( e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} \right) \right] \right\}}{L_p \left( e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)}$	10
$J_w(x) = \frac{\sqrt{\frac{L_p}{Z}}}{W \left( e^{\sqrt{\frac{L_p}{Z}} L} - e^{-\sqrt{\frac{L_p}{Z}} L} \right)} \left\{ \left[ F_{b(0)} \left( e^{\sqrt{\frac{L_p}{Z}} (L-x)} + e^{-\sqrt{\frac{L_p}{Z}} (L-x)} \right) \right] - \left[ F_{b(L)} \left( e^{\sqrt{\frac{L_p}{Z}} x} + e^{-\sqrt{\frac{L_p}{Z}} x} \right) \right] \right\}$	11
$J_s(x) = J_w(x) (1 - \sigma) C_{s(av)} + \omega(T_b) R T_b (C_w(x) - C_{p(av)})$	12
$\frac{(C_w(x) - C_{p(av)})}{(C_s(x) - C_{p(av)})} = \exp\left(\frac{J_w(x)}{k(x)}\right)$	13
$D_b(x) = 6.725E - 6 \exp\left\{0.1546x10^{-3} C_{s(x)} (18.01253) - \frac{2513}{T_b + 273.15}\right\}$	(Koroneos et al., 2007) 14
$\mu_b(x) = 1.234E - 6 \exp\left\{0.0212x10^{-3} C_{s(x)} (18.0153) + \frac{1965}{T_b + 273.15}\right\}$	(Koroneos et al., 2007) 15
$\rho_b(x) = 498.4 m_{f(x)} + \sqrt{[248400 m_{f(x)}^2 + 752.4 m_{f(x)} C_{s(x)} (18.0153)]}$	(Koroneos et al., 2007) 16
$m_{f(x)} = 1.0069 - 2.757E - 4 T_b$	17
$\frac{d(C_{s(x)} F_{b(x)})}{t_f W dx} = -\frac{J_w(x) C_{p(av)}}{t_f} + \frac{J_w(x) C_{s(x)}}{t_f} + \frac{d}{dx} \left( D_b(x) \frac{dC_{s(x)}}{dx} \right)$	18
$C_{p(av)} = \frac{C_{p(0)} + C_{p(L)}}{2}$	19
$C_{p(0)} = \frac{B_s(T_b) R T_b C_{s(0)} e^{\frac{J_w(0)}{k(0)}}}{J_w(0) + B_s(T_b) R T_b e^{\frac{J_w(0)}{k(0)}}}$ and $C_{p(L)} = \frac{B_s(T_b) R T_b C_{s(L)} e^{\frac{J_w(L)}{k(L)}}}{J_w(L) + B_s(T_b) R T_b e^{\frac{J_w(L)}{k(L)}}}$	20, 21
$\frac{dF_{p(x)}}{dx} = -\frac{dF_{b(x)}}{dx}$	22
$F_{p(Total)} = F_{p(L)}$	23
$Rec_{(Total)} = \frac{F_{p(Total)}}{F_{b(0)}} \times 100$	24
$Rej_{observed} = \frac{C_{b(0)} - C_{p(av)}}{C_{b(0)}} \times 100$ $Rej = \frac{Rej_{observed} \exp\left(\frac{J_w(L)}{k(L)}\right)}{1 + Rej_{observed} \left[ \exp\left(\frac{J_w(L)}{k(L)}\right) - 1 \right]}$	Fujioka (2014) 25, 26

