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1 **Optimal reverse osmosis network configuration for the rejection of dimethylphenol from**
2 **wastewater**

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14 **Abstract**

15 Reverse osmosis (RO) has long been recognised as an efficient separation method for treating
16 and removing harmful pollutants, such as dimethylphenol in wastewater treatment. This research
17 aims to study the effects of RO network configuration of three modules of a wastewater
18 treatment system using a spiral-wound RO membrane for the removal of dimethylphenol from
19 its aqueous solution at different feed concentrations. The methodologies used for this research
20 are based on simulation and optimisation studies carried out using a new simplified model. This
21 takes into account the solution-diffusion model and film theory to express the transport
22 phenomena of both solvent and solute through the membrane and estimate the concentration
23 polarization impact respectively. This model is validated by direct comparison with experimental
24 data derived from the literature and which includes dimethylphenol rejection method performed
25 on a small-scale commercial single spiral-wound RO membrane system at different operating
26 conditions. The new model is finally implemented to identify the optimal module configuration

27 and operating conditions that achieve higher rejection after testing the impact of RO
28 configuration.

29 The optimisation model has been formulated to maximize the rejection parameters under optimal
30 operating conditions of inlet feed flow rate, pressure and temperature for a given set of inlet feed
31 concentration. Also, the optimisation model has been subjected to a number of upper and lower
32 limits of decision variables, which include the inlet pressure, flow rate and temperature. In
33 addition, the model takes into account the pressure loss constraint along the membrane length
34 commensurate with the manufacturer's specifications. The research clearly shows that the
35 parallel configuration yields optimal dimethylphenol rejection with lower pressure loss.

36

37 **Keywords:** Spiral-wound Reverse Osmosis; Wastewater Treatment; Dimethylphenol Rejection;
38 Mathematical Modelling; Reverse Osmosis Network Optimisation.

39 **Introduction**

40 Dimethylphenol is one of the phenolic organic compounds which can be certainly found in many
41 industrial (petroleum processing, plastic manufacturing, disinfectants, pesticides, herbicides and
42 resins production) effluents (Gami *et al.*, 2014). A number of agencies such as the Agency of
43 Toxic Substances and Disease Registry (ATSDR) and United States Environmental Protection
44 Agency (EPA) have listed dimethylphenol as a highly toxic compound even in low
45 concentrations and one that, has an ability to remain in the environment for a long period of
46 time. Water UK regulators have set the maximum concentration of phenol in the discharge
47 wastewater of hospitals to be within 10 ppm (Water UK, 2011), while ATSDR has limited the
48 presence of dimethylphenol at a maximum of 0.05 ppm in surface water (ATSDR, 2015).
49 Clearly, much attention has already been paid to establish tight targets for removing this harmful
50 pollutant from industrial effluents before discharging to surface water. Recent, conventional

51 methods of phenolic compounds removal from wastewater include; the microbial degradation,
52 adsorption, incineration, solvent extraction, irradiation, and chemical oxidation such as catalyst
53 wet air oxidation and reverse osmosis (Witek *et al.*, 2006; Mohammed *et al.*, 2016).

54 Reverse Osmosis (RO) technology was initially developed for the desalination of seawater and
55 brackish water to produce drinking water (Greenlee *et al.*, 2009). However, its rapid growth in
56 various applications has rendered RO a commercially attractive separation process for the
57 treatment of industrial effluents (Lee and Lueptow, 2001). Furthermore, RO is now recognised
58 as a promising technology for water recycling and reuse. This is because the use of RO yields
59 low level of the pollutant concentration in the permeate, which in turn accelerates the
60 reclamation of good quality water for yet more applications (Blandin *et al.*, 2016).

61 The configuration of the membrane modules in the RO process has a significant effect on the
62 performance and economics of the process. A graphical-analytical method has been developed
63 by Evangelista (1985) for the design of pressure driven membranes of spiral-wound RO
64 seawater and brackish water plants. This method can predict the number of parallel and series
65 modules either of a straight-through plant or of each section of a tapered plant, as well as the
66 average permeate concentration. El-halwagi (1992) developed a structural representation based
67 on state space approach which includes RO systems by considering the membrane module type
68 and feed specification. Saif *et al.* (2008) implemented a compact representation with a simpler
69 optimization procedure of the general superstructure of El-Halwagi (1992). Sassi and Mujtaba
70 (2012) studied the effect of arrangement of DuPont B-10 hollow fibre membrane modules on the
71 performance of two-stage RO system. Also, the optimisation of each superstructure has been
72 considered using an optimisation-based model for minimising both operating and capital costs.

73 The performance of individual and several spiral-wound RO modules in terms of industrial
74 wastewater treatment has already been studied by considering a range of different operating
75 conditions and different pollutants, such as copper (Chai *et al.*, 1997), nitrate (Cevaal *et al.*,

76 1995; Molinari *et al.*, 2001; Schoeman and Steyn, 2003), secondary treated sewage effluent (Qin
77 *et al.*, 2004), synthetic effluent stream of acrylonitrile, sulphate, ammonium, cyanide and sodium
78 (Bódalo-Santoyo *et al.*, 2004), copper and nickel (Mohsen-Nia *et al.*, 2007), chromium
79 (Mohammadi *et al.*, 2009), di-hydrogen phosphate, sulphite, nitrate and nitrite (Madaeni and
80 Koocheki, 2010) and bisphenol A (Khazaali *et al.*, 2014).

81 However, to the best of authors' knowledge, the superstructure optimisation of spiral-wound
82 reverse osmosis network based on wastewater treatment process for dimethylphenol rejection
83 has not yet been explored. This research therefore aims to obtain the optimal RO configuration
84 from a set of possible configurations, which can achieve higher dimethylphenol rejection under
85 different feed concentrations taking into accounting the allowable pressure loss along the
86 membrane length, as defined by the membrane manufacturer.

87 **Modelling of spiral-wound reverse osmosis**

88 This section shows a simple model that can be used to simulate the phenomenon of solvent and
89 solute transport through the membrane, and one that incorporates the fluid physical properties to
90 predict the rejection of dimethylphenol for a spiral-wound RO process.

91 The Assumptions

92 The following assumptions are made in the proposed model:

- 93 1. The solution-diffusion model is used for mass transport through the module.
- 94 2. The membrane characteristics and the channel geometries are assumed constant.
- 95 3. Validity of the film model theory to estimate the concentration polarization impact.
- 96 4. Constant atmospheric pressure on the permeate channel of 1 atm.
- 97 5. Constant solvent and solute transport parameters and friction factor.
- 98 6. The underlying process is assumed to be isothermal.

100 Governing Equations

101 Based on Assumption 1, the solution-diffusion model is valid to predict the water and solute flux
 102 J_w and J_s (m/s, kmol/m² s) through the membrane as expressed by (Lonsdale *et al.*, 1965).

103
$$J_w = A_w [\Delta P - \Delta \pi_{Total}] \quad (1)$$

104 Where
$$\Delta P = \frac{(P_{f(in)} + P_{f(out)})}{2} - P_p \quad (2)$$

105
$$J_s = B_s (C_m - C_p) \quad (3)$$

106 Where A_w and B_s (m/atm s, m/s) are solvent transport and solute transport parameters
 107 respectively. ΔP , $P_{f(in)}$, $P_{f(out)}$ and P_p (atm) are the transmembrane pressure across the
 108 membrane, inlet and outlet feed pressures and constant permeate pressure (Assumption 4)
 109 respectively.

110 The total osmotic pressure difference $\Delta \pi_{Total}$ (atm) can be described using Eq. (4).

111
$$\Delta \pi_{Total} = (\pi_m - \pi_p) \quad (4)$$

112 Where π_m (atm) is the osmotic pressure of solute at the membrane wall concentration C_m
 113 (kmol/m³). While π_p (atm) is the osmotic pressure at permeate channel regarding the permeate
 114 concentration C_p (kmol/m³). The estimation of the feed and permeate osmotic pressure is carried
 115 out using Eqs. (5) and (6).

116
$$\pi_m = R (T + 273.15) C_m \quad (5)$$

117
$$\pi_p = R (T + 273.15) C_p \quad (6)$$

118 Where R and T (atm m³/kmol K, °C) are the gas constant and constant operating temperature
 119 (Assumption 6) respectively. The concentration of solute at the wall membrane was estimated
 120 based on Assumption 3, which in turn is based on the validity of the film model theory where the

121 solvent flux is linked to the concentration polarization and mass transfer coefficient k (m/s)
 122 based on the following equation:

$$123 \frac{(C_m - C_p)}{(C_b - C_p)} = \exp\left(\frac{J_w}{k}\right) \quad (7)$$

124 C_b and k (kmol/m³, m/s) are the bulk concentration in the feed side and the mass transfer
 125 coefficient for the specified solute respectively. C_b (kmol/m³) is taken as the average value of
 126 feed C_f (kmol/m³) and retentate concentrations C_r (kmol/m³) using Eq. (8).

$$127 C_b = \frac{C_f + C_r}{2} \quad (8)$$

128 The mass transfer coefficient k (m/s) is a function of pressure, concentration, flow rate and
 129 temperature, which is calculated using the proposed equation of Srinivasan *et al.* (2011).

$$130 k = \frac{246,9 D_b Re_b^{0.101} Re_p^{0.803} C_m^{0.129}}{2t_f} \quad (9)$$

131 Where D_b , t_f , Re_b and Re_p are the diffusion coefficient (m²/s), feed channel height (m) and the
 132 Reynolds number along the feed and permeate channels (dimensionless) respectively. The
 133 exponents of Eq. (9) have been estimated experimentally by Srinivasan *et al.* (2011) for the
 134 dimethylphenol aqueous solution. Also, C_m is a dimensionless solute concentration and can be
 135 found from Eq. (10):

$$136 C_m = \frac{C_b}{\rho_w} \quad (10)$$

137 Where ρ_w is the molal density of water (55.56 kmol/m³).

138 The Reynolds number along the feed Re_b and permeate Re_p channels can be calculated from:

$$139 Re_b = \frac{\rho_b de_b Q_b}{t_f W \mu_b} \quad (11)$$

$$140 Re_p = \frac{\rho_p de_p J_w}{\mu_p} \quad (12)$$

141 Where de_b and de_p (m) are the equivalent diameters of the feed and permeate channels
 142 respectively.

143 $de_b = 2t_f$ (13)

144 $de_p = 2t_p$ (14)

145 t_p (m) is the height of permeate channel.

146 The estimation of diffusion coefficient D_b (m²/s), dynamic viscosity (kg/m s), feed density
 147 ρ_b (kg/m³) and permeate density ρ_p (kg/m³) are carried out using water equation of Koroneos
 148 (2007) due to the very dilute aqueous solutions of dimethylphenol used in the experimental work
 149 of Srinivasan *et al.* (2011).

150 $D_b = 6.725E - 6 \exp \left\{ 0.1546E - 3 C_f x 18.01253 - \frac{2513}{T+273.15} \right\}$ (15)

151 $D_p = 6.725E - 6 \exp \left\{ 0.1546E - 3 C_p x 18.01253 - \frac{2513}{T+273.15} \right\}$ (16)

152 $\mu_b = 1.234E - 6 \exp \left\{ 0.0212E - 3 C_f x 18.0153 + \frac{1965}{T+273.15} \right\}$ (17)

153 $\mu_p = 1.234E - 6 \exp \left\{ 0.0212E - 3 C_p x 18.0153 + \frac{1965}{T+273.15} \right\}$ (18)

154 $\rho_b = 498.4 m_f + \sqrt{[248400 m_f^2 + 752.4 m_f C_f x 18.01253]}$ (19)

155 $\rho_p = 498.4 m_f + \sqrt{[248400 m_f^2 + 752.4 m_f C_p x 18.01253]}$ (20)

156 Where, $m_f = 1.0069 - 2.757E - 4 T$ (21)

157 While the bulk feed velocity U_b is calculated using Eq. (22).

158 $U_b = \frac{Q_b}{W t_f}$ (22)

159 Where Q_b and W (m³/s, m) are the bulk feed flow rate calculated using Eq. (23), and the width
 160 of the membrane respectively.

161 $Q_b = \frac{Q_f + Q_r}{2}$ (23)

162 Q_f and Q_r (m³/s) are the feed and retentate flow rates.

163 The process of dimethylphenol rejection is followed by a pressure drop along the membrane
 164 edges. Therefore, the outlet membrane pressure $P_{f(out)}$ (atm) is calculated using the equation of
 165 Sundaramoorthy *et al.* (2011) as follows:

$$166 \quad P_{f(out)} = P_{f(in)} - \frac{bL}{\phi \sinh \phi} \{ (Q_f + Q_r) (\cosh \phi - 1) \} \quad (24)$$

167 Where ϕ, b and L (dimensionless, atm s /m⁴, m) are dimensionless term defined in Eq. (25),
 168 friction parameter and membrane length respectively.

$$169 \quad \phi = L \sqrt{\frac{W b A_w}{\left[1 + \left(\frac{A_w R C_p (T + 273.15)}{B_s} \right) \right]}} \quad (25)$$

170 Therefore, the pressure loss for each element can be calculated using Eq. (26).

$$171 \quad P_{f(lose)} = P_{f(in)} - P_{f(out)} \quad (26)$$

172 Substituting Eq. (26) in Eq. (2) yields:

$$173 \quad \Delta P = P_{f(in)} - \frac{P_{f(lose)}}{2} - P_p \quad (27)$$

174 While, the overall solute and mass balance equations are depicted in the counter of Eqs. (28) and
 175 (29).

$$176 \quad Q_f = Q_r + Q_p \quad (28)$$

$$177 \quad Q_f C_f = Q_r C_r + Q_p C_p \quad (29)$$

178 Where C_f, C_r and C_p (kmol/m³) are the concentration of dimethylphenol in feed, retentate and
 179 permeate channel respectively. Also, Eq. (30) is used to calculate the concentration at the
 180 permeate channel (Al-Obaidi *et al.*, 2017).

181
$$C_p = \frac{C_f B_s}{B_s + \frac{J_w}{\exp(\frac{J_w}{k})}} \quad (30)$$

182 Finally, the rejection parameter of dimethylphenol can be calculated using Eq. (31).

183
$$Rej = \frac{C_f - C_p}{C_f} \times 100 \quad (31)$$

184 The total recovery of the single module can be calculated using Eq. (32).

185
$$Rec = \frac{Q_p}{Q_f} \times 100 \quad (32)$$

186 Where Q_p (m³/s) is the total permeated flow rate calculated using Eq. (33).

187
$$Q_p = J_w A \quad (33)$$

188 Where A (m²) is the effective membrane area.

189 **Module configurations and mathematical modelling**

190 Reverse osmosis membrane systems are typically used as a network of different numbers of
 191 stages that should be designed in a way to meet the requirement of the separation process
 192 including environmental and economic impacts. Here, in order to reduce the number of RO
 193 networks and the complexity of the superstructure problem, the proposed wastewater RO full-
 194 scale plant is designed consisting of only three modules but connected differently to generate
 195 four possible RO networks. Each module holds a maximum of two pressure vessels connected in
 196 parallel, while each pressure vessel holds only one spiral-wound RO membrane type HM4040-
 197 LPE supplied by Ion Exchange, India of 7.85 m² area. The schematic diagrams of four proposed
 198 superstructures of RO network for wastewater treatment can be seen in Fig. 1. These layouts are
 199 essentially similar to the specification of actual networks used for RO seawater desalination
 200 process presented by Abbas (2005).

201 In the series configuration, the concentrated stream of the first membrane element becomes the
 202 feed stream of the subsequent element and so on, while, the permeate streams of three elements
 203 are blended to form the product stream of the plant. Configuration A shows two parallel modules

204 in the first stage and the concentrate streams of these modules are mixed to form the feed of the
 205 second stage module.

206 The objective function for each RO network is to maximize the rejection of dimethylphenol
 207 without exceeding the allowable value of the pressure drop along the membrane length, as
 208 recommended by the manufacturer. The modelling of a single spiral-wound membrane element
 209 has been described in the governing equations section, while the interaction between the stages
 210 and pressure vessels is described in more detail in this section.

211 The complete mathematical equations that describe the overall mass and solute balance
 212 equations of the whole plant with the inlet and outlet streams can be illustrated as follows:

$$213 \quad Q_{f(plant)} = Q_{r(plant)} + Q_{p(plant)} \quad (34)$$

$$214 \quad Q_{r(plant)} = Q_{r(s=n)} \quad s \text{ refers to stage and } n \text{ represents the number of the used stages} \quad (35)$$

$$215 \quad Q_{p(plant)} = \sum_{s=1}^n Q_{p(s)} \quad (36)$$

$$216 \quad C_{r(plant)} = C_{r(s=n)} \quad (37)$$

$$217 \quad Q_{f(plant)} C_{f(plant)} = Q_{r(plant)} C_{r(plant)} + Q_{p(plant)} C_{p(plant)} \quad (38)$$

$$218 \quad Rej_{(plant)} = \frac{C_{f(plant)} - C_{p(plant)}}{C_{f(plant)}} \times 100 \quad (39)$$

$$219 \quad Rec_{(plant)} = \frac{Q_{p(plant)}}{Q_{f(plant)}} \times 100 \quad (40)$$

220 An appropriate simulation model has been designed and developed for a spiral-wound reverse
 221 osmosis membrane module in steady state mode and for a multi-stage plant, which describes the
 222 variation of all the operating parameters along the stages using the gPROMS software (general
 223 Process Modelling System by Process System Enterprise Ltd. 2001). The gPROMS Model
 224 Builder provides a good modelling platform for steady state and dynamic simulation,

225 optimisation, experiment design and parameter estimation of any process. The model equations
226 are solved for a given inlet plant feed flow rate, pressure, dimethylphenol concentration and
227 temperature. The proposed model can predict the variation of all parameters along the stages and
228 pressure vessels. The steady state process model consisting of nonlinear algebraic equations
229 presented earlier can be written in the following compact form:

$$230 \quad f(x, u, v) = 0 \quad (41)$$

231 where, x is the set of all algebraic variables, u is the set of decision variables and v denotes the
232 constant parameters of the process. The function f is assumed to be continuously differentiable
233 with respect to all their arguments.

234

235 **Model Validation**

236 The transport parameters of this model A_w and B_s and the friction parameter b were taken from
237 the experimental work of Srinivasan *et al.* (2011) and shown in Table 1. These values were used
238 in subsequent simulation and optimisation analyses. The experiments were carried out for
239 aqueous solutions of dimethylphenol of concentrations varying from 0.819E-3 to 6.548E-3
240 kmol/m³. The feed was pumped in three different flow rates of 2.166E-4, 2.33E-4 and 2.583E-4
241 m³/s with a set of pressures varying from 5.83 to 13.58 atm for each flow rate. The membrane
242 and module properties used in the calculations are given in Table 1.

243 Fig. 2 provides a comparison between experimental results and model prediction of retentate
244 flow rate, permeate flow rate, retentate pressure, total permeate recovery and dimethylphenol
245 rejection at inlet feed conditions of a set of three inlet feed flow rates of 2.166E-4, 2.33E-4 and
246 2.583E-4 m³/s with inlet feed pressure of 5.83, 7.77, 9.71, 11.64 and 13.58 atm for inlet feed
247 concentration and temperature of 6.548E-4 kmol/m³ and 31.5 °C respectively. Generally, the
248 predicted values of the model correlate well with experimental results over the ranges of

249 pressure and flow rate. This readily shows the suitability of the model to measure the observed
250 rejection data with an acceptable error range.

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Fig. 1. Schematics of different RO configurations studied in this work

RO network performance analysis

The impact of RO network on the rejection of dimethylphenol of three cases of inlet concentration of 1.637, 2.455 and 6.548 kmol/m³ is analysed in this section by estimating the rejection parameter at selected operating conditions of inlet flow rate, pressure and temperature of 4.5E-4 m³/s, 16 atm and 37 °C respectively. The inlet feed flow rate of each element is within the allowable recommended limits set by the manufacturer. The simulation results of four configurations are given in Table 2, which shows the values of dimethylphenol rejection, water recovery and total pressure loss for each selected configuration.

Fig. 2. Comparison of theoretical and experimental values of [a: Retentate flow rate, b: Permeate flow rate, c: Retentate pressure, d: Total permeate recovery and e: Dimethylphenol rejection]

276 Table 2 shows that the proposed four configurations can produce relatively high dimethylphenol
277 rejection values for different inlet feed concentration. However, a single-stage configuration of
278 three parallel modules yields higher values of rejection parameter and production rate at lower
279 pressure loss in comparison with other configurations. This therefore means that the proposed
280 configuration is readily affordable. This cheaper solution achieves a lower pressure drop along
281 the membrane length, which is caused by using the same operating feed flow rate for all the four
282 tested configurations. This is mainly due to the fact that splitting the inlet feed flow rate into
283 three streams in a parallel configuration yields a reduction in the consumption of pressure, which
284 is caused by a lower flow rate in each module. It is the domino effect that increases the rejection
285 and recovery rates. Another immediate advantage of this configuration is the possibility of using
286 the resulting concentrated stream to further increase the recovery rate in a subsequent module
287 due to its high pressure.

288 Another key advantage is the fact that the tapered configurations A and B are relatively similar
289 in their performance of rejection but quite different in their recovery performance. This can be
290 explained by the different impact of configuration type that controls the feed flow rate inside
291 each module.

292 The difference of total recovery that can be achieved for the four configurations is quite clear.
293 Configurations A and D can produce higher quantity of permeate under the same operating
294 conditions than layouts B and C. However, configuration D offers the highest recovery rate due
295 to lower pressure loss along the membrane channel. Table 2 shows that the worst recovery rate is
296 produced using the series configuration C, where it has largely degraded the operating pressure
297 and shows a maximum pressure drop due to an increase in the osmotic pressure in the
298 subsequent modules in spite of having a high feed flow rate. Similar trend was observed by
299 Abbas (2005). The impact of the operating parameters on the performance of RO network is
300 described in more detail below.

301 The effect of the inlet feed concentration on the performance of the RO network is quite similar
302 in all the four configurations studied. Table 2 shows a decrease of the recovery rate and an
303 increase of rejection parameter as a result of increasing the operating feed concentration. This
304 can be attributed to the increase in the osmotic pressure due to an increase in the inlet feed
305 concentration. This reduces the driving force ($\Delta P - \Delta\pi_{Total}$) of permeate flux (Eq. 1). However,
306 the rejection parameter actually increases due to an increase in the inlet feed concentration and
307 this may be due to an increase in the membrane solute isolation intensity. These same results
308 have been confirmed by Al-Obaidi and Mujtaba (2016).

309 Furthermore, the impact of inlet feed concentration on the total pressure loss and retentate flow
310 rate in configuration A can be seen in Fig. 3 at constant initial conditions of feed flow rate,
311 pressure and temperature. The increase of feed concentration of configuration A causes an
312 increase in the pressure drop due to an increase in the rate of concentration polarization. This in
313 turn reduces the quantity of permeate and lifts up the quantity of bulk feed velocity and retentate
314 flow rate, which explains the higher friction and pressure drop.

315 Fig. 4 shows the relation existing between the inlet feed pressure for configuration B with both
316 the total pressure loss and the total permeate flow rate at constant initial conditions of feed
317 concentration, flow rate and temperature. It is not difficult to see that increasing the feed
318 pressure at constant flow rate can readily cause a reduction in the total pressure loss. This is
319 caused by an increase in the permeated flow rate, which reduces the quantity of feed flow rate at
320 the feed channel and retentate stream. The retentate feed pressure will therefore increase, and
321 this is will be followed by a lower pressure loss as can be confirmed in Eq. (24). Fig. 5 shows
322 the impact of inlet feed temperature of the plant on both the total pressure loss and
323 dimethylphenol rejection at constant inlet conditions of feed concentration, flow rate and
324 pressure for configuration C. The feed temperature is expected therefore to have a positive effect
325 on the rejection parameter due to increasing the permeated flow rate.

326 The effect of the inlet feed flow rate on the performance of configuration D at constant initial
327 conditions of concentration, pressure and temperature is shown in Fig. 6. Here, it is not difficult
328 to see that increasing the operating flow rate results in an increase in the total pressure loss of the
329 network. This reduces both the time of residence inside the feed channel and the amount of
330 permeated flow rate. Therefore, the recovery rate decreases as a result of an increase in the feed
331 flow rate.

332 Finally, Fig. 7 shows the relationship existing between the inlet plant feed flow rate as a function
333 to dimethylphenol rejection parameter and the recovery rate of four configurations at inlet feed
334 conditions of 6.548 kmol/m³, 17.7 atm and 32 °C. The simulated results shown in Fig. 7 clearly
335 indicate that the rejection parameter of any RO network increases due to an increase in the inlet
336 feed flow rate. This has the net effect of reducing the concentration polarization impact. While,
337 the recovery rate actually reduces as a result to an increase in the inlet feed flow rate. This is due
338 to a reduction of residence time of the fluid inside the feed channel, which in turn decreases the
339 quantity of permeated water through the membrane.

340 Consequently, any RO network, which yields a lower feed flow rate along its modules, will
341 increase the possibility of gaining a higher recovery rate due to a lowest overall pressure drop.
342 This is quite evident due to different feed flow rates being achieved for different module layouts.
343 It is therefore expected that configuration D does in fact offer a higher recovery rate for the same
344 operating conditions with high rejection due to the lowest pressure drop.

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352 **Fig. 3.** The inlet feed concentration of the plant as a function to the total pressure loss and retentate rate for
353 configuration A at initial conditions of $8.5112E-4 \text{ m}^3/\text{s}$, 19 atm and $35 \text{ }^\circ\text{C}$

354

355

356 **Fig. 4.** The inlet feed pressure of the plant as a function to the total pressure loss and permeate flow rate for
357 configuration B at initial conditions of $5E-4 \text{ m}^3/\text{s}$, $2.455E-3 \text{ kmol}/\text{m}^3$ and $34 \text{ }^\circ\text{C}$

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359

360 **Fig. 5.** The inlet feed temperature of the plant as a function to the total pressure loss and rejection for configuration
361 C at initial conditions of $2E-4 \text{ m}^3/\text{s}$, $6.548E-3 \text{ kmol}/\text{m}^3$ and 15 atm

362

363

364 **Fig. 6.** The inlet feed flow rate of the plant as a function to the total pressure loss and recovery for configuration D
365 at initial conditions of $6.548E-3 \text{ kmol}/\text{m}^3$ and 15.5 atm and $36 \text{ }^\circ\text{C}$

366

367

368

369 **Fig. 7.** The inlet feed flow rate of the plant as a function to the rejection and recovery rate for four
370 RO configurations (A, B, C and D)

371

372 It is worth mentioning that Table 2 confirms that the total recovery of the three modules of
373 wastewater treatment system is in fact higher than what can be achieved in a similar seawater
374 desalination system. This is because the concentration of wastewater feed is lower than seawater
375 feed (not comparable), which means lower osmotic pressure and higher recovery. This finding is
376 in-line with the results of Maskan *et al.* (2000) for a system of two modules of brackish water
377 arranged in different tubular modules configurations.

378

379 **Optimal RO configuration and operating conditions**

380 The objective of this part of the research is to show the development of the RO optimisation
381 framework for the configurations tested (as shown in Fig. 1) based on wastewater treatment
382 spiral-wound RO process and subjected to feed concentration fluctuation. The mathematical
383 model developed in the governing equations section of spiral-wound RO process is used in the
384 design of the RO network in order to achieve high dimethylphenol rejection. This involves a
385 number of different choices of different membrane module configuration. The optimisation
386 technique for RO layout is based on the model equations shown and includes the consideration
387 of other design, physical and economic constraints. This optimisation approach is designed to
388 offer the opportunity to investigate an optimal configuration from a number of alternatives
389 combinations.

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391 **Problem description and formulation**

392 The objective function here is to optimise the rejection of dimethylphenol under different feed
393 concentrations for different RO networks of three elements of spiral-wound membrane type
394 HM4040-LPE supplied by Ion Exchange, India as shown in Fig. 1. This involves four RO
395 configurations and allows the underlying optimizer to facilitate the selection of the optimal RO

418 Also, the optimisation problem entails the following constraints of a single spiral-wound RO
419 membrane, which satisfy the maximum and minimum practical bounds of operating conditions:

$$Q_f^L \leq Q_f \leq Q_f^U$$

$$P_{f(in)}^L \leq P_{f(in)} \leq P_{f(in)}^U$$

$$T^L \leq T \leq T^U$$

420 The limits of the decision variables of inlet feed flow rate, pressure and temperature of a single
421 RO membrane are given in Table 1 and constrained by the membrane manufacturer. It is to be
422 noted that the optimisation procedure of the four configurations will be carried out in a way that
423 permits the estimation of the pressure required by each module.

424 **RO networks optimisation results**

425 The optimisation results of four selected RO networks are shown in Fig. 1 at three different feed
426 concentration and presented in Table 3. This shows the optimum decision variables of each
427 layout and its performance regarding the overall dimethylphenol rejection, the maximum
428 pressure loss occurring in the RO element and the total pressure loss for the whole configuration.
429 Table 3 shows that the four RO configurations can attain a rejection parameter between 95.6 to
430 99.25 % at different operating conditions. It is worth noting that each RO configuration has its
431 specific optimum operating condition that guarantees the highest dimethylphenol rejection while
432 taking into account the constraint of a maximum pressure loss of 1.3817 atm along the
433 membrane module. Having said this, it is also worthwhile noting that all the RO configurations
434 hit the upper limit of feed temperature to achieve the objective function. This confirms again the
435 importance of temperature and its contributions in the underlying design (Fig. 5). Table 3 clearly
436 shows that the parallel configuration D has the largest dimethylphenol rejection for all the tested
437 feed concentrations.

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439 The goal of maximizing the rejection parameter whilst constraining the optimisation problem
440 within the allowable pressure drop leads to a reduction of the inlet feed flow rate due to its
441 valuable impact on the pressure drop. It is the small cross-flow velocity in the feed channel
442 which helps reduce the frictional pressure drop.

443 Table 3 also shows that configurations A and D require a higher feed pressure than in
444 comparison with configuration B and C in order to optimize their rejection parameter. The
445 rationale behind this is that a higher feed flow rate requires, a higher operating pressure for
446 substituting the higher loss of pressure at such configurations. Nevertheless, the optimisation is
447 carried out with a pressure loss constraint, which has restricted the possible choice for the inlet
448 feed flow rate that can achieve the higher rejection. Therefore, the optimizer may choose
449 configurations B and C for ensuring a lower feed pressure albeit yielding marginally lower
450 rejections.

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452 **Conclusions**

453 The treatment of dimethylphenol aqueous solutions using a multi-stage RO network based on a
454 spiral-wound module is mathematically modelled to simulate and optimize the rejection
455 parameter commensurate with the limits of operation and the constraints of both the module and
456 RO layout. The simulation and optimization methodologies developed were based on the
457 solution-diffusion model constrained by the concentration polarization impact. The consistency
458 and sensitivity of this new model has been tested against experimental data of dimethylphenol
459 rejection from the literature using a pilot-scale RO system of a single spiral-wound RO
460 membrane element. The results compare well with published results with an acceptable
461 correlation error for most operating parameters. The impact of the main operating parameters of
462 feed pressure, flow rate and temperature on the rejection were analysed for different RO
463 networks. An optimization study has been carried out to measure the capability of different RO

464 networks to reject dimethylphenol from its aqueous solutions at three different inlet feed
465 concentrations constrained by the manufacturer's specification of module pressure loss and the
466 upper and lower limits of the operating conditions. Specifically, the optimization results have
467 shown that the parallel configuration can attain the highest rejection parameter within the lowest
468 pressure loss in comparison to other configurations.

469 Further work is planned to investigate the optimal design of RO network for pollutants of high
470 solute transport values such as NDMA (N-nitrosodimethylamine) nitrosamine when
471 implementing the multi-stage arrangement that could involve permeate reprocessing required for
472 improving the purity of the permeate.

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577 **Tables**

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Table 1. Specifications of the spiral-wound membrane element

Make	Ion Exchange, India
Membrane type and configuration	Hydramem, HM4040-LPE, Spiral-wound, Low pressure application, TFC Polyamide
Feed and permeate spacer thickness (t_f) (t_p) (m)	0.8 and 0.5
Effective membrane area (m ²)	7.85
Membrane sheet length (L) and width (W) (m)	0.934 and 8.4
Maximum operating temperature (°C)	40
Maximum operating pressure (atm)	24.7717
Maximum pressure drop per element (atm)	1.3817
Maximum and minimum feed flow rate (m ³ /s)	1E-4 – 1E-3
A_w (m/ atm s)	9.7388E-7
B_s (dimethylphenol) (m/s)	1.5876E-8
b (atm s/m ⁴)	9400.9

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Table 2. The simulation results of four RO networks

Feed concentration $\times 10^3$, kmol/m ³	Scenario	Rej_{plant}	Rec_{plant}	Total configuration $P_{f(lose)}$ atm
1.637	A	97.7616	64.7493	3.2898
	B	97.7069	55.2476	4.7183
	C	97.7649	49.4304	8.4956
	D	97.7267	66.5223	0.8743
2.455	A	98.0408	63.3045	3.3446
	B	97.9696	53.9999	4.7401
	C	98.0050	48.3503	8.5561
	D	98.0184	64.7607	0.8859
6.548	A	98.5153	57.9802	3.5490
	B	98.4268	49.3336	4.8243
	C	98.4190	44.1557	8.7946
	D	98.5049	58.7340	0.9257

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Operating conditions: 6.548E-3 kmol/m³, 4.5E-4 m³/s, 16 atm and 37 °C

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Table 3. The optimisation results of dimethylphenol for five scenarios of RO networks

Feed concentration $\times 10^3$, kmol/m ³	Configuration	Decision variables			Max. pressure loss of element, atm	Total pressure loss of configuration, atm	$Re_{j_{plant}}$
		$Q_{f(plant)}$ (m ³ /s)	$P_{f(in)(plant)}$ (atm)	$T_{(plant)}$ (°C)			
1.637	A	4.5111E-4	20.2758	40	1.3817	2.4561	98.3568
	B	2.0648E-4	15	40	1.3817	1.6394	96.9203
	C	2.0648E-4	15	40	1.3817	2.1404	95.5991
	D	7.2239E-4	24.7717	40	1.3764	1.3764	98.9794
2.455	A	4.5947E-4	21.7534	40	1.3826	2.3753	98.5478
	B	2.0568E-4	15	40	1.3817	1.6468	97.2615
	C	2.0567E-4	15	40	1.3817	2.1831	96.2038
	D	7.1786E-4	24.7717	40	1.3754	1.3754	99.0559
6.548	A	4.5198E-4	21.9687	40	1.3826	2.4909	98.9045
	B	2.0249E-4	15	40	1.3817	1.6761	97.8881
	C	2.0249E-4	15	40	1.3817	2.3420	97.3488
	D	7.0132E-4	24.7717	40	1.3724	1.3724	99.2509

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