Evaluation of phenol removal via a spiral wound reverse osmosis process with different feed concentrations: simulation study

Mudhar A. Al-Obaidi, Samir N. Mustafa and Kawther H. Malek

ABSTRACT
Reverse osmosis (RO) process is progressively engaged in various industrial applications as a promising separation process in favour of classical methods. In this study, an earlier one-dimensional distributed model of RO process, developed by the author, is used to simulate the transport phenomena of phenol removal. The proposed model represented the process parameters as a function of longitudinal variation along the x-coordinate of feed side. The transport parameters of the membrane are optimised by the gEST parameter estimation tool of gPROMS. The model is verified against phenol removal experimental data for a pilot-scale spiral wound RO (SWRO) treatment system. The model has been used to explore the effects of key operating parameters on the phenol removal for five feed concentration cases.

Key words | parameter estimation, phenol removal, simulation, spiral wound reverse osmosis (SWRO), wastewater treatment

HIGHLIGHTS
- A distributed model of RO process is used to investigate the process performance.
- The transport parameters are optimised using the gEST parameter estimation tool.
- The model has been validated against experimental data from the literature.
- The effect of the operating conditions on phenol removal is investigated.
- Increasing operating pressure beyond a certain value will deteriorate the removal.

NOMENCLATURE

- $A_w$ Solvent transport coefficient (m atm$^{-1}$ s$^{-1}$).
- $b$ Feed and permeate channels friction parameter (atm s m$^{-1}$).
- $B_s$ Solute transport coefficient (m s$^{-1}$).
- $C_{(b(x))}$ Phenol concentration in any point along the x-axis of the feed channel (kmol m$^{-3}$).
- $C_{(b(0))}$ Inlet phenol concentration of the feed channel (kmol m$^{-3}$).
- $C_{(b(L))}$ Outlet phenol concentration of the feed channel (kmol m$^{-3}$).
- $C_{(p(0))}$ Average permeate phenol concentration in the permeate channel (kmol m$^{-3}$).
- $C_{(p(L))}$ Inlet permeate phenol concentration of the permeate channel (kmol m$^{-3}$).
- $C_{(p(w))}$ Outlet permeate phenol concentration of the permeate channel (kmol m$^{-3}$).
- $C_{(w(x))}$ Phenol concentration at the membrane wall in any point along the x-axis of the feed channel (kmol m$^{-3}$).
- $D_{(b(x))}$ Diffusivity parameter of feed in any point along the x-axis of the feed channel (m$^2$ s$^{-1}$).
- $F_{(b(x))}$ Feed flow rate in any point along the x-axis of the feed channel (m$^3$ s$^{-1}$).
- $F_{(b(0))}$ Inlet feed flow rate of the feed channel (m$^3$ s$^{-1}$).
It is worth noting that the current research serves a precise purpose to explore the performance of a spiral wound RO (SWRO) system for the elimination of phenol from synthesised wastewater. Phenol is a very toxic compound even at low concentrations in the wastewater of several industrial effluents from oil, coal, pesticides, dyes and pharmaceutical production plants (Mahajan et al. 1980; Othman et al. 2017; Naguib & Badawy 2020). The operating conditions have a considerable influence on the performance of the RO process including that of the solute removal and water recovery on the variation of feed parameters. The analysis of the effects of feed parameters on the performance of seawater RO desalination process has previously been investigated in several studies. For example, Abbas (2005) used a simple lumped model to simulate the process of an industrial seawater SWRO treatment system and studied the influence of the operating flow rate and pressure on the overall performance of removal and water recovery. Also, Kaghazchi et al. (2010) addressed the influence of operating pressure on the performance of industrial seawater RO plants made of SW membrane module type FilmTec SW30HR-380 of 35 m² effective membrane area. The above two studies show that increasing the operating pressure (low to medium values) and flow rate has a helpful influence on solute removal. However, raising the feed pressure beyond a specific value reduces the removal parameter. Additionally, Jiang et al. (2014) analysed the performance of a seawater SWRO process type SW30HR-380 while varying the feed pressure, flow rate, temperature, and concentration using a one-dimensional model. The results show that the removal parameter slowly and non-linearly increases due to growing feed pressure and flow rate. The same results also depict that it decreases as a consequence of any growth in feed concentration and temperature.

In the field of RO wastewater treatment process, Mohammadi et al. (2009) showed a steady increase of chromium removal as a result of increasing the feed flow rate and pressure for a pilot plant scale of a SWRO module type 2521 TE produced by a Korean CSM company. The results show an inconsiderable impact of chromium feed concentration when removed. On the other hand, the impact of temperature shows an optimum value, which attends a maximum removal.

Khazaali et al. (2014) investigated the effect of operating pressure, flow rate, concentration and pH on the removal of aqueous solutions of bisphenol A (BPA) using a low-pressure polyamide RO module of 0.446 m² membrane area. They have shown that the solute removal increases as a consequence of an increase in the pressure and flow rate. The
results also show critical values of pressure and flow rate for a maximum removal. Interestingly, the removal of BPA reduces when the feed concentration increases, despite low feed concentration attaining low solute removal. Generally, the impact of operating parameters on phenol removal using a SWRO system has not been addressed fully. Two examples can be found in the available literature.

The first example relates to Li et al. (2010), who assessed the influence of feed pressure, flow rate, temperature, concentration and pH on the performance of seven nanofiltration (NF) and RO membranes to remove phenol in phenolic-containing made wastewater. The results show insignificant influence of feed concentration and feed flow rate on phenol removal, especially for the SWRO process. However, the phenol removal declines remarkably with temperature. Additionally, the phenol removal actually increases at low and medium pressures, but it more or less stays the same at higher pressures.

The second example relates to Tabassi et al. (2014), who used a laboratory scale SWRO thin film composite membrane type SG 2514TF of 0.6 m² area from GE Osmonics Company to explore the effect of feed parameters on phenol removal from aqueous solutions relying on the irreversible thermodynamic model developed by Spiegler and Kedem. The results show an increase in phenol removal as a consequence of growing the feed flow rate, pressure, and feed concentration.

Al-Obaidi et al. (2017b) presented a specific one-dimensional distributed model following the irreversible thermodynamic principles for the elimination of phenol from wastewater using a SWRO system. The model was used to simulate process performance within a narrow range of operating conditions.

It is clear therefore that more work is needed to study the impact of feed conditions on phenol removal for a SWRO process, as well a more detailed assessment of process performance for phenol removal given a wide range of feed conditions. More importantly, the solution-diffusion model is characterised by investigating only two transport parameters, which produces more accurate prediction results compared to those from the irreversible thermodynamics model, which uses three transport parameters. In the respect, Mujtaba (2012) confirmed that the solution-diffusion model is simpler and more accurate for estimating membrane transport phenomena. Therefore, the core aim of this study is to carry out a comprehensive simulation of a SWRO process for gaining a deeper examination of the effect of feed conditions on phenol removal. The work will take into account the earlier one-dimensional distributed model developed by the author and based on the solution-diffusion principles. This work will consider a wide range of feed conditions in line with the manufacturer design limits. The previous study of Al-Obaidi et al. (2017b) did not include a parameter estimation, which is always used to yield the best model’s parameters. This research deals with this heads on in that it describes a comprehensive model, which uses the parameter estimation tool of gPROMS, to accomplish four objectives: a) to measure the accuracy of the proposed model for predicting phenol removal and process parameters against experimental data, b) to specifically forecast the values of the transport parameters of the membrane and the friction factor for each inlet feed concentration, c) to evaluate the effects of three main operating conditions namely feed flow rate, pressure, and temperature (in a wide range) on phenol removal for five cases of inlet feed concentration.

MODELLING OF SWRO PROCESS

Al-Obaidi et al. (2017b) have already developed a comprehensive one-dimensional model for a single SWRO process and which includes the physical property equations. This model is used to study the change of operating parameters with spatial dimension along the x-coordinate of feed side and to evaluate the elimination of chlorophenol from wastewater, based on a single SWRO process. This initial research has provided the motivation for applying the model, this time, for the removal of phenol from wastewater using the same process. For the convenience of the reader, the model assumptions are as follows:

(a) The solution-diffusion model is used to characterise the water and solute fluxes.
(b) Constant membrane characteristics and channel geometries.
(c) The friction parameter is utilised to identify the pressure drop in the x-coordinate of feed channel relying on Darcy’s law.
(d) 1 atm pressure along the permeate channel.
(e) Fixed phenol concentration in the permeate side and calculated as the mean of inlet and outlet permeate phenol concentrations.
(f) Isothermal separation process.

Code for the steady state model has been written and solved in the gPROMS (Process System Enterprise Ltd 2003), where the membrane is distributed into a specific number of segments of equal intervals (Δx) along the x-coordinate. Therefore, specified parameters of feed flow rate,
Table 1 | Modelling of the spiral wound RO of Al-Obaidi et al. (2017b)

<table>
<thead>
<tr>
<th>Model equations</th>
<th>Specifications</th>
<th>Eq. no.</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ F_{b(x)} = \left{ F_{b(0)} - (W \theta x \Delta P_{b(0)}) + \left( W \theta b \left( \frac{x^2}{2} \right) F_{b(0)} \right) + \left( W \theta b \left( \frac{W \theta b}{\ell} \right)^{0.5} \left( \frac{x^2}{2} \right) (\Delta P_{b(x)} - \Delta P_{b(0)}) \right) \right} ]</td>
<td>Feed flow rate at any point along the x-coordinate</td>
<td>1</td>
</tr>
<tr>
<td>[ \theta = \frac{A_w B_x}{B_x + R T_b A_w C_{p(aw)}} ]</td>
<td>Parameter in Equation (1)</td>
<td>2</td>
</tr>
<tr>
<td>[ U_{b(x)} = \frac{F_{b(x)}}{\ell W} ]</td>
<td>Velocity at any point along the x-coordinate</td>
<td>3</td>
</tr>
<tr>
<td>[ P_{b(x)} = \left{ P_{b(0)} - (b x F_{b(0)}) + \left( b W \theta \left( \frac{x^2}{2} \right) (\Delta P_{b(x)}) \right) - \left[ b^2 W \theta \left( \frac{x^2}{6} \right) F_{b(0)} \right] - \left[ b^2 W \theta \left( \frac{W \theta b}{\ell} \right)^{0.5} \left( \frac{x^2}{6} \right) (\Delta P_{b(x)} - \Delta P_{b(0)}) \right) \right} ]</td>
<td>Feed pressure at any point along the x-coordinate</td>
<td>4</td>
</tr>
<tr>
<td>[ \Delta P_{b(x)} = \Delta P_{b(0)} - (b x F_{b(0)}) - \left[ \left( \frac{W \theta b}{\ell} \right)^{0.5} b x (\Delta P_{b(x)} - \Delta P_{b(0)}) \right] ]</td>
<td>Pressure difference between the feed and permeate channels at any point along the x-coordinate</td>
<td>5</td>
</tr>
<tr>
<td>[ \Delta P_{b(0)} = P_{b(0)} - P_p ]</td>
<td>Pressure difference between the feed and permeate channels at x = 0</td>
<td>6</td>
</tr>
<tr>
<td>[ J_{w(x)} = \theta \left{ \Delta P_{b(0)} - (b x F_{b(0)}) \right} - \left[ \left( \frac{W \theta b}{\ell} \right)^{0.5} b x (\Delta P_{b(x)} - \Delta P_{b(0)}) \right] ]</td>
<td>Water flux at any point along the x-coordinate</td>
<td>7</td>
</tr>
<tr>
<td>[ J_{s(x)} = B_x (C_{w(x)} - C_{p(aw)}) ]</td>
<td>Solute flux at any point along the x-coordinate</td>
<td>8</td>
</tr>
<tr>
<td>[ \frac{(C_{w(x)} - C_{p(aw)})}{(C_{b(x)} - C_{p(aw)})} = \exp \left( \frac{J_{w(x)}}{k_{(x)}} \right) ]</td>
<td>Wall solute concentration at any point along the x-coordinate</td>
<td>9</td>
</tr>
<tr>
<td>[ k_{(x)} = 1.177 \left( \frac{U_{b(x)} D_{b(x)}}{\ell W} \right)^{0.3333} ]</td>
<td>Mass transfer coefficient of solute at any point along the x-coordinate (Wankat 1990)</td>
<td>10</td>
</tr>
<tr>
<td>[ D_{b(x)} = 6.725E - 6 \exp \left{ 0.1546E - 3 C_{b(x)} (18.012) - \frac{2513}{T_b + 273.15} \right} ]</td>
<td>Diffusivity at any point along the x-coordinate (Koroneos et al. 2007)</td>
<td>11</td>
</tr>
<tr>
<td>[ \frac{C_{b(x)}}{\ell W} \frac{dF_{b(x)}}{ds} + \frac{F_{b(x)}}{\ell W} \frac{dC_{b(x)}}{ds} = \frac{d}{ds} \left[ D_{b(x)} \frac{dC_{b(x)}}{ds} \right] - \frac{(J_{w(x)} C_{p(aw)})}{\ell} + \frac{(J_{s(x)} C_{b(x)})}{\ell} ]</td>
<td>Bulk solute concentration at any point along the x-coordinate (Lee et al. 2010)</td>
<td>12</td>
</tr>
<tr>
<td>[ C_{p(aw)} = \frac{C_{p(0)}}{2} ]</td>
<td>Average permeate solute concentration</td>
<td>13</td>
</tr>
</tbody>
</table>

(continued)
pressure, solute concentration, and temperature with one atmospheric permeate pressure, the proposed model is able to estimate the longitudinal difference of all associated parameters in the feed and permeate sides along the x-coordinate. However, the constants used in the model include the membrane transport parameters of water and solute, and the friction factor. These are required to be estimated before solving the model, as shown more specifically under ‘Parameter estimation’. The corresponding model equations are provided in detail in Table 1.

EXPERIMENTAL APPARATUS AND PROCEDURE

This is based on a pilot-scale SWRO treatment system of one thin-composite membrane practised by Srinivasan et al. (2010) in the experiments of low-concentration feed solutions of phenol of specific concentrations, as described below.

Table 2 shows the features of the SW module. The experiments were carried out for five groups of inlet feed concentrations of 2.125, 4.25, 6.375, 8.5 and 10.6 × 10⁻³ kmol m⁻³, where the feed was pumped at a constant feed flow rate of 3.33 × 10⁻¹ m³ s⁻¹ (Marcovecchio et al. 2005). Also, for each group of inlet feed concentrations, the experiments were carried out for a set of inlet feed pressures of 4.93, 6.9, 8.9, 10.9, 12.8 and 14.8 atm with a range of 31.5–34.5 °C of operating temperature.

PARAMETER ESTIMATION

Solving any model equations, such as the one developed for RO membrane, necessitates allocating the unknown parameters and feed conditions. In the simulation study, the experimental data of Srinivasan et al. (2010) are employed to predict the optimum values of unknown parameters for each run of experiments. These are then deployed with the known parameters to estimate the removal of phenol

| Make | Ion Exchange, India |
| Module configuration and membrane material | SW and commercial TFC (thin film composite) |
| Membrane area (A), module width (W), length (L), and diameter | 0.75 m², 1.6667 m, 0.45 m, and 0.0635 m |
| Feed (t_f) and permeate t_p spacers thickness | 0.85 mm and 0.78 mm |

Table 1 | Model equations

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Eq. no.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeate solute concentrations at x = 0 and x = L (Al-Obaidi et al. 2020)</td>
<td>14 15</td>
</tr>
<tr>
<td>Permeate flow rate at any point along the x-coordinate</td>
<td>16</td>
</tr>
<tr>
<td>Water recovery</td>
<td>17</td>
</tr>
<tr>
<td>Solute removal (Srinivasan et al. 2010)</td>
<td>18</td>
</tr>
</tbody>
</table>

| Table 2 | Membrane features and geometry

| Make | Ion Exchange, India |
| Module configuration and membrane material | SW and commercial TFC (thin film composite) |
| Membrane area (A), module width (W), length (L), and diameter | 0.75 m², 1.6667 m, 0.45 m, and 0.0635 m |
| Feed (t_f) and permeate t_p spacers thickness | 0.85 mm and 0.78 mm |
under the specified feed conditions. Specifically, the parameter estimation tool of the gEST in the gPROMS is employed to forecast the unknown parameters of $A_w$ (water permeability constant), $B_s$ (solute permeability constant), and $b$ (friction factor).

The principle of parameter estimation is characterised by minimising the sum of square errors (SSE) between the model prediction and observational data of retentate concentration, retentate flow rate, retentate pressure, average permeate concentration, solute removal and total permeate flow rate. This is already carried out by an initial guestimate of the required parameter that would be altered until reaching an optimal value of the lowest possible SSE. The mathematical optimisation solver tool called MXLKHD (Maximum Likelihood) is used to carry out the parameter estimation in the gPROMS software suite. Specifically, Successive Quadratic programming (SQP) technique was successfully employed to solve the optimisation problem, which was addressed as a Non-Linear Programming (NLP) problem (Jarullah et al. 2011).

The optimisation problem of parameter estimation can be expressed as:

- Given: feed phenol concentration $C_{b(0)}$, pressure $P_{b(0)}$, feed flow rate $F_{b(0)}$, and temperature $T_b$.
- Obtain: Model constants include water permeability constant $A_w$, solute permeability constant $B_s$, and friction factor $b$.
- Minimising: SSE
- s.t.: process model and process constraints.

For instance, the mathematical expression of SSE can be formulated as follows:

$$\text{SSE} = \sum_{i=1}^{N_{\text{Data}}} \left[ C_{b,L}^{\text{Exp}} - C_{b,L}^{\text{Cal}} \right]^2$$

(1)

$C_{b,L}^{\text{Exp}}$ and $C_{b,L}^{\text{Cal}}$ denote the experimental and model prediction of the retentate concentration, respectively.

The mathematical expression of the parameter estimation is as follows:

$$\text{Min} \quad \text{SSE}$$

$$A_w, B_s, b$$

s.t. Equality constraints:

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

Inequality constraints:

$$A_w^L \leq A_w \leq A_w^U$$

$$B_s^L \leq B_s \leq B_s^U$$

$$b^L \leq b \leq b^U$$

The parameter estimation results for the membrane transport parameters and friction factor of $A_w$, $B_s$, and $b$, respectively, for each run of experiments are given in Table 3. The same parameters are also estimated for the whole experiments and for each group of inlet feed concentration as reported in Table 3.

**MODEL VALIDATION**

Figure 1 shows a simple comparison between the model estimations of several operating parameters of the SWRO process against the observational data of five cases of operating feed phenol concentration carried out by Srinivasan et al. (2010). The operating parameters investigated include the retentate phenol concentration, average permeate phenol concentration, phenol removal, retentate flow rate, outlet permeate flow rate and retentate pressure. Mostly, a plausible corroborations between the model estimated values and observational over the ranges of operating parameters can be affirmed.

**INFLUENCE OF OPERATING CONDITIONS ON PHENOL REMOVAL**

The feed pressure, flow rate, and temperature parameters are highlighted as important factors, which control the removal of the RO process. It is imperative to explore the influence of feed parameters on RO process performance and more so for the elimination of highly toxic organic compounds. In this respect, the model shown in Table 1 is deployed to forecast the process. Clearly, the model is sensitive to different parameters of the process in so far as the phenol removal for the RO plant of a single SW module is concerned. This is why a more detailed analysis of the effect of operating parameters on phenol removal is required based on the experiments achieved by Srinivasan et al. (2010). These use five cases of inlet feed concentration of $2.125 \times 10^{-3}$, $4.25 \times 10^{-3}$, $6.375 \times 10^{-3}$, $8.5 \times 10^{-3}$, and $10.6 \times 10^{-4}$ kmol m$^{-3}$ with the following operating
Table 3 | Parameter estimation results of the gPROMS

<table>
<thead>
<tr>
<th>Case</th>
<th>Cb0, EO3</th>
<th>Pb(0)</th>
<th>Tb</th>
<th>Aw</th>
<th>B_1</th>
<th>b</th>
<th>A_w</th>
<th>B_1</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.125</td>
<td>4.93</td>
<td>32.5</td>
<td>1.578×10^{-6}</td>
<td>2.049×10^{-6}</td>
<td>13,010.4</td>
<td>1.3974×10^{-6}</td>
<td>1.838×10^{-6}</td>
<td>12,999</td>
</tr>
<tr>
<td>2</td>
<td>2.125</td>
<td>6.9</td>
<td>33.1</td>
<td>1.406×10^{-6}</td>
<td>1.850×10^{-6}</td>
<td>13,042.6</td>
<td>1.289×10^{-6}</td>
<td>1.046×10^{-6}</td>
<td>12,969.8</td>
</tr>
<tr>
<td>3</td>
<td>2.125</td>
<td>8.9</td>
<td>33</td>
<td>1.394×10^{-6}</td>
<td>1.827×10^{-6}</td>
<td>13,486.9</td>
<td>8.5</td>
<td>14.8</td>
<td>33.5</td>
</tr>
<tr>
<td>4</td>
<td>2.125</td>
<td>10.9</td>
<td>33.4</td>
<td>1.444×10^{-6}</td>
<td>1.708×10^{-6}</td>
<td>13,536.4</td>
<td>1.289×10^{-6}</td>
<td>1.046×10^{-6}</td>
<td>12,969.8</td>
</tr>
<tr>
<td>5</td>
<td>2.125</td>
<td>14.8</td>
<td>34</td>
<td>1.274×10^{-6}</td>
<td>1.047×10^{-6}</td>
<td>12,909.7</td>
<td>6.375</td>
<td>14.8</td>
<td>34</td>
</tr>
</tbody>
</table>

For the whole experiments:

\[ A_w = 1.1803 \times 10^{-6} \]
\[ B_1 = 1.0408 \times 10^{-6} \]
\[ b = 12,973.9 \]

parameters of upper and lower feed pressure, flow rate, and temperature of (4–20 atm), \((5 \times 10^{-5} - 1 \times 10^{-3} \text{ m}^3\text{ s}^{-1})\), and \((20–40 \degree \text{C})\), respectively. The specified limits of operating conditions are within the permissible recommended range of the manufacturer. The model transport coefficients \(A_w, B_1\) and \(b\) have been assumed constant for each case of inlet feed concentration in the simulation study, as reported in Table 3.

The individual and interactive influence of operating parameters on phenol removal for low and high inlet feed concentration, case 1 and case 5, respectively, can be shown in the three-dimensional response surface plots of Figures 2–6. Most importantly, the optimal conditions of operating parameters that lead to a maximum phenol removal can be determined for each case of inlet feed concentration, as detailed in the following section.

At low feed concentration of \(2.125 \times 10^{-3}\) kmol m\(^{-3}\) (case 1), the response of phenol removal to the deviation in both inlet feed pressure and flow rate is shown in Figures 2 and 5 at 34 \degree \text{C} of operating temperature. Note that the range of feed flow rate examined is quite large, as depicted in Figures 2 and 5.

For the range of low to medium inlet feed flow rates \((5 \times 10^{-5} - 3 \times 10^{-4} \text{ m}^3\text{ s}^{-1})\), Figure 2 depicts that the influence of feed pressure on the elimination of phenol is quite variable, as it is associated with two different behaviors against the removal parameter. At low operating pressure of up to 9 atm, the phenol removal increases as a result of an increase in the pressure. This is because of the growth in the driving force of water flux, which in turn lessens the phenol concentration at the permeate side. However, beyond the pressure of 9 atm, the phenol removal decreases up to the higher feed...
On the other hand, Figure 3 depicts the same tested operating parameters of feed pressure for a medium and high inlet feed flow rate range between \(3.3 \times 10^{-4} - 1 \times 10^{-3} \text{ m}^3 \text{s}^{-1}\). Here, the phenol removal is steadily improved due to an increase in the pressure. This can be ascribed to the influence of high feed flow rate, which causes a reduction in the wall membrane concentration. The high feed flow rate positively diminishes the impact of concentration polarisation by increasing the turbulence inside the module. The net effect of all this is an elevation of the flux of water even when increasing the pressure drop due to an increase in the feed flow rate. More importantly, running the process at high feed flow rate and low pressure actually deteriorates the removal parameter (Figure 3). This depicts that the positive effect of feed pressure is negligible even with a lower residence time of the fluid inside the module. Also, it can be noted that the optimum phenol removal for the second range of feed flow rate of \(3.3 \times 10^{-4} - 1 \times 10^{-3} \text{ m}^3 \text{s}^{-1}\) has been achieved within a range of 13–20 atm. This is comparable with the first lower range of feed flow rate of \(5 \times 10^{-5} - 5 \times 10^{-4} \text{ m}^3 \text{s}^{-1}\), which was conducted between 7.5 and 9 atm, as shown in Figure 2.

In summary, running the process, at high inlet feed flow rate and low feed concentration and constant temperature of 34°C can yield an optimum phenol removal with higher inlet operating pressures.

Figure 4 displays the influence of operating temperature on the phenol elimination for the same set of feed pressures tested. It is detected that the increase of feed temperature has a positive influence on removal parameter especially for the range of temperatures tested. The reduction in solution viscosity and density when increasing the phenol diffusion parameter are the main causes for the phenol removal increase. Another conclusion that can be drawn from Figure 4 is that increasing the temperature from 20°C to 40°C has a weighty impact on phenol removal at high feed pressures compared to low operating pressures. This is ascribed to the influence of the feed pressure, which is considered as the main key parameter of the RO process. However, the simulation results shown in Figure 4 are based on the assumption of constant water and solute transport parameters for the range of operating temperatures of 20–40°C tested.

For the high inlet feed concentration of \(10.6 \times 10^{-3} \text{ kmol} \text{ m}^{-3}\) (case 5), Figures 5 and 6 represent the simulation outputs of the change in pressure and flow rate at operating temperature of 34°C. Firstly, it is noted that growing the feed concentration to \(10.6 \times 10^{-3} \text{ kmol m}^{-3}\) would increase phenol removal for all the pressures tested. Interestingly, despite the fact that growing the feed concentration causes a growth in the concentration polarisation and phenol concentration, this is not the only factor affecting the removal process.
concentration at the permeate side, the increase of permeate concentration is incomparable with the growth of feed concentration in the feed side. This leads to an increase of the phenol removal in line with Equation (18) of Table 1.

Same results were detected for the three kinds of membranes and used by Gómez et al. (2009).

In addition, Figures 5 and 6 show that any increase in the feed flow rate would promote phenol removal. This is
due to reducing of the osmotic pressure and the increase of the mass transfer coefficient, which positively aids to limit the concentration polarisation effect and feed concentration at the membrane surface. Having said this, it is possible to use a range of higher inlet feed flow rates to assure higher phenol removal (Figure 6).

For low ranges of feed flow rate of $5 \times 10^{-5} - 3 \times 10^{-4}$ m$^3$ s$^{-1}$, Figure 5 shows that the maximum phenol removal is achieved between 7.5 and 9 atm, where a steady reduction beyond this pressure is observed. This reduction is the result of the increase of the bulk concentration and associated osmotic pressure of the feed side. This lessens the water flux via the membrane pores. The optimum phenol removal is carried out between 10.5 and 20 atm for the second range of feed flow rates of $3.5 \times 10^{-4} - 1 \times 10^{-3}$ m$^3$ s$^{-1}$, with a steady increasing of removal parameter when the feed pressure is increased.

The above simulation results have demonstrated the need to carry out an optimisation study to explore the optimum phenol removal of a singular SWRO process especially at different feed concentrations.

**CONCLUSIONS**

In this study, a one-dimensional steady-state accurate model was applied to explore the influences of the operating conditions on the removal of phenol from synthesised wastewater. The reliability of the model was verified in contradiction to real observational data of phenol removal from the open literature using SWRO process. A sensitivity analysis was then conducted to evaluate the influence of three feed parameters, within the maximum and minimum manufacturers' bounds of feed pressure, flow rate and temperature, on phenol removal for five cases of inlet feed concentration. One of the key findings of this research was that for any inlet feed concentration and low range of feed flow rate conditions, increasing the operating pressure
beyond a certain value results in actually deteriorating phenol removal. However, the same has not been observed for high inlet feed flow rate conditions, where the removal phenol parameter showed a steady increase.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

REFERENCES

Tabassi, D., Mnif, A. & Hamrouni, B. 2014 Influence of operating conditions on the retention of phenol in water by reverse osmosis SG membrane characterized using Spiegler-Kedem model. Desalination and Water Treatment 52, 1792–1803.

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