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

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Abstract

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

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

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

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

Introduction

Dimethylphenol is one of the phenolic organic compounds which can be certainly found in many industrial (petroleum processing, plastic manufacturing, disinfectants, pesticides, herbicides and resins production) effluents (Gami *et al.*, 2014). A number of agencies such as the Agency of Toxic Substances and Disease Registry (ATSDR) and United States Environmental Protection Agency (EPA) have listed dimethylphenol as a highly toxic compound even in low concentrations and one that, has an ability to remain in the environment for a long period of time. Water UK regulators have set the maximum concentration of phenol in the discharge wastewater of hospitals to be within 10 ppm (Water UK, 2011), while ATSDR has limited the presence of dimethylphenol at a maximum of 0.05 ppm in surface water (ATSDR, 2015). Clearly, much attention has already been paid to establish tight targets for removing this harmful pollutant from industrial effluents before discharging to surface water. Recent, conventional methods of phenolic compounds removal from wastewater include; the microbial degradation, adsorption, incineration, solvent extraction, irradiation, and chemical oxidation such as catalyst wet air oxidation and reverse osmosis (Witek *et al.*, 2006; Mohammed *et al.*, 2016).

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

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

The performance of individual and several spiral-wound RO modules in terms of industrial wastewater treatment has already been studied by considering a range of different operating conditions and different pollutants, such as copper (Chai *et al.*, 1997), nitrate (Cevaal *et al.*, 1995; Molinari *et al.,* 2001; Schoeman and Steyn, 2003), secondary treated sewage effluent (Qin *et al.,* 2004), synthetic effluent stream of acrylonitrile, sulphate, ammonium, cyanide and sodium (Bódalo-Santoyo *et al.,* 2004), copper and nickel (Mohsen-Nia *et al.,* 2007), chromium (Mohammadi *et al.,* 2009), di-hydrogen phosphate, sulphite, nitrate and nitrite (Madaeni and Koocheki, 2010) and bisphenol A (Khazaali *et al.,* 2014).

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

Modelling of spiral-wound reverse osmosis

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

The Assumptions

The following assumptions are made in the proposed model:

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

Governing Equations

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

$$J_w = A_w[\Delta P - \Delta\pi_{Total}] \tag{1}$$

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

$$J_s = B_s\left(C_m - C_p\right) \tag{3}$$

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

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

$$\Delta\pi_{Total} = \left(\pi_m - \pi_p\right) \tag{4}$$

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

$$\pi_m = R\ (T + 273.15)\ C_m \tag{5}$$

$$\pi_p = R\ (T + 273.15)\ C_p \tag{6}$$

Where R and T (atm m³/kmol K, °C) are the gas constant and constant operating temperature (Assumption 6) respectively. The concentration of solute at the wall membrane was estimated based on Assumption 3, which in turn is based on the validity of the film model theory where the solvent flux is linked to the concentration polarization and mass transfer coefficient k (m/s) based on the following equation:

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

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

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

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

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

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

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

Where ρ_w is the molal density of water (55.56 kmol/m^3).

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

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

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

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

$$de_b = 2t_f \quad (13)$$

$$de_p = 2t_p \quad (14)$$

t_p (m) is the height of permeate channel.

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

$$D_b = 6.725E-6\ exp\left\{0.1546E-3\ C_f\, x18.01253\ -\frac{2513}{T+273.15}\right\} \quad (15)$$

$$D_p = 6.725E-6\ exp\left\{0.1546E-3\ C_p\, x18.01253\ -\frac{2513}{T+273.15}\right\} \quad (16)$$

$$\mu_b = 1.234E-6\, exp\left\{0.0212E-3\ C_f\, x18.0153 + \frac{1965}{T+273.15}\right\} \quad (17)$$

$$\mu_p = 1.234E-6\, exp\left\{0.0212E-3\ C_p\, x18.0153 + \frac{1965}{T+273.15}\right\} \quad (18)$$

$$\rho_b = 498.4\, m_f + \sqrt{\left[248400\, m_f^2 + 752.4\, m_f\, C_f\, x18.01253\right]} \quad (19)$$

$$\rho_p = 498.4\, m_f + \sqrt{\left[248400\, m_f^2 + 752.4\, m_f\, C_p\, x18.01253\right]} \quad (20)$$

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

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

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

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

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

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

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

$$P_{f(out)} = P_{f(in)} - \frac{bL}{\emptyset \sinh \emptyset}\left\{\left(Q_f + Q_r\right)(cosh\emptyset - 1)\right\} \tag{24}$$

Where $\emptyset, b$ and L (dimensionless, atm s /m^4, m) are dimensionless term defined in Eq. (25), friction parameter and membrane length respectively.

$$\emptyset = L\sqrt{\frac{W\ b\ A_W}{\left[1+\left(\frac{A_W\ R\ C_p\ (T+273.15)}{B_S}\right)\right]}} \tag{25}$$

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

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

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

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

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

$$Q_f = Q_r + Q_p \tag{28}$$

$$Q_f\ C_f = Q_r\ C_r + Q_p\ C_p \tag{29}$$

Where C_f, C_r and C_p (kmol/m^3) are the concentration of dimethylphenol in feed, retentate and permeate channel respectively. Also, Eq. (30) is used to calculate the concentration at the permeate channel (Al-Obaidi *et al.*, 2017).

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

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

$$Rej = \frac{C_f - C_p}{C_f} \; x100 \tag{31}$$

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

$$Rec = \frac{Q_p}{Q_f} \; x100 \tag{32}$$

Where Q_p (m^3/s) is the total permeated flow rate calculated using Eq. (33).

$$Q_p = J_w \; A \tag{33}$$

Where A (m^2) is the effective membrane area.

Module configurations and mathematical modelling

Reverse osmosis membrane systems are typically used as a network of different numbers of stages that should be designed in a way to meet the requirement of the separation process including environmental and economic impacts. Here, in order to reduce the number of RO networks and the complexity of the superstructure problem, the proposed wastewater RO full-scale plant is designed consisting of only three modules but connected differently to generate four possible RO networks. Each module holds a maximum of two pressure vessels connected in parallel, while each pressure vessel holds only one spiral-wound RO membrane type HM4040-LPE supplied by Ion Exchange, India of 7.85 m^2 area. The schematic diagrams of four proposed superstructures of RO network for wastewater treatment can be seen in Fig. 1. These layouts are essentially similar to the specification of actual networks used for RO seawater desalination process presented by Abbas (2005).

In the series configuration, the concentrated stream of the first membrane element becomes the feed stream of the subsequent element and so on, while, the permeate streams of three elements are blended to form the product stream of the plant. Configuration A shows two parallel modules in the first stage and the concentrate streams of these modules are mixed to form the feed of the second stage module.

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

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

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

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

$$Q_{p(Plant)} = \sum_{s=1}^{n} Q_{p(s)} \tag{36}$$

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

$$Q_{f(plant)}\, C_{f(plant)} = Q_{r(plant)}\, C_{r(plant)} + Q_{p(plant)}\, C_{p(plant)} \tag{38}$$

$$Rej_{(plant)} = \frac{C_{f(plant)} - C_{p(plant)}}{C_{f(plant)}}\, x100 \tag{39}$$

$$Rec_{(plant)} = \frac{Q_{p(plant)}}{Q_{f(plant)}}\, x100 \tag{40}$$

An appropriate simulation model has been designed and developed for a spiral-wound reverse osmosis membrane module in steady state mode and for a multi-stage plant, which describes the variation of all the operating parameters along the stages using the gPROMS software (general Process Modelling System by Process System Enterprise Ltd. 2001). The gPROMS Model Builder provides a good modelling platform for steady state and dynamic simulation, optimisation, experiment design and parameter estimation of any process. The model equations are solved for a given inlet plant feed flow rate, pressure, dimethylphenol concentration and temperature. The proposed model can predict the variation of all parameters along the stages and pressure vessels. The steady state process model consisting of nonlinear algebraic equations presented earlier can be written in the following compact form:

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

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

Model Validation

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

Fig. 2 provides a comparison between experimental results and model prediction of retentate flow rate, permeate flow rate, retentate pressure, total permeate recovery and dimethylphenol rejection at inlet feed conditions of a set of three inlet feed flow rates of 2.166E-4, 2.33E-4 and 2.583E-4 m^3/s with inlet feed pressure of 5.83, 7.77, 9.71, 11.64 and 13.58 atm for inlet feed concentration and temperature of 6.548E-4 kmol/m^3 and 31.5 °C respectively. Generally, the predicted values of the model correlate well with experimental results over the ranges of pressure and flow rate. This readily shows the suitability of the model to measure the observed rejection data with an acceptable error range.

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]

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

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

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

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

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

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

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

Finally, Fig. 7 shows the relationship existing between the inlet plant feed flow rate as a function to dimethylphenol rejection parameter and the recovery rate of four configurations at inlet feed conditions of 6.548 kmol/m^3, 17.7 atm and 32 °C. The simulated results shown in Fig. 7 clearly indicate that the rejection parameter of any RO network increases due to an increase in the inlet feed flow rate. This has the net effect of reducing the concentration polarization impact. While, the recovery rate actually reduces as a result to an increase in the inlet feed flow rate. This is due to a reduction of residence time of the fluid inside the feed channel, which in turn decreases the quantity of permeated water through the membrane.

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

Fig. 3. The inlet feed concentration of the plant as a function to the total pressure loss and retentate rate for configuration A at initial conditions of 8.5112E-4 m³/s, 19 atm and 35 °C

Fig. 4. The inlet feed pressure of the plant as a function to the total pressure loss and permeate flow rate for configuration B at initial conditions of 5E-4 m³/s, 2.455E-3 kmol/m³and 34 °C

Fig. 5. The inlet feed temperature of the plant as a function to the total pressure loss and rejection for configuration C at initial conditions of 2E-4 m³/s, 6.548E-3 kmol/m³ and 15 atm

Fig. 6. The inlet feed flow rate of the plant as a function to the total pressure loss and recovery for configuration D at initial conditions of 6.548E-3 kmol/m³ and 15.5 atm and 36 °C

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

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

Optimal RO configuration and operating conditions

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

Problem description and formulation

The objective function here is to optimise the rejection of dimethylphenol under different feed concentrations for different RO networks of three elements of spiral-wound membrane type HM4040-LPE supplied by Ion Exchange, India as shown in Fig. 1. This involves four RO configurations and allows the underlying optimizer to facilitate the selection of the optimal RO network that can achieve the required higher rejection of dimethylphenol. The planned outcome of this part of the research is the ability to predict a set of optimum operating conditions for a fixed RO framework. The problem of optimisation will be subjected to process and module constraints commensurate with the maximum allowable pressure drop for each element of 1.3817 atm. The last, but not least, constraint was chosen to meet the economic and technical requirements. Also, the optimisation technique utilizes the lower and upper limits of the membrane constraints of inlet pressure, flow rate and temperature as shown in Table 1. Finally, the best optimum design of RO network will be the one that yields higher dimethylphenol rejection and at the same time meets the constraints of the process for three cases of inlet feed concentration of 1.637, 2.455 and 6.548 kmol/m³ respectively.

The objective function is set to maximize the rejection of dimethylphenol at different feed concentration:

$$\underset{Q_{f(plant)},\, P_{f(in)(plant)},\, T_{(plant)}}{\text{Max}} \quad Rej$$

Subject to:

Equality constraints:

Process Model: $f(x, u, v) = 0$

Inequality constraints:

$$Q_{f(plant)}{}^{L} \leq Q_{f(plant)} \leq Q_{f(plant)}{}^{U}$$

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

$$T_{(plant)}{}^{L} \leq T_{(plant)} \leq T_{(plant)}{}^{U}$$

Where, U and L are the upper and lower limits of the selected RO network.

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

$$Q_f{}^L \leq Q_f \leq Q_f{}^U$$

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

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

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

RO networks optimisation results

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

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

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

Conclusions

The treatment of dimethylphenol aqueous solutions using a multi-stage RO network based on a spiral-wound module is mathematically modelled to simulate and optimize the rejection parameter commensurate with the limits of operation and the constraints of both the module and RO layout. The simulation and optimization methodologies developed were based on the solution-diffusion model constrained by the concentration polarization impact. The consistency and sensitivity of this new model has been tested against experimental data of dimethylphenol rejection from the literature using a pilot-scale RO system of a single spiral-wound RO membrane element. The results compare well with published results with an acceptable correlation error for most operating parameters. The impact of the main operating parameters of feed pressure, flow rate and temperature on the rejection were analysed for different RO networks. An optimization study has been carried out to measure the capability of different RO networks to reject dimethylphenol from its aqueous solutions at three different inlet feed concentrations constrained by the manufacturer's specification of module pressure loss and the upper and lower limits of the operating conditions. Specifically, the optimization results have shown that the parallel configuration can attain the highest rejection parameter within the lowest pressure loss in comparison to other configurations.

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

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Tables

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

Table. 2. The simulation results of four RO networks

Feed concentration x10^3, kmol/m³	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

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

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

Feed concentration x10^3, kmol/m³	Configuration	Decision variables			Max. pressure loss of element, atm	Total pressure loss of configuration, atm	Rej_{plant}
		$Q_{f(plant)}$ (m³/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