Simulation results of reverse osmosis mathematical models

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1 Introduction

In this document, the simulation results for three models of an RO process based on the studies of [1]–[3] have been explained. Two dynamics model and one steady state model have been analyzed and the effect of inputs on the outputs are investigated.

2 Steady-state analysis

The data needed to build the model is based on the information of Table 1 in study of [1]. The results of steady state response of the outputs have been illustrated in the following figures.

Table 1. The specific of feed water

Variable	Value
Feed permeate flow rate Q_f	$3\left(\frac{\mathrm{m}^3}{\mathrm{h}}\right)$
Feed pressure P_f	21.37 (bars)
Feed temperature C_f	25
Feed concentration C_f	10190 (ppm)

Spiral wound membranes are usually considered as cross flow separator to model its filtration process. The permeate flow rate through the membrane is strong function of the difference between feed pressure and osmotic pressure and is estimated by following equation

$$\mathrm{Q}_p = A_{\mathrm{perm}} S_e (\mathrm{TCF})(\mathrm{FF}) \left[\left(P_f - \frac{\Delta P_{fc}}{2} - P_p\right) - \left(\mathrm{CPF}\frac{\pi_f + \pi_b}{2} - \pi_p\right)\right] \tag{1}$$

Where A_{perm} the permeability of the membrane is, S_e is the membrane active surface area and both parameters are available from the RO membrane data sheet. In the RO process, higher the feed water temperature, higher the permeate flow rate. So a temperature correction factor (TCF) is introduced in the equation and it is approximated by the formulas provided by the DOW membrane manufacturer company.

$$\text{TCF} = \begin{Bmatrix} \exp\left[2640\left(\frac{1}{198} - \frac{1}{273 + T_w}\right)\right], T_w = 25^{\circ}\text{C} \\ \exp\left[3020\left(\frac{1}{198} - \frac{1}{273 + T_w}\right)\right], T_w < 25^{\circ}\text{C} \end{Bmatrix} \tag{2}$$

T_w is the feed water temperature. FF is the membrane fouling factor. Its value is unity for new membrane and decreases as the RO filtration time increases. P_f is the pressure of feed water entering the membrane module. ΔP_{fc} is the pressure drop along the membrane module (feed side pressure e concentrate side pressure) during the filtration process and is approximated by empirical formula as follows

$$\Delta P_{\text{fc}} = 0.756\left(\frac{Q_c + Q_f}{2}\right)^{1.7} \tag{3}$$

CPF is concentration polarization factor and is given by following empirical relation as follows

$$\text{CPF} = e^{(0.7Y)} \tag{4}$$

Y is the recovery ratio. π is the osmotic pressure of solution at a given salinity and temperature and is calculated by following practical short approximation reported in the

$$\pi = \begin{Bmatrix} \frac{C(T + 320)}{491000}, C < 20000\text{mg}/l \\ \frac{0.0117C - 34}{14.23} \cdot \frac{(T + 320)}{345}, C > 20000\text{mg}/l \end{Bmatrix} \text{bars} \tag{5}$$

T is the feed water temperature and C is the salinity in PPM or mg/l. From above equations permeate flow rate is calculated. Concentration of the salt in the filtered water is calculated by using following equation:

$$C_p = B_{\text{salt}} S_e(\text{TCF})\left[\text{CPF}\left(\frac{C_{\text{fc}}}{Q_p}\right)\right] \tag{6}$$

B_{salt} is the salt permeability of the membrane and is evaluated from manufacturer's data. Se is membrane active area. C_{fc} is the average concentration of the water on the concentrate side of the mem- brane module and is calculated by following formula.

$$C_{fc} = \frac{C_f + C_c}{2}, C_{\text{fc}} = C_f \ln\left(\frac{1}{1 - Y}\right)/Y \tag{7}$$

By making use of mass balance equation brine concentrate is calculated by following equation.

$$Q_f C_f = Q_p C_p + Q_c C_c \tag{8}$$

In the below figures the results for various test of the model based on the above equations are presented.

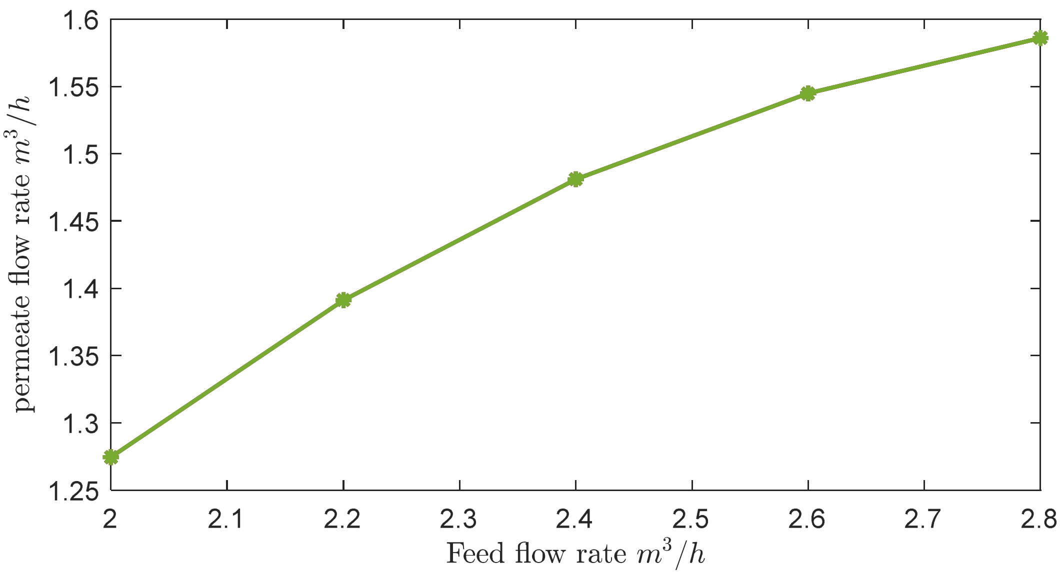

Figure 1. Permeate flow rate steady state response based on the change in feed flow rate.

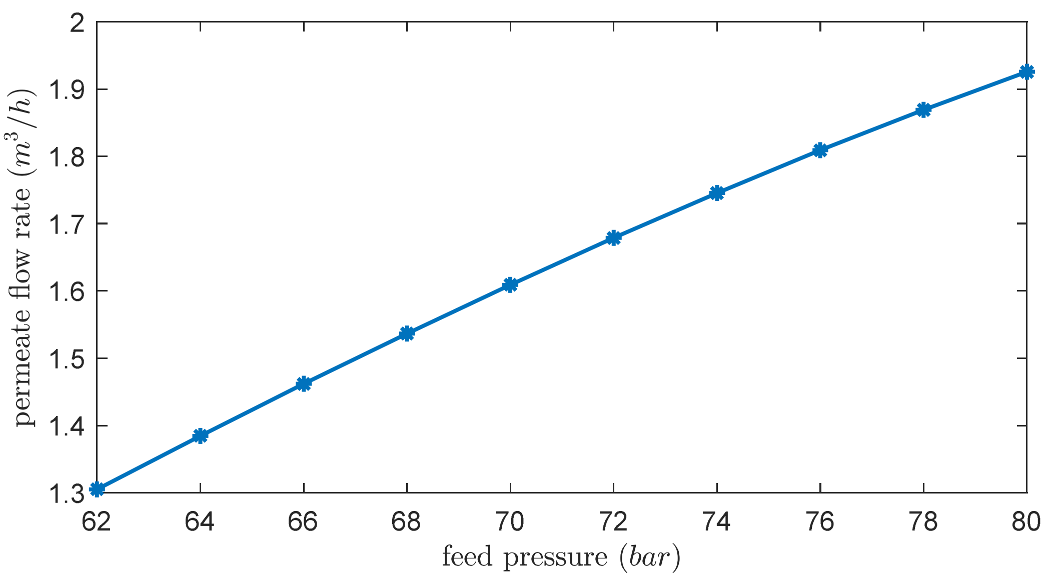

Figure 2. The changes in the steady state response of permeate flow rate based on the changes in feed pressure

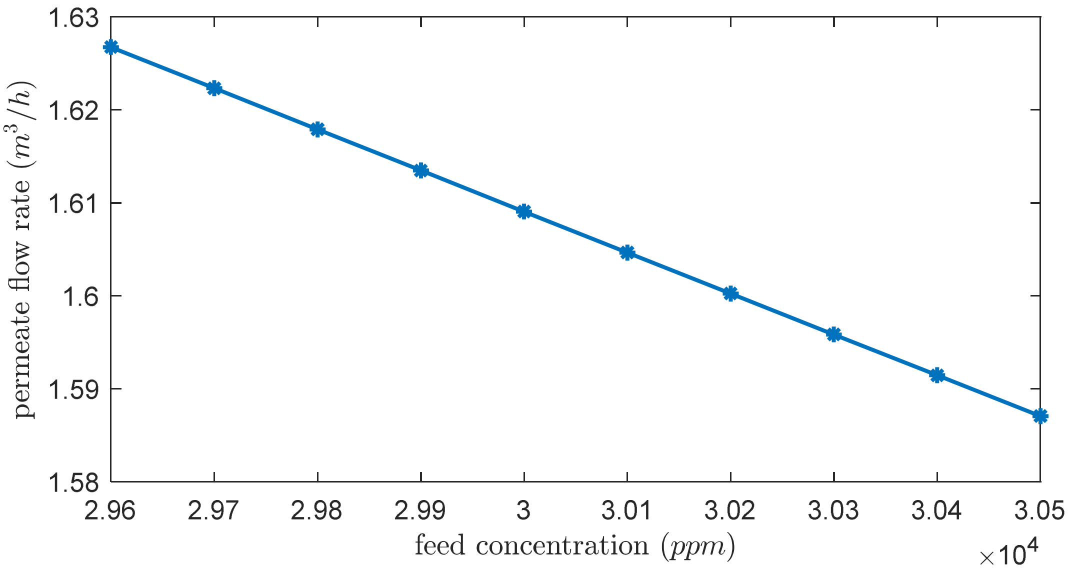

Figure 3. Changes in the permeate flow rate steady state response based on the changes in feed concentration

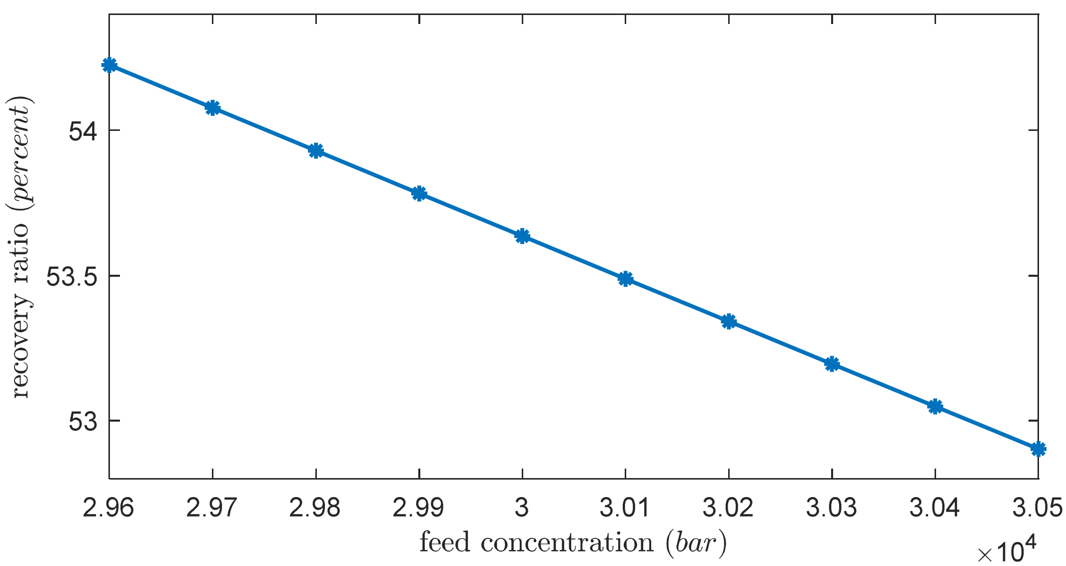

Figure 4. Changes in recovery ratio based on the feed concentration

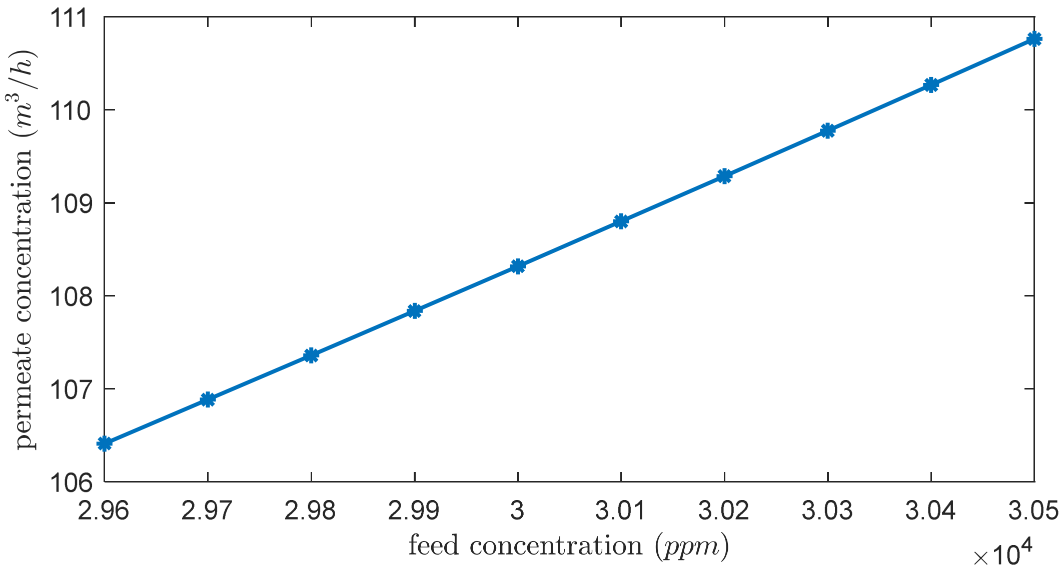

Figure 5. The changes in permeate concentration steady state response based on the feed concentration changes

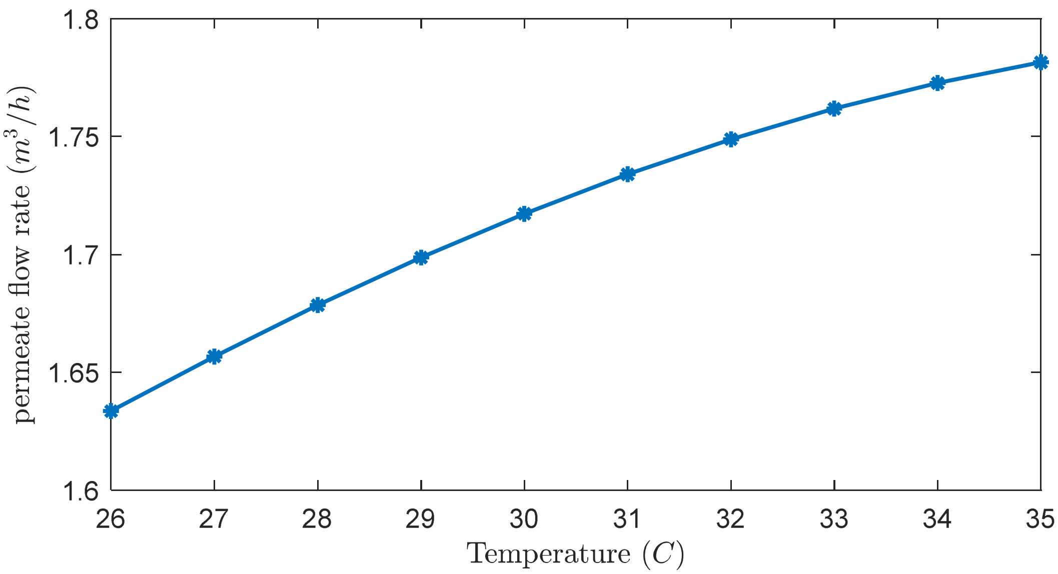

Figure 6. Changes in permeate flow rate steady state response based on the changes in various values for temperature.

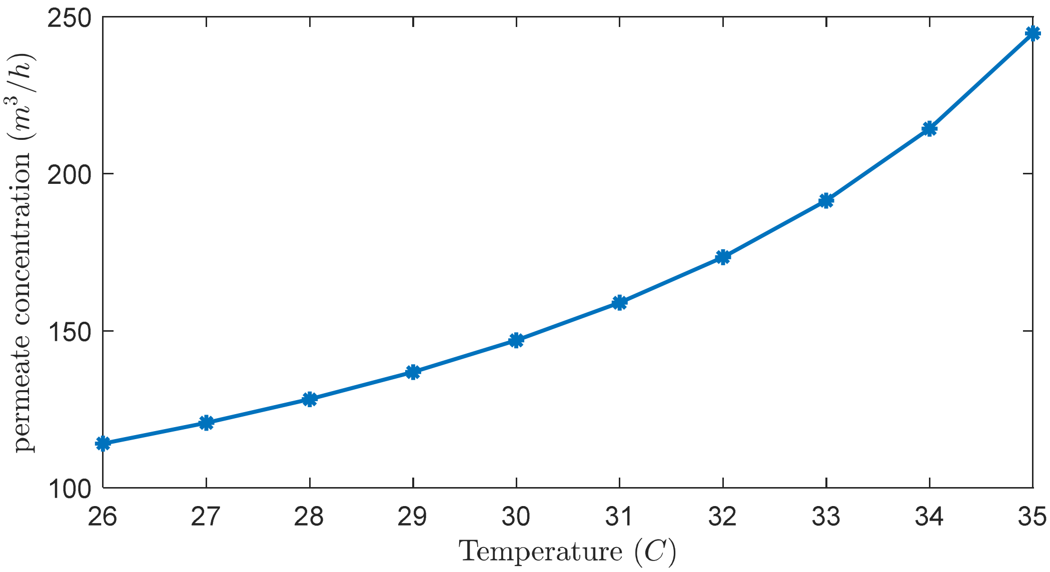

Figure 7. The effect of changing feed temperature on the permeate concentration steady state values.

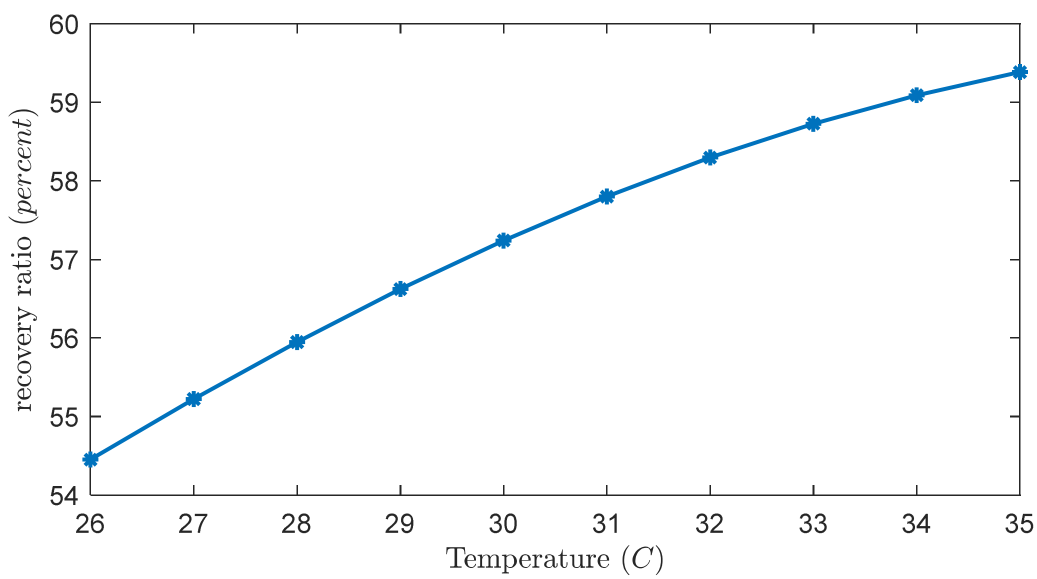

Figure 8. The changes in recovery ratio based on the changes in feed temperature

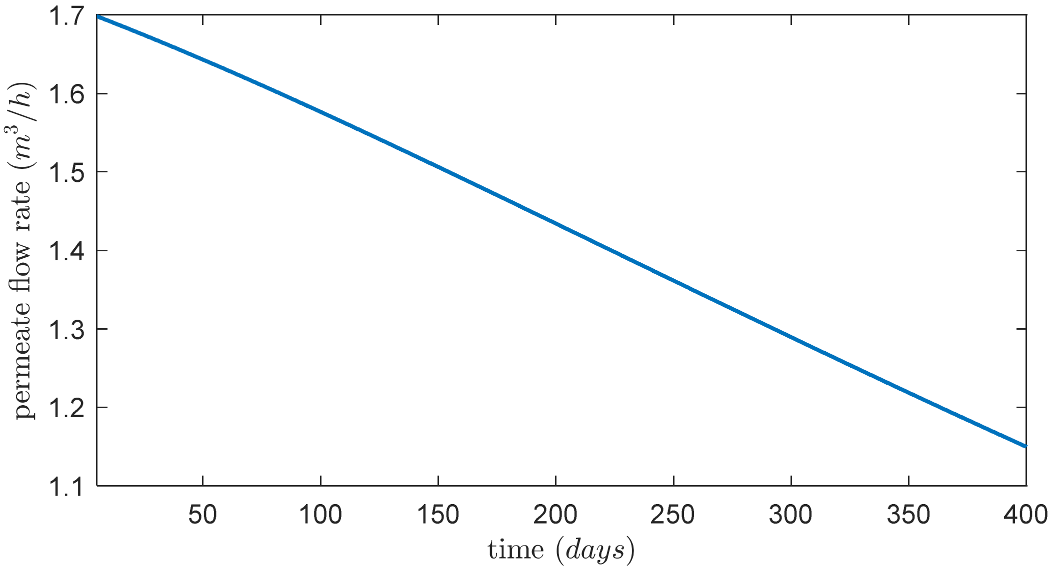

Figure 9. The effect of fouling on the permeate flow rate steady state response

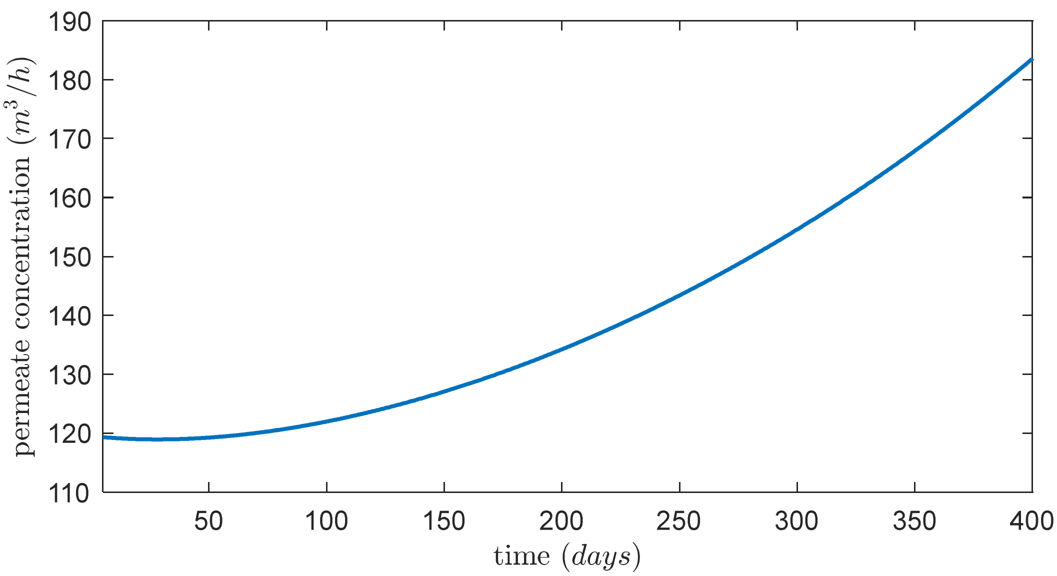

Figure 10. The effect of fouling on the permeate concentration steady state response

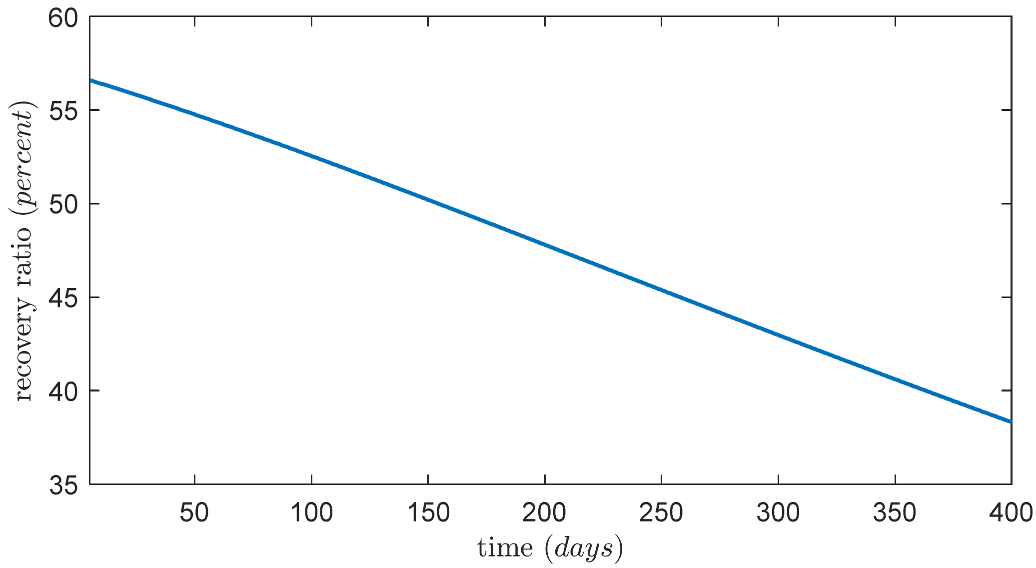

Figure 11. The effect of fouling on the recovery ratio during the 400 days.

2.1 Dynamic simulation of the reverse osmosis process

The following equations have been used to build a simple model [2].

name	Representation
Minimum and maximum brine flow rates	$F_{bmin} = F_f - F_{pmax}$ $F_{bmax} = F_f - F_{pmin}$
Minimum and maximum permeate flow rates	$F_{pmax} = \frac{R_r max}{R_f}$ $F_{pmin} = \frac{R_{rmin}}{100} F_f$
Brine flow rate	$F_b = F_{bmax} - \left(\frac{F_{b_b max} - F_{bmin}}{H_{max} - H_{min}}\right) H_{max} + \left(\frac{F_{bmax} - F_{bmin}}{H_{max} - H_{min}}\right) H$
Trans membrane pressure	$\Delta P = \frac{P_f + P_b}{2} - P_p$
Inherent reject valve characteristics	$F_b = R^{\left[\left(\frac{H}{100}\right)-1\right]} \sqrt{P_b - P_{bo}}$
Brine pressure	$P_b = R^{2\left[1-\left(\frac{H}{100}\right)\right]} F_b^2 + P_{bo}$
Water passage	$F_m = K_w(\Delta P - \Delta\pi) A_{em} T_m$
Salt passage	$F_s = K_s(C_f - C_p) A_{em} T_s$
Effective membrane area	$A_{em} = n_v n_e A_m$
Arrhenius equation	$T_m = e^{a_T\left(\frac{T_f - T_{ref}}{T_f}\right)}$

	$T_s = e^{b_T\left(\frac{T_f - T_{ref}}{T_f}\right)}$
Net osmotic pressure	$\Delta\pi = \frac{\pi_f + \pi_b}{2} - \pi_p$
Feed osmotic pressure	$\pi_f = 75.84 \times 10^3 C_f$
Brine osmotic pressure	$\pi_b = 75.84 \times 10^3 C_b$
Permeate osmotic pressure	$\pi_b = 75.84 \times 10^3 C_p$

The model is simulated based on the provided information in Table 2.

Table 2. Simulation model inputs

Simulation model input parameters for testing nominal operation of the RO process.

Variable	Value
Feed flow, F_f [kg/s]	50
Feed pressure, P_f [kPa]	5883.99
Feed concentration, C_f [ppm]	41350
Feed temperature, T_f [°K]	301.65
Salt rejection, *SR* [%]	97.94
Recovery rate, R_r [%]	44.44
Minimum recovery rate, R_{rmin} [%]	10
Maximum recovery rate, R_{rmax} [%]	50
Reject valve percentage opening, *H* [%]	47.6507

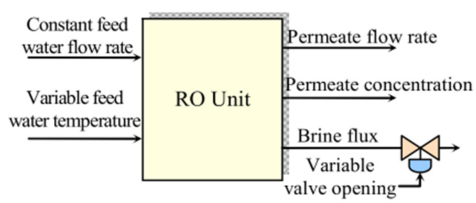

Figure 12. block diagram of Ro unit

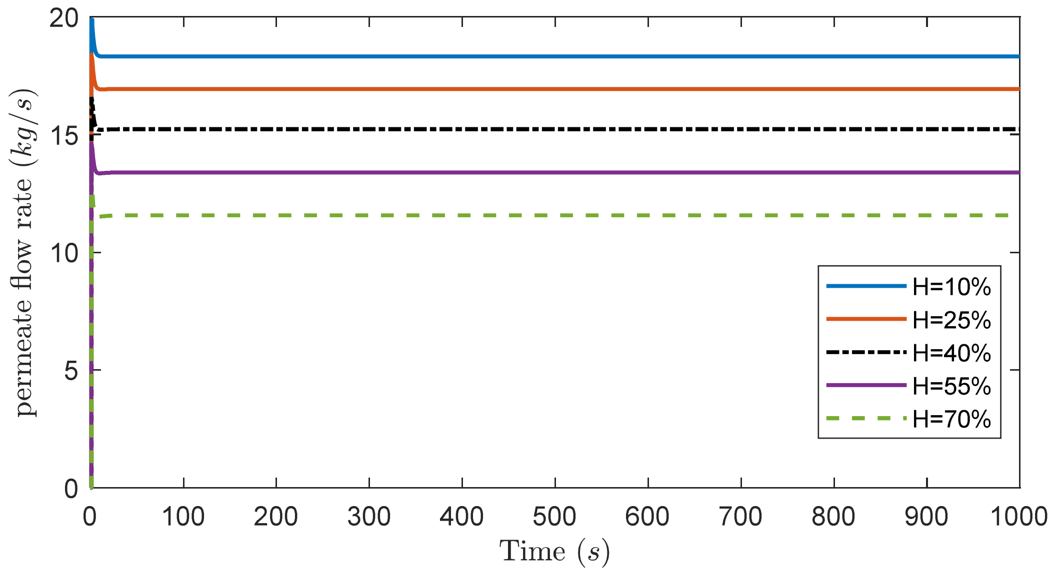

Figure 13. Change in transient response of permeate flow rate based on the opening of the valve at brine side

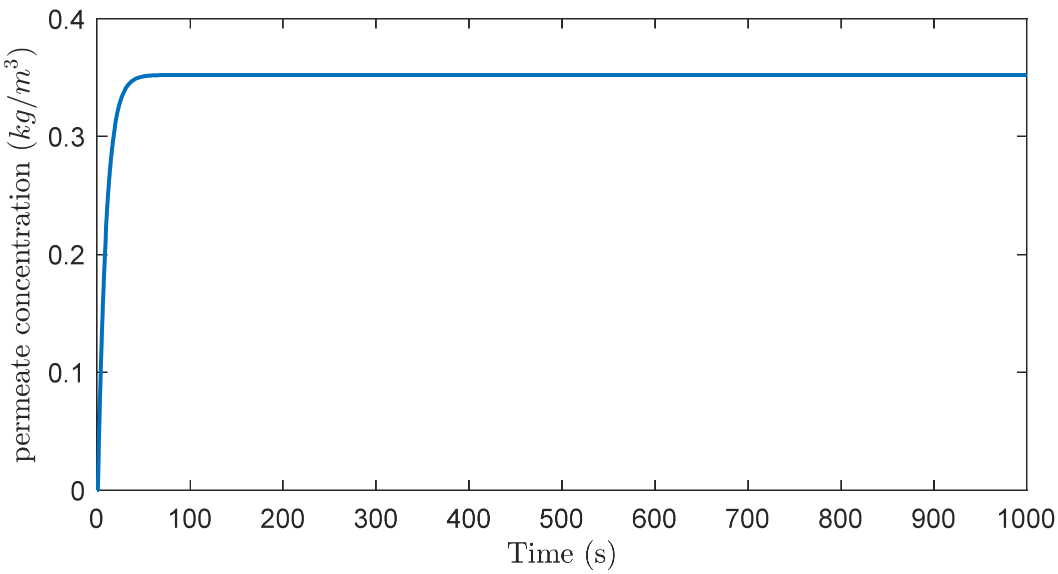

Figure 14. Transient response for permeate concentration

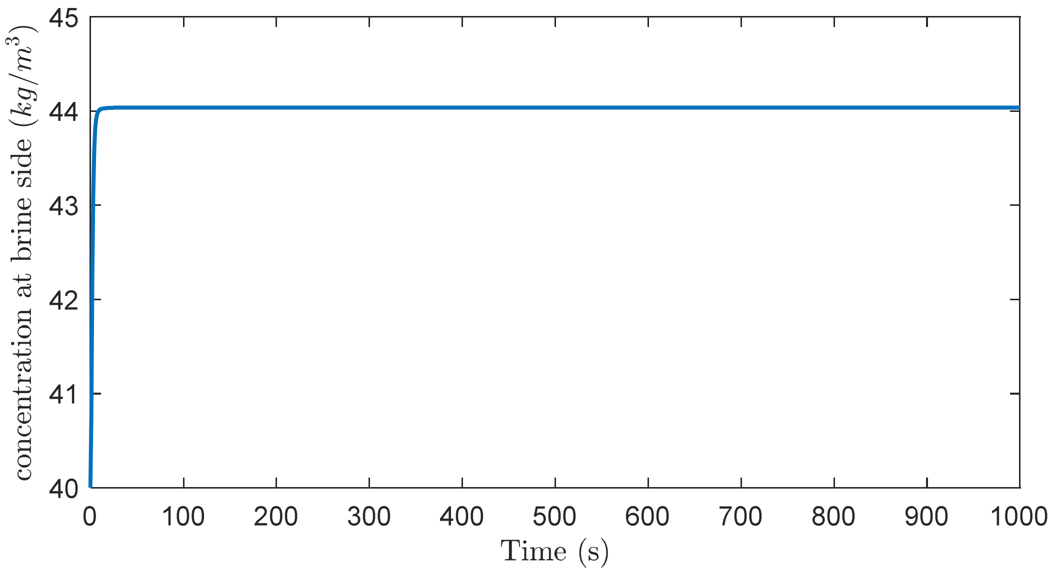

Figure 15. Transient response for brine concentration

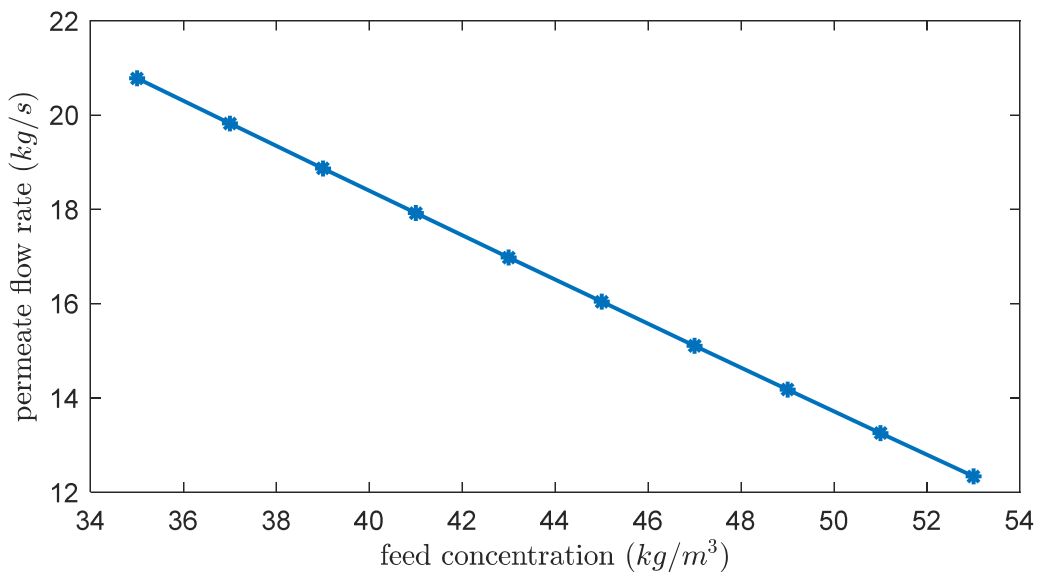

Figure 16. Change in steady state response of permeate flow rate by changing the feed concentration

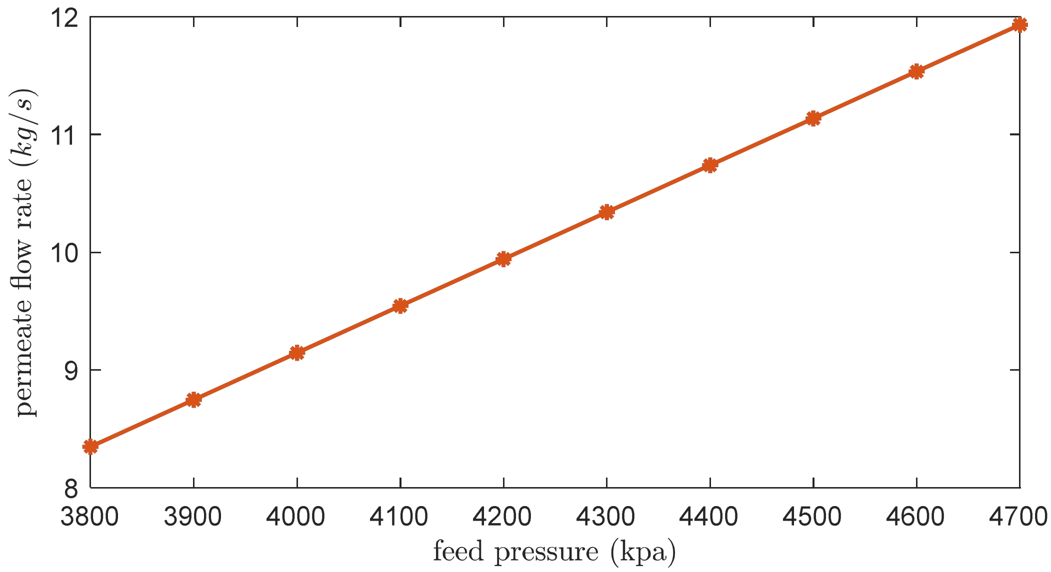

Figure 17. Change in the steady state response of permeate flow rate by changing in the feed pressure

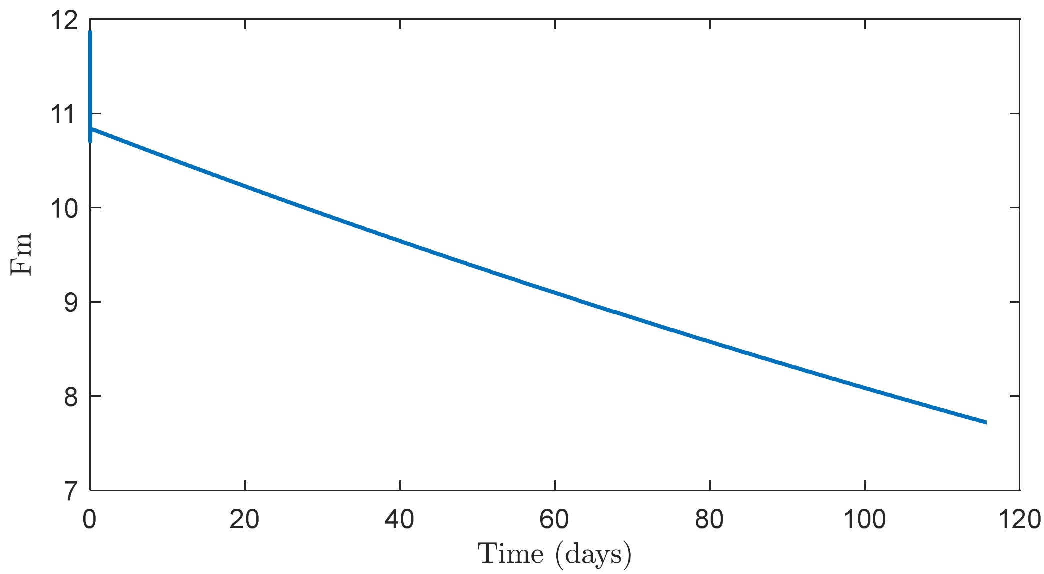

Figure 18. The effect of fouling based on the days elapsed on the membrane water passage

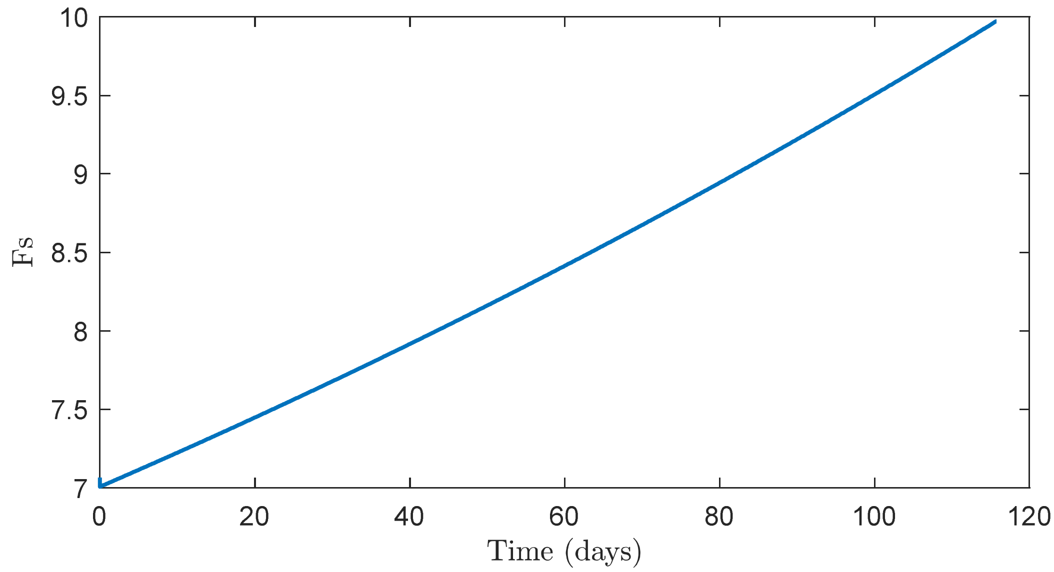

Figure 19. The effect of fouling based on the days elapsed on the membrane salt passage

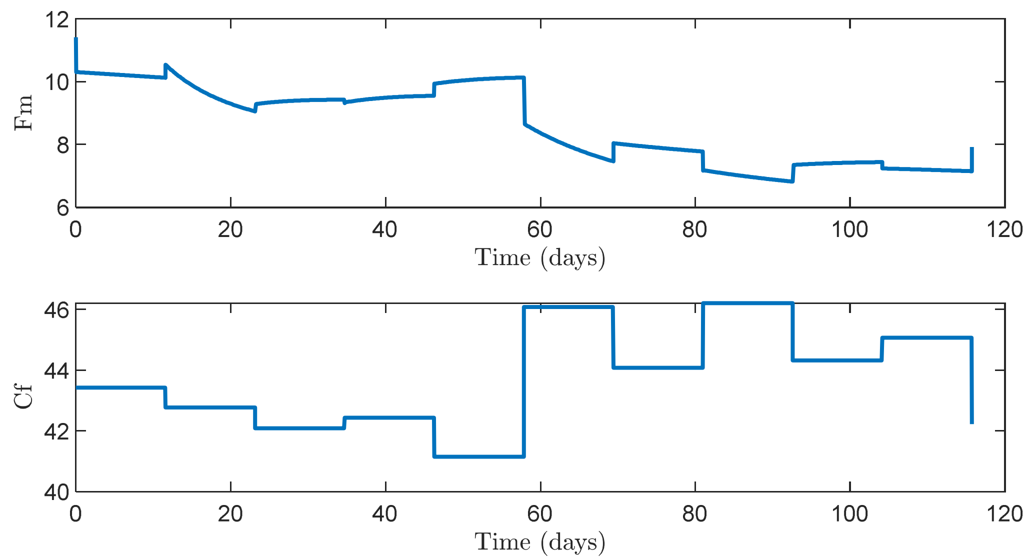

Figure 20.change in water passage by changing in feed concentration by considering fouling effect

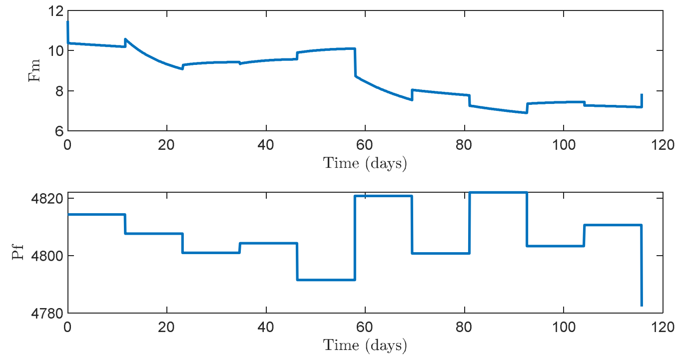

Figure 21.change in water passage by changing in feed pressure by considering fouling effect

2.2 Dynamic simulation of the reverse osmosis process

The model has been created based on the following equations provided in [3].

Descripition	The mathematical expression
Dynamic axial water flux	$\frac{\mathrm{d}J_{\mathrm{w}(x)}}{\mathrm{d}t} = \left\{\left(A_{\mathrm{w}}\left(\left(P_{\mathrm{b}(x)} - P_{\mathrm{p}}\right) - RT_{\mathrm{b}(x)}\left(C_{\mathrm{w}(x)} - C_{\mathrm{p}(x)}\right)\right)\right) - J_{\mathrm{W}(x)}\right\}\left(\frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W\Delta x}\right)$
Dynamic axial solute flux	$\frac{\mathrm{d}_{\mathrm{s}(x)}}{\mathrm{d}t} = \left\{\left(B_{\mathrm{s}}\exp\left(\frac{J_{\mathrm{w}(x)}}{k_{(x)}}\right)\left(C_{\mathrm{b}(x)} - C_{\mathrm{p}(x)}\right)\right) - J_{s(x)}\right\}\left(\frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W\Delta x}\right)$
Dunamic axial membrane wall concentration	$\frac{\mathrm{d}C_{\mathrm{w}(x)}}{\mathrm{d}t} = \left\{\left(C_{\mathrm{p}(x)} + \exp\left(\frac{J_{\mathrm{w}(x)}}{k_{(x)}}\right)\left(C_{\mathrm{b}(x)} - C_{\mathrm{p}(x)}\right)\right) - C_{\mathrm{w}(x)}\right\}\left(\frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W\Delta x}\right)$
Pressure difference along the membrane	$\Delta P_{\mathrm{b}(x)} = \left(P_{\mathrm{b}(x)} - P_{\mathrm{p}}\right)$
Dynamic axial feed flow rate	$\frac{\mathrm{dF}_{\mathrm{b}(x)}}{\mathrm{d}t} = \left[\left\{-W\left(A_{\mathrm{W}}\left(\left(P_{\mathrm{b}(x)} - P_{\mathrm{p}}\right) - RT_{\mathrm{b}(x)}\exp\left(\frac{J_{\mathrm{w}(x)}}{k_{(x)}}\right)\left(C_{\mathrm{b}(x)} - C_{\mathrm{p}(x)}\right)\right)\right)\right\} - \frac{\mathrm{d}F_{\mathrm{b}(x)}}{\mathrm{d}x}\right]\left(\frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W}\right)$
Dynamic axial feed pressure	$\frac{\mathrm{d}P_{\mathrm{b}(x)}}{\mathrm{d}t} = \left[-bF_{\mathrm{b}(x)} - \frac{\mathrm{d}P_{\mathrm{b}(x)}}{\mathrm{d}x}\right]\left(\frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W}\right)$
Axial permeated flow rate	$F_{\mathrm{p}(x)} = J_{\mathrm{w}(x)}W\Delta x$
Dynamic axial molar flux of feed	$\frac{\mathrm{d}C_{\mathrm{b}(x)}}{\mathrm{d}t} = -\frac{C_{\mathrm{b}(x)}}{t_{\mathrm{f}}W}\frac{\mathrm{d}F_{\mathrm{b}(x)}}{\mathrm{d}x} - \frac{F_{\mathrm{b}(x)}}{t_{\mathrm{f}}W}\frac{\mathrm{d}C_{\mathrm{b}(x)}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}\left[D_{\mathrm{b}(x)}\frac{\mathrm{d}C_{\mathrm{b}(x)}}{\mathrm{d}x}\right] - \frac{J_{\mathrm{w}(x)}C_{\mathrm{p}(x)}}{t_{\mathrm{f}}}$
Dynamic axial molar flux of permeate	$\frac{\mathrm{d}C_{\mathrm{p}(x)}}{\mathrm{d}t} = -\frac{c_{\mathrm{p}(x)}}{t_{\mathrm{p}}W}\frac{\mathrm{d}F_{\mathrm{p}(x)}}{\mathrm{d}x} - \frac{F_{\mathrm{p}}(x)}{t_{\mathrm{p}W}}\frac{\mathrm{d}C_{\mathrm{p}(x)}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}\left[D_{\mathrm{p}(x)}\frac{\mathrm{d}C_{\mathrm{p}(x)}}{\mathrm{d}x}\right] + \frac{J_{\mathrm{w}(x)}C_{\mathrm{p}(x)}}{t_{\mathrm{f}}}$
Dynamic axial feed temprature	$\frac{\mathrm{d}T_{\mathrm{b}(x)}}{\mathrm{d}t} = \left[\frac{F_{\mathrm{b}(x)}\left(T_{\mathrm{b}(0)} - T_{\mathrm{b}(x)}\right)}{t_{\mathrm{f}}W\Delta x}\right] - \left[\frac{J_{\mathrm{w}(x)}\left(T_{\mathrm{b}(x)} - T_{\mathrm{p}(x)}\right)}{t_{\mathrm{f}}}\right]$
Dynamic axial permeate temprature	$\frac{\mathrm{d}T_{\mathrm{p}(x)}}{\mathrm{d}t} = \left[\frac{J_{\mathrm{w}(x)}\left(T_{\mathrm{b}(x)} - T_{\mathrm{p}(x)}\right)}{t_{\mathrm{f}}}\right]$
Axial mass transfer coefificient	$k_{(x)}\mathrm{de}_{\mathrm{b}} = 147.4D_{\mathrm{b}(x)}\mathrm{Re}_{\mathrm{b}(x)}^{0.13}\ \mathrm{Re}_{\mathrm{p}(x)}^{0.739}\ C_{\mathrm{m}(x)}^{0.135}$

The model is simulated based on the following information.

Table 3. the characteristics of feed flow

Variable	*Value*
Feed permeate flow rate Q_f	2.166e-4 $\left(\frac{m^3}{s}\right)$
Feed pressure P_f	15 (atm)
Feed temperature T_f	35 C
Feed concentration C_f	0.77e-3 $kmol/m^3$

Table 4

Specifications of constant parameters and differential variables at $t = 0$.

Parameter	Value
Feed spacer thickness (t_f)	0.8 mm
Permeate channel thickness (t_p)	0.5 mm
Module length (L)	0.934 m
Module width (W)	8.4 m
Molal density of water (ρ_w)	55.56 kmol/m^3
Gas law constant, (R)	0.082 (atm m^3/°K kmol)
Permeate pressure (P_p)	1 atm
Feed channel friction parameter (b)	8529.45 $\left(\frac{\text{atm s}}{\text{m}^4}\right)$
Solvent transport coefficient (A_w)	9.5188×10^{-7} $\left(\frac{\text{m}}{\text{atm s}}\right)$
Solute transport coefficient (B_s) (chlorophenol)	8.468×10^{-8} $\left(\frac{\text{m}}{\text{s}}\right)$

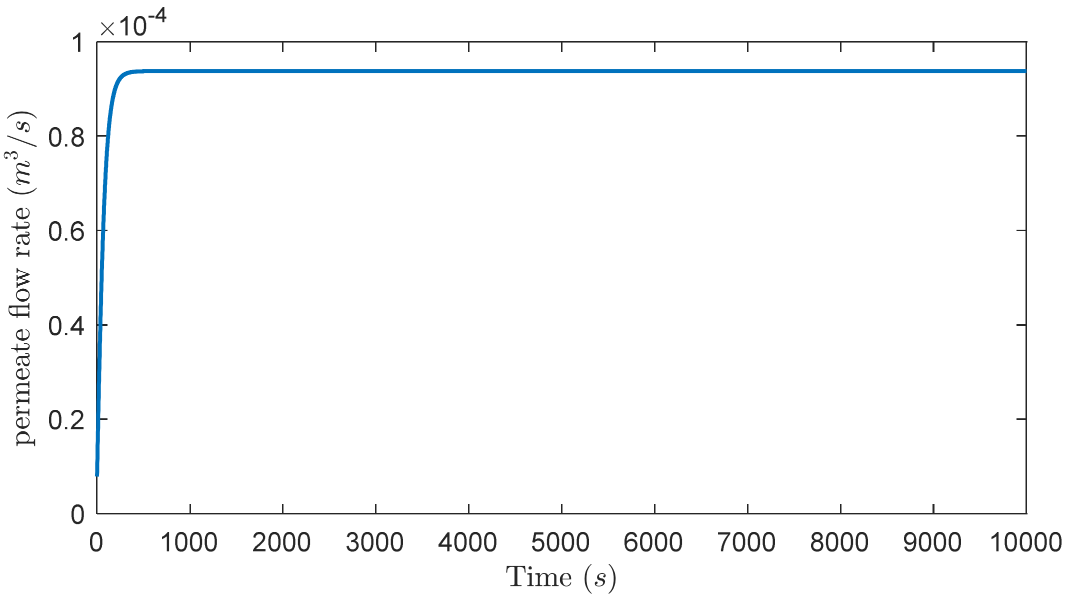

Figure 22. The permeate flow rate response

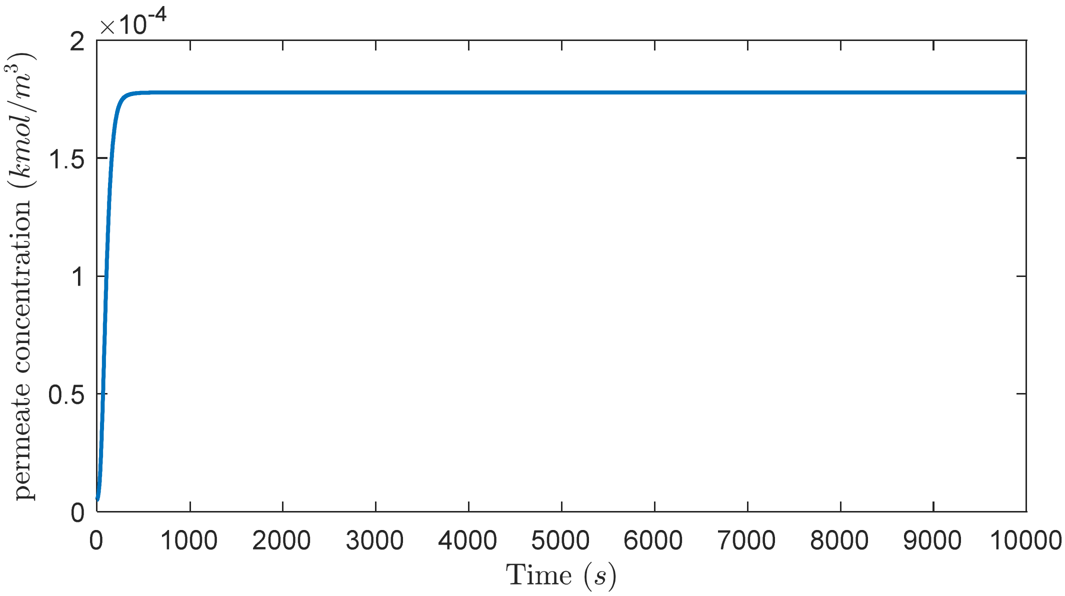

Figure 23. The permeate concentration response

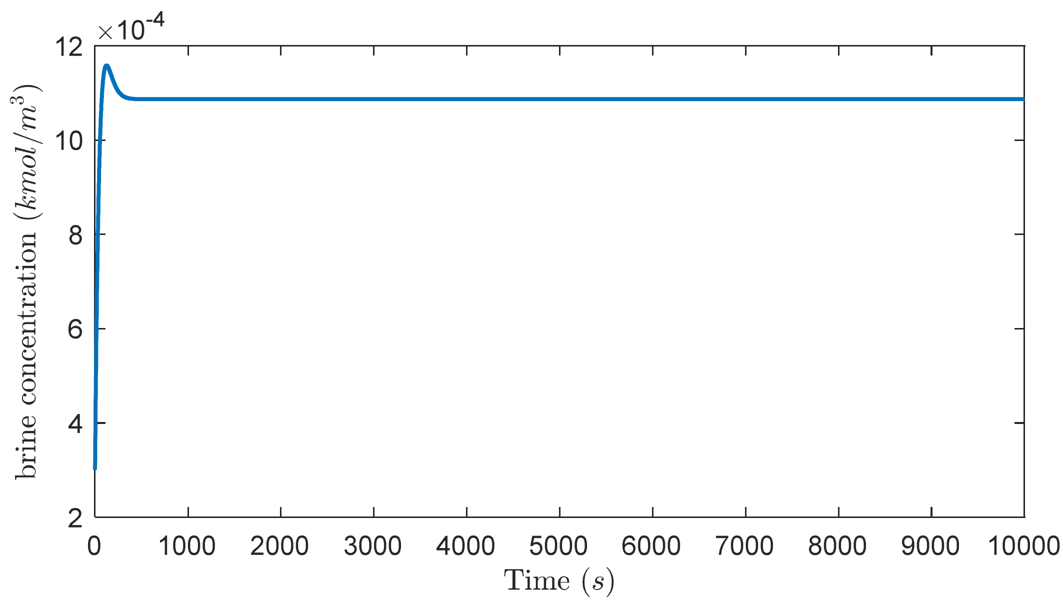

Figure 24. The response of brine concentration.

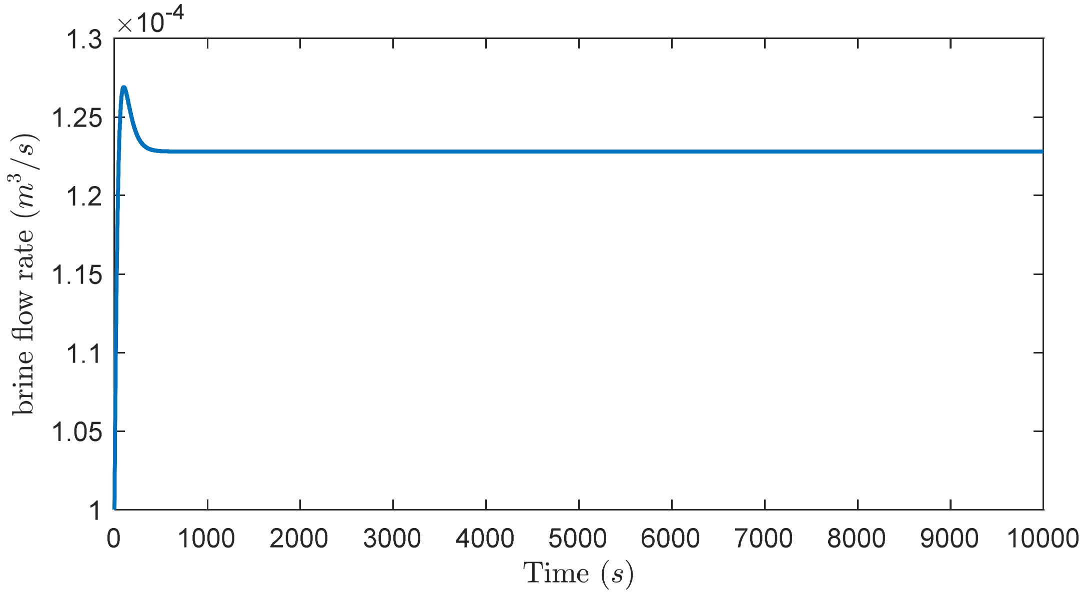

Figure 25. The brine flow rate

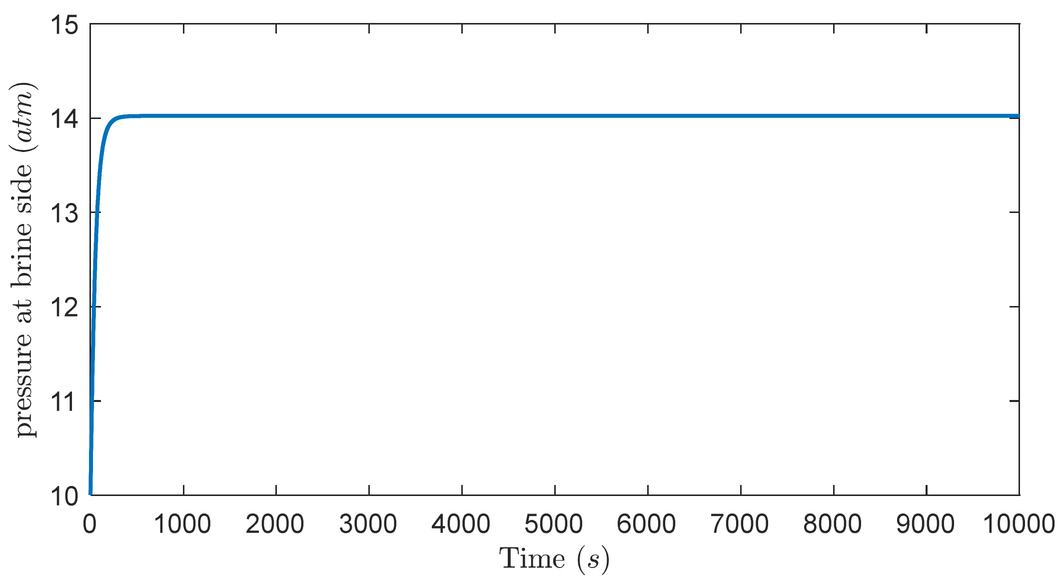

Figure 26. The brine pressure

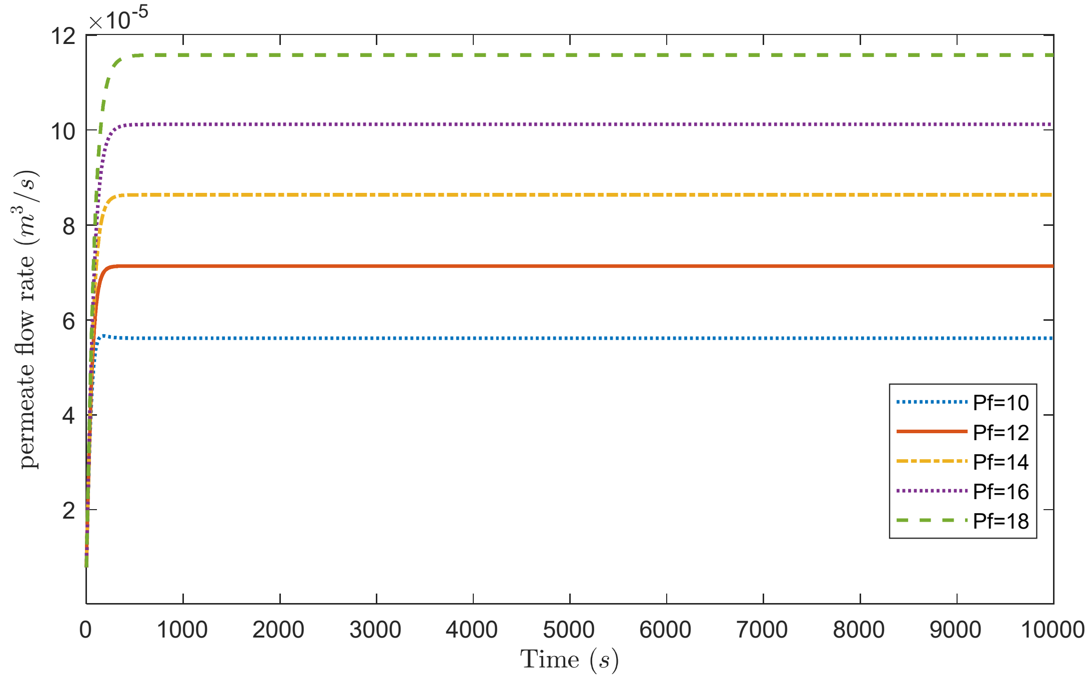

Figure 27. Permeate flow rate dynamic behavior based on the variation of feed pressure

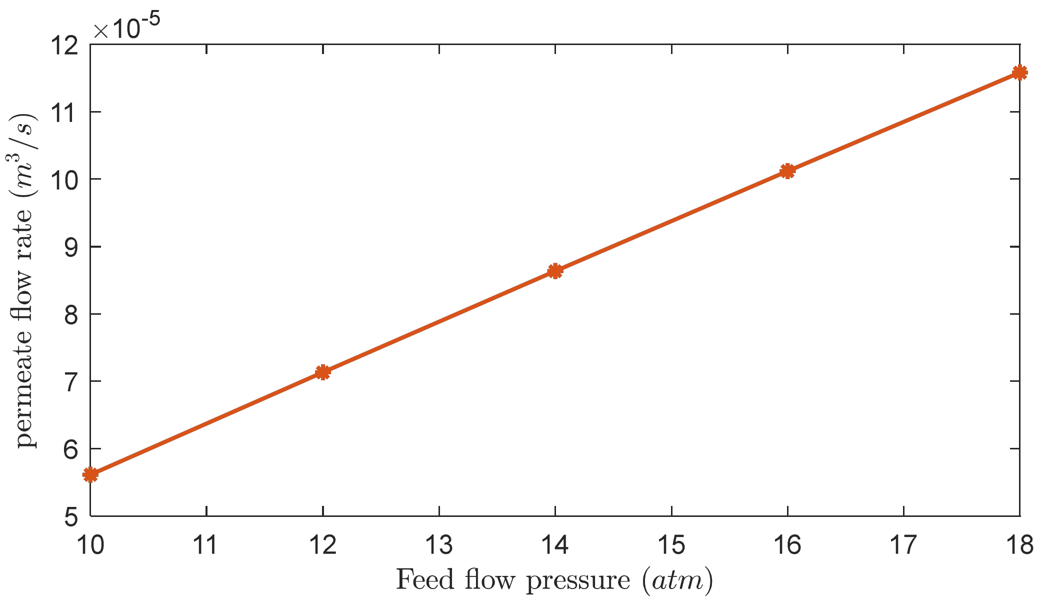

Figure 28. The changes of permeate flow rate based on the feed flow pressure

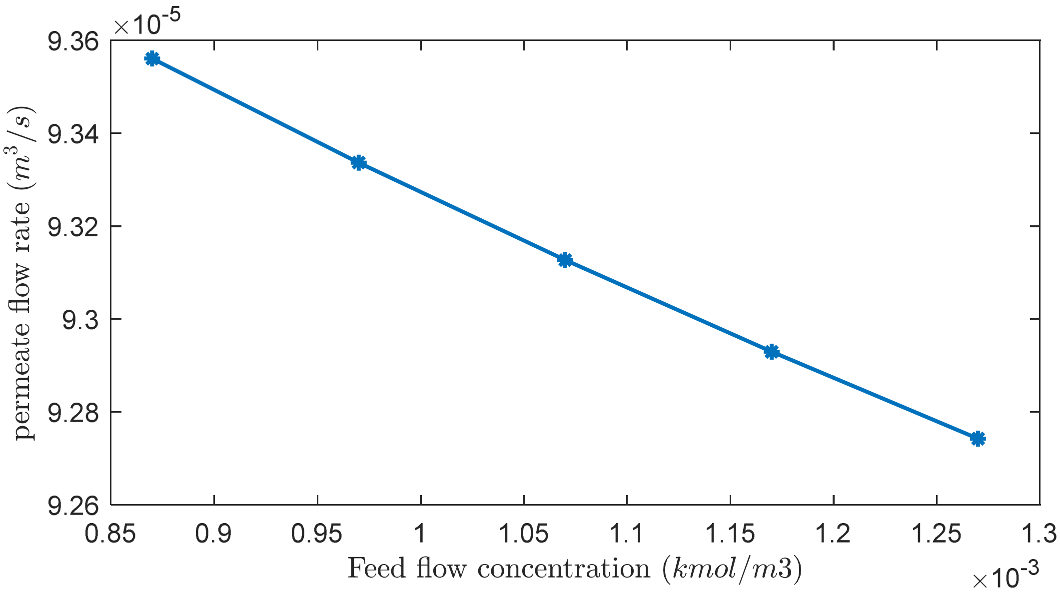

Figure 29. The changes on the steady state response based on the changes of feed flow concentration

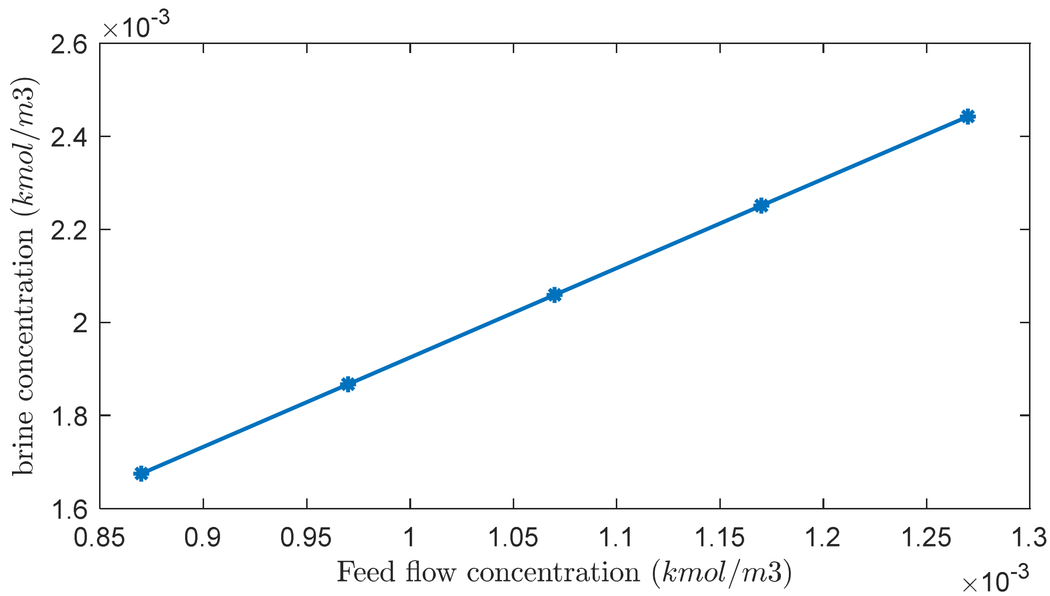

Figure 30. The changes on the brine concentration steady state response based on the feed flow concertation

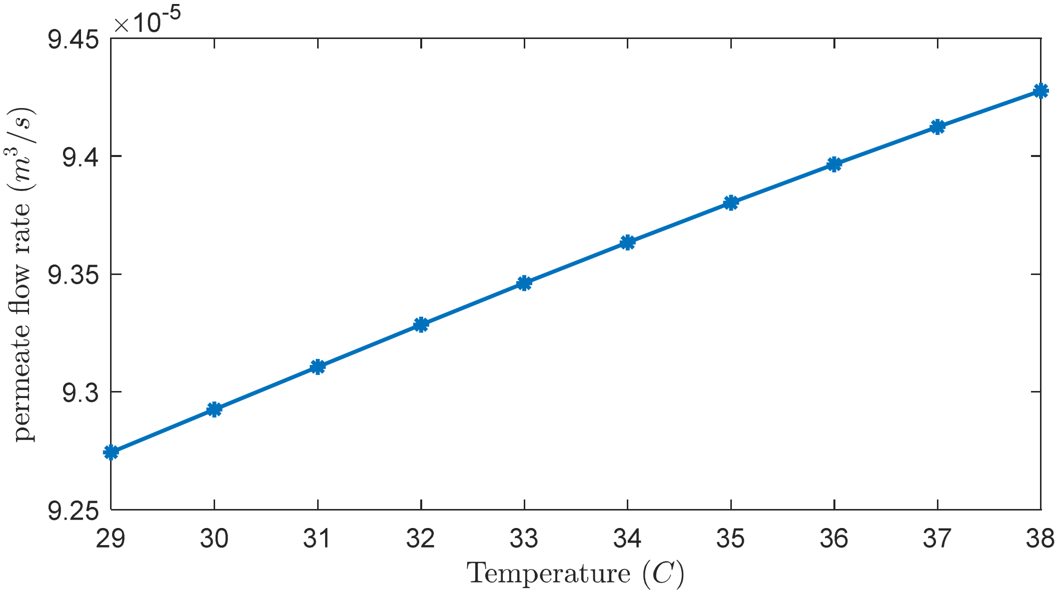

Figure 31. Changes on the permeate flow rate based on the changes in the temperature

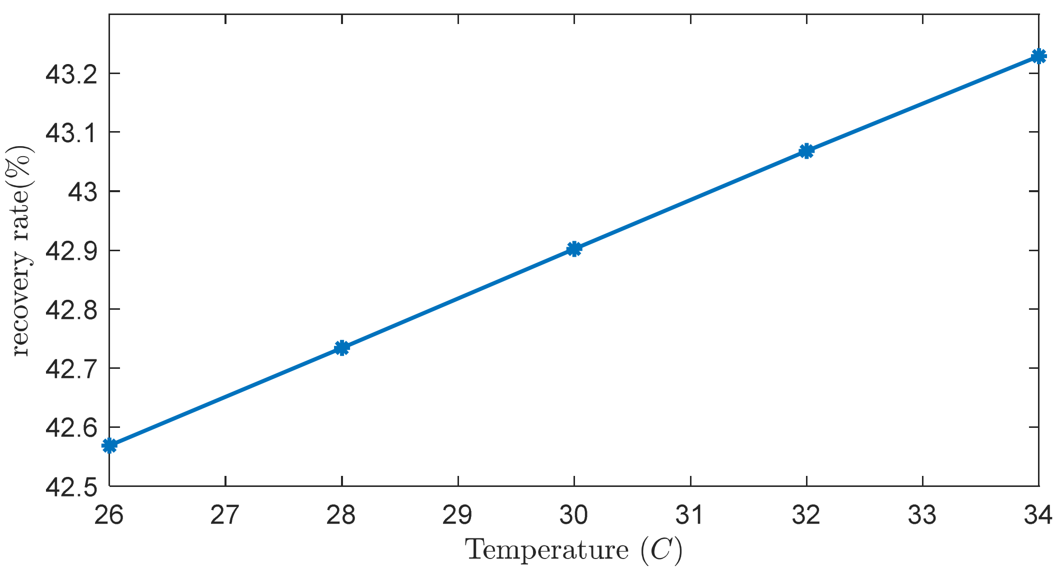

Figure 32. changes in recovery ratio based on the changes in temperature

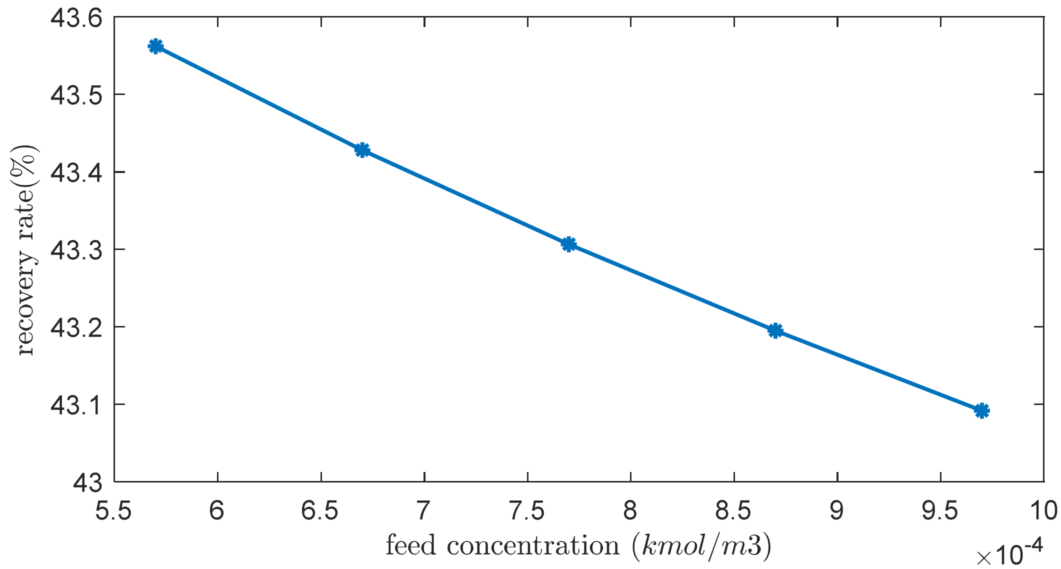

Figure 33. The recovery rate change based on the feed concentration changes

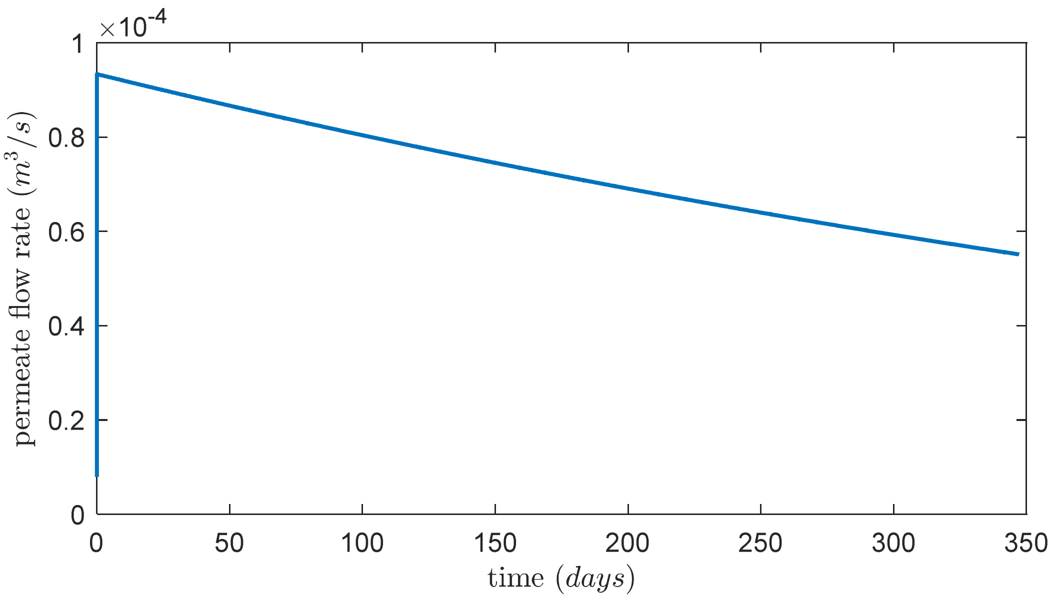

Figure 34. The permeate flow rate by considering the effect of fouling

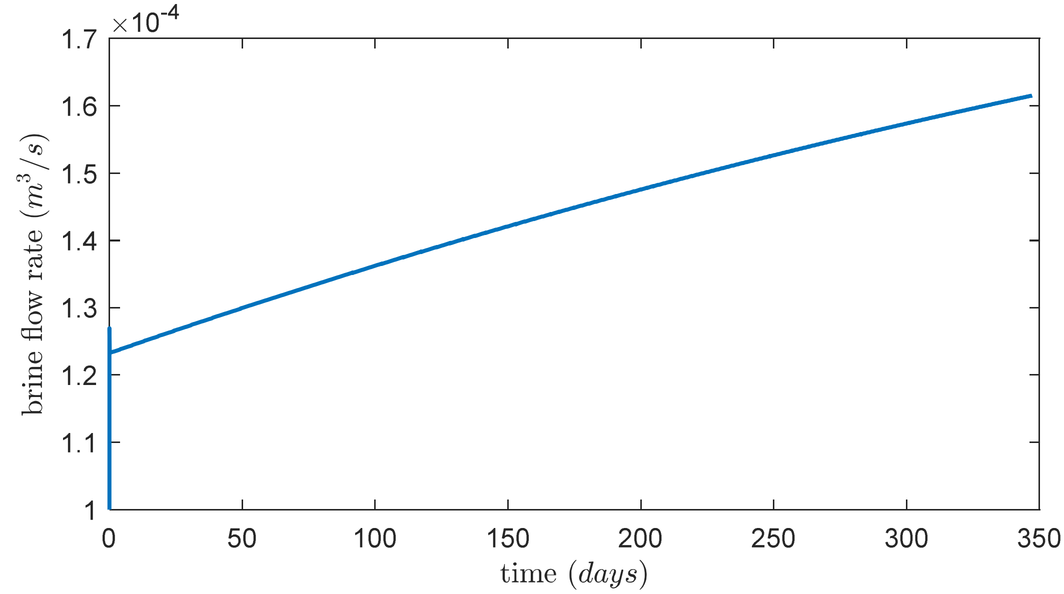

Figure 35. The brine flow rate by considering the fouling effect

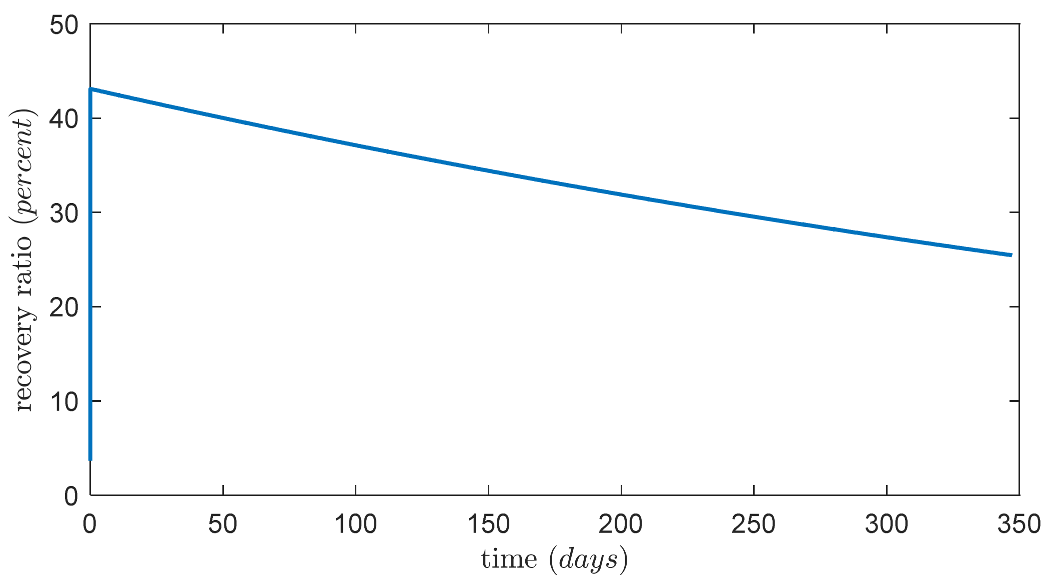

Figure 36. The effect of fouling on the recovery ratio during 350 days.

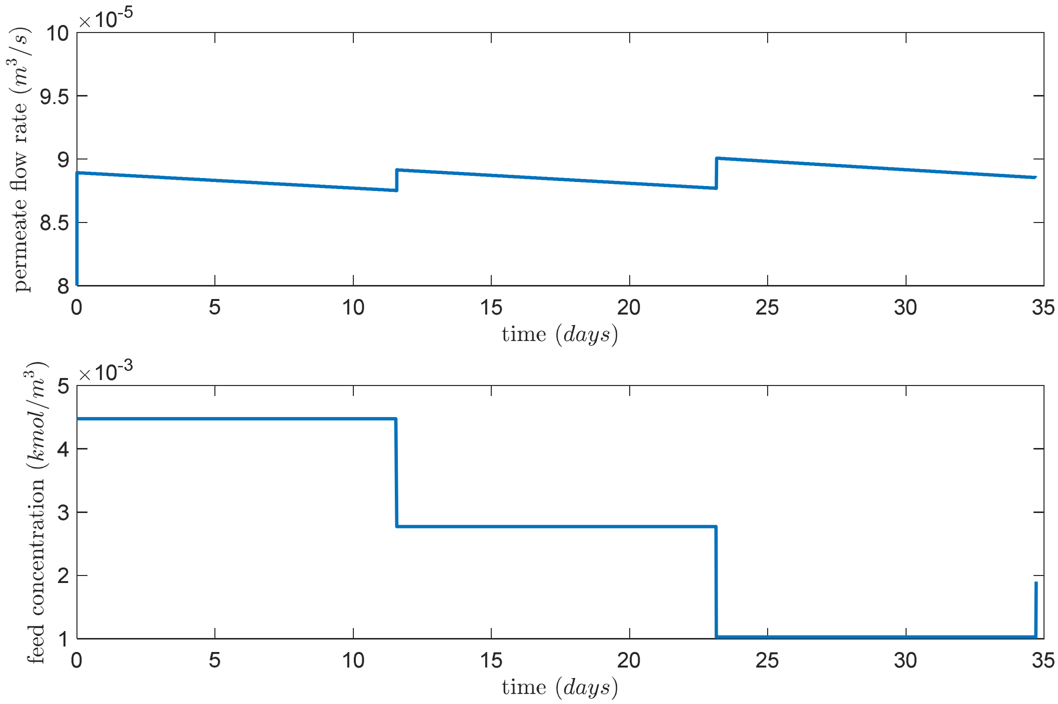

Figure 37. Permeate flow rate changes based on the changes in feed concentration and fouling

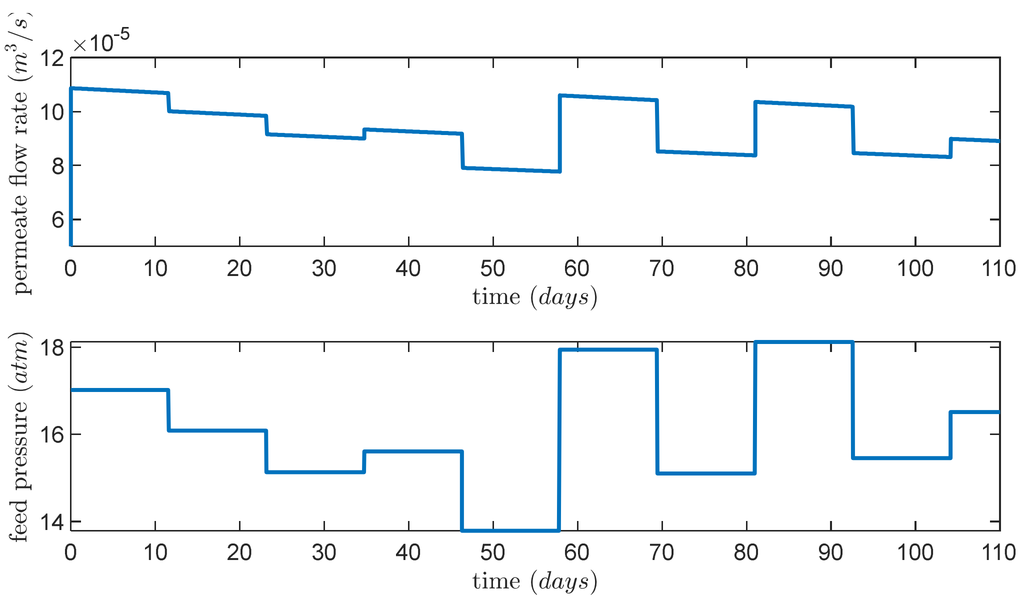

Figure 38. Permeate flow rate changes based on the changes in feed pressure and fouling