

51 (2013) 2755–2767 March



Development of a transient model for the desalination of sea/brackish water through reverse osmosis

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Received 4 April 2012; Accepted 9 September 2012

ABSTRACT

Mathematical models that adequately represent steady state and transient behaviour of desalination process comprising of equalisation tank, reverse osmosis (RO) system using a constant rate of transfer of diffusing substance per unit area of the cylinder surface and a potable water tank system are developed. A solute mass transport model is solved using the partial differential equation parabolic elliptical numerical technique using Crank–Nicholson method is inbuilt. Solution of this model shows decline in the permeate flux in the RO membrane. The theoretical transient and steady state models are compared with experimental results. The comparison shows that both the transient and steady state models are matching with the experimental results. A Transfer function model has also been developed to represent input–output relations. The decrease in flux in the RO membrane was compared with the experimental results.

Keywords: Desalination; Modelling; Membrane; Reverse osmosis; Multivariable

1. Introduction

Scarcity of fresh water due to global warming, seasonal anomaly and deterioration in quality of underground water has lead to extensive research on desalination process. Production of potable water from brackish and seawater sources started from 1950s. Desalination is a separation process used to reduce the amount of dissolved salts in seawater or brackish water to a usable or potable level by distillation (multi stage flash (MSF), multiple effect evaporation, vapour compression, or by membrane processes such as electrodialysis reversal, nano-filtration, membrane distillation, forward osmosis and reverse osmosis (RO). Out of all these, RO [1] using cellulose acetate or polyamide membranes, is a widely used desalination process and was chosen as the cost of production is reduced by the use of energy efficient techniques.

Models that adequately describe the performance of RO membranes are very important since these are needed in the design of RO processes. In literature, many mathematical models for desalination have been reported. Murkes and Bohman [2] developed a steady state model relating permeate flux to basic design parameters to study membrane performance underflow at different regions. Slater et al. [3] presented a transient membrane mass transfer model for a small-scale RO unit using non-linear differential

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equations representing feed conditions, flux, solute concentrations and rejections. Alatiqi et al. [18] identified a Multi-Input Multi-Output (MIMO) transfer function model for the desalination process from experimental data for closed-loop control. Transient models for membrane fouling phenomena were presented by Fountoukidis et al., Jacob et al. and Hoek et al. [4-6]. Davis and Leighton [7] presented theories describing transport of concentrated boundary layer under laminar flow. Masihide and Shoji [8] estimated transport parameters of RO membranes for seawater desalination. Performance of RO systems was predicted (2005) using feed forward neural network. Multi-solute transport was explained by a 2D mathematical model (2005) for RO system. Dynamic models membrane concentration polarisation (2007) of described by Nerst-Planck equation and film theory was developed by Chaabane et al. [9]. Senthilmurugan et al. [10] formulated models of RO using spiral-wound and had estimated parameters using numerical techniques. Hyun-Je et al. [11] presented a simplified model of RO system and Chen et al. [12] proposed a dynamic model of RO for seawater desalination. Sobana and Panda [13] presented a review on modelling, identification and control of desalination systems using RO technology. All these models describe either steady state mass transfer phenomena or transient dynamics of membrane concentration polarisation and can be used to evaluate process performance. In case of sudden demand of potable water from city (or with changes in the feed composition), the throughput needs to be increased that needs a transient model to predict system performance and recovery ratios of the RO process. It is observed that there is a lack of modelling information that will directly help to construct transfer function models for synthesising controllers. Few works (Constrained model predictive control, [19]; Advanced control for MSF desalination plant, [20]; Decentralised control of MSF desalination, [21]; Model predictive control of a RO desalination unit, [22]) on the control of desalination process were reported based on transfer function models that were developed mostly from experimental data. Hence, a dynamic model for a RO desalination unit from theoretical background is aimed at the present work. A simple schematic of a RO scheme is presented in Fig. 1. Raw water is pre-treated and stored temporarily in an equalisation tank from which it is pumped using high pressure to the tubular membrane chamber made of DOW FILMTECH SW30HR380 of diameter 2.5 inches to overcome osmotic pressure barrier that cause solvent (potable water) to transport from feed to permeate side. The performance of the process depends on pressure,



Fig. 1. Schematic of a RO desalination process.

temperature and concentration of dissolved solids. Stable operation of RO processes using spiral membrane needs analysis of its mathematical model to improve plant performance, efficiency, safety and reliability.

Naturally, the measured variables in the process are flow rate and concentration of dissolved solids in product water, the manipulated variable is pressure on feed water side and the load is flow rate of feed water as it varies according to demand. The objective of this work is to develop a simplified steady state mass transfer model and transient dynamics including concentration polarisation for construction of a simple control strategy for this process.

Thus the rest of the paper is organised as follows. Experimental set-up has been described in Section 2 under methodology. Section 2 discusses the theoretical preliminaries of steady state mass transfer model. A transient model representing dynamics of permeate characteristics for RO system is also developed in this section. Section 3 presents results on validation of model and also the influence of parameters on the performance of the process under steady state and transient behaviour. At the end, conclusion is drawn.

2. Methodology

2.1. Experimental set-up

A seawater-based desalination plant has been installed in Narippaiyur village of Ramanathapuram district, Tamil Nadu, India, with a capacity of 3.80 MLD of drinking water. This is the first desalination plant for the production of potable water in South Asia. The arrangement of the experimental set-up is shown in Fig. 2.

2.1.1. Filters and pumps

A well with an inner diameter of 1,000 mm is dug in the sea and is covered with a basket with small holes



Fig. 2. Process flow scheme of desalination plant at TWAD, Ramanathapuram, Tamil Nadu.

and mesh $(100 \times 15 \text{ mm glass-reinforced plastic [GRP]})$ material) so that fish and algae are not allowed to enter inside the well which is connected to an equalisation tank of $70 \operatorname{sq} m \times 7 \operatorname{m}$ by two pipes (GRP material) of inner diameter of 450 mm and the length of 450 m. The pipe is connected to the equalisation tank with certain slope so that the height of water in the equalisation tank is equal to the height of sea. The tank is equipped with three vertical turbines and two horizontal centrifugal pumps (capacity $450-500 \text{ m}^3/\text{h}$) that deliver water to filters section with a pressure of $3-3.5 \text{ kg/cm}^2$. Three dual-media filters of 3 m diameter and 7 m height, with a capacity of 120–170 m³/h and filled with sand and gravels are employed in series as primary filters to remove coarse particles and suspended solids from water. The dirt and turbidity are also reduced to some extent at first and second stages of filters. Water then enters into the third stage of filter, polished dual media filters (PDMF) where suspended solids, dirt and turbidity are reduced to yield colourless and odourless water.

After PDMF, water enters to cartridge filter to eliminate particles more than 5μ after which it is pumped (discharge pressure >50 kg/cm²) to RO sections.

2.1.2. RO section

ROs operate over a pH range of 2–11 pH with excellent performance in terms of flux, salt, organic rejection, microbiological resistance and with free chlorine tolerance of less than 0.1 ppm. Water permeability and solute permeability characteristics depend on the performance of membrane. The feed water is allowed to enter in the inner most radius of the spiral RO section. The permeate comes out through the outermost layer of the RO. The ions are attracted by the polyamide material of membrane. The TDS reduces from 40,000 to 500 ppm for running (operation) time of 12 h through 168 ROs (spiral bound) of 1 m length each. A RO consists of 30 membranes leafs. Each leaf is made up of two membrane sheets glued together 2758

back to back with a permeate spacer in between them. The consistent glue line of about 1.5 inches wide seals the inner (permeate) side of the leaf against the outer (feed/concentrated) side. The leaves are rolled up with a sheet of feed spacer between each of them (shown in Fig. 3), which provide the channel for feed and concentration to flow. The permeate (p) and brine (b) from all the RO's are collected and passed to the opposite direction of the feed water entering section of RO. The brine from the RO section is collected that amounts to approximately 50% of feed. A schematic process flowsheet (Fig. 4) describes flow rates of different streams in the entire plant. About 70% of brine is recirculated to feed-mixing tank. Rest of the brine can be used for recovery of salts. Ten percentage of feed goes to precipitate or forms scale that gets adhered to membrane. An amount of about 35-40% of feed goes to permeate tank and can be used for potable purpose.

To boost the feed water pressure from 51 to 60 kg/cm^2 , centrifugal type of energy recovery devices (electromechanically operated butterfly dump valve and a flow control valve) are used by taking (energy conservation/recovered) the energy from the brine stream. The structures of mathematical models (steady and transient) for each of the units of the plant are formulated in Section 2.2.

2.2. Mass transfer model

The permeate (p) (due to vertical component of velocity) comes out along the surface of membrane while the concentrated brine (due to horizontal component of velocity) flows axially through the membrane. The RO process can be thought of comprising of a grey box model (Fig. 5) with one input or manipulated variable, several disturbance and design variables and output or control variables. Models that predict separation characteristics also minimise the number of experiments that must be performed to describe a particular system. Models that adequately

describe the performance of RO membranes are very important since these are needed in the design of RO processes.

Due to transverse diffusion across the walls of RO tubes (cylindrical), the permeate comes out and gets accumulated in the product tank. The axial flow stream goes as rejection or brine.

2.2.1. Basic mass transfer model: steady state

This model assumes that membrane tubes are arranged in single stack in parallel to constitute a module. Raw feed enters at flow rate Q_{f0} and a solute concentration C_{f0} that mixes in an equalisation tank. Recycle streams of permeate and retentate also enter in this tank resulting a mixed feed (*c*) with concentration of C_f that is pumped (with a pressure P_f) to the RO module. Thus, there are two velocity components (one horizontally and the other acts vertically along the membrane axis) of the feed stream.

The permeate (p) (due to vertical component of velocity) comes out along the surface of membrane while the concentrated brine (due to horizontal component of velocity) flows axially through the membrane. Steady sate model helps us to calculate variables associated to each stream at the exit of each equipment/unit. It is evident from Fig. 1 that there are mostly four units: mixing, RO, permeate and brine tanks. Let us develop equations for each unit.

Permeate stream:

The permeate flux is given by

$$J_{W} = K_{W}(\Delta P - (\pi_{mT} - \pi_{p}))$$

= $K_{W}((P_{mT} - P_{p}) - (\pi_{mT} - \pi_{p}))$ (1)

where K_W is hydraulic permeability or water mass transfer coefficient; suffix *F* is for feed, mT is for combined or mixed feed in equalisation tank, *P* is for pressure, p stands for permeate and π is the osmotic pressure and is given by Vant Hoff's relation as



Fig. 3. Representation of cross sectional view of RO membrane.



Fig. 4. Schematic liquid flow and pressure flow schemes in desalination process.



Fig. 5. Block diagram of RO process.

 $\pi = \phi\left(\frac{n}{v}\right) R_{\rm g} T$

where ϕ = osmotic pressure coefficient,

n = number of moles of dissolved solute,

v = volume of the mixer,

 R_{g} = gas constant and T = temperature.

Under isothermal condition, the above equation is reduced to

$$\pi = \beta C$$

where *C* is the molar concentration and $\beta = \phi R_g T$. Concentration of permeate (*C*_p) can be found from Eq. (2).

As the impermeable solutes accumulate inside the membrane surface, a laminar boundary layer is formulated for which concentration polarisation is given by

$$\frac{C_{\rm mT} - C_{\rm p}}{C_{\rm B} - C_{\rm p}} = \exp\left(\frac{J_{\rm W}}{K_{\rm CP}}\right) = \alpha \tag{2}$$

where $C_{\rm B}$ is the concentration of bulk stream inside the membrane and $K_{\rm CP}$ is the concentration polarisation mass transfer coefficient and is given by

$$K_{\rm CP} = \frac{0.023C_{\rm mT} N_{\rm Re}^{0.83} N_{\rm Sc}^{0.33}}{2L} \tag{3}$$

With Reynolds number $N_{\text{Re}} = \frac{\rho d_m u}{\mu}$ and Schmidt number $N_{\text{Sc}} = \frac{\mu}{\rho D_L}$ where d_m = diameter of RO membrane, D_L is the liquid diffusivity, μ is the viscosity of liquid and u = liquid velocity, L = length of RO tube and ρ = liquid density.

Thus, the volumetric flux, in Eq. (1), can be rewritten as

$$J_{W} = K_{W}((P_{mT} - P_{p}) - \beta(C_{mT} - C_{p}))$$

= $K_{W}((P_{mT} - P_{p}) - \beta\alpha(C_{b} - C_{p}))$ (4)

where $C_{\rm B}$ is the bulk liquid concentration inside the membrane and can be calculated as

$$C_{\rm B} = \frac{C_{\rm mT} + C_{\rm b}}{2} \tag{5}$$

with C_{mT} as feed concentration and C_b as concentration of retentate (brine) at the exit of RO module. *Mixing tank*:

Eq. (1) may be used to obtain permeate flux (J_W) . Eq.

(4) is then applied to get permeate concentration (C_p).

With this value of $C_{\rm p}$, bulk concentration of liquid, $C_{\rm B}$ can be calculated using Eq. (2). Retentate concentration ($C_{\rm b}$) can be found from Eq. (5).

Permeate flow can be related as

$$Q_{\rm p} = J_{\rm W} S_{\rm a} \tag{6}$$

where $S_a = W(dz) = \frac{a}{L}dz$ = surface area of membrane. where a = area, *L* = length along RO, *z* = thickness of RO, *W* = width of RO.

Combined flow is

$$Q_{\rm mT} = Q_{\rm F} + p'Q_{\rm p} + (1 - b')Q_{\rm b} \tag{7}$$

where p' = fractional flow of permeate added to equalisation tank and 1 - b' = fractional flow of retentate added to equalisation tank.

Brine tank:

To calculate brine flux the following equation can be used

$$J_{\rm b} = K_{\rm S}(\beta C_{\rm mT} - C_{\rm p}) \tag{8}$$

Thus, $Q_b = J_b S_a$

With this value of Q_{b} , flow rate of combined feed stream can be calculated using Eq. (7). Osmotic pressure is a function of temperature and concentration.

The osmotic pressure can be calculated by $\pi = (0.6955 + 0.0025T) \times 10^8 \times \frac{C_i}{\rho_i}$ where C_i is concentration (kg/m³) and ρ is density at interface at temperature T (°C). The density can be given by $\rho = 498.4$ m $+\sqrt{(248400 \text{ m}^2 + 752.4 \text{ mC})}$ where constant m is given by $m = 1.0069 - 2.757 \times 10^{-4}T$. Salt concentration (C) at the membrane wall is $C_i = C_p + (C_{Fc} - C_p) \times \exp\left(\frac{l_w}{K_s} \times 1,000\right)$. The mass transfer coefficient $K_s = 1.101 \times 10^{-4}u_b^{0.5}$ where u_b is velocity (m/s) of brine.

RO section:

Thus, the volumetric permeate flux is $J_{\rm P} = J_{\rm W}/\rho_{\rm P}$ = $K_{\rm W}((P_{\rm Fc} - P_{\rm P}) - \beta\alpha(C_{\rm B} - C_{\rm P}))/\rho_{\rm P}$. With the development of cake layer on the membrane, the permeate flux is $J_{\rm W} = \frac{\Delta P - \Delta \pi}{\mu(R_{\rm m} + R_{\rm C})}$ where $R_{\rm m}$ is membrane resistance and $R_{\rm C}$ is resistance imparted by cake layer deposited over the membrane surface and is given by $R_{\rm C} = \alpha M_{\rm d} = \left[\frac{45(1-\varepsilon)}{\rho_{\rm c} d_{\rm p}^2 \varepsilon^3}\right] M_{\rm d}$ where $\rho_{\rm c}$ is particle cake density and $a_{\rm p}$ is particle radius. $\mu = \frac{\eta}{\rho}$, with η as viscosity and ρ as density of fluid. Cake layer can be calculated from $\delta_{\rm c} = \left[\frac{(4/3)\pi a_{\rm p}^3}{1-\varepsilon}\right] M_{\rm C}$ where $M_{\rm C}$ is the total number of particles per unit area accumulated in the cake layer. At pH = 7.1, $M_{\rm d} = 8.56 \,{\rm g/m^2}$, = 2.71 × 10⁻¹⁵ m/kg and $\delta_{\rm c} = 20$ for seawater. Mindler and Epstein [14] approximated C_{CW} (concentration at the interface of cake and liquid) with the following relation $\frac{C_{CW}}{C_B} = 1.33 \exp(\frac{\gamma}{0.75} \frac{y}{\delta}) C_p$ with $\gamma = \frac{2V_{mT}(N_{Sc})^{2/3}}{fu_x}$ and *f* as friction factor for turbulent flow [15]. Eq. (2) can be solved to get concentration profile along RO membranes.

2.2.2. Transient model

The system considered here consists of an equalisation feed tank, a RO membrane module and a product collection tank. Feed enters the membrane module through a feeding pump and a part (1 - b') of concentrated brine that comes out (axially) from RO is recycled to equalisation tank. Similarly, a part of the permeate (radially) that comes out through membrane gets recycled to the equalisation tank. After developing the steady state balance equations, one needs to formulate the transient dynamics around the tanks and RO module to design safe and efficient control of the system. The transient dynamics are derived as follows:

2.2.2.1. *Feed/equalisation tank*. The transient mass balance equation around the mixing tank becomes

$$V_{\rm mT} \frac{dC_{\rm mT}}{dt} = V_{\rm s0} \frac{dC_{\rm s0}}{dt} + bV_{\rm b0} \frac{dC_{\rm b0}'}{dt} + (1-p)V_{\rm p0} \frac{dC_{\rm p0}'}{dt} - V_{\rm mm} \frac{dC_{\rm mm}}{dt}$$
(9)

With initial conditions as:

at
$$t = 0, V_{mT} = V_{s0}$$
 and C_{mm}
= $[V_{s0} + bV_{b0} + (1 - p)V_{p0}]/V_{mm}$ (9a)

If we want to maintain a constant holdup in equalisation tank, assume, V_{mT} = constant, the Laplace transformed continuity equation of the integrated system becomes

$$\begin{split} C_{\rm mT}(s) = & \frac{(V_{\rm s0}/V_{\rm mm})C_{\rm s0}(s)}{s(V_{\rm mT}/V_{\rm mm}) + 1} + \frac{(1-p)(V_{\rm p0}/V_{\rm mm})C_{\rm p0}(s)}{s(V_{\rm mT}/V_{\rm mm}) + 1} \\ & + \frac{(1-b)(V_{\rm b0}/V_{\rm mm})C_{\rm b0}(s)}{s(V_{\rm mT}/V_{\rm mm}) + 1} \end{split}$$

or,
$$C_{mT}(s) = \frac{V_{so}C_{so}(s)}{sV_{mT} + V_{mm}} + \frac{[1-b]V_{bo}}{sV_{mT} + V_{mm}} + \frac{[1-p]V_{po}}{sV_{mT} + V_{mm}}$$
(9b)

Three streams (seawater, exit stream from brine tank and exit flow from permeate tank) are considered to be entering the mixing tank from which a single stream goes out as mixed flow. Volumetric flow rates of the streams are V_{so} , V_{bo} and V_{po} in m³/h. Similarly, the height (h_{mt}) of liquid is related to inlet flow rates around the mixing tank as

$$h_{\rm mt}(s) = \frac{C_{\rm so}R_{\rm mt}/C_{\rm mm}}{R_{\rm mt}A_{\rm mt}(s) + 1} V_{\rm so}(s) + \frac{C_{\rm bo}'R_{\rm mt}/C_{\rm mm}}{R_{\rm mt}A_{\rm mt}(s) + 1} \\ \times [1 - b]V_{\rm bo}(s) + \frac{C_{\rm po}'R_{\rm mt}/C_{\rm mm}}{R_{\rm mt}A_{\rm mt}(s) + 1} \\ \times [1 - p]V_{\rm po}(s)$$
(9c)

where *s* is Laplace variable.

2.2.2. Membrane module: concentration polarisation. Fluid transport through the cylindrical porous membrane (of length *L* and radius *R*) is assumed to have axial (u_x or horizontal) and radial (u_y or vertical) components of velocity. It is also assumed that with the transport of fluid-feed, a boundary layer (thick in solute and in laminar flow) is formed along the inner-side of membrane leaving behind a bulk stream of fluid flowing axially along the centre of the membrane tubes. The radial component gives rise to permeate flow. The concentration polarisation that is developed due to separation of boundary layer is given by

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial y^2} - u_y \frac{\partial C}{\partial y} - u_x \frac{\partial C}{\partial x}$$
(10)

with initial conditions:

$$C = 0 \text{ at } t = 0 \tag{10a}$$

$$\frac{\partial C}{\partial y} = 0$$
 at $y = 0$

and boundary conditions:

$$C = C_0 \text{ at } x = 0, \tag{10b}$$

$$D_L \frac{\partial C}{\partial y} = u_y C - V_P C_P$$
 at $y = L$

The solution of the above PDE equation has been achieved as

$$C = \frac{2}{L} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi y}{L}\right) \sin\left(\frac{n\pi x}{L}\right) e^{-\kappa^2 D_L U t}$$
(10c)

where $U = \sqrt{u_x^2 + u_y^2}$ and $u_y = \frac{\nabla P}{2\eta L} (4R^2 - y^2)$ and $u_x = u_m(\frac{R^2 - x^2}{R^2})$ and $\kappa^2 = \frac{dy^2}{y} = (\frac{n\pi}{L})^2 = \text{constant}$ ($\approx 0.1, 0.2, \dots, 1.0$). The value u_m is the fluid velocity at centre of the membrane tube.

Permeate flux J_W is given by

$$J_{\rm W} = K_{\rm W}[(P_{\rm mT} - P_{\rm P}) - (\beta \pi_{\rm mT} - \pi_{\rm P})]$$
(11)

Using Vant Hoff relation, the above equation can be rewritten as

$$H_{\rm W} = K_{\rm W}[(P_{\rm mT} - P_{\rm P}) - (\beta C_{\rm mT} - C_{\rm P})RT]$$
(12)

Differentiating (w.r. to *t*) the above equation,

$$\frac{dJ_{W}}{dt} = K_{W} \left[\frac{d\Delta P}{dt} - \beta \frac{dC_{mT}}{dt} RT \right]$$
(13)

Substituting $\frac{dC_{mT}}{dt}$ from Eq. (9), we get from Eq. (13)

$$\frac{dJ_{W}}{dt} = K_{W} \left[\frac{d\Delta P}{dt} - \beta \left\{ \frac{V_{\rm so} \frac{dC_{\rm so}}{dt} + bV_{\rm bo} \frac{dC_{\rm bo}}{dt} + (1-p)V_{\rm po} \frac{dC_{\rm po}}{dt} - V_{\rm mm} \frac{dC_{\rm mm}}{dt} \right\} RT \right]$$
(14)

2.2.2.3. *Production of brine*. Material balance for the production of brine or retentate is given by

$$\frac{\mathrm{d}m_{\mathrm{b}}}{\mathrm{d}t} = F_{\mathrm{mm}} - F_{\mathrm{b}} - F_{\mathrm{p}} - F_{\mathrm{c}} \tag{15}$$

$$\frac{dC_{b}}{dt} = \frac{[V_{mm}(C_{mm} - C_{b}) - V_{P}(C_{P} - C_{b}) - V_{bo}(C_{bt}) - V_{ci}(C_{ci})]}{V_{bt}}$$
(16)

The brine flow rate is given by

$$F_{\rm b} = K_{\rm bo} \sqrt{(p_{\rm b} - p_{\rm bo})} \tag{17}$$

with K_{b0} and p_{b0} as valve characteristics. The above transient equations can be linearised around the operating point from where the concentration dynamics is given by

$$C_{bt}(s) = \frac{V_{mm}}{sV_{bt} + V_{bo}} C_{mm}(s) - \frac{V_{pi}}{sV_{bt} + V_{bo}} C_{pi}(s) - \frac{V_{ci}}{sV_{bt} + V_{bo}} C_{ci}(s)$$
(18)

In the above equation, *C* represents concentration, *V* represents volumetric flow rate, suffix b is for brine,

p for permeate, i for inlet and o for outlet streams. The height of liquid in the tank can be given as

$$h_{\rm bt}(s) = \frac{C_{\rm bi}R_{\rm bt}/C_{\rm bo}}{R_{\rm bt}A_{\rm bt}s + 1} V_{\rm bi}(s) \tag{19}$$

2.2.2.4. Product tank. After the solute comes out of RO, it mixes with the streams of brine. The other stream, containing solvent or permeate or product water gets accumulated/collected in the product tank at a rate Q_p . A part of the product water flow may be withdrawn (Q_w) as per demand or it can also be recirculated (p part) to the feed tank. The continuity equation for the product tank becomes

$$[1-p]Q_{\rm p}C_{\rm p} - Q_{\rm w}C_{\rm w} = \frac{\rm d}{{\rm d}t}(Q_{\rm w}C_{\rm w})$$
(20)

$$\frac{C_{\rm pt}(s)}{C_{\rm pi}(s)} = \frac{V_{\rm mm} - V_{\rm bi} - V_{\rm co}}{sV_{\rm pt} + (V_{\rm mm} - V_{\rm bi} - V_{\rm co})}$$
(21)

and liquid height is given by

$$\frac{h_{\rm pt}(s)}{V_{\rm pi}(s)} = \frac{c_{\rm pi}R_{\rm pt}/C_{\rm po}}{R_{\rm pt}A_{\rm pt}(s) + 1}$$

rate of change of mass can be balanced using mass flow rates as

$$\frac{\mathrm{dm}_{\mathrm{p}}}{\mathrm{d}t} = F_{\mathrm{p}} - F_{\mathrm{pc}} \tag{22}$$

Eqs. (10c) and (22) are basically lumped equations representing the flow dynamics of permeate.

2.2.2.5. *Cake deposition module*. Due to transverse section of flow, solids get deposited on the walls of membrane. As a result, layers of cake build up. After formulating mass balance, and introducing deviation variables and finally taking Laplace transform, we can get following equation.

$$M_{\rm c}(s) = \frac{K_{\rm b}}{s^2} [C_{\rm b}(s) - C_{\rm s}(s)]^{\rm m}$$
(23)

 $K_{\rm b} = K_{\rm c} \ \psi \ S_{\rm p}$ and in this case, m = 1.

 C_{1}

Cake resistance is given by

$$\frac{R_{\rm c}(t)}{m_{\rm c}(t)} = \frac{\alpha}{A_{\rm m}} \tag{24}$$

For p=0 and r=0, Eq. (4) reduces to $C_{\rm fc}(t) = \frac{C_t}{Q_{\rm f0}}[1-e^{-t/\tau}]$, where $\tau = V_{\rm f0}/Q_{\rm f0}$. The multivariable block diagram of the integrated system (comprising of feed tank, RO membranes and Product tank) can be constructed.

2.2.2.6. *Pump module*. The osmotic pressure exerted by the fluid is

$$\frac{\Delta P_{\rm a}}{C_{\rm m}/C_{\rm f}} = 2RT \left(1 - \frac{C_{\rm p}}{C_{\rm m}}\right) C_{\rm f} \tag{25}$$

These mechanistic models (developed as above) are helpful in steady state as well as transient simulation for model validation and formulation of linear-

Table 1

Values of the normal operating conditions of the plant (seawater near Ramanathapuram, Tamil Nadu, India)

Serial no.	Variables	Value	
1.	Concentration of feed in the equalisation tank	40,000 mg/L	
2.	Concentration of feed to RO module	41,350 mg/L	
3.	Flow rate of feed to RO module		
4.	Volume of feed water 4.4944 n		
5.	Flow rate of mixed feed water 0.05 m ³ /s		
6.	Permeate (due to vertical component of velocity) comes	0	
	out along the surface of the membrane the value is 1 if the permeate is recycled, $\%$		
7.	Concentrated brine (due to horizontal component of velocity)	72.5	
	flows axially through the membrane, the value is 1 if the brine is recycled, $\%$		
8.	Concentration of permeate from the RO module	800 mg/L	
9.	Flow rate of permeate from the RO module	0.022 m ³ /s	
10.	Concentration of brine from the RO module	70,000 mg/L	
11.	Flow rate of brine from the RO module		

Table 2 Important technical details of the RO plant

	echinical details of the KO plant		
Serial no.	Parts	Specification	Specification
1.	Seawater intake mouth	Intake mouth covering mesh size	100*15 mm slots
2.	Connecting pipe from intake mouth to equalisation tank	Inner diameter and outside diameter	450 mm, 490 mm
3.	Feed pump motor	Speed	2,900 rpm
	squirrel gauge induction type	Rating	30 KW, 415 V 3 phase
4.	Feed pump (vertical centrifugal type)	Head	49/39 m of WC
5.	RDMF (horizontal)	i. Sand mesh size 14"	400 mm
		height	150 mm
		ii. Gravel 1/8"*1/16"	150 mm
		height	150 mm
		iii. Gravel 1/4"*1/8" height	600 mm
		iv. Gravel 3/8"*1/4"	3,000 mm
		v. Gravel 3/4"*3/8"	7,000 mm
		vii. Diameter	
		viii. Length	
6.	PDMF (horizontal)	i. Anthracite height	300 mm
		ii. Gravel 1/8"*1/16" height	100 mm
		iii. Gravel 1/4"*1/8" height	100 mm
		iv. Gravel 3/8"*1/4"	100 mm
		v. Gravel 3/4"*3/8"	600 mm
		vi. Refilling freq	5 year once
		vii. Diameter	3,000 mm
_		viii. Length	7,000 mm
7.	Disc filter: 2" ADF	1. Disc element: polyethylene	15-25 s
		11. Flusing cycle time	25 m°/h
		111. Max flow rate	10 bar
0		iv. Max working pressure	
8.	Cartridge filter	Material: polypropylene	
		11. Filter element size	2.6"OD1.1"ID 40" length
0	E	iii. No. of catridge element/filter	30 nos.
9.	Energy recovery device	1. Material: duplex stainless steel	150
		11. Feed flow	158 cu.m/ h
10		iii. Brine flow	79 cu.m/ h
10.	HP pump	1. Centrifugal pump	
		11. Total discharge head	634 m of WC
11		III. Suction pressure min	5 m of WC
11.	HP pump motor rating	BHEL	450 KW, 2,980 rpm
12	RO membrane	i Type Filmtech SW30HR380	50 HZ, 6.6 KV, 5 ph
12.	no membrane	Outer material: polyamide	
		Centre material: polysulphone	
		ii Length	1 meter
		iii. Outer diameter	8″
		iv. One vessel length (6 ROS)	6.6 meter
		v. Vessel inner dia	210 mm
		vi. Top most vessel pressure	2 kg/cm^2
		vii. Feed flow/vessel	$6 \text{ m}^3/\text{h}$
		viii. Permeate flow/vessel	$5 \text{ m}^3/\text{h}$
		ix. Brine flow/vessel	$1.5 {\rm m}^3/{\rm h}$
		,	,

ised multi-input multi-output models for controller synthesis.

3. Result and discussion

In this section, the above theoretical model is simulated and output is obtained. When the plant is running under steady operating condition, permeate flow is calculated for different values of pump pressures. These calculated values are compared with that observed experimentally. Similarly, in a step, disturbance (from 1 to 60 bar) in the feed pressure is given and permeate flow rate and concentration and brine flow rate are observed, from the model equations, to have transient behaviour.

Table 1 shows the normal operating condition of the plant. Table 2 gives the technical specification of the plant. Percentage of salt rejection is found to be 99.5%. Designed recovery is calculated as 50%.

3.1. Model Validation

The theoretical response is obtained after simulating the model as per Fig. 6. The mathematical models are validated in two different modes. (i) Steady state (Fig. 6(b)) and (ii) transient/startup mode. When the plant was running at steady state, pump pressure data was collected. These are treated as input data to RO module. Using these data, output (flow rate) from RO is calculated using Eq. (8). These calculated outputs are plotted (Fig. 6(b)) against pump pressure and are compared with the same (measured flow rate from exit of RO) against pump inputs. Calculated error between the two curves is found to be 0.5041. When the plant was in the startup mode, pump pressure data (input) are collected and outputs (flow rate and concentration) from exit of permeate tank (as described in Fig. 6(a, c and d) are recorded. Same variables (flow rate and concentration from permeate tank) from model equations are calculated after simulating (a step input of 60 bar is provided as ΔP of pump to calculate outputs from permeate tank) the developed model. The recorded (experimental) and theoretically calculated values (simulated) are compared in Fig. 6(a) and (d). It is found that both the responses are in close agreement and the errors (mean squared error, MSE) calculated between the curves are 4.2893 (Fig. 6(a)), 7.868 (Fig. 6(c)) and 3.3281 (Fig. 6(d)). The error or deviation between the theoretical and experimental values in Fig. 6, has been found in terms of R^2 . In case of permeate flow rate (Fig. 6(a)), R^2 is found to be 0.9293; for brine flow rate (Fig. 6(c)), R^2 is found to be 0.9962; for permeate concentration (Fig. 6(d)), R^2 is calculated to be 0.9795. R^2 gives amount of variability in the data explained or accounted by the model. In all the above results, R^2 is found to be closure to 1, proving that the present model is in close agreement with the experimental data.



Fig. 6. Comparison of permeate flow rate and concentration with respect to theoretical (model) and experimental values [validation of model with experimental values: unsteady state results are in (a), (c) and (d): steady state result is in (b)].



Fig. 7. Concentration profile along the radial length of RO membranes with different initial concentration.

Eq. (10c) can be used to find concentration of permeate. Fig. 7 shows concentration profiles along the radius of RO. Streams at the centre of RO contains initial concentration, C_{f0} which is plotted in *y* axis. The concentration declines as radial length increases from centre of membrane. With different values of C_{f0} , the concentration profiles are plotted in Fig. 7.

Eqs. (9)–(23) are solved in MATLAB and the transient responses of flow rate and concentration at the exit of RO module and the potable water tank and brine are plotted (Fig. 8) for step disturbance in feed streams of respective units. The steady state results



Fig. 9. Comparison of computed permeate flow-rates for different feed flow-rates using present model and model by Chen-Jen Lee et al. [12].

of permeate flow rate (F_p) for various values of feed flow rate are computed using present model and are compared with the same from Chen-Jen Lee et al. [12]. It is found that the results from the present study are in close agreement with that of Chen-Jen Lee et al. [12]; thus, the model has been validated. It can be seen (Fig. 9) that the permeate flow rates from Chen et al. [12]. behaves linearly with feed flow rate; while those from the present model show little



Fig. 8. Time profile of streams under nominal operating conditions (0–800 s) followed by same with 10% change (after 800 s) in feed-flow rate in raw feed [for permeate (a) flow rate and (b) concentration, for brine (c) flow rate and (d) concentration].

non-linearity, establishing the fact that permeate flow rate changes with feed flow rate nonlinearly. Moreover, recovery calculated from Chen-Jen Lee et al. [12] is 10%, whereas it is 40% as obtained from the present model.

3.2. Linearised model

Thus, the desalination system developed here has two manipulated inputs and three measured outputs. The inputs to the multivariable system are pump pressure (P) and ratio ($R_{\rm FB}$) of flow rates of seawater feed to that of brine stream as it enters the equalisation tank (as shown in Fig. 1). The outputs to the multi-input multi-output system are permeate concentration, flow rate and pH. The transfer function of the developed model is given by Eq. (26)

$$\begin{bmatrix} Q_p \\ C_p \\ pH_p \end{bmatrix} = \begin{bmatrix} \frac{1.52388 * 10^{-5}e^{-0.55s}}{0.716153s + 1} & \frac{0.092857e^{-0.3666s}}{1.1875s + 1} \\ \frac{-5.176 * 10^{-6}e^{-0.55s}}{0.717834s + 1} & \frac{-16.0482e^{-0.233s}}{3.31s + 1} \\ \frac{1.167 * 10^{-6}e^{-0.55s}}{7s + 1} & \frac{1.1857 * 10^{-6}e^{-0.15s}}{2.5s + 1} \end{bmatrix} \begin{bmatrix} \Delta P \\ R_{FB} \end{bmatrix}$$
(26)

Tong et al. [16] used engineering equation solver to obtain results from a steady state and transient model for desalination system. Chaaben et al. [17] derived a MIMO transfer function for desalination plant from existing models. The models presented here are unique and novel as they represent a real plant. These models can be used for process control purpose.

4. Conclusion

A comprehensive mechanistic mathematical model representing individual units of desalination process is formulated from first principles of mass transfer. The integrated system is of multivariable type in nature and is represented as having two inputs, namely, pump pressure and ratio of flow rates of seawater feed to that of brine stream; and three outputs, namely, permeate concentration, flow rate and pH. The steady state and transient behaviour of the model are validated using practical industrial data. Permeate flow rates are calculated from steady state model equations for different values of pump pressures to validate steady state behaviour of the process by comparing similar industrial data obtained practically. Similarly, flow rates and concentrations of permeate stream are calculated for step changes in inputs using transient model and are validated using similar data recorded from experiment. Thus, the developed model has been validated. The linearised model is useful for further study for safe operation and control of the process.

Nom	Nomenclature				
$A_{\rm bt}$	—	area of the brine tank in m ²			
$A_{\rm m}$	—	area of the membrane = 0.10367 m^2			
A _{mt}	—	area of the mixing tank in m ²			
b	—	percentage of brine recycled to mixing tank			
		taken from the brine tank (25)			
C _b		density of brine in $kg/m^3 = 1,064$			
$C_{\rm bi}$	_	concentration of brine at the inlet of the brine			
		tank in mg/ml			
C_{bo}		concentration of brine at the outlet of the brine			
		tank in mg/ml			
$C_{\rm bo}$	—	concentration of brine recycle stream to mixing			
		tank in mg/ml			
$C_{\rm bt}$	—	concentration of brine in brine tank in mg/ml			
$C_{\rm c}$	—	concentration of brine from the RO module in			
		mg/ml			
$C_{\rm ci}$	_	concentration of cake in mg/ml			
$C_{\rm f}$	—	feed water concentration in mg/ml			

 $C_{\rm mm}$ concentration of the exit stream from mixing tank entering into the membrane module.

- concentration of feed in the equalisation tank in $C_{\rm mt}$ mg/ml
- C_{p} concentration of permeate from the RO module in mg/ml
- concentration of permeate inflow to the C_{pi} permeate tank in mg/ml
- C_{pt} concentration of permeate in the permeate tank in mg/ml
- $C_{\rm s}$ saturation constant = 0.369 kg/m^3
- concentration of seawater entering into the $C_{\rm so}$ mixing tank in mg/ml
- concentration of permeate recycle to mixing C_{po} tank, mg/ml
- $C_{\rm w}$ concentration of potable water in mg/ml
- height of brine in the brine tank in m $h_{\rm bt}$
- height of seawater in mixing tank in m $h_{\rm mt}$
- height of liquid in permeate tank in m hpt
 - rate constant of bulk crystallisation = $8.52 \times 10^{-9} \text{ m}^3/\text{s}$
 - solute mass transfer coefficient, m²/s
- water mass transfer coefficient, m²/s K_{w}
- mass of cake in kg M_{c}

 $K_{\rm c}$

 $K_{\rm s}$

Р

Qp

- % permeate (due to vertical component of velocity) comes out along the surface of the membrane the value is 1 if the permeate is recycled (=40%)
- P_{b} brine pressure, kg/m^2
- feed water pressure, kg/m² $P_{\rm f}$
- permeate pressure, kg/m² $P_{\rm p}$
- brine flow rate in m³/h $Q_{\rm b}$
- flow rate of brine from the RO module in m³/h $Q_{\rm c}$
- feed water flow rate in m³/h $Q_{\rm f}$
 - flow rate of permeate from the RO module in m³/h

- $Q_{\rm w}$ flow rate of potable water in m³/h
- *R* concentrated brine (due to horizontal component of velocity) flows axially through the membrane, the value is 1 if the brine is recycled
- R_{bt} resistance of the value in the brine tank (for liner value $R_{bt}=1$)
- $R_{\rm c}$ resistance of the cake in the membrane, Pa s m⁻¹
- $R_{\rm m}$ resistance of membrane, Pa s m⁻¹
- R_{mr} resistance of the exit valve from mixing tank (for linear valve R_{mt} =1)
- $R_{\rm pt}$ resistance of the exit valve from permeate tank (for linear valve $R_{\rm pt}$ =1)
- $S_{\rm p}$ surface area of active sites on bulk crystallisation = $0.5 \, {\rm m}^2$
- $V_{\rm bo}$ volumetric flow rate of brine output from brine tank in m³/h
- $V_{\rm bt}$ volume of brine tank in m³
- $V_{\rm ci}$ volumetric flow rate of cake in m³/h
- V_{co} volumetric flow rate of the cake in m³/h
- $V_{\rm mm}$ volumetric flow rate of mixing tank water entering the RO module in m³/h
- $V_{\rm mT}$ volume of mixing tank in m³
- $V_{\rm pi}$ volumetric flow rate of the inlet stream to the permeate tank
- *V*_{po} volumetric flow rate of permeate from the output of the permeate tank in m³/h
- $V_{\rm pt}$ volume of permeate tank in m³
- $V_{\rm so}$ volumetric flow rate of seawater to the mixing tank in m³/h

Suffix and prefix

- b brine
- c cake
- f feed
- i interface or inlet
- m membrane or mixing
- p permeate
- r recycle
- s solute
- t tank
- w water

Greek symbols

- Ψ deposition probability of crystals = 0.7
- η viscosity of seawater in kg/m.sec
- α specific cake resistance = 4.15×10^{14} m/kg

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