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Optimal Design of Reverse Osmosis-Based Water Treatment Systems

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We address the problem of optimal design of reverse osmosis (RO)-based water treatment systems. A superstructure optimization method is proposed to solve the problem, where the superstructure for a RO system is structurally enhanced with additional features. We formulate the problem as mixed-integer nonlinear program which is solved to yield optimal results. A case study on desalination is considered in this work, and the numerical results obtained using our approach are validated using a commercial simulation tool. We further extend the problem by considering the effects of degradation of membrane performance over time and solve it by representing the problem as a two-stage stochastic program. This new approach is highly useful for identifying minimum cost robust designs for membrane-based water purification systems, which are especially important in desalination applications. © 2012 American Institute of Chemical Engineers *AIChE J,* 58: 2758–2769, 2012
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Introduction

Clean fresh water is a critical raw material and process fluid in the chemical and process industry, and from a design standpoint, traditionally viewed as cheap and plentiful. In the last few years, there have been significant shortages in the supply of industrial freshwater in both the developing as well as the established markets, along with more stringent environmental regulations on wastewater discharge. This has led to more opportunities for managing the available water resources and wastewater disposal more efficiently. Desalination, which is used for providing potable water in some parts of the world, is a major and growing application, where improved system design is important. This research is directed toward developing a systematic approach for the design of robust, continually operated water treatment systems at minimum cost.

Reverse osmosis (RO) and nanofiltration membrane technologies have been used effectively for water treatment in a number of applications. The cost of using RO for applications such as desalination is mostly lower than using more expensive distillation techniques and it is also simple and modular to operate.[1] These systems are also easily adjusted to change feed quality and product quality requirements. The principles behind RO and other membrane based technologies can be found in the FILMTEC^{TM} technical manual.[2] In these water treatment systems, a membrane system forms the major part of the network, typically where a set of membrane elements are placed in pressure vessels that are arranged in a certain way.[2] There are different membrane types (e.g., high flux, fouling resistant, high rejection) that are manufactured to cater to different industrial, municipal, and commercial applications. The performance of such treatment systems can be improved not only by increasing the separation efficiencies of the membranes used but also by deciding on the optimal configuration of the various pressure vessels containing the membrane elements and deciding on the number and type of membranes to be present in these. There has been considerable work in the past that has focused on designing optimal water treatment networks based on membrane technology. El-Halwagi[3] presented a mixed-integer nonlinear programming (MINLP) formulation based on a state space representation for the synthesis of optimal RO systems for waste reduction. This idea was modified by Voros et al.,[4] who solved a seawater desalination problem by formulating it as a nonlinear program (NLP). Zhu et al.[5] extended the original state space representation to design optimal and flexible RO networks using an iterative solution procedure taking into account the variations in feed characteristics and system performance. These authors, as also See et al.,[6] were able to determine an optimal membrane maintenance/regeneration schedule. The effect of reducing the number of membrane elements within a pressure vessel and changing the system configuration on the system economics in nanofiltration plants was studied by Wessels et al.[7]

The problem of cost optimizing systems with different types of spiral wound membranes elements was addressed by Lu et al.[8,9] who used the initial idea by El-Halwagi.[3] Their method is able to select the optimal network configuration along with the optimal membrane type to use. However, there have been relatively few articles that use detailed modeling of spiral wound membranes in an optimization

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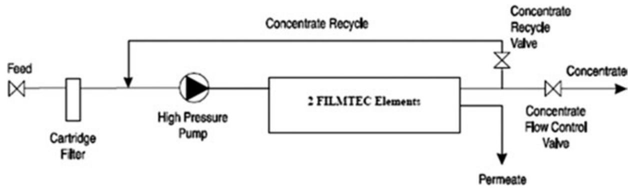

Figure 1. Single module system with two membrane elements.

framework and this work focuses on designing systems with such membranes, as it is common industrial practice. Vince et al.[10] have used such spiral wound membranes and have captured both economic and the environmental objectives in designing optimal membrane networks using an MINLP model. We extend such work by incorporating certain new features in the design and using an improved model.

This work deals with the design of optimized RO-based water treatment systems with spiral wound membranes. Here, we use a mathematical programming-based approach to predict a minimum cost (capital and operating) RO membrane network that is able to meet both product demand and quality requirements of customers. This overcomes the limitations of simulation-based software tools (ROSA: RO system analysis, CADIX: computer-assisted design for ion exchange). In such simulators, the design has to be decided based on experience of the designer or based on heuristics[2] and then input in the software manually to test its validity. The current ROSA and CADIX technology is a manual, change a variable at time, run, evaluate results approach. CADIX has a wizard approach to design with relooping. Although these are industry standards for design assistance, neither allows for systems solution nor optimization on cost objectives. The proposed optimization tool based on this work will be able to synthesize a design based on system constraints so that the overall cost of the network is minimized.

The Synthesis Problem

The problem involves the optimal design and operation of a water treatment network. This network consists of a set of RO pressure vessels through which water can be passed. Each pressure vessel has a certain number of spiral wound membrane elements inside it arranged in series. A membrane element removes the pollutants from the incoming raw water stream under an applied pressure, giving rise to a clean water stream (permeate) and a contaminant enriched stream (concentrate). The schematic of a single module system with two membrane elements (see FILMTEC™ technical manual[2]) is given in Figure 1.

The pressure differential is a primary driver of the permeate and solute fluxes across a membrane element. The arrangement of the elements in the pressure vessel is such that the concentrate from a membrane element becomes the feed of the subsequent membrane element and the permeate from each of the membrane elements is collected in a central permeate tube. Each pressure vessel normally has two outlets—permeate obtained from the outlet of the permeate tube, and concentrate (or reject) from the end of the pressure vessel. In this work, we allow for a part of the permeate to be withdrawn from the first membrane element inside the vessel effectively giving rise to three outlets from a pressure vessel. The pressure vessels are usually arranged in parallel which gives rise to a single stage. We have a multistage system when the concentrate from a stage becomes the feed for a subsequent set of parallel pressure vessels (or stage). Sometimes the concentrate from subsequent stages in recirculated back to initial stages for enhancing the recovery of the system. A two stage system with concentrate recycle is shown in Figure 2 (see FILMTEC™ technical manual[2]).

A permeate staged system arises when the permeate from a stage is sent to the next stage for further purification. In this case, each stage is termed as a "pass."

The RO system can be operated in batch as well as continuous modes and each of the modes of operation has its advantages and disadvantages.[2] In this work, we consider continuously operating treatment systems. The goal is to synthesize a network interconnecting the pressure vessels and deciding on the flows between them to minimize the total capital and operating costs of the water treatment. In this work, we neglect the effects of pretreatment and post-treatment processes for the given RO membrane network. The novelty in this work is that the structural representation of the treatment system is enhanced in an optimization framework by incorporating the feature of withdrawing permeate from the front end of a pressure vessel (in this case, from the first element) in the superstructure, thereby allowing new solutions to the design problem. We have also combined together many other structural features such as feed bypasses, recirculation streams, and designed the system for multiple feeds and sinks. The self-recycle streams (that is, permeate or concentrate from a pressure vessel being sent back to the same vessel) in this work are also modeled rigorously so that their physical validity is ensured. We have not dealt with the concept of pressure exchangers directly—instead the pressures required at different pressure vessels are obtained as a result of the optimization. The model can easily be extended to account for the pressure exchange equipment.

We assume we have the following data:

1. Number and flow rates of raw water source streams.
2. Number and type of contaminants present in the source streams.
3. Number of permeate and concentrate sinks with required product demand and quality constraints.
4. Membrane parameters including water permeability of membranes, solute diffusivities, and fouling factor.
5. Pressure drops across membrane elements.
6. Upper limit on transmembrane pressure of membrane elements.
7. Maximum permeate flux for a membrane element.
8. Maximum feed flux.
9. Bounds on element recovery.

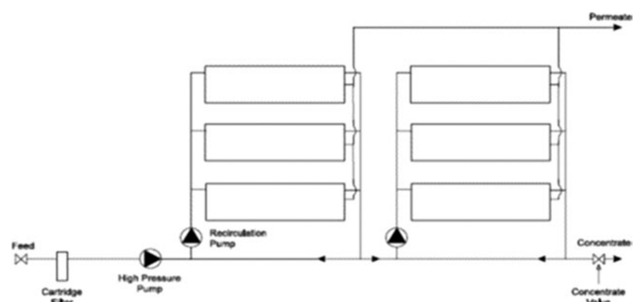

Figure 2. Two stage system with concentrate recirculation.

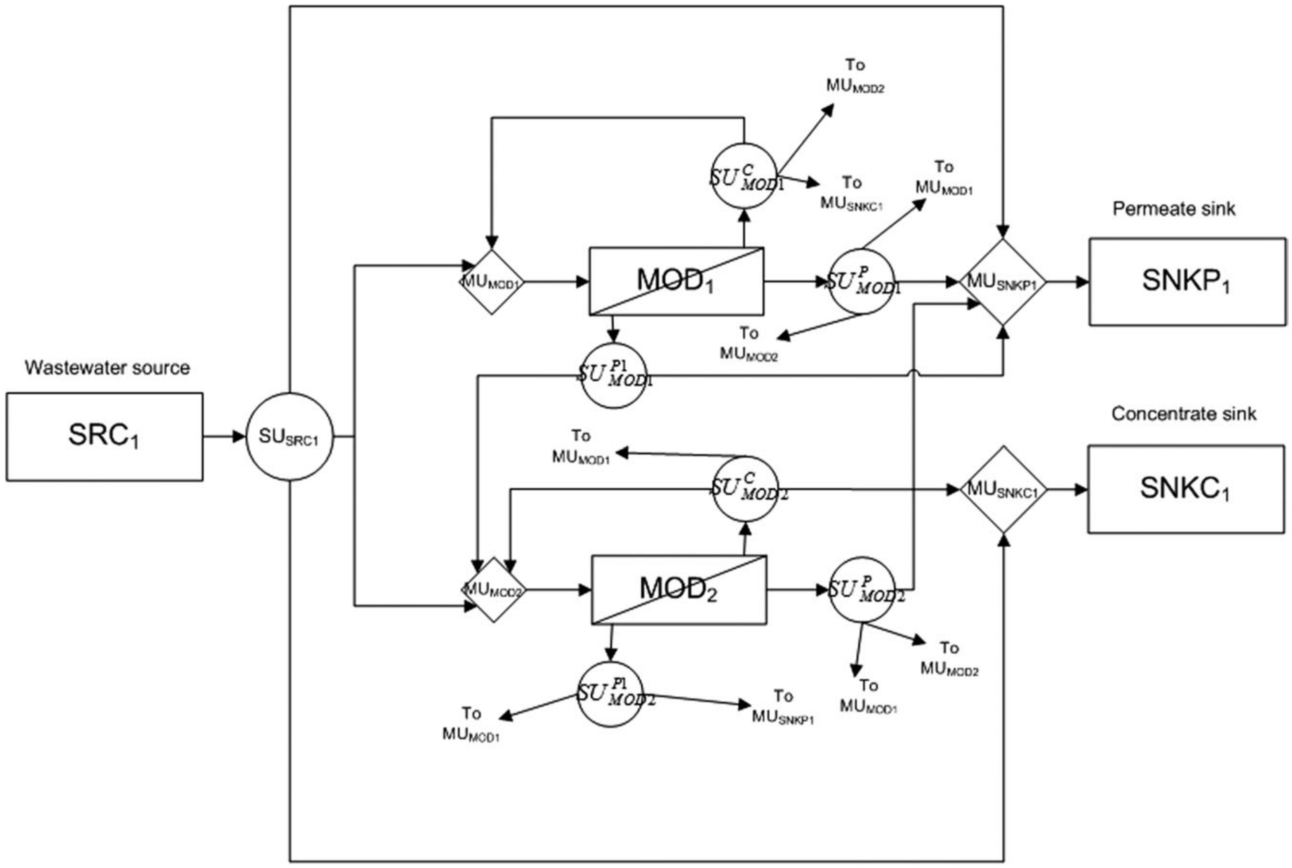

Figure 3. Superstructure for a wastewater treatment system with two treatment blocks.

10. Maximum area of a membrane element.
11. Temperature of the system.

The synthesis procedure determines the optimal values of the following variables in the design:

(a) Flow between various units in the system and their respective contaminant composition.

(b) Inlet and outlet pressure for a pressure vessel inside a treatment block.

(c) Number of pressure vessels parallel in a treatment block and the number of membrane elements in the pressure vessels within each block.

(d) Transmembrane pressure, transmembrane-osmotic pressure, pressure drop, permeate-back pressure, and inlet and outlet pressure for the individual membrane elements inside a pressure vessel.

(e) Contaminant concentration for feed, permeate, and concentrate for a membrane element.

(f) Inlet flow, permeate flow, concentrate flow for a membrane element.

(g) Membrane element recoveries.

(h) Water and solute fluxes for a membrane element.

(i) Membrane element areas.

(j) Rejection ratios for membrane elements.

Synthesis Methodology

To design an optimal wastewater treatment network, we propose a systematic superstructure optimization approach, where we initially construct a superstructure containing a number of design alternatives. The idea is that the optimization engine extracts the optimal design from this superstructure with respect to the specified objective function and imposed constraints. A superstructure of a treatment system with two treatment blocks, a single feed source, one permeate sink, and one concentrate sink is shown in Figure 3.

The blocks MOD_1 and MOD_2 represent the two treatment blocks that can be used for the waste treatment. Each treatment block consists of a number of pressure vessels in parallel. Each pressure vessel inside a particular treatment block has the same number of membrane elements inside it. The blow-up of a treatment block is shown in Figure 4.

The treatment blocks ($t \in$ MOD) are connected to each other and also to the wastewater sources (SRC) and the treated water sinks (SNK) with the help of mixers (MU) and splitters (SU). In Figure 3, we have a single wastewater stream coming from source (SRC_1) present at the inlet of the network and this transfers the effluent it carries to the splitter (SU_{SRC_1}). This splitter is connected to the various mixers in the system. The mixers MU_{MOD_1} and MU_{MOD_2} are present at

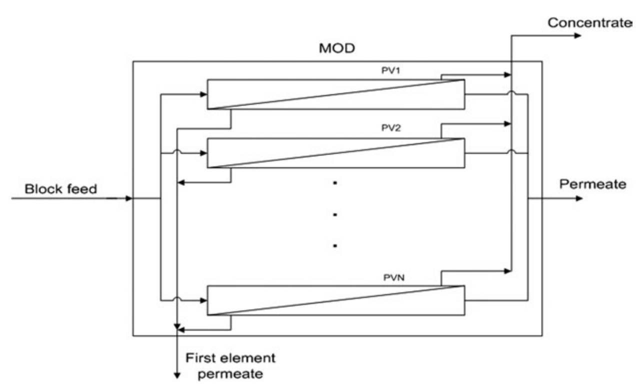

Figure 4. Blow-up of a treatment block.

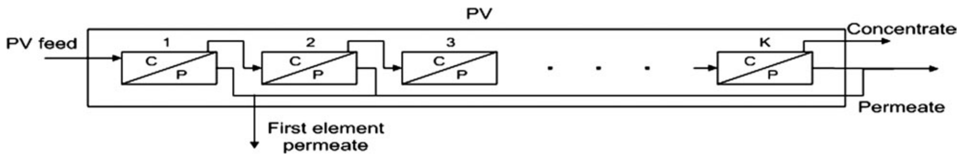

Figure 5. Arrangement of membrane elements inside a pressure vessel.

the inlet of the treatment blocks, whereas the mixer MU_{SNKP_1} mixes the permeate streams and directs the mixed stream to the sink $SNKP_1$ and the mixer MU_{SNKC_1} mixes the concentrate streams and directs it to the sink $SNKC_1$. As can be seen in Figure 3, each treatment block t is also connected to three splitters, SU_t^P, SU_t^C, and SU_t^{P1}. The permeate streams coming out of the permeate tube of each pressure vessel inside the treatment block t are combined and are directed to splitter SU_t^P. Similarly, the concentrate streams coming out of each pressure vessel inside a treatment block t are combined and sent to splitter SU_t^C. The flow to splitter SU_t^{P1} from a treatment block t is actually the sum of the flows of the permeates withdrawn from the first membrane element of all the pressure vessels inside the treatment block t. This is done because the permeate from the first element in a pressure vessel is purer than those from the subsequent elements and mixing it with the final permeate product can help reach product quality constraints more efficiently. All the pressure vessels inside a treatment block behave identically and handle identical flows and compositions. The detailed structure of a pressure vessel is shown in Figure 5.

All the splitters in the network direct water to the various mixers in the system. It is to be noted that the permeate streams are not sent to the concentrate sinks and the concentrate streams are not sent to the permeate sinks. Finally, in this network, there is also an option of bypassing the feed wastewater directly to the mixers placed before the sinks. This superstructure is easily generalized for a system with *N* treatment blocks.

To design the system, we first represent the superstructure in Figure 3 using a MINLP model (see Model Section) and it is optimized with respect to an objective function (usually total cost of network). This yields a design with the optimal network configuration and values of the variables that we are interested in. The following steps are involved in the optimal synthesis of the RO membrane network:

1. Gather the relevant data to characterize the equipment in the system to be designed.
2. Choose a number of treatment blocks (we limit it usually to $N \leq 10$) for practical reasons and select the number of membrane elements to be present inside each pressure vessel of a treatment block. The number of membrane elements inside each pressure vessel in a certain treatment block is taken to be the same. This step allows the designer some freedom in building up the superstructure and helps the optimization procedure.
3. Input the values of various parameters required in the model and set known bounds on various operating and design variables of the system. The model used to represent the RO network design problem is a MINLP (see Model Section), where the integer variables correspond to the number of pressure vessels inside each treatment block.
4. Solve the MINLP model using a standard MINLP solver package. An alternate approach to directly solving the MINLP model is as follows:

(a) Convert the MINLP model into a nonlinear programming model by relaxing the integer variables. The number of pressure vessels in the treatment block obtained from solving the relaxed NLP problem (P′) using any standard NLP solver may now be noninteger.

(b) Fix the integer variables in the original MINLP model to the nearest integer value greater than the optimal value of the corresponding variable obtained by solving the relaxed NLP model (P′) thus converting model (P) into an NLP termed as (P-NLP). We optimize the model (P-NLP) with any standard NLP solver to obtain a solution with integer values of the pressure vessels. This solution would be suboptimal to the original MINLP model (P).

5. As a result of this optimization, the solver will select certain treatment blocks from the superstructure and predict the optimal values of required operating conditions and design variables so that performance limits and process constraints are satisfied. Using the network configuration as obtained after the optimization, the number of stages and passes can be decided by the designer based on the flow of the concentrate and permeate streams obtained from the optimization results.

Model

We use total flows and contaminant compositions of the streams to formulate the material balance equations for each unit in the system. Nonconvex bilinear terms are present in these flow balance equations and are responsible for giving rise to multiple local optimal solutions to the design problem.[11] Certain assumptions are made before modeling the system:

1. The contaminant concentrations are assumed to be measured with respect to the solution volume (for example, mg L^{-1} of solution).
2. The model equations are written for a single solute (j = NaCl), although the model can be extended for multiple solutes.

The units in the system are modeled as follows:

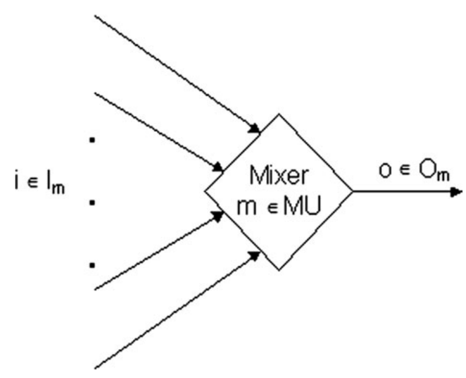

Figure 6. Mixer unit.

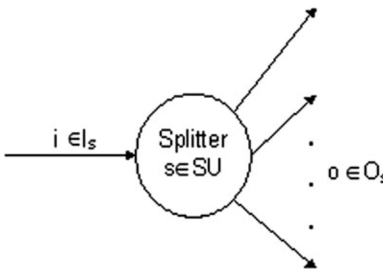

Figure 7. Splitter unit.

Mixers

In Figure 6, a mixer $m \in \mathrm{MU}$ is shown consisting of a set of inlet streams i that are specified in the index set I_{m}, and an outlet stream $o \in O_{\mathrm{m}}$. The overall material balance for the mixer m is given by Eq. 1 and the flow balances for each contaminant j in that mixer are given in Eq. 2.

$$F^o = \sum_{i \in I_{\mathrm{m}}} F^i \quad \forall \mathrm{m} \in \mathrm{MU},\ o \in O_{\mathrm{m}} \tag{1}$$

$$F^o C_j^o = \sum_{i \in I_{\mathrm{m}}} F^i C_j^i \quad \forall m \in \mathrm{MU},\ o \in O_{\mathrm{m}}, j = \mathrm{NaCl} \tag{2}$$

Here, F_i is the total flow of stream i (in kg s^{-1}) and C_j^i is the concentration of contaminant j (in ppm) in stream i. The individual contaminant balance equations contain nonconvex bilinear terms.

Splitters

As shown in Figure 7, a splitter $s \in \mathrm{SU}$ consists of an inlet stream $i \in I_{\mathrm{s}}$ and a set of outlet streams o specified in the index set O_{s}. The contaminant composition in the streams leaving the splitter is equal to the composition in the inlet stream. The following linear equations model the splitter s

$$F^i = \sum_{o \in O_{\mathrm{s}}} F^o \quad \forall s \in SU,\ i \in I_{\mathrm{s}} \tag{3}$$

$$C_j^o = C_j^i \quad \forall s \in \mathrm{SU}, \forall o \in O_{\mathrm{s}},\ i \in I_{\mathrm{s}}, j = \mathrm{NaCl} \tag{4}$$

Treatment blocks

As shown in Figure 8, a treatment block $\mathrm{t} \in \mathrm{MOD}$ consists of a number of pressure vessels (PVs) in parallel. Each block has an inlet stream $i \in I_{\mathrm{t}}$ and outlet streams $o \in O_{\mathrm{t}} = \{p_{\mathrm{t}}, c_{\mathrm{t}}, p1_{\mathrm{t}}\}$. p_{t} is combined stream of the permeate streams from the permeate tube of each pressure vessel inside block t, c_{t} is the combined stream of the concentrates from the pressure vessels of treatment block t, and $p1_{\mathrm{t}}$ is the combination of the permeate flows withdrawn from the first element of each pressure vessel inside block t. The inlet stream to a treatment block t is divided equally into (n_t^v) pressure vessels. All pressure vessels inside a particular treatment block are assumed to be identical and are modeled with identical flows, fluxes, recoveries, areas, solute concentrations, and pressures. The following equations are used to model the overall block

$$F^i = n_{\mathrm{t}}^v \cdot F_{\mathrm{t}}^{\mathrm{in}} \quad \forall t, i \in I_{\mathrm{t}} \tag{5}$$

$$F^o = n_t^v \cdot F_{\mathrm{out}}^{\mathrm{o}} \quad \forall t, \forall o \in O_{\mathrm{t}} \tag{6}$$

$$F^i = \sum_{\mathrm{o}} F^{\mathrm{o}} \quad \forall t, i \in I_t, \forall o \in O_{\mathrm{t}} \tag{7}$$

$$F^i C_j^i = \sum_{o} F^o C_j^o \quad \forall t, i \in I_t, \forall o \in O_{\mathrm{t}}, \mathrm{j} = \mathrm{NaCl} \tag{8}$$

where $F_{\mathrm{t}}^{\mathrm{in}}$ is the flow rate of stream into a pressure vessel inside treatment block t, whereas $F_{\mathrm{out}}^{\mathrm{o}}$ is the flow rate of stream o coming out of a pressure vessel inside treatment block t.

The inlet flow to each pressure vessel is passed through a series of spiral wound membrane elements. All the pressure vessels inside a particular block t are assumed to have the same number of membrane elements (K_{t}) in series. The overall flow and solute balance across the membrane element is given by the following equations

$$\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{in}} = \mathrm{Fe}_{k_{\mathrm{t}}}^{p} + \mathrm{Fe}_{k_{\mathrm{t}}}^{c} \quad \forall t, k = 1..K_{\mathrm{t}} \tag{9}$$

$$\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{in}} \mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{in}} = \mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{p}} \mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{p}} + \mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{c}} \mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{c}} \quad \forall t, k = 1..K_{\mathrm{t}}, \mathrm{j} = \mathrm{NaCl} \tag{10}$$

Here, $\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{in}}$, $\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{p}}$, and $\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{c}}$ are the flow rates of feed, permeate, and concentrate, respectively, for a membrane element k inside a pressure vessel inside treatment block t, whereas $\mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{in}}$, $\mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{p}}$,and $\mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{c}}$ are the solute concentrations in the respective streams.

There are a number of articles to describe the transport of solvent and solutes across membrane elements.[12–14] We use a simplified, and commonly used, set of equations to describe the transport phenomena. Membrane scaling effects are neglected in the model.

The permeate flow across a membrane is given by

$$\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{p}} = (J_{k_{\mathrm{t}}}^{\mathrm{w}} + J_{k_{\mathrm{t}}}^{\mathrm{j}}) S_{\mathrm{M}}^{t} \quad \forall t, k = 1..K_{\mathrm{t}}, \mathrm{j} = \mathrm{NaCl} \tag{11}$$

where $J_{k_{\mathrm{t}}}^{\mathrm{w}}$ and $J_{k_{\mathrm{t}}}^{j}$ are the water and solute flux, respectively, across membrane element k inside a pressure vessel in treatment block t. S_M^{t} is the area of a single membrane element in treatment block t.

The permeate and the water recovery for a single membrane element are related by

$$\mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{p}} = r_{k_{\mathrm{t}}} \mathrm{Fe}_{k_{\mathrm{t}}}^{\mathrm{in}} \quad \forall t, k = 1..K_{\mathrm{t}} \tag{12}$$

where $r_{k_{\mathrm{t}}}$ is the recovery of membrane element k inside a pressure vessel in treatment block t.

The solute rejection for a membrane is also taken as a variable and computed as

$$\mathrm{RR}_{\mathrm{j},k_{\mathrm{t}}} = 1 - \frac{\mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{p}}}{\mathrm{Ce}_{\mathrm{j},k_{\mathrm{t}}}^{\mathrm{in}}} \quad \forall t, k = 1..K_{\mathrm{t}}, \mathrm{j} = \mathrm{NaCl} \tag{13}$$

$\mathrm{RR}_{k_{\mathrm{t}}}^{\mathrm{j}}$ is the rejection of solute j in membrane element k inside a pressure vessel in treatment block t.

The water and solute flux across a membrane element are computed as

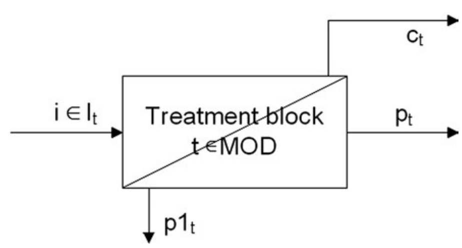

Figure 8. Treatment block.

$$J_{k_t}^{w} = A.(\Delta P_{k_t} - \Delta\pi_{k_t}) \quad \forall t, k = 1 \ldots K_t \tag{14}$$

$$J_{k_t}^{j} = B_j.Ce_{j,k_t}^{w} \quad \forall t, k = 1 \ldots K_t, j = NaCl \tag{15}$$

Here, A is the water permeability across an membrane element, ΔP_{k_t} is the transmembrane pressure across membrane element k inside a pressure vessel in treatment block t, $\Delta \pi_{k_t}$ is the osmotic pressure difference across membrane element k inside a pressure vessel in treatment block t, B_j is the solute j permeability, and $Ce_{j,kt}^{w}$ is the solute j concentration at the feed side outer wall of membrane element k inside a pressure vessel in treatment block t.

The solute flux across a membrane element is also dependant on the total permeate flow across the membrane

$$J_{k_t}^{j} S_M^{t} = Fe_{j,k_t}^{p}.Ce_{j,k_t}^{p} \quad \forall t, k = 1..K_t, j = NaCl \tag{16}$$

The average feed-concentrate concentration at the feed side wall of a membrane element is simply calculated as

$$Ce_{j,k_t}^{w} = \frac{Ce_{j,k_t}^{in} + Ce_{j,k_t}^{c}}{2} \quad \forall t, k = 1 \ldots K_t, j = NaCl \tag{17}$$

The transmembrane pressure is given by

$$\Delta P_{k_t} = P_{k_t}^{in} - P_t^{p} - \frac{\Delta p_{k_t}^{drop}}{2} \quad \forall t, k = 1..K_t \tag{18}$$

Here, $P_{k_t}^{in}$ is the pressure of inlet feed to membrane element k inside a pressure vessel in treatment block t, P_t^{P} is the permeate back-pressure inside membrane elements in treatment block t, $\Delta\ p_{k_t}^{drop}$ is the pressure drop on the feed side of membrane element k inside a pressure vessel in treatment block t.

The transmembrane osmotic pressure across a membrane element inside block t is approximated by the Van't Hoff relation[10]

$$\Delta\pi_{k_t} = \frac{2RT\rho}{M_{NaCl}} \cdot (Ce_{j,k_t}^{w} - Ce_{j,k_t}^{p}) \quad \forall t, k = 1..K_t, j = NaCl \tag{19}$$

where, R is the gas constant, T is the temperature of system, M_{NaCl} is the molar mass of the solute NaCl, and ρ is the density of the solution being handled in the elements. The membrane is assumed to be isothermal.

The membrane water permeability is computed as a function of the temperature and the fouling factor in the following equation

$$A = A_{ref} \cdot FF \cdot TCF \tag{20}$$

where A_{ref} is the water permeability across a membrane at reference temperature, FF is the fouling factor, and the temperature correction factor (TCF) is given by

$$TCF = e^{\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)} \tag{21}$$

Here, E is the membrane activation energy and T_0 is the reference temperature.

The flow rate, pressure, and the solute concentration in the feed inlet to a membrane element are connected to the flow rate of the concentrate, pressure, and the concentrate solute concentration of the previous element, respectively.

$$Fe_{k_t+1}^{in} = Fe_{k_t}^{c} \quad \forall t, k = 1 \ldots K_t - 1 \tag{22}$$

$$P_{k_t+1}^{in} = P_{k_t}^{in} - \Delta p_{k_t}^{drop} \quad \forall t, k = 1 \ldots K_t - 1 \tag{23}$$

$$Ce_{j,k_t+1}^{in} = Ce_{j,k_t}^{c} \quad \forall t, k = 1 \ldots K_t - 1, j = NaCl \tag{24}$$

The inlet operating variables to a pressure vessel inside a treatment block are matched up with the corresponding operating variables of the first membrane element in that pressure vessel as given

$$Fe_{k_t}^{in} = F_t^{in} \quad \forall t, k = 1 \tag{25}$$

$$Ce_{j,k_t}^{in} = C_j^{i} \quad \forall t, i \in I_t, k = 1, j = NaCl \tag{26}$$

$$P_{k_t}^{in} = P_t^{in} \quad \forall t, k = 1 \tag{27}$$

Here, P_t^{in} is the pressure of inlet feed to treatment block t.

A part of the permeate is withdrawn from the first membrane element of a pressure vessel and is represented as follows

$$F_{out}^{p1_t} \leq Fe_{k_t}^{p} \quad \forall t, k = 1 \tag{28}$$

The concentrate and end permeate withdrawn from a pressure vessel are calculated using the following equations

$$F_{out}^{c_t} = Fe_{k_t}^{c} \quad \forall t, k = K_t \tag{29}$$

$$F_{out}^{p_t} = \sum_{k_t} Fe_{k_t}^{p} - F_{out}^{p1_t} \quad \forall t \tag{30}$$

The pressures in the different outlet streams from a pressure vessel are given by

$$P_{out}^{c_t} = P_{k_t}^{in} - \Delta p_{k_t}^{drop} \quad \forall t, k = K_t \tag{31}$$

$$P_{out}^{p_t} = P_t^{p} \quad \forall t \tag{32}$$

$$P_{out}^{p1_t} = P_t^{p} \quad \forall t \tag{33}$$

where P_{out}^{o} ($o = p_t, c_t, p1_t$) is the pressure of stream o coming out of a pressure vessel inside treatment block t. We have assumed that the pressure inside the permeate tube remains constant.

The solute concentrations in the various outlet streams from a treatment block are given by the following equations

$$Ce_{j,k_t}^{c} = C_j^{c_t} \quad \forall t, k = K_t, j = NaCl \tag{34}$$

$$Ce_{j,k_t}^{p1_t} = C_j^{p1_t} \quad \forall t, k = K_t, j = NaCl \tag{35}$$

$$F^{p_t} C_j^{p_t} = n_t^{v} \sum_{k_t} Fe_{k_t}^{p} Ce_{j,k_t}^{p} - F^{p1_t} C_j^{p1_t} \quad \forall t, j = NaCl \tag{36}$$

We have the overall flow and solute balances for the entire system as follows

$$\sum_{sr} \sum_{i \in I_{SU_{sr}}} F^{i} = \sum_{snkp} \sum_{o \in O_{MU_{snkp}}} F^{o} + \sum_{snkc} \sum_{o \in O_{MU_{snkc}}} F^{o} \tag{37}$$

$$\sum_{sr} \sum_{i \in I_{SU_{sr}}} F^{i} C_j^{i} = \sum_{snkp} \sum_{o \in O_{MU_{snkp}}} F^{o} C_j^{i} + \sum_{snkc} \sum_{o \in O_{MU_{snkc}}} F^{o} C_j^{i} \qquad j = NaCl \tag{38}$$

The self-recycle flow constraints state that the concentrate recycle flow from a treatment block back to the same

Table 1. Process and Membrane Parameters

Process and Membrane Parameters	Value
Pure water permeability A_{ref} (10^{-9} kg m^2 s^{-1} Pa^{-1})	12
Salt permeability constant B (10^{-5} kg m^2 s^{-1})	15
Maximum membrane element area (m^2)	40.9
Temperature (K)	293
E (J mol^{-1})	25000
R (J mol^{-1} K^{-1})	8.314
T_0 (K)	298
ρ (kg m^{-3})	1000
M_{NaCl} (kg mol^{-1})	0.0585
FF	0.85
Element pressure drop (bar)	0.2
Maximum permeate backpressure (bar)	0.3
Maximum element recovery (%)	14.7
Maximum applied TMP per element (bar)	41.3
Maximum element feed flow rate (kg s^{-1})	4.2
Maximum element permeate flow rate (kg s^{-1})	0.347
Maximum element water flux (kg s^{-1} m^{-2})	0.008

treatment block should not exceed the sum of the inlet flows into the mixer preceding the treatment block (except the recycle flow) minus the sum of the permeate streams withdrawn from that treatment block. Similar constraints are also then written for the self-recycling permeate streams to ensure validity of the recycle flows. These are given in Eqs. 39 and 40.

$$\sum_{\substack{i \in I_{\mathrm{MU_t}} \\ i \in O_{\mathrm{SU_t^C}}}} F^i = \sum_{\substack{o \in I_{\mathrm{MU_t}} \\ o \notin O_{\mathrm{SU_t^C}}}} F^o - F^{p_t} - F^{p1_t} \qquad \forall t \tag{39}$$

$$\sum_{\substack{i \in I_{\mathrm{MU_t}} \\ i \in O_{\mathrm{SU_t^P}}}} F^i = \sum_{\substack{o \in I_{\mathrm{MU_t}} \\ o \notin O_{\mathrm{SU_t^P}}}} F^o - F^{c_t} - F^{p1_t} \qquad \forall t \tag{40}$$

Objective function

In process synthesis, the optimization problem is usually to minimize the sum of the annualized capital cost of the design and operating cost of the system. In this model, we use surrogates for the cost of capital and operating costs in a simplified objective that minimizes the sum of the number of elements in the system (measure of annualized capital cost) and the inlet feed flow into the system (measure of operating cost). The objective function is shown in Eq. 41.

$$\min \quad z = \sum_t n_t^v . K_t + \sum\nolimits_{\mathrm{sr}} \sum\nolimits_{i \in I_{\mathrm{SU_{sr}}}} F^i \tag{41}$$

The term $\sum_t n_t^v . K_t$ is the total number of membrane elements in the network, whereas the term $\sum_{\mathrm{sr}} \sum_{i \in I_{\mathrm{SU_{sr}}}} F^i$ stands for the sum of all feeds from all external sources into the system.

Equal weights have been assigned to both summation terms in the objective function, as they are of the same order of magnitude for the case study considered in this work.

The flow rate and quality (contaminant concentration) restrictions on various streams in the system are modeled by imposing numerical bounds on the different variables in the model. Eqs. 1–41 comprise the MINLP model (P) that is to be solved.

Case Study

The case study considered in this work is taken from Vince et al.[10] The problem is to design a RO membrane network that is able to produce 405.1 kg s^{-1} (35,000 m^3 d^{-1}) of water with less than 0.3 g L^{-1} NaCl contaminant. The feed is assumed to be brackish surface supply water with silt density index (SDI) $<$ 5 and with a concentration of 3 g L^{-1}. BW30LE-440 membranes are used for this desalination process. The relevant process parameters (including the membrane specific parameters) and bounds are taken from Vince et al.[10] and the FILMTEC™ technical manual[2] and some of them have been modified and are given in Table 1.

Initially, we choose a superstructure with two treatment blocks, one with seven membrane elements in its pressure vessels (block $\mathrm{MOD_1}$) and the other containing eight membrane elements in its pressure vessels (block $\mathrm{MOD_2}$). The superstructure is identical to the one shown in Figure 3. We formulate the model using the mathematical programming application AIMMS® and solve it on an Intel 1.83 GHz machine with 1 GB memory. We optimize the model with an objective of minimizing the sum of number of elements in the system and the feed water consumption, to yield an optimal design as shown in Figure 9. The flows in the streams shown in this figure are in kg s^{-1}. The optimal objective value is 2059.4 found after 20 iterations of the MINLP solution algorithm. The MINLP model (P) corresponding to this problem has two integer variables, 304 continuous variables and 299 constraints and solves using the AOA solver in AIMMS® in 3.02 CPUsecs. The relaxed NLP model (P′) for this problem has 306 continuous variables and 299 constraints. The total time taken to solve the model (P) using the heuristic in Model Section is 0.08 CPUsecs and leads to the same solution of 2059.4. Larger models would take longer but the ability to solve a substantially sized system quickly appears feasible. A global optimal solver could also have been used to solve the problem although the focus of the study was not on globally optimizing such membrane-based water treatment systems.

Figure 9 shows that we need only one stage to achieve the required product purity. The optimal number of pressure vessels in the treatment block is 203, with each pressure vessel

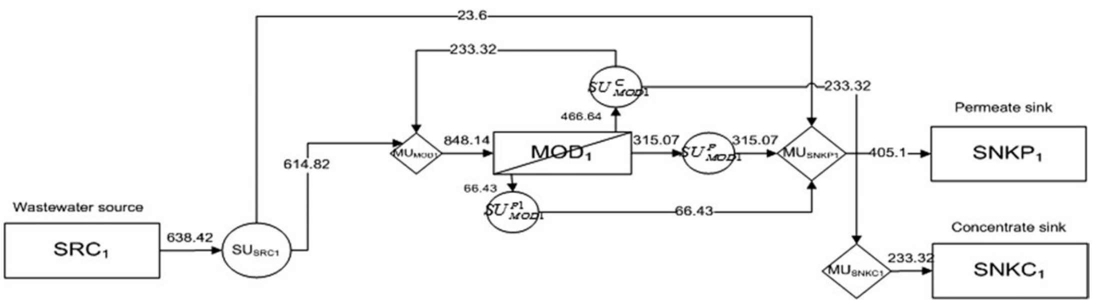

Figure 9. Optimal network configuration for case study.

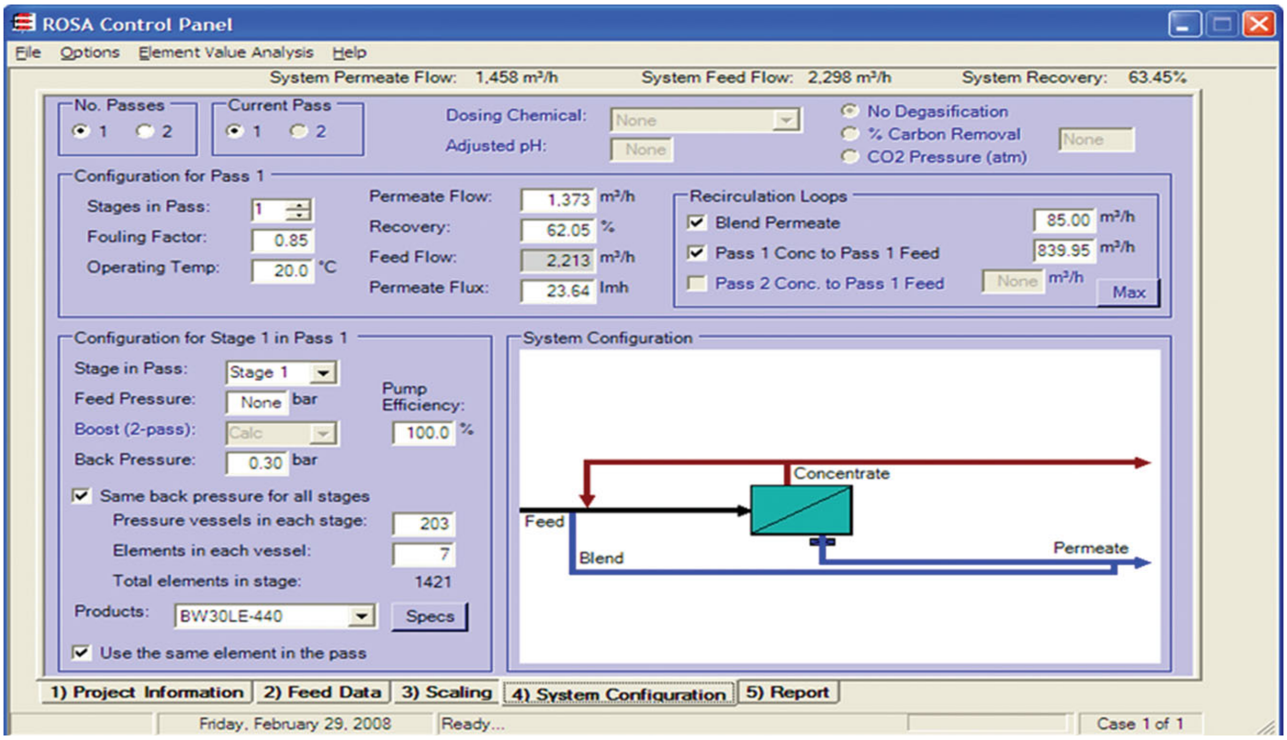

Figure 10. Input screen shot from ROSA.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

containing seven membrane elements. The total recovery in the system is 63.45%. It can be seen here that the optimization chooses to withdraw a part of the permeate from the first membrane element of each of the pressure vessels.

We validated this synthesized design in ROSA by inputting the number of stages, passes, operating temperature, number of pressure vessels in each stage, number of elements in a pressure vessel, total system recovery, product flow rate, permeate backpressure, feed bypass flow rate, concentrate recycle, and feed solute concentration in the ROSA simulator and find that the operating conditions output by the software (not shown here) are quite close to the ones predicted by the optimization model. The system configuration input into ROSA is given in Figure 10.

The system configuration output from ROSA is given in Figure 11.

Table 2 provides the overall results obtained from ROSA.

We then used the Dow water solutions heuristics described in the FILMTEC^{TM} technical manual[2] to design the system using the inputs from Table 1 and the flux data from the FILMTEC^{TM} manual,[2] we find that the method given in the FILMTEC^{TM} technical manual[2] predicts a total number of 1421 elements in the stage; 203 pressure vessels

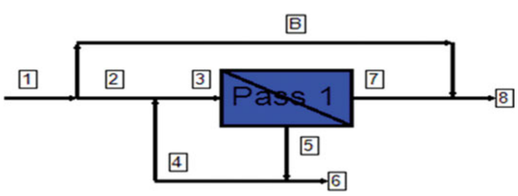

Figure 11. System design from ROSA.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

each with seven elements. These results are close to what the optimizer predicts with the simplified objective function.

It is also possible to find a better solution to the design problem by testing out pressure vessels with a different number of membrane elements. To study the effect of using fewer numbers of membrane elements inside the pressure vessels, we again build a superstructure with two treatment blocks—one with five elements inside its pressure vessels (block MOD_1) and the other with six elements inside its pressure vessels (block MOD_2). On optimizing the system with the given data, we obtain the network configuration shown in Figure 12.

This is a two stage system with treatment block MOD_1 being Stage 1 and MOD_2 being Stage 2 and in this case, the overall system recovery is 77.22%, the total number of pressure vessels with five elements (block MOD_1) is 180, whereas the total number of pressure vessels in Stage 2 (with six membrane elements) is 78. On comparing with the network in Figure 9, we find that although the network in Figure 12 has more pressure vessels, it has fewer total elements, leading to a lower objective value of 1892.56. This configuration also has lower number of membrane elements and higher recovery than the design obtained using heuristics. Note that all the solutions for this case study may be termed as suboptimal or near optimal as the MINLP solver terminates after 20 iterations.

System Design Under Uncertainty

There are uncertainties during the operation of a RO system. For instance, the feed conditions (such as quantity and quality) may change during network operation, the membrane performance can go down due to fouling effects, or product demand and quality may change among other things. A traditional engineering approach to handle uncertainties

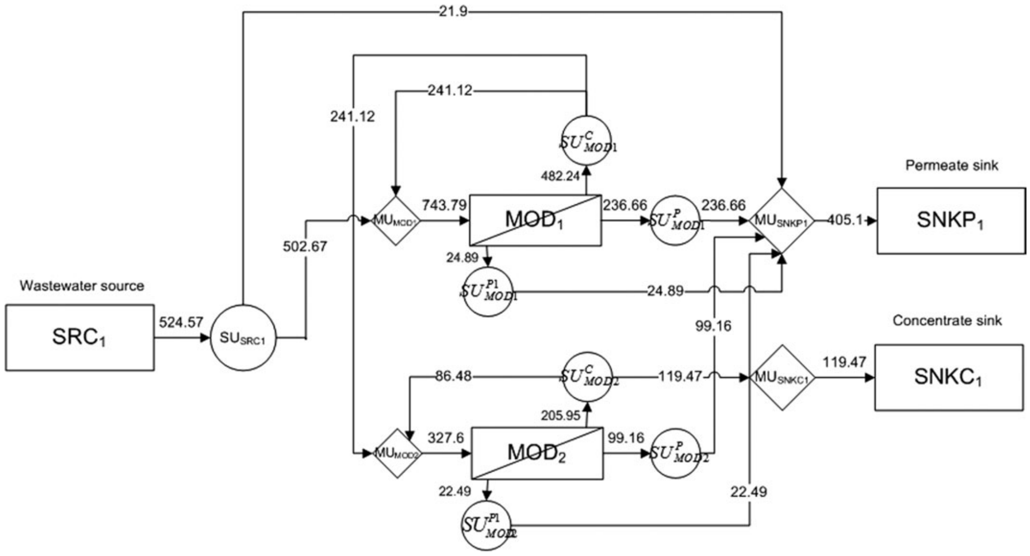

Figure 12. Optimal network configuration for case study with fewer membrane elements in pressure vessels.

would use specified over-design and other guidelines to modify a base design. We can also use a systematic approach to ensure that the proposed system network is designed to be robust and optimal from the beginning, accounting for the uncertainties. Zhu et al.[5] proposed an iterative solution procedure for designing a system which would be feasible under different feed and fouling conditions. We propose a stochastic programming approach for designing a network that is feasible and optimal in the face of uncertainty. In a stochastic programming approach,[15] the emphasis is on achieving optimality accounting for the fact that the recourse variables can be adjusted for each parameter realization.[16–18] The advantage of a two-stage stochastic programming approach is that we can obtain a design that is optimal over various given scenarios without an iterative scheme. In the first stage, the design variables including the number of pressure vessels in the treatment blocks, the maximum flows possible in the streams in the system, and the areas of the membrane elements in the pressure vessels are fixed, whereas the second stage variables that include the flows, concentrations, and pressures can be changed after uncertain operating conditions have changed. The goal is to construct a system that will have minimum capital and operating cost over the lifetime of the network operating under uncertain conditions ensuring that contaminant levels in the product must always fall below specified limits.

In this work, we consider the membrane fouling factor to be the only uncertain parameter in the system, which is assumed to be independent to the configuration of the membranes and the pressure vessels. This is an example of an uncertain parameter that takes on different values at different points of time during network operation. Because the

Table 2. System Operation Results from ROSA

Raw Water TDS	3000.02 mg L^{-1}	% System Recovery (8/1)	63.45%
Water Classification	Surface Supply SDI < 5	Fouling Factor (Pass 1)	0.85
Feed Temperature	20.0°C		
Pass #	Pass 1		
Stage #	1		
Element type	BW30LE-440		
Pressure vessels per stage	203		
Elements per pressure vessel	7		
Total number of elements	1421		
Pass average flux	23.64 lmh		
Stage average flux	23.64 lmh		
Permeate back pressure	0.30 bar		
Booster pressure	0.00 bar		
Chemical dose	–		
Energy consumption	0.82 kWh m^{-3}		
Pass 1			
Stream #	Flow (m^3 h^{-1})	Pressure (bar)	TDS (mg L^{-1})
1	2298.00	0.00	3000.02
2	2213.00	0.00	3000.02
3	3052.95	14.03	4317.65
4	839.95	10.86	7780.66
5	1679.85	10.86	7780.66
6	839.90	10.86	7780.66
7	1373.10	–	80.98
B	85.00	0.00	3000.02
8	1458.10	0.00	251.14
7/2	% Recovery	62.05	

Table 3. Scenario Uncertain Parameter Values and Probabilities

Scenario (sn)	1	2	3
Fouling factor (FF_{sn})	0.85	0.8	0.9
Probability (P_{sn})	0.5	0.3	0.2

integrated network is highly interconnected, changes in the uncertain parameters can adversely affect all parts of the network, and for certain values of the uncertain parameters, it may not be possible to operate the network without violating the product quality restrictions or the operating limits on the flows, contaminant levels, and fluxes in the system. To avoid this situation, we have to take into account the uncertainty in the system at the time of designing the network.

It is important to take into account the effect of fouling at the design stage itself, as it is one of the major factors that affects system performance over a period of time. We assign discrete values to the fouling factor, thereby creating a finite number of scenarios to characterize the uncertainty in which the fouling factor can take on these different values, and thus, convert the two-stage stochastic program into its multiscenario deterministic equivalent. These discrete values are average values over periods of time even though the fouling shows transient behavior. Probabilities are assigned to the occurrence of each scenario which is used to optimize a weighted objective function. In the design problem, apart from minimizing the cost, we also have to ensure that the product demand is met and the concentrations of the contaminants in the product stream must be less than specified levels at all times. For this, we have to take some decisions at both stages of the two-stage stochastic program.

Decisions pertaining to the first stage, which have to be taken before the appearance of uncertainty in the system are, (1) the maximum water flow rate allowed in each stream, (2) the number of pressure vessels in each treatment block, and (3) membrane areas of the individual elements inside the pressure vessels in the treatment blocks. These decisions correspond to the design variables in the problem and once chosen, these variables remain fixed throughout the duration of operation of the network and cannot be altered during operation. The second stage decisions among others are the flows of water to be pumped through each pipe in the network. These can be changed during network operation depending on the values taken by the uncertain parameters at any point of time. The problem at hand is to mathematically model the network as a multiscenario problem and optimize the model so as to determine the optimal first and second stage decisions that minimize the total cost of the network.

To model the network operating under uncertainty, we first represent the uncertainty in the system through the use of scenarios. The operation of the network is divided into different scenarios, where it is assumed that the fouling factors take on different known discrete values in each scenario, with specified probabilities assigned to the occurrence of each scenario. The model in Model Section is extended to form a multiscenario MINLP model and solved using the method given in Synthesis Methodology Section. All the variables in the system with the exception of the membrane element areas (S_M^t), number of pressure vessels in the treatment blocks (n_t^v), are now defined for each scenario (sn). We also introduce an additional variable $\hat{F^i}$ to denote the maximum flow capacity of a stream i. An additional constraint is added to the model

$$\hat{F^i} \geq F^i_{\text{sn}} \quad \forall i, \forall \text{sn} \tag{42}$$

which states that the maximum flow rate in that stream should be greater than or equal to the flow in that stream in every scenario (F^i_{sn}). We also modify the objective function to include the effect of the maximum flow capacity of each stream as attributing in part to the annualized capital cost.

The new objective function is:

$$\min \quad z' = \sum_t n_t^v.K_t + \sum_{\text{sn}} p_{\text{sn}} \sum_{\text{sr}} \sum_{i \in I_{\text{SU}_{\text{sr}}}} F^i_{\text{sn}} + \sum_i \hat{F^i} \tag{41a}$$

In this objective, we can see that probabilities are assigned to the raw water feed used in different scenarios to compute the expected operating cost. The annualized capital cost is the first stage cost and is a function of the total number of membrane in the system and the maximum flow capacity of each connection. The multiscenario model includes the constraints (1)–(40) written for each scenario, Eqs. 42 and 41a.

We apply this stochastic programming approach to solve the case study with three different scenarios. In the superstructure corresponding to this case study, there are two treatment blocks: MOD_1 with pressure vessels with seven membrane elements inside each, and MOD_2 with pressure vessels containing eight membrane elements each. The fouling factor is assigned three different average values and the corresponding probabilities are computed using the fractions of the time the fouling factor takes these values over the entire period of operation. Table 3 shows the different scenarios for the case study.

On solving the MINLP model corresponding to the case study with different fouling factors (with two integer variables, 935 continuous variables, 986 constraints), we obtain the network structure shown in Figure 13. After 20 iterations of the

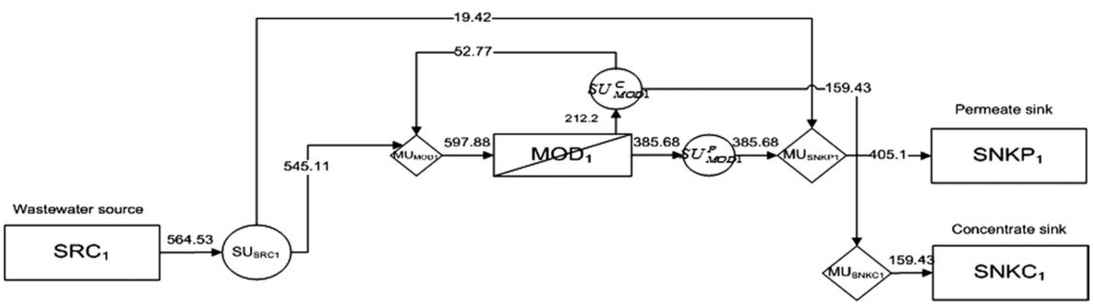

Figure 13. Optimal network structure for case study accounting for changes in membrane fouling factor during operation.

AIMMS® AOA solver (11.8 CPUsecs), the best found locally optimal objective value for the MINLP model is 5696.3.

The maximum allowed flows in the connections are shown in this figure. It is to be noted that the number of pressure vessels in the treatment block MOD_1 (with each pressure vessel containing seven membrane elements) increases from 203 in Figure 9 to 235 in Figure 13 to obtain the required product with the given purity because of the changes in membrane efficiencies that is reflected in the changing fouling factors. However, as the maximum water flow from the source is decreased the recoveries are now increased.

Conclusions and Future Work

A new framework has been developed to address the problem of designing cost optimized and robust RO systems for desalination. We followed a superstructure optimization approach, where the structural representation is enhanced by including the possibility of permeate withdrawal from both ends of a pressure vessel. The effects of uncertainty in the membrane performance are also considered by formulating and solving the problem as a stochastic program. Cost functions to represent the capital costs (including costs of pressure exchangers and pipes) and the operating costs (e.g., electricity consumption) can be incorporated in the model to make it more detailed in the future. We can also choose to withdraw permeate at the end of different elements within a pressure vessel instead of at the first element. Future work would also include implementing a more detailed model for multicomponent systems along with creating of good initial points for solving the optimization models.

Acknowledgments

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Notation

Indices

c_t = concentrate from treatment block t
j = contaminant
i, o = stream/connection/pipe
k = membrane element
m = mixer
p_t = permeate from treatment block t
$p1_t$ = permeate extracted from the first membrane elements inside treatment block t
s = splitter
sn = scenario
sr = source
snkc = permeate sink
snkp = concentrate sink
t = treatment block

Sets

I_m = set of inlet streams into mixer m
I_s = inlet stream into splitter s
I_t = inlet stream into treatment block t
MU = set of mixers
O_m = outlet stream from mixer m
O_s = outlet streams from splitter s
O_t = outlet streams from treatment block t
SN = set of scenarios
SNK = set of treated water sinks
SRC = set of wastewater sources
SU = set of splitters
MOD = set of treatment blocks

Parameters

A = water permeability across membrane elements
A_{ref} = water permeability across membrane at reference temperature
B_j = solute permeability
E = membrane activation energy
FF = fouling factor
K_t = number of membrane elements inside each pressure vessel in treatment block t
M_{NaCl} = molar mass of NaCl
N = total number of treatment blocks
R = gas constant
T = temperature of system
T_0 = reference temperature
TCF = temperature correction factor
ρ = density of solution
$\Delta p^{drop}_{k_t}$ = pressure drop on the feed side of membrane element k inside a pressure vessel in treatment block t

Continuous variables

C^k_j = concentration of contaminant j in stream k
$C^{p1_t}_{out,j}$ = solute j concentration in stream $p1_t$ coming out of pressure vessel in treatment block t
Ce^{in}_{j,k_t} = concentration of contaminant j in feed into membrane element k inside a pressure vessel in treatment block t
Ce^{p}_{j,k_t} = concentration of contaminant j in permeate from membrane element k inside a pressure vessel in treatment block t
Ce^{c}_{j,k_t} = concentration of contaminant j in concentrate from membrane element k inside a pressure vessel in treatment block t
Ce^{w}_{j,k_t} = solute j concentration at the feed side outer wall of membrane element k inside a pressure vessel in treatment block t
$\hat{F}^i$ = maximum flow rate allowed in stream i
F^i = flow rate of stream i
$Fe^{in}_{k_t}$ = flow rate of feed into membrane element k inside a pressure vessel in treatment block t
$Fe^{p}_{k_t}$ = flow rate of permeate from membrane element k inside a pressure vessel in treatment block t
$Fe^{c}_{k_t}$ = flow rate of concentrate from membrane element k inside a pressure vessel inside treatment block t
F^{in}_t = flow rate of stream into a pressure vessel inside treatment block t
F^o_{out} = flow rate of stream o coming out of a pressure vessel inside treatment block t
$J^w_{k_t}$ = water flux across membrane element k inside a pressure vessel in treatment block t
$J^j_{k_t}$ = solute j flux across membrane element k inside a pressure vessel in treatment block t
P^{in}_t = pressure of inlet feed to treatment block t
$P^{in}_{k_t}$ = pressure of inlet feed to membrane element k inside a pressure vessel in treatment block t
P^p_t = permeate back-pressure inside membrane elements in treatment block t
P^o_{out} = pressure of stream o coming out of a pressure vessel inside treatment block t
r_{k_t} = recovery of membrane element k inside a pressure vessel in treatment block t
$RR^j_{k_t}$ = rejection of solute j in membrane element k inside a pressure vessel in treatment block t
S^t_M = area of a single membrane element in a pressure vessel in treatment block t
ΔP_{k_t} = transmembrane pressure across membrane element k inside a pressure vessel in treatment block t
$\Delta\pi_{k_t}$ = osmotic pressure difference across membrane element k inside a pressure vessel in treatment block t

Integer variables

n^v_t = number of pressure vessels inside treatment block t

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