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Multi-objective optimization of reverse osmosis desalination units using different adaptations of the non-dominated sorting genetic algorithm (NSGA)

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Abstract

Multi-objective optimization using genetic algorithm (GA) is carried out for the desalination of brackish and sea water using spiral wound or tubular modules. A few sample optimization problems involving two and three objective functions are solved, both for the operation of an existing plant (which is almost trivial), as well as, for the design of new plants (associated with a higher degree of freedom). The possible objective functions are: maximize the permeate throughput, minimize the cost of desalination, and minimize the permeate concentration. The operating pressure difference, ΔP, across the membrane is the only important decision variable for an *existing* unit. In contrast, for a new plant, ΔP, the active area, A, of the membrane, the membrane to be used (characterized by the permeability coefficients for salt and water), and the type of module to be used (spiral wound/tubular, as characterized by the mass transfer coefficient on the feed-side), are the important decision variables. Sets of non-dominated (equally good) Pareto solutions are obtained for the problems studied. The binary coded elitist non-dominated sorting genetic algorithm (NSGA-II) is used to obtain the solutions. It is observed that for maximum throughput, the permeabilities of both the salt and the water should be the highest for those cases studied where there is a constraint on the permeate concentration. If one of the objective functions is to minimize the permeate concentration, the optimum permeability of salt is shifted towards its lower limit. The membrane area is the most important decision variable in designing a spiral wound module for desalination of brackish water as well as seawater, whereas ΔP is the most important decision variable in designing a tubular module for the desalination of brackish water (where the quality of the permeate is of prime importance). The results obtained using NSGA-II are compared with those from recent, more efficient, algorithms, namely, NSGA-II-JG and NSGA-II-aJG. The last of these techniques appears to converge most rapidly.

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Keywords: Multi-objective optimization; Elitist non-dominated sorting genetic algorithm; Jumping genes; Genetic algorithm; Optimization; Desalination; Brackish water; Seawater; Reverse osmosis; Membranes

1. Introduction

Desalination of seawater and brackish water is routinely used nowadays for overcoming the huge scarcity of potable water in different parts of the world. Desalination involves the reduction of the concentration of the total dissolved solids (TDS) to less than about $200 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$ ($200\,\mathrm{mg\,L^{-1}}$). Brackish water has a much lower TDS ($<10{,}000 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$) than seawater ($>30{,}000 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$). This difference in the TDS is associated with substantial differences in the osmotic pressures associated with these operations, leading to large variations in the operating pressure differences across the reverse osmosis (RO) membrane. The largest desalination plant in the world treating brackish water (Lohman, 1994) is located at Yuma, AZ, USA. This has a capacity of $275{,}000\,\mathrm{m^3\,day^{-1}}$. It

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Nomenclature

a	permeability coefficient for water ($m\,h^{-1}\,bar^{-1}$)
A	active area of membrane (m^2)
b	permeability coefficient of salt ($m\,h^{-1}$)
b_π	osmotic coefficient (Eqs. (A2.4) and (A2.10)) ($m^3\,bar\,kg^{-1}$)
C	salt concentration ($kg\,m^{-3}$)
Cost	operating cost of desalination unit ($\$\,h^{-1}$)
C_{ele}	cost of electricity ($\$\,kW^{-1}\,h^{-1}$)
C_{main}	maintenance cost of membrane ($\$\,m^{-2}\,h^{-1}$)
C_{mem}	capital cost of membrane ($\$\,m^{-2}\,h^{-1}$)
C_{pump}	capital cost of the pump ($\$\,h^{-1}$)
d_h	hydraulic diameter of channel (m)
D_{AB}	mass diffusivity of salt (A) through water (B) ($m^2\,h^{-1}$)
f_i	ith objective function ($m^3\,h^{-1}$; $\$\,h^{-1}$; $kg\,m^{-3}$)
H	penalty parameter defined in Eq. (3)
I_{dist}	crowding distance
I_{rank}	rank
J_w	volumetric flux of water ($m\,h^{-1}$)
J_s	mass flux of salt ($kg\,m^{-2}\,h^{-1}$)
k_s	mass transfer coefficient of salt in feed side ($m\,h^{-1}$)
l_{chrom}	length of chromosome
l_{substr}	length of substring
l_{aJG}	string length of jumping gene
m	defined in Eq. (A2.14)
n	exponent for the pumping cost (Eq. (A2.13))
N_{gen}	generation number
N_{gmax}	maximum number of generations
N_p	total number of chromosomes in the population
p_c	crossover probability
p_{JG}	jumping gene probability
p_m	mutation probability
P	pressure, bar
Pen	penalty parameter (Eq. (3))
Q_w	volumetric flow rate (throughput) ($m^3\,h^{-1}$)
R	observed rejection
Re	Reynolds' number
Sc	Schmidt number
Sh	Sherwood number
T	temperature of the feed (°C)
v	velocity of water in feed channel ($m\,h^{-1}$)
W_{base}	reference value of power for estimating pumping cost (Eq. (A2.13)) (kW)

Subscript/superscript

b	bulk
bw	brackish water
d	desired
L	lower bound
p	permeate
ref	reference, Yuma plant (Lohman, 1994)
s	salt
sw	seawater
U	upper bound

Greek letters

Δ	difference
η	efficiency of the pump
ν	kinematic viscosity of salt solution ($m^2\,h^{-1}$)
π	osmotic pressure (bar)
ρ	density of seawater ($kg\,m^{-3}$)

uses spiral wound cellulose acetate membranes to treat raw water having $3100 \times 10^{-3}\,kg\,m^{-3}$ TDS and produces permeate water having a TDS less than $200 \times 10^{-3}\,kg\,m^{-3}$. The largest desalination plant in the world processing seawater (Ayyash, 1994) operates in Jeddah, Saudi Arabia. This has a capacity of $56{,}800\,m^3\,day^{-1}$ and treats water having a TDS of approximately $44{,}000 \times 10^{-3}\,kg\,m^{-3}$.

RO has several advantages over other desalination processes such as distillation, evaporation and electro-dialysis (Ho & Sirkar, 1992). The main advantages of RO over other desalination processes are its simple design, lower maintenance costs, easier de-bottlenecking, simultaneous removal of both organic and inorganic impurities, low discharge in the purge stream, and energy savings. RO is a rate-governed pressure-driven process. The solvent flux depends upon the applied pressure difference, trans-membrane osmotic pressure difference, concentration of feed, permeability coefficients of salt and water, and the extent of concentration polarization. The flux increases (at the expense of high concentration polarization) with an increase in the operating pressure difference and permeability coefficients, and decreases with an increase in the salt concentration.

Rigorous optimal design (or operation) of RO modules will help in reducing their cost. Attempts have been made to obtain optimal designs of RO units considering cost as the single objective function. Wiley, Fell and Fane (1985) have carried out the optimal design of membrane modules for brackish water desalination using the Rosenbrock (1960) hill climb method without constraints, with Palmer's (Palmer, 1969) axis rotation method. Sequential quadratic programming (SQP; Gill, Murray, & Wright, 1991) has been used by Maskan, Wiley, Johnston, and Clements (2000) to find optimal networks of reverse osmosis modules. These studies involve the optimization of only a single objective function, which may, at times, be taken as a weighted-average of several conflicting objective functions. The assignment of values of the weighting factors is subject to considerable controversy. Like most problems, the design of RO modules is also associated with several non-commensurate, objective functions that need to be optimized simultaneously in the presence of a few constraints. Such problems are best handled using multi-objective optimization (MOO) techniques. In such problems, a set of several equally good (non-dominated) optimal solutions is often obtained (instead of a single optimal point), called a Pareto set. The basic advantage of MOO formulations is that the decision-maker is not confined to look at only a single mathematically optimal solution (usually that involving the minimum cost), but he/she can examine a set of efficient solutions using a judgment of the trade-offs involved, refining his/her final decision (Mavrotas & Diakoulaki, 1998; Deb, 2001). Indeed, Pareto sets are becoming an 'increasingly effective way to determine the necessary trade-offs between conflicting objective functions' (D.E. Goldberg in Deb, 2001). The use of a single objective function which is a weighted-average of several objectives also has the drawback that certain optimal solutions may be lost since they may never be explored, particularly when the non-convexity of the objective function gives rise to a duality gap (Goicoechea, Hansen, & Duckstein, 1982). Unfortunately, there is no study on the optimal design of RO modules in the literature using multiple objective functions, though a parallel study (Yuen, Aatmeeyata, Gupta, & Ray, 2000) on beer dialysis (minimizing the alcohol content of beer to give low-alcohol beer, while maximizing the taste chemicals in the product) has been reported. Optimal RO design in desalination involves the selection of membrane material, module geometry (viz., plate and frame, tubular, spiral wound, or hollow-fiber), membrane area, quality of product, solvent recovery (i.e., water), operating pressure difference across the membrane, and the throughput (Bhattacharyya, Williams, Ray, & McCray, 1992; Parekh, 1988). One should be able to select optimal module parameters that provide the highest possible throughput (first objective function) while simultaneously minimizing the cost of desalination (second objective function). These are conflicting (and non-commensurate) requirements. Clearly, desalination through RO provides an excellent opportunity for multi-objective optimization studies.

Over the last few years, scientists, engineers and economists have used AI-based evolutionary techniques, particularly, genetic algorithms (GA; Deb, 1995; Goldberg, 1989; Holland, 1975), extensively to solve optimization problems involving single objective functions. This basic algorithm, *s*imple GA or SGA (Goldberg, 1989), offers advantages (Deb, 2001; Holland, 1975) over more traditional optimization approaches (e.g., several search techniques, Pontryagin's principle, SQP, etc.), in some cases. Moreover, it has the advantage that it does not require good initial guesses for the values of the 'decision variables'. It uses a population of several points simultaneously along with probabilistic operators, viz., reproduction, crossover and mutation, inspired by natural genetics. In addition, SGA has the advantage that it uses only the values of the objective functions and not any derivatives, as required by gradient search techniques. In the early algorithms, binary coding was used for representing the continuous decision variables, i.e., these variables were represented/coded as a series (string) of binary numbers (and then mapped into real numbers for use in model equations). This is an unavoidable compromise and causes problems (Deb, 2001), e.g., it slows down the computing speed and, at times, renders convergence impossible. Modifications (e.g., real coded GAs, the jumping gene adaptation, etc.) are becoming available but each technique has its own limitations.

Several workers have extended SGA to solve multi-objective optimization problems. Any of these techniques, reviewed recently by Deb (2001) and Coello Coello, Veldhuizen and Lamont (2002), can be used to obtain the Pareto fronts. A popular algorithm for such problems is the non-dominated sorting genetic algorithm (NSGA), developed by Deb and coworkers (Deb, 2001). Two versions of this technique are available, NSGA-I (Srinivas & Deb, 1995) and NSGA-II (Deb, Pratap, Agarwal, & Meyarivan, 2002). Bhaskar, Ray, and Gupta (2000) have reviewed the variety of multi-objective optimization problems in chemical engineering that have been solved in the last decade using NSGA-I (as well as the earlier optimization studies using traditional techniques). NSGA-II introduces the concept of elitism (Deb, 2001) and has been applied recently to solve two highly computationally intensive problems in chemical engineering, namely, the multi-objective optimization of an industrial fluidized-bed catalytic cracker unit (FCCU; Kasat, Kunzru, Saraf, & Gupta, 2002) and the unsteady operation of a steam reformer (Nandasana, Ray, & Gupta, 2003). An important feature of NSGA-II is that the best members are selected from a combined pool of parents and daughters (generated by crossover and mutation of the parents), and these become the parents for the next generation. Elitism reduces the diversity of the gene pool, but offers several advantages (Deb, 2001). Kasat and Gupta (2003), inspired by the concept of jumping genes (JG or transposons; McKlintock, 1987; Stryer, 2000) in biology, developed the jumping gene (JG) operator for use with SGA/NSGA. This macro–macro mutation operation in the binary-coded NSGA-II-JG speeds up the optimization of FCCUs by almost an eight-fold factor, and provides the *global* optimal Pareto front for the test problem, ZDT4 (Deb, 2001; Zitzler, Deb, & Thiele, 2000), which could not be solved satisfactorily using the binary-coded NSGA-II. The JG operator helps improve the diversity of the gene pool and, thus, counteracts the negative effect of elitism. A further adaptation of NSGA-II-JG has been presented by Guria, Verma, Mehrotra, and Gupta, 2005). This is referred to as NSGA-II-mJG (modified JG). This algorithm has been found to speed up the convergence to the global optimal solutions for problems involving networks, as for example, froth flotation circuits (Guria et al., 2005) for mineral processing. More recently, Bhat, Saraf, and Gupta (2005) further adapted this concept and proposed NSGA-II-aJG (adapted JG), which could solve ZDT4 even more efficiently. This adaptation has been applied successfully by Khosla, Saraf, and Gupta (2005) for the multi-objective optimization of fuel oil blending operations. Details of NSGA-II-JG as well as NSGA-II-aJG are given in Appendix A.

The present work involves the simulation of the desalination plant (Lohman, 1994) at Yuma, followed by the formulation and solution of a few multi-objective optimization problems for desalination using RO modules. The binary coded NSGA-II (Deb, 2001; Deb et al., 2002) is used. The results are then compared with those obtained with NSGA-II-JG and NSGA-II-aJG so as to study the efficiency of these algorithms. The optimization is carried out both at the *operating stage* (Lohman, 1994; optimization of the operating conditions in an existing unit) as well as at the design stage (optimization of a new plant), to illustrate the variety of optimization problems that can be solved. The optimal solutions of the first problem are also compared with the actual operating point of the existing unit (Lohman, 1994). The methodology is quite general and can be used for other plants as well. It may be mentioned that this is the first application of the multi-objective elitist NSGA-II with the jumping gene adaptations in the area of membrane separation processes.

2. Formulation

2.1. Model of the reverse osmosis (RO) process

Various mathematical models are available that describe the local behavior and performance of the RO process. The transport through RO membranes is well described by the widely accepted solution diffusion model (Lonsdale, Merten, & Riley, 1965; Rautenbach, 1986; Soltanieh & Gill, 1981). The detailed equations (for isothermal operation) are given in Appendix B. The permeate flux, J_w (=Q_w/A), the permeate quality, C_p, and the cost, Cost, the three important variables that are used as objectives in this study, are given by

$$J_w = a\left[\Delta P - b_\pi\left(C_b - \frac{bC_b\exp(J_w/k_s)}{J_w + b\exp(J_w/k_s)}\right)\exp(J_w/k_s)\right] \quad \text{(a)}$$

$$C_p = \frac{bC_b}{b + J_w\exp(-J_w/k_s)} \quad \text{(b)} \qquad (1)$$

$$\text{Cost} = C_{mem}A + C_{main}A + C_{pump}\left(\frac{Q_w\Delta P}{W_{base}\eta}\right)^n + \frac{C_{ele}Q_w\Delta P}{\eta} \quad \text{(c)}$$

The variables in Eq. (1) are defined in the Nomenclature. The volumetric flow rate, Q_w, of the permeate can be expressed in terms of four *design* variables: the area, A, of the membrane, the permeability coefficient, a, of water, the permeability coefficient, b, of the salt, and the feed-side liquid film mass transfer coefficient, k_s (Brian, 1965, 1966; Kimura & Sourirajan, 1968; Sherwood, Brian, Fisher, & Dresner, 1965; Sirkar, Dang, & Rao 1982). The values of k_s depend upon the hydrodynamics on the feed side (Ohya & Taniguchi, 1975; Ohya, Nakajima, Takagi, Kagawa, & Negishi, 1977; Perry, Green, & Malony, 1997; Rao & Sirkar, 1978; Shock & Miquel, 1987; Stanojevic, Lazarevic, & Radic, 2003; Taniguchi, 1978; Taniguchi & Kimura, 2005; Taniguchi, Kurihara, & Kimura, 2001; Wiley et al., 1985), and may be estimated for different RO modules (e.g., plate and frame, spiral wound, hollow-fiber, and tubular) using the correlations summarized in Appendix B. The throughput, Q_w, also depends on one *operating* condition: the pressure difference, ΔP, across the membrane. The solute concentration, C_b, in the feed and the temperature, T, of operation, are usually specified (constants).

Eq. (1a) is an implicit nonlinear algebraic equation that can easily be solved numerically to give J_w and Q_w for a set of values of C_b, T, A, a, b, k_s and ΔP, b_π can be estimated using Eqs. (A2.17) and (A2.18). The secant method (Ray & Gupta, 2004) is used to solve this equation. This method requires lower and upper bounds (estimates) of J_w, as well as two initial guesses of this root. The values of C_p and the cost can then be evaluated using Eqs. (1b) and (1c), respectively.

2.2. Multi-objective optimization

The plant at Yuma, AZ, USA (Lohman, 1994) uses a spiral wound module and treats brackish water. The parameters characterizing this unit first need to be estimated ('tuned'). This is done using the following available information (Lohman, 1994): $A = 3.93072 \times 10^5\ \mathrm{m^2}$; $Q_w = 275{,}000\ \mathrm{m^3\ day^{-1}} = 11{,}458\ \mathrm{m^3\ h^{-1}}$; $\Delta P = 27.6$ bar; $C_b = 3.1\ \mathrm{kg\ m^{-3}}$; observed rejection = 97%; $C_p = 0.2\ \mathrm{kg\ m^{-3}}$ and $T = 25\,^\circ\mathrm{C}$. The exact value of k_s depends on the geometric parameters of the element (i.e., the number of leaves, the thickness of spacers, the porosity of the feed spacer and the membrane thickness) and the physical properties (mainly, density, kinematic viscosity and mass diffusivity) of the salt solution, and is estimated using Eq. (A2.9). Details of different types of spiral wound modules are given by Shock and Miquel (1987). We have used values corresponding to a FilmTec FT 30 spiral wound module (Shock & Miquel, 1987) in the present study. The 'tuned' values of the two unknown parameters, a and b, are obtained by curve-fitting the operating data, as $1.80 \times 10^{-3}\ \mathrm{m\ bar^{-1}\ h^{-1}}$ and $5.04 \times 10^{-4}\ \mathrm{m\ h^{-1}}$, respectively. A simple two-objective optimization problem for the (operating) plant at Yuma (referred to as *operating-stage* optimization) is first solved (Problem 1). The optimal value of the single decision variable, ΔP, is to be obtained. Since the permeabilities, a and b, depend primarily on the membrane, and since the latter is the same for all values of ΔP, the tuned values of these parameters are used. Thus, for this problem, values of C_b, b_π, A, a, b, T, and the module are specified. Two objective functions are used: maximization of the permeate flow rate, Q_w, and minimization of the *Cost*. The permeate concentration, C_p, is

Table 1
Details of the several optimization problems studied

Problem no.	1	2	3	4	5
Module	Spiral wound (FilmTec FT30)	Spiral wound (FilmTec FT30)	Tubular module (PCI)	Spiral wound (FilmTec FT30)	Tubular module (PCI)
k_s (m h^{-1})	Eq. (A2.9) (Shock & Miquel, 1987)	Eq. (A2.9) (Shock & Miquel, 1987)	Eqs. (A2.15) and (A2.16) (Wiley et al., 1985)	Eq. (A2.9) (Shock & Miquel, 1987)	Eqs. (A2.15) and (A2.16) (Wiley et al., 1985)
Feed	Brackish water	Brackish water	Brackish water	Sea water	Brackish Water
Operating/design	Operating (Yuma)	Design	Design	Design	Design
C_b (kg m^{-3})	3.1 (Lohman, 1994)	3.1 (Lohman, 1994)	3.1 (Lohman, 1994)	35.0	3.1 (Lohman, 1994)
b_π (m^3 bar kg^{-1})	0.789[b]	0.789[b]	0.789[b]	0.781[b]	0.789[b]
Values (existing) or bounds (new)					
ΔP (bar)	10–50	10–50	10–50	75–250	10-50
$10^{-5}A$ (m^2)[a]	3.93072 (Lohman, 1994)	1.0–4.0	2.0–4.0	1.0–4.0	2.0-4.0
$10^3 a$ (m^3 m^{-2} bar^{-1} h^{-1})	1.8 (Shock & Miquel, 1987)	0.5–5.0	0.2–1.0	0.5–5.0	0.2-1.0
$10^4 b$ (m^3 m^{-2} h^{-1})	5.04 (Shock & Miquel, 1987)	0.1–1.0	0.08–0.3	0.1–1.0	0.08-0.3
$C_{p,d}$[c] (kg m^{-3})	0.2	0.2	0.2	–	–

[a] $10^3 a = 1.8$ represents $a = 1.8 \times 10^{-3}$, etc.
[b] Calculated from Eqs. (A2.17) and (A2.18).
[c] $C_{p,d}$ is used as an objective function in Problem 5 (and not used as a constraint in Problem 4).

constrained to lie below a desired value, $C_{p,d}$. This problem, relevant to the operation of the existing plant at Yuma, can be written mathematically, as:

Problem 1. Yuma plant; specified C_b, b_π, A, a, b, T; FilmTec FT 30 spiral wound module

$$\begin{aligned}
&\text{Max } f_1(\Delta P) \equiv \frac{Q_w}{Q_{w,ref}} \quad \text{(a)}\\
&\text{Min } f_2(\Delta P) \equiv \frac{\text{Cost}}{\text{Cost}_{ref}} \quad \text{(b)}\\
&\text{Subject to (s.t.)}:\\
&\text{Model equations (Appendix 2)} \quad \text{(c)}\\
&\text{Bounds}: \quad \Delta P_L \le \Delta P \le \Delta P^U \quad \text{(d)}\\
&\text{Constraint}: \quad C_p \le C_{p,d} \quad \text{(e)}
\end{aligned} \tag{2}$$

In Eq. (2), $Q_{w,ref}$ and Cost$_{ref}$ (=11,458 m^3 h^{-1} and \$ 2904 h^{-1}, respectively), estimates for the currently operating Yuma plant using Eq. (1), are used to normalize the two objective functions, ΔP_L and ΔP^U are the lower and upper bounds on ΔP (values given in Table 1) and $C_{p,d}$ is taken as 0.2 kg m^{-3}. Eq. (A2.9) is used to estimate k_s (for any Q_w), while the Cost is given only by the second (constant for all Q_w, since A is constant) and fourth terms of the right hand side of Eq. (1c) (since the remaining two terms are already 'sunk' for an existing/operating plant; see discussion in Appendix B). It may be noted that the normalization constant, Cost$_{ref}$, is evaluated using all four terms in Eq. (1c) (this is unimportant since Cost$_{ref}$ is a constant anyway).

We could also study the optimization of desalination units under more flexible *design* conditions (for new units). The decision variables, then, are not only ΔP, but also the membrane parameters, namely, A, a, b and, the membrane module (k_s). The membrane permeability coefficients, a and b, are related to the thickness of the membrane and its properties, namely, the diffusivities of salt and water in the membrane, the partition coefficient of the solute in the membrane, the feed temperature and, the nature of the concentration polarization, and can be considered as decision variables directly. A is the membrane area and can vary continuously. k_s depends on the hydrodynamics associated with the membrane module, and can be estimated using the correlations in Appendix B for any desired module. Two, two-objective optimization problems are being studied here using two different modules (so that the results can be compared), namely, the FilmTec FT 30 spiral wound module (Shock & Miquel, 1987), and the PCI tubular module (Wiley et al., 1985):

Problems 2 and 3. (design stage; specified C_b, module, T):

$$\begin{aligned}
&\text{Max } f_1(\Delta P, A, a, b) \equiv \frac{Q_w}{Q_{w,ref}} \quad \text{(a)}\\
&\text{Min } f_2(\Delta P, A, a, b) \equiv \frac{\text{Cost}}{\text{Cost}_{ref}} \quad \text{(b)}\\
&\text{Subject to (s.t.)}:\\
&\text{Model equations (Appendix B)} \quad \text{(c)}\\
&\text{Bounds}: \quad \Delta P_L \le \Delta P \le \Delta P^U, \qquad A_L \le A \le A^U,\\
&\qquad a_L \le a \le a^U, \qquad b_L \le b \le b^U \quad \text{(d)}\\
&\text{Constraint}: \quad C_p \le C_{p,d} \quad \text{(e)}
\end{aligned} \tag{3}$$

The values of the normalization constants, $Q_{w,ref}$ and Cost$_{ref}$, are taken to be the same as in Problem 1 (since these are constants anyway; this does not matter, as discussed earlier). Table 1 gives the details. Problem 4 is also described by Eq. (3), but corresponds to the desalination of *sea water* using a

Table 2
Computational parameters used for Problems 1–5

Problem no.	1	2	3	4	5	4(JG)	4(aJG)
N_{gmax}	500	1000	1000	1000	10000	1000	1000
N_p	100	100	100	100	100	100	100
l_{substr}	32	32	32	32	32	32	32
l_{chrom}	32	128	128	128	128	128	128
p_c	0.90	0.99	0.98	0.90	0.80	0.98	0.98
p_m	0.01	0.001	0.01	0.02	0.015	0.001	0.001
p_{JG}	–	–	–	–	–	0.80	0.80
l_{aJG}	–	–	–	–	–	–	12
Random seed number[a]	0.765	0.765	0.765	0.765	0.765	0.765	0.765
H	10^5	10^5	10^5	–	–	–	–

[a] Random numbers are generated using the Knuth (1997) portable subtractive pseudo-random number generator.

FilmTec FT30 spiral-wound module. Because the salt concentration in sea water is high, the constraint on C_p is omitted for this problem. In Problems 2–4, all four terms on the right hand side of Eq. (1c) are used to estimate the Cost (see discussion in Appendix B).

The constraint on C_p in Problems 1–3 (Eqs. (2e) and (3e)) is taken care of using a penalty function approach (Deb, 1995, 2001). We add (for minimization of an objective function) or subtract (for maximization) a penalty, Pen, given by

$$\text{Pen} \equiv H\left[1-\left(\frac{C_p}{C_{p,d}}\right)\right] \tag{4}$$

to both the objective functions (in Eqs. (2) and (3)). In Eq. (4), the penalty, Pen, is taken to be a very large number (compared to the values of the two objective functions) whenever the value of C_p is above $C_{p,d}$, but Pen is zero when C_p is below $C_{p,d}$ (Deb, 1995, 2001). Table 2 gives the values of H used. Its value is large enough so that the solutions do not change with a further increase of H.

The NSGA-II (Kasat et al., 2002), NSGA-II-JG (Kasat & Gupta, 2003) and NSGA-II-aJG (Bhat et al., 2005) codes available to us maximize *all* the objective functions. A popular transformation for an objective function, f, that has to be minimized, to one involving the fitness function, F, that has to be maximized, is given by

$$F=\frac{1}{1+f} \tag{5}$$

This transformation does not alter the optimal solutions (Deb, 1995, 2001).

3. Results and discussion

The NSGA-II computer code was tested on a few test problems (Deb, 2001) to make sure that it was free of errors. Problem 1 (Table 1) was run with a single chromosome using $\Delta P_L = \Delta P^U = 27.6$ bar. The following optimal values were obtained: $Q_w = 11458.0\,\text{m}^3\,\text{h}^{-1}$ and Cost = \$ 2904.0 h^{-1}, the same as actually used (simulation values) in the plant. This confirms that the code finally used for optimization is free of errors. Several other standard tests, described by Kasat et al. (2002) were also tried. The best values of the computational parameters were then obtained for the different problems. These are given in Table 2.

In Problem 1, there is only one degree of freedom (a selected value of J_w determines the complete solution) and so the solution of Eq. (2) can be obtained analytically. It is found that as ΔP increases, Q_w increases and the Cost goes down, a characteristic of a Pareto set. This problem is a relatively trivial one and so detailed results are not being presented here (but can be supplied on request), and this problem is not pursued further.

Problem 2 is a more interesting, design-stage multi-objective optimization problem, involving more than a single degree of freedom. Pareto sets are obtained, as shown in Fig. 1a. The CPU time taken for this problem (as well as all others, using any of the adaptations of NSGA-II) for 1000 generations, and using 100 chromosomes is 1 min (on a Pentium IV, 1.7 GHz, 256 MB RAM). The mean value of the crowding distance, $I_{i,dist}$ (see Step 3c in Appendix A), as well as the standard deviation of these values, in any generation, can be used to get an idea of the degree of convergence of the Pareto set. Details of this method are described in Kasat and Gupta (2003). Alternatively, an eye estimate can be used to get an idea of when the Pareto set has stopped changing (converged) from generation to generation, and if the ‘spread’ of the points in the set are near-uniform (the standard deviation of $I_{i,dist}$ can be used for this). The two approaches give *nearly* similar results. Fig. 1d and e show that the optimal module must have the maximum permissible permeability coefficients (a and b) for the FilmTec FT30 spiral wound membrane. This is not surprising. What is interesting is that the increase in Q_w is first achieved by an increase in the value of membrane area, A, to its maximum permissible value (with ΔP being constant at an intermediate value of about 33 bar). Thereafter, Q_w and the Cost both increase because of the increase in ΔP (with the membrane area, A, being constant at its maximum specified value). This indicates that Q_w is more sensitive to A than to ΔP. It may be mentioned that the constraint on C_p in Problem 2 can be replaced by an additional term in the Cost that accounts for the decrease in the

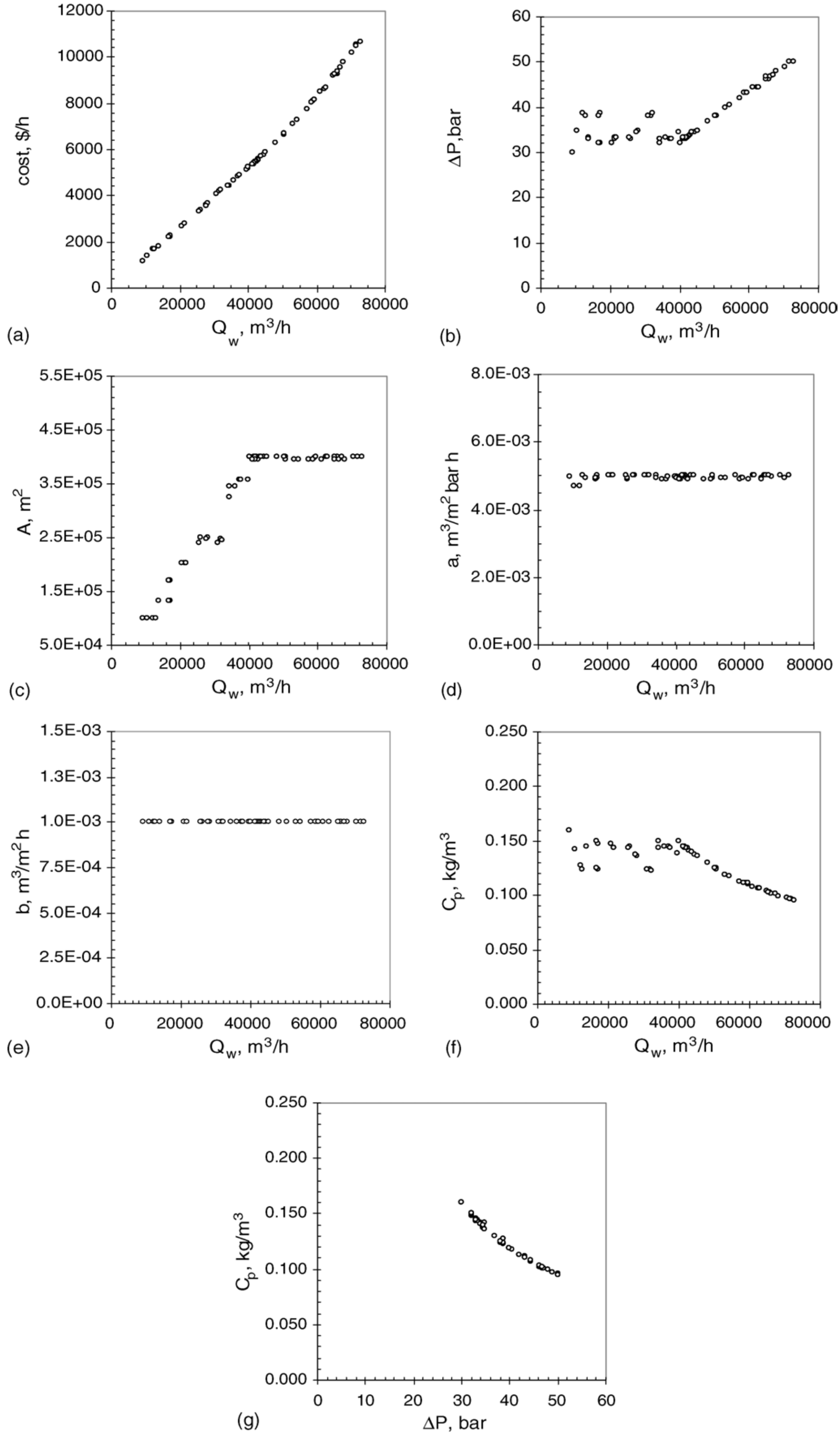


Fig. 1. Optimal solutions for Problem 2 (see Table 1 for details).

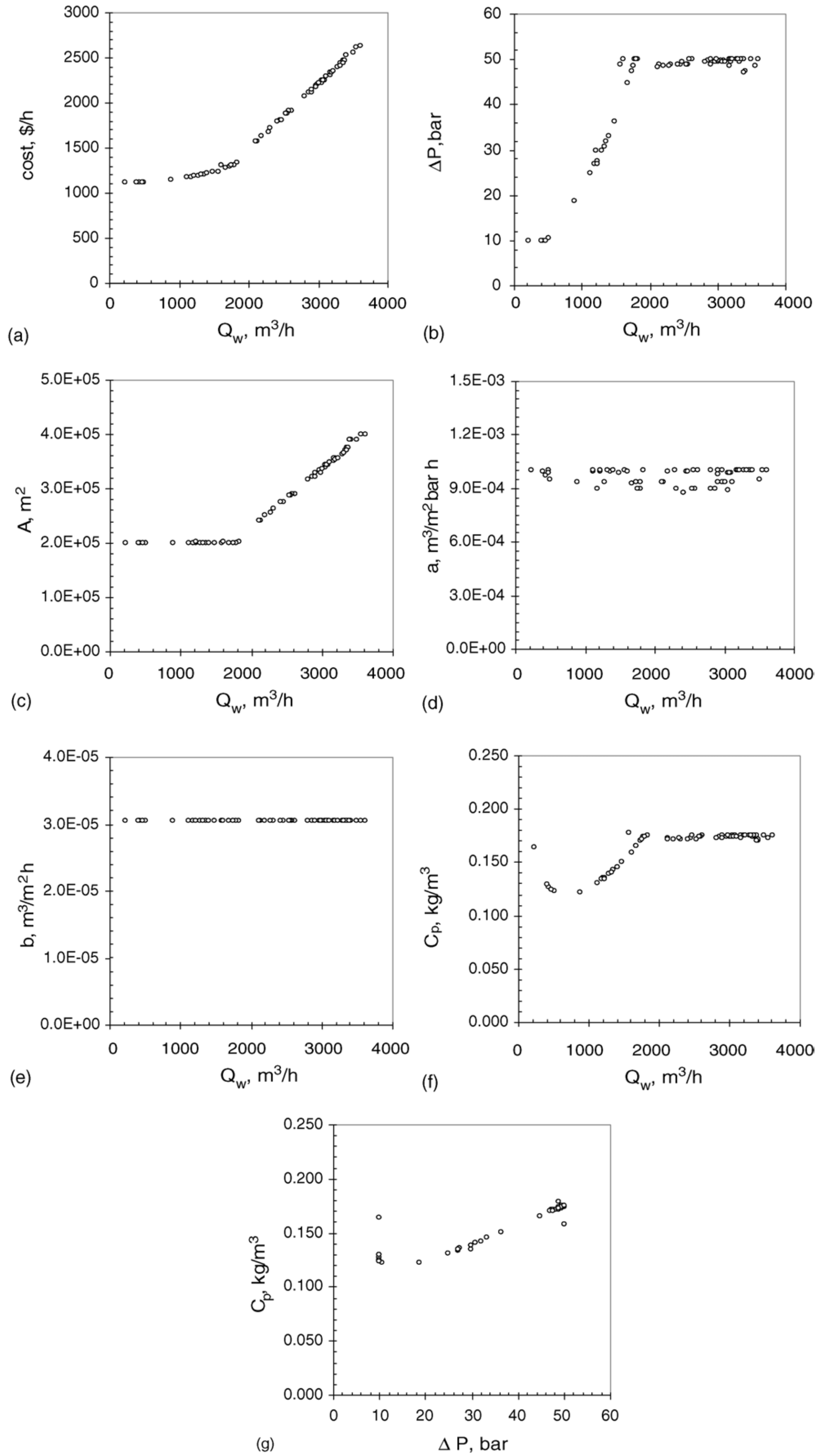


Fig. 2. Optimal solutions for Problem 3 (see Table 1 for details).

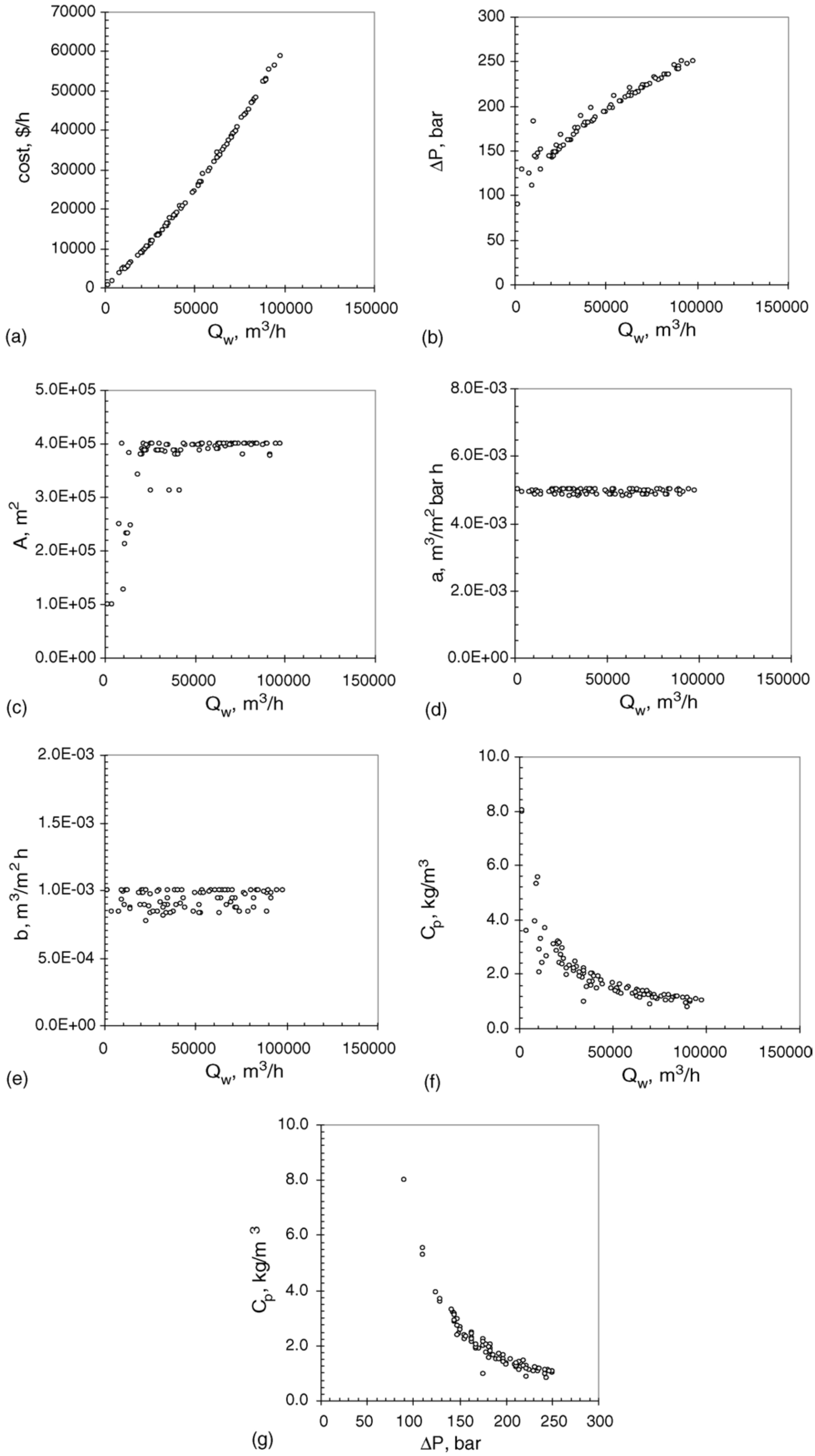


Fig. 3. Optimal solutions for Problem 4 (see Table 1 for details).

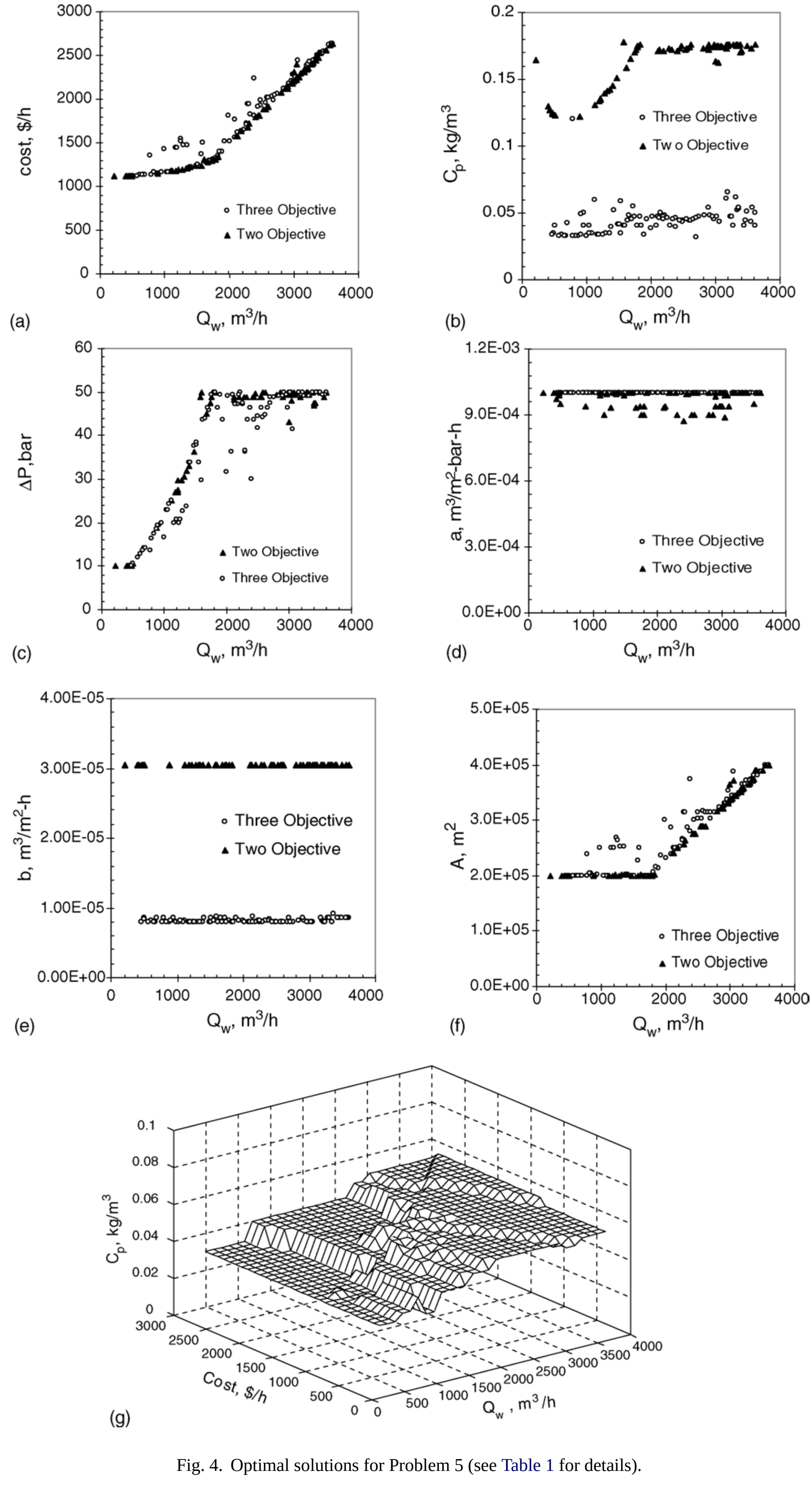


Fig. 4. Optimal solutions for Problem 5 (see Table 1 for details).

value of the permeate concentration when its specification is violated. This, and several other interesting optimization problems, can be solved but are not presented since the aim is to present results of only a few simple problems.

Fig. 2 shows results for the design-stage two-objective optimization problem for the desalination of brackish water using a different module, namely the PCI tubular module. Fig. 2a shows the Pareto set. Fig. 2d and e show that the optimal values of the permeabilities of water and salt must have the maximum possible values. This is similar to observations from Fig. 1 (for the spiral wound module). In the case of the PCI module, the increase in Q_w is first achieved by an increase of ΔP to its maximum possible value (with the membrane area being constant at its minimum specified value). Thereafter, Q_w and Cost both increase with an increase in the membrane area (with the ΔP being constant at its upper limit). This indicates that Q_w is more sensitive to ΔP than to A for this module. The contrast in the behaviors of the results for the two modules is clearly brought out in Figs. 1 and 2. The value of C_p remains almost constant after ΔP attains

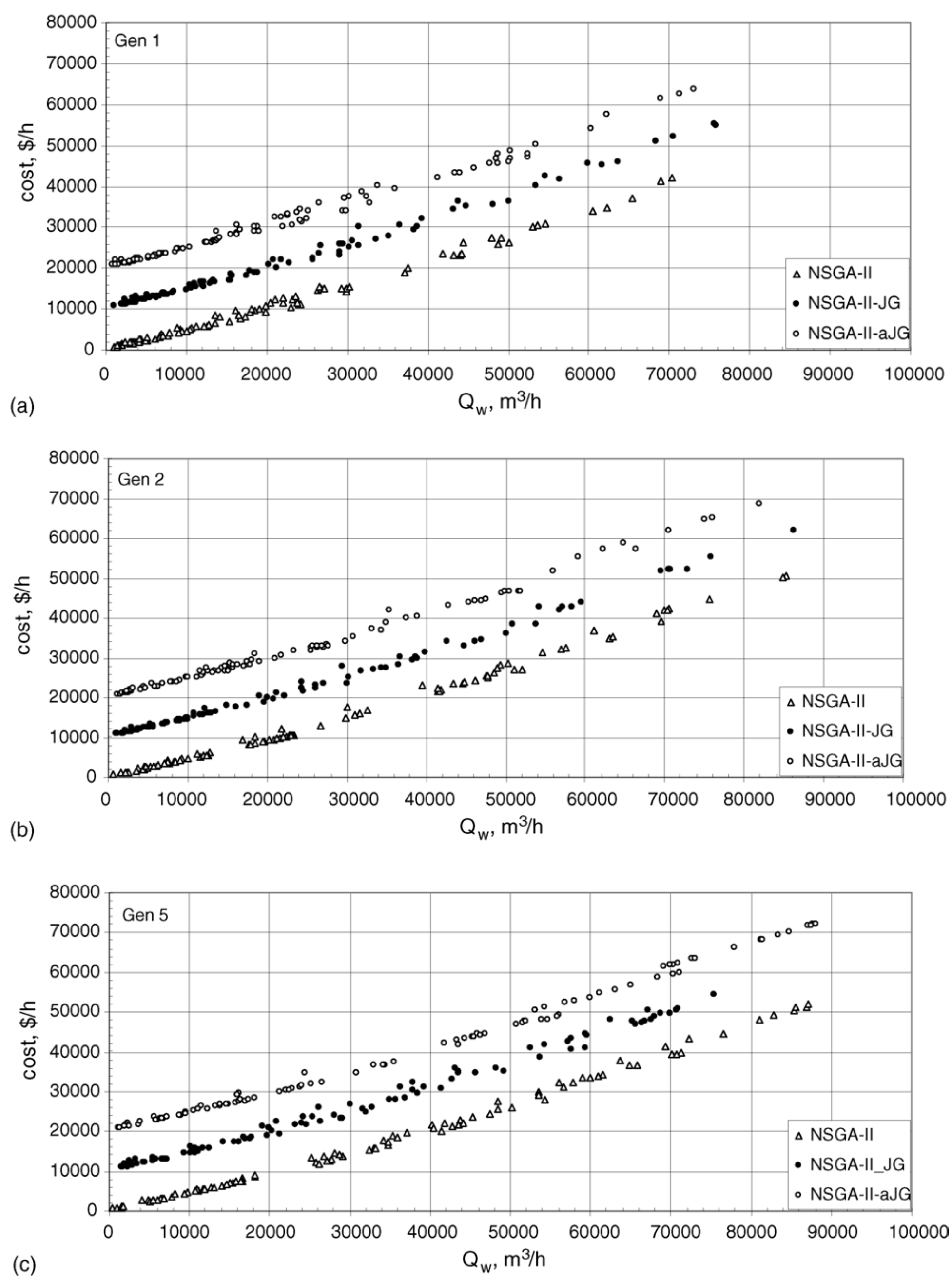
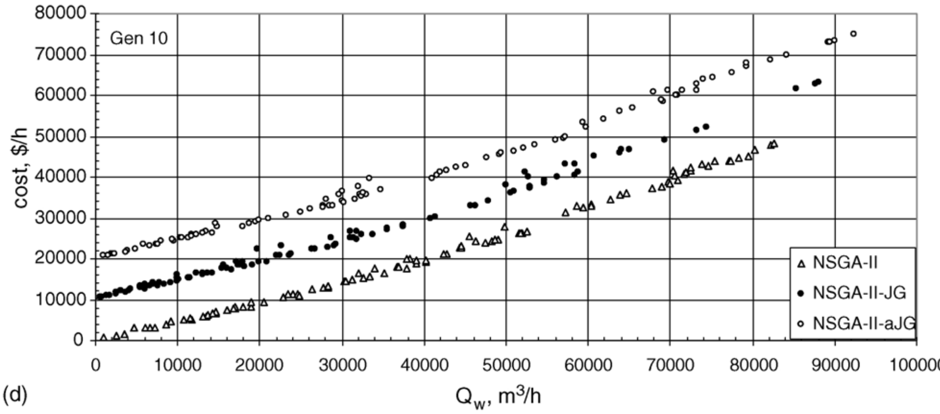
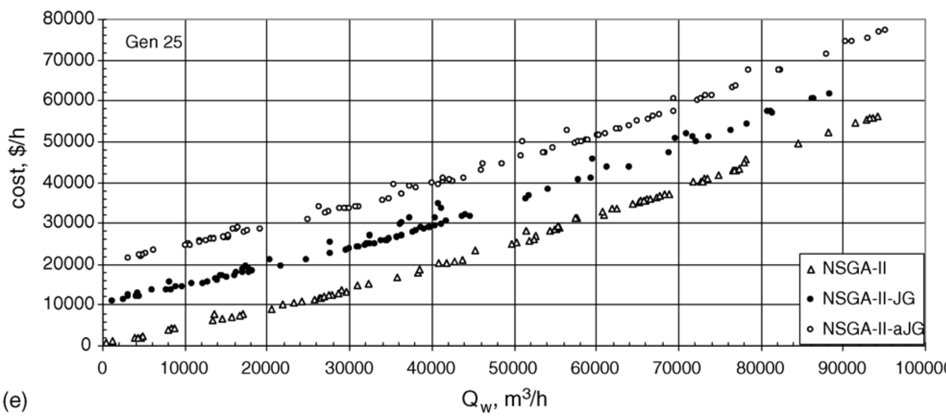


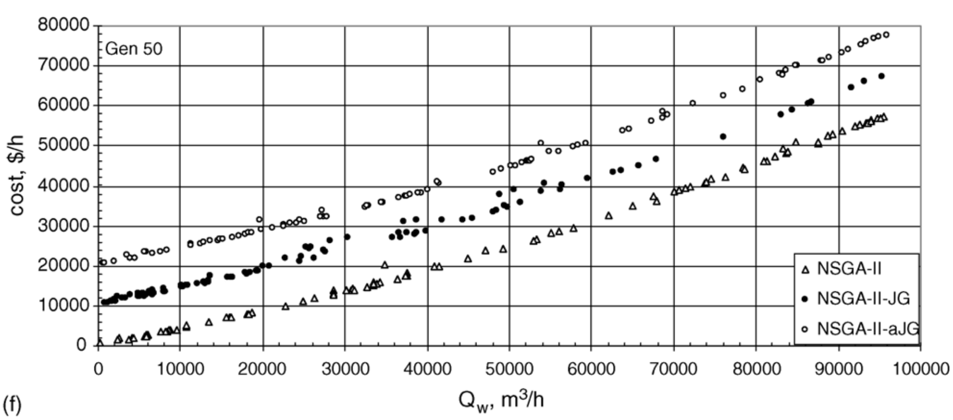
Fig. 5. Optimal Pareto solutions for Problem 4 using NSGA-II, NSGA-II-JG and NSGA-II-aJG (results for NSGA-II-JG and NSGA-II-aJG are displaced upwards by 10,000 and 20,000 $\$\,h^{-1}$, respectively, on the ordinate so that the plots can be easily compared).



(d)



(e)



(f)

Fig. 5. (*Continued*).

its maximum value. This is consistent with intuitive expectations. A small amount of scatter is observed in the optimal values of ΔP, A, a and b in Figs. 1 and 2. It is clear that differences in these four decision variables compensate for each other, and do not affect the Pareto set much. This is a characteristic of problems associated with several degrees of freedom, and such insensitivity of the Pareto set to scatter in a few decision variables has been encountered earlier in real-life studies (Bhaskar et al., 2000; Sareen & Gupta, 1995; Tarafder, Rangaiah, & Ray, 2005). It is known that GA does not guarantee optimality of the final solutions (Deb, 2001) and a few sub-optimal points/solutions are almost always encountered. However, one can easily infer the optimal Pareto solution from the results generated. One way of eliminating the scatter is to express the decision variables as low-order polynomials (Sareen & Gupta, 1995), and obtain optimal values of the coefficients used. These would give *near-optimal* solutions that are more useful. It is interesting to observe from Figs. 1 and 2 that spiral wound modules give higher throughputs than tubular ones (for similar values of the operating variables), of course at higher costs.

Fig. 3 presents the Pareto set for the design-stage, two-objective optimization of a *sea water* desalination unit using the FilmTec FT 30 spiral wound module (Problem 4, Table 1).

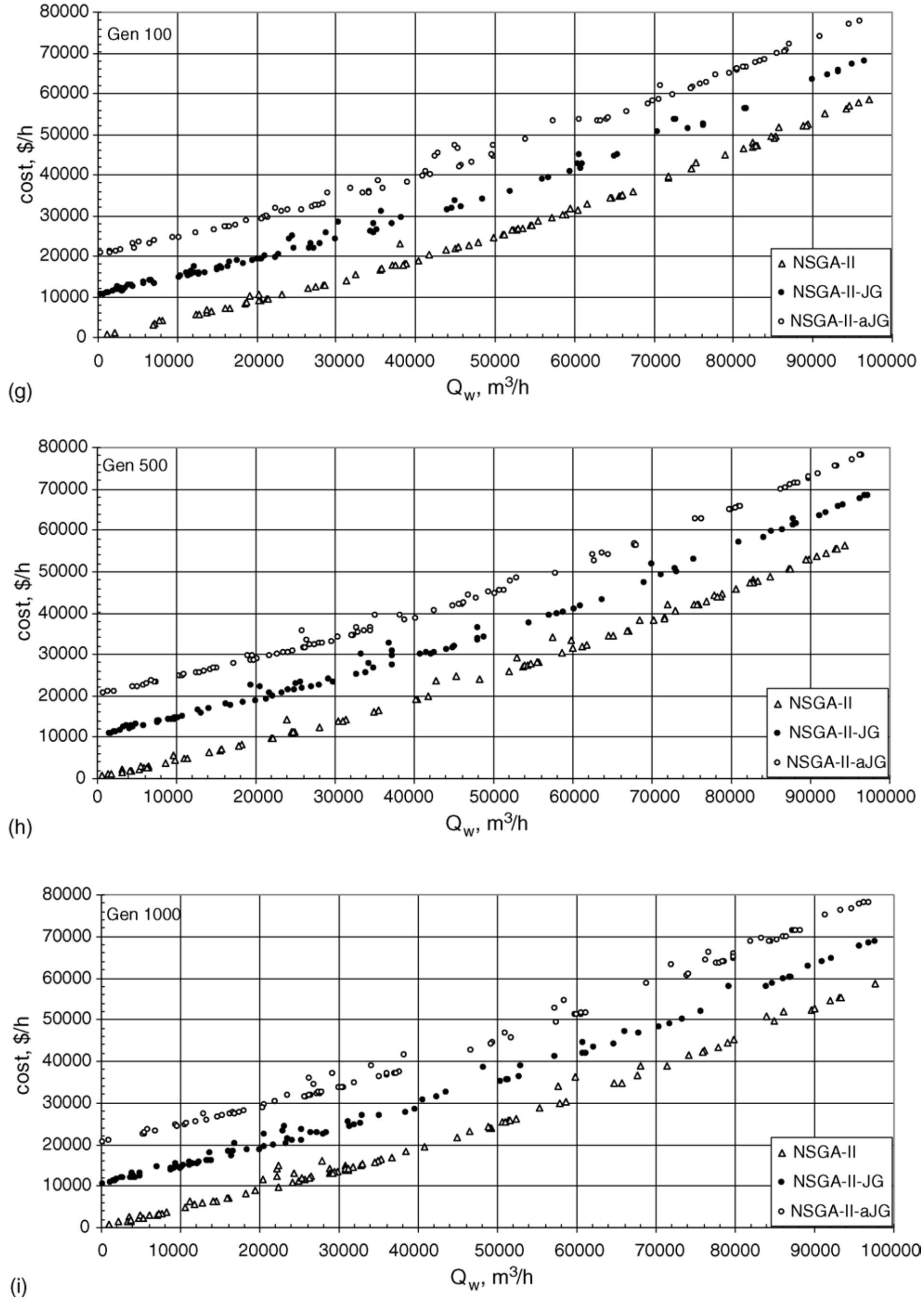


Fig. 5. (*Continued*).

Here, the bounds of the membrane permeability coefficients of water and salt (i.e., a and b) of Problem 2 are used, but much higher ranges of ΔP are imposed for obvious reasons. In this case, Q_w increases initially because of the increase in both the membrane area, A, as well as ΔP. After the maximum area of the membrane is attained, a further increase in Q_w is obtained due to the increase in ΔP. Small amounts of scatter in the decision variables, mainly, ΔP, A, a and b is observed, but the final Pareto set is insensitive to these variations. The qualitative similarity of the optimal solutions for the two cases (Problems 2 and 4, involving different ranges for ΔP) for treating brackish water and sea water, respectively, using the FilmTec FT 30 spiral wound membrane is to be noted, and contrasted to the results for the PCI tubular module (Problem 3).

The occurrence of a minimum in C_p in Problem 3 (Fig. 2) suggests that we can take the minimization of C_p as a third objective function. We, therefore, solve the following three-objective optimization problem (at the design stage):

Problem 5. (design stage; specified C_b, T, PCI module):

$$\begin{aligned}
&\text{Max } f_1(\Delta P, A, a, b) \equiv \frac{Q_w}{Q_{w,\mathrm{ref}}} \quad \text{(a)}\\
&\text{Min } f_2(\Delta P, A, a, b) \equiv \frac{\mathrm{Cost}}{\mathrm{Cost}_{\mathrm{ref}}} \quad \text{(b)}\\
&\text{Min } f_3(\Delta P, A, a, b) \equiv C_p \quad \text{(c)}\\
&\text{Subject to (s.t.)}:\\
&\text{Model equations (Appendix B)} \quad \text{(d)}\\
&\text{Bounds}: \quad \Delta P_L \le \Delta P \le \Delta P^U, \qquad A_L \le A \le A^U,\\
&\qquad\qquad a_L \le a \le a^U, \qquad b_L \le b \le b^U \quad \text{(e)}
\end{aligned} \tag{6}$$

The Cost is estimated for Problem 5 using all four terms on the right in Eq. (1c). The reference values of $Q_{w,\mathrm{ref}}$ and $\mathrm{Cost}_{\mathrm{ref}}$, are the same as in Problem 1.

Fig. 4 shows the results of Problem 5. The optimal points in Fig. 4a and b, together, comprise a three-dimensional Pareto *surface*. A 3D plot involving the objective functions is shown in Fig. 4g. Since the cost increases (worsens) (and C_p increases (worsens), albeit slightly) as Q_w increases (improves) over the entire range of the latter, the optimal solution has the characteristics of a Pareto set. In the 3D plot, some peaks are observed because of the outliers in Fig. 4a and b, but a general increase is observed from the low Q_w–low C_p–low Cost end to the high Q_w–high C_p–high Cost end. This problem is, clearly, more meaningful. A decision maker can be provided these results, and may be asked to select an appropriate 'preferred' solution. The results of the three-objective Problem 5 are also compared with those of the two-objective Problem 3 in Fig. 4. It is seen that the degree of scatter increases with the introduction of the third objective function to Problem 3. The optimal values of C_p for Problem 5 are always lower than those obtained in Problem 3 because this variable is being minimized (Eq. (6c)). This forces the membrane permeability coefficient of the salt, b, to take on its lowest value (Fig. 4e), while a shifts to its upper limit (Fig. 4d) (as compared with the two-objective problem with the constraint on the permeate concentration (Problem 3)). Other optimal parameters for the three-objective problem, viz., ΔP, a and A, vary with Q_w (Fig. 4c, d and f) almost in a similar manner as compared to the two-objective problem.

Two recent improvements of NSGA-II (Deb, 2001; Deb et al., 2002), namely, NSGA-II-JG (Kasat & Gupta, 2003) and NSGA-II-aJG (Bhat et al., 2005), have been used to solve one of the problems (Problem 4) to see if the jumping gene (JG) adaptations provide any advantage. The best values of the computational parameters have been obtained for all these techniques, and are listed in Table 2. Fig. 5 shows the development of the Pareto set over the generations using the three codes (the values of the cost for NSGA-II-JG and NSGA-II-aJG have been increased by 10,000 and 20,000 $\$\,h^{-1}$, respectively, to displace their plots vertically, so that they can be compared easily), while Table 3 gives numerical values at a few generations. It is observed from Fig. 5 as well as Table 3 that the 'range' of the Pareto set (minimum and maximum

Table 3
Comparison of the characteristics of the Pareto solutions obtained from the three techniques (Problem 4)

Generation no.	NSGA-II range[a] from	NSGA-II range to	NSGA-II mean of $I_{i,\mathrm{dist}}$	NSGA-II S.D. of $I_{i,\mathrm{dist}}$	NSGA-II-JG range from	NSGA-II-JG range to	NSGA-II-JG mean of $I_{i,\mathrm{dist}}$	NSGA-II-JG S.D. of $I_{i,\mathrm{dist}}$	NSGA-II-aJG range from	NSGA-II-aJG range to	NSGA-II-aJG mean of $I_{i,\mathrm{dist}}$	NSGA-II-aJG S.D. of $I_{i,\mathrm{dist}}$
1	986.71	70344.35	1.3218	1.4925	1012.79	75788.65	1.3219	1.4925	710.57	73049.41	1.3219	1.4926
2	579.52	85304.78	0.8682	1.1361	1012.79	86334.10	1.0611	1.4814	1083.95	81857.83	0.9461	1.2159
5	481.77	87069.66	0.6376	1.0412	1488.75	75420.80	0.6374	1.0552	1094.22	88141.74	0.6465	1.0969
10	1024.68	82648.16	0.6702	1.0592	563.21	88040.48	0.6591	1.0575	888.33	92471.25	0.6479	1.0202
20	299.41	94172.77	0.7008	1.1051	1135.63	88375.73	0.7074	1.1067	**3003.17**	**95147.50**	0.6726	1.0708
30	299.27	93857.76	0.7121	1.1176	583.53	82762.29	0.7250	1.1120	496.72	92996.29	0.6966	1.0854
40	284.37	93715.16	0.7151	1.1254	279.90	92911.11	0.7286	1.1274	1213.76	92604.98	0.7088	1.1062
50	291.27	95544.68	0.7164	1.1211	773.29	95409.55	0.7284	1.1320	546.01	95966.83	0.7232	1.1118
60	276.33	95925.77	0.7211	1.1234	**309.11**	**96586.80**	**0.7309**	1.1310	1058.69	96659.94	0.7280	1.1348
70	1216.87	94054.49	0.7201	1.1387	952.87	95970.74	0.7327	1.1321	4003.01	96625.17	**0.7301**	**1.1344**
80	276.05	96060.30	0.7249	1.1255	1099.54	95440.73	0.7340	1.1334	417.34	83193.50	0.7326	1.1377
90	**279.8616**[b]	**96361.52**	**0.7312**	**1.1519**	308.86	96146.71	0.7315	1.1336	782.38	96890.85	0.7301	1.1432
100	1190.24	97027.84	0.7321	1.1371	308.90	96507.96	0.7324	1.1338	390.20	95974.30	0.7298	1.1350
500	621.21	94407.30	0.7371	1.1457	641.36	97289.16	0.7387	**1.1444**	871.73	96562.55	0.7342	1.1360
1000	1041.78	97586.34	0.7380	1.1463	221.76	97568.99	0.7388	1.1489	233.83	96782.56	0.7348	1.1394

[a] Values of Q_w ($m^3\,h^{-1}$).
[b] Entries in bold-face are satisfactory, i.e., values are almost as good as for the 1000th generation.

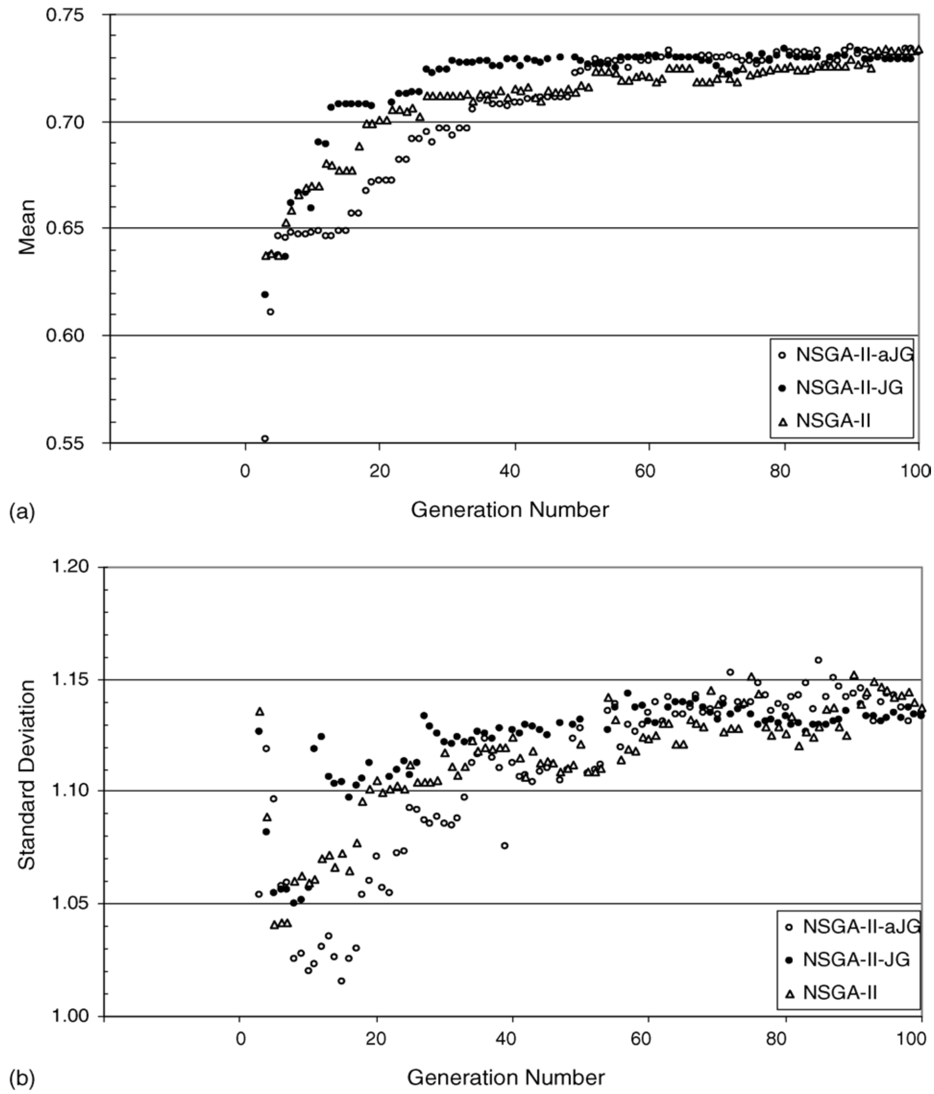


Fig. 6. Mean and standard deviation of $I_{i,dist}$ for the Pareto solutions (shown in Fig. 5) of Problem 4 (for $N_{gen} \geq 3$).

values of Q_w) increases with the generation number, with the range of NSGA-II-aJG becoming satisfactory (i.e., almost the same as that at the 1000th generation) at the 20th generation itself, faster than for NSGA-II and NSGA-II-JG. Another characteristic of the Pareto sets is the distribution/spread of the several points. Two parameters describe this aspect of the Pareto sets: the *mean* distance between consecutive points (note that the same number of chromosomes are used for all three techniques), and the *standard deviation* of these distances. Kasat and Gupta (Kasat & Gupta, 2003) have suggested the use of the mean and the standard deviation of $I_{i,dist}$ (see Appendix A) in any generation for this purpose. Fig. 6 and Table 3 show these parameters for the three techniques, at different generations. Fig. 6a and Table 3 show that the mean value of $I_{i,dist}$ is lower at the beginning (after some initial large values). This is because the range (of the Pareto set) is smaller and the same number of points is present in all generations. It is found that the mean and standard deviation of $I_{i,dist}$ (and the range) do not change much above about 80–100 generations. This can be taken as an indication that convergence has been attained (in fact, this can be used for all previous results, even though higher values of N_{gmax} have actually been used). Interestingly, the mean and standard deviation of $I_{i,dist}$ at the 100th generation are almost the same for all the three algorithms. Fig. 6 and Table 3 show that there are oscillations in both these parameters, even for as high a value of N_{gen} as 80. Similar oscillations in the behavior of the Pareto set have been observed earlier, though qualitatively. It is also observed that the mean and the standard deviation of $I_{i,dist}$ converge *faster* to their final converged value for NSGA-II-aJG than for the other two techniques (see italicized entries in Table 3). This means that this technique is the least expensive, computationally (since the computational time to achieve convergence is directly proportional to the number of generations necessary). It may be added that one could improve the 'spread' of the Pareto sets by using the ε–constraint method (Deb, 2001), in which we replace one objective function (in this case, Q_w) by an equality constraint and solve the resulting optimization problem (with a single objective function, in this case) several times over for several constant values of Q_w. This methodology has its own problems (Deb, 2001).

4. Conclusions

A few two-objective (maximizing the throughput while minimizing the cost) and three-objective optimization problems (maximizing throughput while minimizing the cost as well as the permeate concentration) are studied for the desalination of brackish water and sea water. Pareto optimal sets of equally good non-dominated solutions are obtained. The optimal solutions for spiral wound modules are compared to those for tubular modules. The membrane area, A (design parameter), is the most important decision variable in the desalination of brackish water and seawater using spiral wound modules. In contrast, the applied pressure, ΔP (operating parameter), is the most important decision variable in the desalination of brackish water using tubular modules. Three AI-based algorithms, NSGA-II, NSGA-II-JG and NSGA-II-aJG, are used to obtain the optimal solutions and it is observed that NSGA-II-aJG is the most rapid of these algorithms if one is interested in obtaining reasonable, near-optimal solutions with a small computational effort.

Acknowledgement

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Appendix A. Binary coded elitist non-dominated sorting genetic algorithm, NSGA-II (Deb, 2001; Deb et al., 2002) with the jumping gene operators, JG (Kasat & Gupta, 2003) and aJG (Bhat et al., 2005)

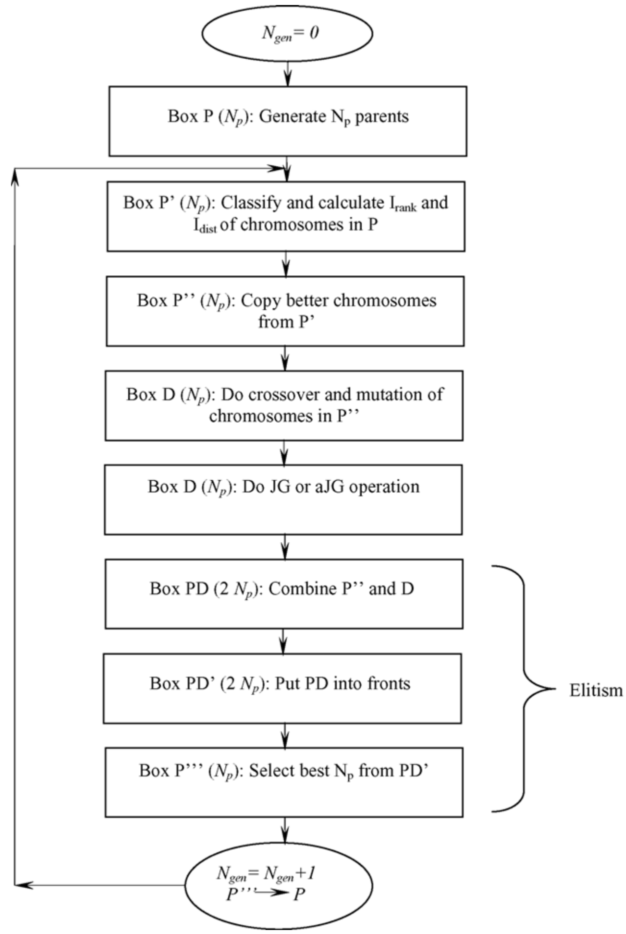

Fig. A1. Flow chart of NSGA-II and the JG adaptations.

1. Generate box, P, of N_p binary-coded parent chromosomes (see flowchart in Fig. A1), using a sequence of random numbers (e.g., a chromosome representing two decision variables, each represented by five binaries could be 11010 10110). Map each chromosome into a set of real values of the decision variables. Use the model equations to compute the values of all the objective functions (for each chromosome).
2. Classify these chromosomes into fronts based on non-domination (Deb, 2001) as follows:
   (a) create new (empty) box, P', of size, N_p;
   (b) transfer the ith chromosome from P to P', starting with the first;
   (c) compare chromosome, i, with each member, j, in P', one at a time;
   (d) if i dominates j (i.e., all objective functions of i are superior to/better than those of j), remove j from P' and put it back in P at its place;
   (e) if i is dominated by j, remove i from P' and put it back in P at its place;
   (f) if i and j are non-dominated (i.e., at least one objective function of i is inferior to that of j, while all others are superior), keep both i and j in P'. Explore all j in P';
   (g) repeat, sequentially, for all chromosomes in P. P' constitutes the first front or sub-box (of size $\leq N_p$) of non-dominated chromosomes. Assign all chromosomes in this front $I_{i,rank} = 1$;
   (h) create subsequent fronts in (lower) sub-boxes of P' using the chromosomes remaining in P. Compare these members *only* with members present in the current sub-box. Assign all chromosomes in the individual sub-boxes, $I_{i,rank} = 2, 3, \ldots$ Finally, all N_p chromosomes are in P', boxed into one or more fronts.
3. Evaluate the crowding distance, $I_{i,dist}$, for the ith chromosome in any front using:

(a) rearrange all chromosomes in front, j, in ascending order of the values of any one of their fitness functions, F_k;
(b) find the largest cuboid (rectangle for two fitness functions) enclosing i, that just touches its nearest neighbors in the F-space;
(c) $I_{i,dist} \equiv 1/2$ (sum of all sides of this cuboid);
(d) assign large values of $I_{i,dist}$ to solutions at the boundaries to make them important.

4. Copy the better of the N_p chromosomes of P' in a new box, P'' (‘better’ parents). Use:
(a) select any pair, i and j, from P' (randomly, irrespective of fronts);
(b) identify the better of these two chromosomes. i is better than j if (for minimization of all fitness functions):

$$I_{i,\text{rank}} \neq I_{j,\text{rank}} : I_{i,\text{rank}} < I_{j,\text{rank}},$$

$$I_{i,\text{rank}} = I_{j,\text{rank}} : I_{i,\text{dist}} > I_{j,\text{dist}};$$

(c) copy (without removing from P') the better chromosome in a new box, P'';
(d) repeat till P'' has N_p members;
(e) copy all of P'' in a new box, D, of size N_p;
Not all of P' need be in P'' or D.

5. Carry out crossover and mutation (Deb, 1995) of chromosomes in D. This gives a box of N_p daughter chromosomes:
(a) *Crossover*: randomly select two chromosomes and a random crossover site (say, after the third position) and exchange the binaries as shown below:

$$\begin{array}{l} 110\,|\,10\ \ 10110 \\ 011\,|\,11\ \ 11010 \end{array} \rightarrow \begin{array}{l} 110\,|\,11\ \ 11010 \\ 011\,|\,10\ \ 10110 \end{array}$$

(b) *Mutation*: for *each* binary in *each* chromosome, generate a random number and check (using p_m) if it needs to be changed by this operator. If yes, switched it over (from 0 to 1 or vice versa).

6. Do JG or aJG operation: select a chromosome (sequentially) from D, say 110|10 10|110.
Check if JG/aJG operation is needed, using a random number and p_{JG}. If yes:
(a) generate a random number between 0 and 1;
(b) multiply this by l_{chrom}, the total number of binaries in the chromosome. Round off to convert into an integer. This represents the position of the beginning of a transposon (say, at the end of the third binary in the above chromosome);
(c) JG or aJG:
- JG: generate another similar random number and identify a second location (end of the JG) in the selected chromosome (say, the after the seventh binary);
- aJG: fix the second end of the JG using the specified string length, l_{aJG} (say $l_{aJG} = 4$; so place a marker at the end of the 3 + 4 = seventh binary) of the jumping gene (Bhat et al., 2005);

(d) replace the set of binaries between these two locations by a new set of binaries (use random numbers). For example, we may get 110|00 11|110

7. Copy all N_p members of P'' and all the N_p members of D into box PD (elitism). Box PD has $2N_p$ chromosomes.
8. Reclassify these $2N_p$ chromosomes into fronts (box PD′) using *only* non-domination (see Step 2 above).
9. Take the best N_p from box PD′ and put into box P'''.
10. This completes one generation. Stop if criteria are met.
11. Copy P''' into starting box, P. Go to Step 2 above.

Appendix B. Model equations

The volumetric flux, J_w (Lonsdale et al., 1965; Rautenbach, 1986; Sherwood, Brian, & Fischer, 1967; Soltanieh & Gill, 1981) of the solvent is represented phenomenologically by

$$J_w = a(\Delta P - \Delta\pi) \tag{A2.1}$$

while the mass flux, J_s, of the solute is given by

$$J_s = b(C_{\text{wall}} - C_p) \tag{A2.2}$$

In the presence of concentration polarization (Sherwood et al., 1967), J_w, at steady state, is also given by

$$J_w = k_s \ln \frac{C_{\text{wall}} - C_p}{C_b - C_p} \tag{A2.3}$$

We use

$$\Delta\pi = b_\pi(C_{\text{wall}} - C_p) \tag{A2.4}$$

to estimate the osmotic pressure across the membrane. We can also write the solute flux as

$$J_s = J_w C_p \tag{A2.5}$$

Combining Eqs. (A2.1)–(A2.3) (eliminating C_{wall}), we obtain, finally (Rautenbach, 1986):

$$J_w = a\left[\Delta P - b_\pi\left(C_b - \frac{bC_b \exp(J_w/k_s)}{J_w + b\exp(J_w/k_s)}\right)\exp(J_w/k_s)\right] \tag{A2.6}$$

and

$$C_p = \frac{bC_b}{b + J_w \exp(-J_w/k_s)} \tag{A2.7}$$

The observed rejection is given by

$$R = 1 - \frac{C_p}{C_b} \tag{A2.8}$$

Estimation of mass transfer coefficient, k_s

Spiral wound module (Shock & Miquel, 1987)

$$Sh = 0.065\, Re^{0.865}\, Sc^{0.25} \tag{A2.9}$$

where, $Sh = \dfrac{k_s d_h}{D_{AB}}$, $\quad Re = \dfrac{d_h v}{\nu}$ and $Sc = \dfrac{\nu}{D_{AB}}$

The hydraulic diameter of a spiral wound module depends on the channel height, the specific surface area of the spacer and the void fraction. Details for various membranes are given by Shock and Miquel (1987).

For brackish water, the kinematic viscosity, ν, can be estimated from the data given by Sourirajan (1970) for the NaCl–H_2O system at 25 °C:

$$\nu = 0.0032 + 3.0 \times 10^{-6} C + 4.0 \times 10^{-9} C^2 \tag{A2.10}$$

The mass diffusivity, D_{AB} (NaCl–H_2O; $T = 25$ °C), is estimated as $5.5 \times 10^{-6}\,\mathrm{m^2\,h^{-1}}$ at $C = 3.1\,\mathrm{kg\,m^{-3}}$ (Sourirajan, 1970).

For seawater, D_{AB}, μ and ρ (Sekino, 1994; Taniguchi & Kimura, 2005; Taniguchi et al., 2001) can be estimated from the following equations:

$$D_{AB} = 6.725 \times 10^{-6} \exp\left(0.1546 \times 10^{-3} C - \frac{2513}{273.15 + T}\right) \tag{A2.11}$$

$$\mu = 1.234 \times 10^{-6} \exp\left(0.00212 C - \frac{1965}{273.15 + T}\right) \tag{A2.12}$$

and

$$\rho = 498.4m + \sqrt{248000m^2 + 752.4mC} \tag{A2.13}$$

$$\text{where, } m = 1.0069 - 2.757 \times 10^{-4} T \tag{A2.14}$$

B.1. Tubular module (Wiley et al., 1985)

For laminar flow, i.e., for $Re \leq 2100$ in a circular tube, the Leveque relationship (Perry et al., 1997):

$$Sh = 1.62\left(Re\, Sc \frac{d}{l}\right)^{0.33} \tag{A2.15}$$

and for turbulent flow, i.e., for $Re \geq 2100$ (Perry et al., 1997; Wiley et al., 1985):

$$Sh = 0.023 Re^{0.8}\, Sc^{0.33} \quad \textit{for } Sc < 1,$$
$$Sh = 0.023 Re^{0.875}\, Sc^{0.25} \quad \textit{for } 1 \leq Sc \leq 1000,$$
$$Sh = 0.0096 Re^{0.91}\, Sc^{0.35} \quad \textit{for } Sc > 1000 \tag{A2.16}$$

B.2. Estimation of the osmotic coefficient (Sourirajan, 1970)

The osmotic pressure, π, is obtained from the data given by Sourirajan (1970) for the NaCl–H_2O system at 25 °C (concentration range: 0–49.95 kg m^{-3}) and is correlated as:

$$\pi = 0.7949C - 0.0021C^2 + 7.0 \times 10^{-5} C^3 - 6.0 \times 10^{-7} C^4 \tag{A2.17}$$

Therefore, the osmotic coefficient, b_π, can be obtained as

$$b_\pi = \frac{\pi}{C} \tag{A2.18}$$

B.3. Estimation of the cost

The cost of production of desalinated water is given by the following equation (Maskan et al., 2000):

$$\text{Cost} = C_{\text{mem}} A + C_{\text{main}} A + C_{\text{pump}} \left(\frac{Q_w \Delta P}{W_{\text{base}} \eta}\right)^n + \frac{C_{\text{ele}} Q_w \Delta P}{\eta} \tag{A2.19}$$

Substituting the appropriate cost coefficients and $\eta = 0.6$, one obtains (Maskan et al., 2000; Perry et al., 1997)

$$\text{Cost} = 1.946 \times 10^{-3} A + 3.57 \times 10^{-3} A + 0.0943 \left(\frac{Q_w \Delta P}{1611.36}\right)^{0.67} + 2.315 \times 10^{-3} Q_w \Delta P \tag{A2.20}$$

The first and third terms on the right hand side of Eq. (A2.20) are not used in evaluating the ‘Cost’ for the operating-stage optimization Problem 1, since they represent ‘sunken’ capital that is already invested in an existing unit.

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