

Synthesis of near-optimal topologically constrained property-based water network using swarm intelligence

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Abstract The sustainability of water resources is one of the major concerns of the world. Industries are finding ways to minimize water costs and to reduce water pollution through efficient use of supplies. One of effective solutions is the use of water pinch technology or process integration techniques. Property integration emerged as the third trend of process integration technique (aside from energy and mass integration) to solve the problem of water network synthesis by considering physical stream properties such as pH or resistivity. Various techniques have been done to solve this property-based problem. In this pa-

per, mixed integer non-linear programming (MINLP) problems with topological constraints is studied. Nowadays, various evolutionary algorithms are also used to solve such MINLP problems. In this study, particle swarm optimization is used to solve the property integration problem. A comparison is made between this algorithm and commercial genetic algorithm (GA) applications. Particle swarm optimization is observed to perform favorably compared to GA.

Keywords Process integration · Property integration · Mixed integer non-linear programming · Particle swarm optimization

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Introduction

Population growth and world economic progress lead to a large amount of freshwater (FW) usage while the supply of this resource remains constant. Consequently, an enormous volume of wastewater (WW) is released into the environment. The reduction of water consumption by industry is needed for sustainability. One of the promising solutions for water conservation is via the use of process integration (PI) techniques. PI techniques can be broadly categorized into graphical insight-based (often known as pinch analysis) and mathematical-based approaches, in which the graphical technique was initially developed to minimize energy use by maximizing waste heat recovery during the energy crisis in the 1970s (Hohmann 1971; Linnhoff et al. 1982).

Mass integration was then developed by the analogy based on thermal pinch technique to reuse the industrial solvents efficiently (El-Halwagi and Manousiou-

thakis 1989; El-Halwagi 1997). The mass integration technique was later extended to its special case of water reuse/recycle network by Wang and Smith (1994). Many recent works on water network have then been reported, either based on the graphical insight-based techniques or mathematical-based approaches. The main advantage of graphical pinch analysis technique is the identification of network targets, i.e. FW and WW flowrates, ahead of detailed network design. (Dhole et al. 1996; Olesen and Polley 1997; Sorin and Bedard 1999; Polley and Polley 2000; Hallale 2002; El-Halwagi et al. 2003; Manan et al. 2004; Aly et al. 2005; Foo et al. 2005; Prakash and Shenoy 2005a, b).

Despite the advantage of being able to set targets ahead of design, the graphical water pinch approach often suffers from the limitation of being cumbersome due to its graphical nature. Mathematical-based techniques, on the other hand, serves as a good supplement tool in handling more complex systems, as well as in offering different options during network synthesis. The early work of mathematical-based optimization approach for water network synthesis was reported by Takama et al. (1980a, b, 1981) based on superstructure approach. After the seminal work of Takama et al., various other mathematical-based optimization approaches were presented. Alva-Argáez (1998, 1999) developed the integrated approach combining the insights from water pinch and mathematical programming in handling the mass transfer-based water network synthesis problems. The combined use of pinch and linear programming (LP) techniques was later presented by Jacob et al. (2002). Optimization approach based on non-linear programming (NLP) was later presented for mass transfer-based processes (Rossiter and Nath 1995; Yang et al. 2000; Abebe et al. 2003) and for non-mass transfer-based processes (Dunn et al. 2001). Huang et al. (1999) and Benko et al. (1999 2000) individually developed the mathematical-based approach to include water treatment in the total water network synthesis. Bagajewicz et al. utilized LP and algorithmic procedures for the design of water network, for both single (Savelski and Bagajewicz 2000a, b, 2001; Gómez et al. 2001) and multiple impurities (Bagajewicz et al. 2000; Bagajewicz and Savelski 2001; Savelski and Bagajewicz 2003). More recent works on this area are dominated by the advanced mathematical optimization approaches, such as fuzzy logic programming (Tan 2002; Tan and Cruz 2004), genetic algorithm (Tsai and Chang 2001; Li et al. 2003; Prakotpol and Srinophakun 2004; Shafiei et al. 2004; Lavric et al. 2005) and random search optimization approaches (Poplewski et al. 2002; Poplewsk and Jeżowski 2005). Mathematical-based optimization ap-

proach serves as a supplementary tool to graphical pinch approach in addressing more complex systems, such as system with many water-using processes (typically more than ten streams), multiple impurities problems (Wang et al. 2003) and mass load uncertainty (Koppol and Bagajewicz 2003), or to evaluate zero discharge possibility (Koppol et al. 2003).

From the above description, one notices that different computational approaches have been proposed to solve the various mathematical models. Generally, LP is used for simple water network problem and its optimality is guaranteed. However, when other considerations such as network complexity are considered in the model, the result is a mixed integer non-linear programming (MINLP) problem due to the additional binary value. The difficulty in solving a MINLP problem is that global optimum cannot be guaranteed by conventional deterministic algorithms. To date, evolutionary algorithms (EAs) have been applied to solve MINLP problem in water network synthesis problem, with genetic algorithm (GA) being the most established EA technique (Tsai and Chang 2001; Shafiei et al. 2004; Prakotpol and Srinophakun 2004; Wu and Chang 2003; Chungsiriporn et al. 2006). However, GA has some limitations in terms of success rate and solution quality such as convergence time and error (Elbeltagi et al. 2005; Abido 2002; Yin et al. 2006). This calls for the development of a new algorithm so that the problem can be handled more efficiently.

Besides, the above-mentioned studies focused on water reuse/recycle have been mainly based on mass concentration. In some cases water quality that is in concern for reuse and recycles is defined by physical properties such as density, turbidity, color, pH, etc. Thus, the conventional mass integration techniques based on component tracking is inapplicable. Besides, due to the environment regulation that limits the discharge of the certain properties, the reuse/recycle of streams based on properties tracking is necessary. Property integration was recently introduced for this purpose, which can be defined as a holistic approach to the allocation and manipulation of streams and processing units, based on the tracking, adjustment, assignment and matching of functionalities throughout the process (El-Halwagi et al. 2004). It is important to consider that component-based problem is different from property-based problem. The component balance may be satisfied but property balance might be violated. In considering material reuse/recycle based on property context, it is necessary to define the property operator, a surrogate property that enables the conservative tracking of stream properties. Various re-

search have focused on this (Shelley and El-Halwagi 2000; El-Halwagi et al. 2004; Kazantzi and El-Halwagi 2005), with some property operators summarized by Foo et al. (2006), as shown in Table 1.

This study focuses on the use of particle swarm optimization (PSO) technique in solving the MINLP model in a property-based water reuse/recycle network. The objective is to find the minimum FW flow-rate for each connected reuse/recycle stream. Since pipe, pump cost, and different elevation of processes are considered, different topological constraints can be introduced. Within a water reuse/recycle network, network complexity may be constrained for the following reasons:

- Safety, reliability and operability
- Capital cost
- Total environmental impact, measured on a life cycle basis, arising from network retrofit and operation (Ku-Pineda and Tan 2006)
- Plant layout
- Forbidden and compulsory stream matches

A case study of water minimization in the semiconductor industry adapted from literature (Ng et al. 2006) is used as demonstration. A different network possibilities using PSO for property integration are given at the end part of this study. As will be shown, PSO can handle the limitation of previous reported works such as GA.

Problem statement

This research is focused on the new application of PSO to MINLP model of single-component water/wastewater minimization retrofit problem with network topology constraints. The reason for the use of binary variables is to limit the topology of the water reuse network to trade off the water savings and capital cost arising from network complexity. This MINLP model cannot be solved by graphical approaches such as pinch analysis and the use of a heuristic algorithm is preferable.

Particle swarm optimization

Particle swarm optimization is similar to other EAs in terms of searching procedure. This method was proposed by Kennedy and Eberhart (1995) and it is inspired by the behavior of social animals. This is done with particles in multidimensional space that have a position and a velocity. In PSO, each solution is a particle in the swarm and is considered as an agent which is similar to a chromosome in GA (El-beltagi et al. 2005). There are three factors that make the particle move. First, each particle based on its experiences moves together to next better position till the posting place is reached. This is called self-influence. Second, each particle based on the optimum position of all the particles in the flock chooses the optimum position where the best particle is currently installed. This is called global swarm influence. Third, the particle tends to continue its current motion as a result of momentum influence. Thus, by combining these three influences the new updated position of the particles is found. The best next position is considered to be a new starting position until the optimum point is realized. The trajectory of the particle is attracted by three factors moving in space as shown in Fig. 1. These factors are represented in three dimensions as self-influence, swarm influence and momentum.

The flow chart of PSO algorithms is depicted in Fig. 2. In PSO, the initial value is generated randomly and the fitness of the population is evaluated by updating the position of each particle. The mathematical form translated this velocity and position update is shown below (Kennedy and Eberhart 1995).

$$\mathbf{V}_i + 1 = a \times \mathbf{V}_i + b \times R1 \times (\text{pbest} - \mathbf{X}_i) + c \times R2 \times (\text{gbest} - \mathbf{X}_i) \tag{1}$$

$$\left. \begin{aligned} \mathbf{X}_i + 1 &= d \times \mathbf{X}_i + e \times \mathbf{V}_i + 1 \\ \mathbf{V}_{\max} &\geq \mathbf{V}_i \geq -\mathbf{V}_{\max} \end{aligned} \right\} \tag{2}$$

Table 1 Various forms of property operator (Foo et al. 2006)

Property of mixture	Mixing rule	Operator
Density ($\bar{\rho}$)	$\frac{1}{\bar{\rho}} = \sum_i \frac{x_i}{\rho_i}$	$\psi(\rho_i) = \frac{1}{\rho_i}$
Reid vapor pressure ($\overline{\text{RVP}}$)	$\overline{\text{RVP}} = \sum_i x_i \text{RVP}_i^{1.44}$	$\psi(\text{RVP}_i) = \text{RVP}_i^{1.44}$
Material content (\bar{M})	$\bar{M} = \sum_i x_i M_i$	$\psi(M_i) = M_i$
Electric resistivity (\bar{R})	$\frac{1}{\bar{R}} = \sum_i \frac{x_i}{R_i}$	$\psi(R_i) = \frac{1}{R_i}$
Viscosity (μ)	$\log(\bar{\mu}) = \sum_{i=1}^N x_i \log(\mu_i)$	$\psi(\mu_i) = \log(\mu_i)$
Paper reflectivity (\bar{R}_{∞})	$\bar{R}_{\infty} = \sum_i x_i R_{\infty,i}^{5.92}$	$\psi(R_{\infty,i}) = \sum_i x_i R_{\infty,i}^{5.92}$

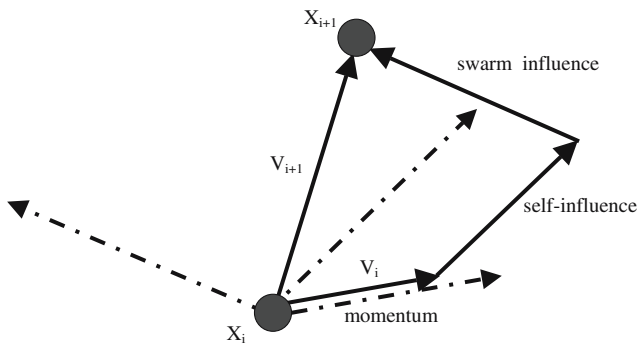


Fig. 1 Particle trajectory in PSO model (adapted from Hassan et al. 2005)

where a , b , and c are the constant parameters ranging from 0 to 2, $R1$ and $R2$ are the random numbers between 1 and 0, \mathbf{V} and \mathbf{X} are velocity and posi-

tion, respectively, subscript i is the current state of the particle, and $pbest$ and $gbest$ are the local best and global best, respectively. A detailed description of these parameters is given by many researchers (El-beltagi et al. 2005; Kennedy and Eberhart 1995). A brief description of each term in the equation is depicted in Table 2.

Particle swarm optimization has been applied in many areas such as electrical engineering, project management and civil engineering. Some of these PSO applications are shown in Table 3.

Model

This section describes MINLP models for the design of simplified water reuse networks based on the source/sink water allocation concept. Similar models have been developed for mass-exchange based formulations (Bagajewicz and Savelski 2001).

Subscripts

- i index for water source
- j index for water sink

Parameters

- Ψ_{fresh} property operator of FW
- $\Psi_{out,i}$ property operator of water source (i)
- $\Psi_{max,in,j}$ maximum property operator of water sink (j)
- $\Psi_{min,in,j}$ minimum property operator of water sink (j)
- S_i flowrate of water source (i)
- D_j flowrate of water sink (j)
- N maximum number of reuse streams allowed
- F desired total FW consumption

Decision variables

- f_j freshwater flowrate supplied to demand (j)
- w_i wastewater flowrate from source (i)
- r_{ij} flowrate of water reused from source (i) to demand (j)
- b_{ij} binary switching variable for the link from source (i) to demand (j)

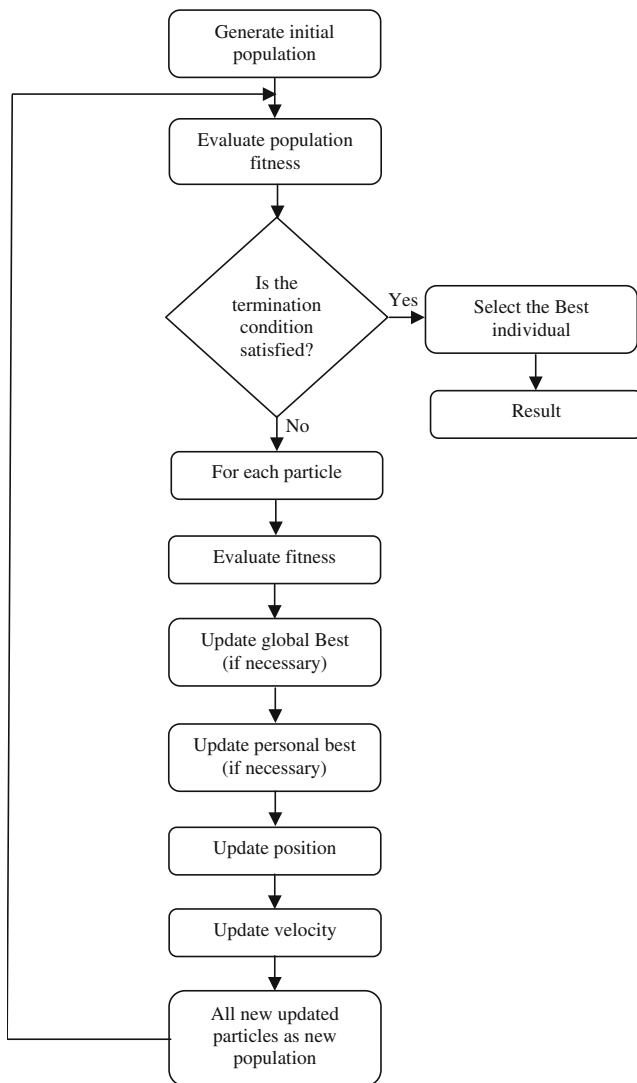


Fig. 2 Generic PSO algorithms

Table 2 Description of terms in velocity update equation (1)

Term	Description
$a \times \mathbf{V}_i$	Momentum influence of current velocity
$b \times R1 \times (pbest - \mathbf{X}_i)$	Self-influence or attraction of particles to pbest
$c \times R2 \times (gbest - \mathbf{X}_i)$	Flock influence or attraction of particles to gbest

Table 3 Some applications of PSO

Method	Author	Year	Application
Improved PSO	Abido	2002	Optimal power flow through fuel cost minimization, voltage profile improvement, and voltage stability enhancement
Simple PSO	Zhang et al.	2005	Minimizing project duration for construction management to schedule the resource-constrained project
Self-adaptive chaotic PSO	Chuanwen and Bompard	2005	Designing optimal dispatch of a hydroelectric plant
Hybrid PSO	Yin et al.	2006	Optimal task assignment with reasonable time in distributed systems
Hybrid PSO	El-Dib et al.	2006	Maximum loading of power system through solving the problem of voltage stability
Hybrid PSO	Tan	2006	Selection of optimal pollution prevention and control techniques for clay brick production

MINLP model

$$\sum_i \sum_j b_{ij} \leq N \tag{8}$$

The objective function is to minimize the total amount of FW used in the system:

$$\min \sum_j f_j \tag{3}$$

The problem is subject to several constraints. The water balance for each source is given by

$$w_i + \sum_j b_{ij} r_{ij} = S_i \quad \forall i \tag{4}$$

The water balance for each sink is given by

$$f_j + \sum_i b_{ij} r_{ij} = D_j \quad \forall j \tag{5}$$

The property limit of each water sink must be met at the maximum property load by the mixed stream supplied to it:

$$f_j \Psi_{\text{fresh}} + \sum_i \Psi_{\text{out},i} b_{ij} r_{ij} \leq D_j \Psi_{\text{max},in,j} \quad \forall j \tag{6}$$

However, the property limit of each water sink must be met at the minimum property load by the mixed stream supplied to it:

$$f_j \Psi_{\text{fresh}} + \sum_i \Psi_{\text{out},i} b_{ij} r_{ij} \geq D_j \Psi_{\text{min},in,j} \quad \forall j \tag{7}$$

The property operator is selected so that the mixing rules in Eqs. 6 and 7 are applicable. Some operators are shown in Table 1. The model split is based on the LP of El-Halwagi et al. (2003) except for the insertion of the binary variables b_{ij} . This modification makes the model non-linear, but is necessary to be able to consider topological constraints on the water reuse network. For example, a maximum number of water reuse streams N may be specified to prevent the resulting network from being too complicated:

Finally, all variables in the system are non-negative:

$$f_i, w_j, b_{ij}, r_{ij} \geq 0 \quad \forall i, j \tag{9}$$

This model thus allows the minimum water consumption to be found in a network of specified complexity.

Case study

A literature case study from Ng et al. (2006) is used to test the performance of PSO. It involves water minimization in a semiconductor process plant where the resistivity (R) is the property in concern for water reuse/recycle. Resistivity constitutes an index of the ionic content of aqueous streams. Candidates for water reuse/recycle include two water sources and two water sinks. The unintegrated FW demand of the process amounts to 1,700 gal/min. The property operator of the resistivity is given in the Eq. 10).

$$\Psi = 1/R \tag{10}$$

This kind of plant consumes a large amount of high purity FW and discharges a huge amount of WW. The process stream flowrates and the property are shown in Table 4. The solution of the problem by pinch analysis or LP gives a minimum FW demand of 562.5 gal/min, with three reuse streams when no restriction is placed on network topology, is shown in Fig. 3 (Ng et al. 2006). These conventional targeting methods cannot be used when topological constraints to the networks are added although heuristic network synthesis method can be used for these purposes. PSO coded in Visual

Basic for Applications® is used to solve the case study. The parameter to be used in PSO algorithms is given in Table 5. The recommended parameters used in Table 5 are guided by literature review (Trelea 2003) and have been adjusted based on preliminary tests.

Since the optimum FW consumption by pinch analysis (Ng et al. 2006) needs three links, the alternative networks considered in this work will be limited to less than three links, i.e. $N = 2$ and 1. This is to demonstrate how the number of reuse/recycle streams can be reduced by taking into consideration the network capital cost, location of individual processes, etc. The company has to trade off the amount of FW saving and capital cost. The different reuse streams and FW consumption are conducted by PSO and GA with number of links.

Two-link network

The first objective is to minimize FW usage with a maximum of two streams. The average solution found by PSO over ten trials was 782 ± 189 gal/min, a 54% reduction relative to the baseline target (the unintegrated FW demand of 1,700 gal/min). The material balances were satisfied to within $\pm 1\%$ in the final solution. Since different network topologies require different freshwater flowrates, the final results from the different test runs vary somewhat. The best network design found among the ten runs is shown in Fig. 4. On the other hand, the average solution found using GA with the same number of function evaluations was $1,286 \pm 188$ gal/min, which was a 24% reduction relative to the baseline. Also, material balance errors of up to 5% in sink, source, and property load equations were found in the solutions. The optimum result from ten runs is shown in Fig. 5. It is also noted that the FW

Table 5 Parameters in PSO

Parameter	Tuning value
a	0.85
b	1.5
c	1.5
d	1
e	1
μ	145
Number of particles	20
Maximum number of iterations	10,000

consumption resulting from PSO algorithm is much lower than the solution formed by GA. Moreover, the fitness evolution of FW and WW is shown Fig. 6. It also shows that the algorithms approach the final solution in about 3,000 iterations.

One-link network

The second case is limited to one link only ($N = 1$). For both PSO and GA, ten runs with the same number of function evaluations were done. The FW consumption by PSO with this limit is $1,086 \pm 47$ gal/min, a 36% reduction compared to baseline. The variation of FW consumption is depending on the network that is obtained from the ten runs. The network design of the frequent and optimum FW requirement is shown in Fig. 7. The evolution of the algorithm solution for FW and WW is shown in Fig. 8. It can be seen that the algorithms converged in about 200 iterations. On the other hand, the result from GA is $1,230 \pm 213$ gal/min. The network design is shown in Fig. 9.

On the basis of the two case studies, the solution found by PSO is better than the result obtained by GA for solving the property-based water reuse/recycle network. The different water consumption with

Table 4 Process water unit in the semiconductor industries (Ng et al. 2006)

Source	F (gal/min)	R (k Ω cm)	Sink	F (gal/min)	R (k Ω cm)
Class I–II water	650	14,000	Backgrinding	1,000	16,000
Class III–IV water	600	12,000	Marking	700	10,000
Freshwater	?	18,000			

Fig. 3 Optimum network with unlimited topology (Ng et al. 2006)

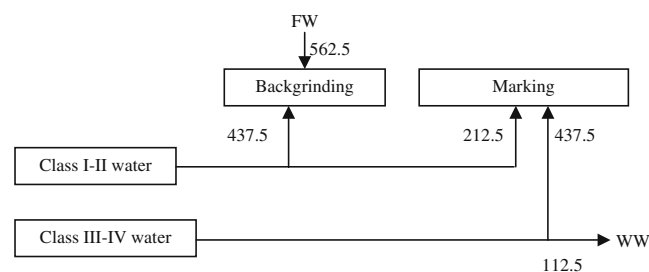


Fig. 4 Optimum network with two limited links achieved by PSO

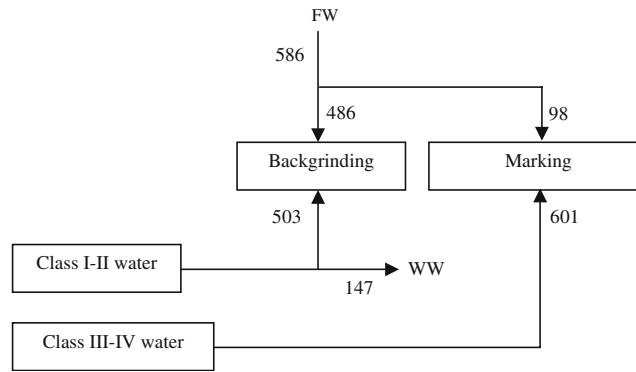
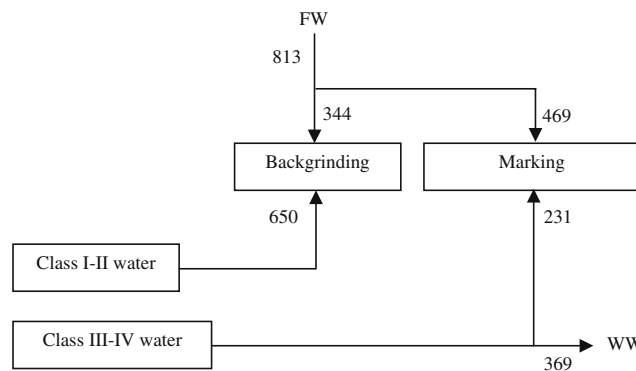


Fig. 5 Optimum network with two limited links achieved by GA



different desired links is solved by PSO and is depicted in Fig. 10. A comparison between PSO and GA shows that PSO provides a better performance than GA in all cases tested, in terms of speed and solution quality. Remarkably, the result formed by GA for maximum of two links violates the common sense of FW versus link because the FW requirement of two links must be less than or equal to one link limit. But in this case, the result of two links is higher than that of one link, clearly indicating that the GA has found a local or false

optimum. A summary of result of PSO and GA is shown in Table 6. The existence of local optimal is a common result in the non-linear model.

There is possibility to solve this MINLP model by deterministic methods because it can be decomposed into linear model when the binary variables are replaced by real values (0 and 1). The result achieved by each LP is always an optimum solution, but many trials are needed, especially for large problems. Thus, it is impractical to solve this MINLP model by decomposition into LP for all possible topologies. For instance, given m sources and n sinks of water in a process plant, the number of trials (N_{trial}) required to solve is given in the equation.

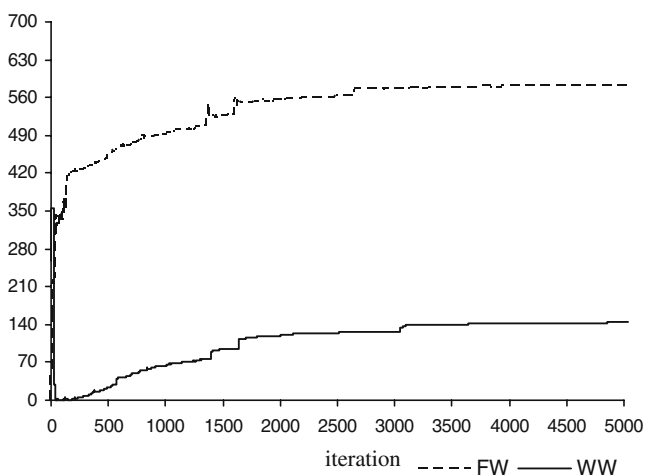


Fig. 6 Evolution of best solution in case 1

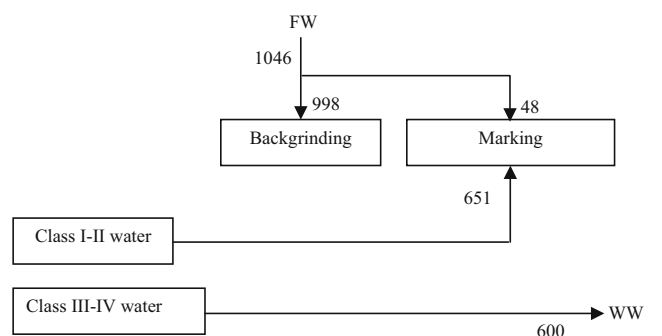


Fig. 7 Optimum network with one-limited links achieved by PSO

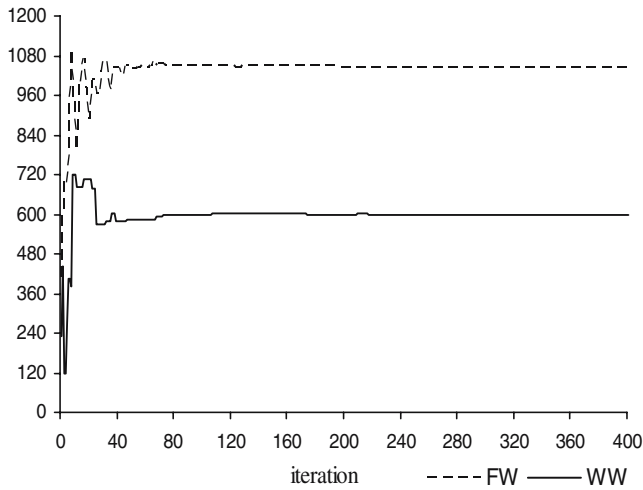


Fig. 8 Evolution of best solution in case 2

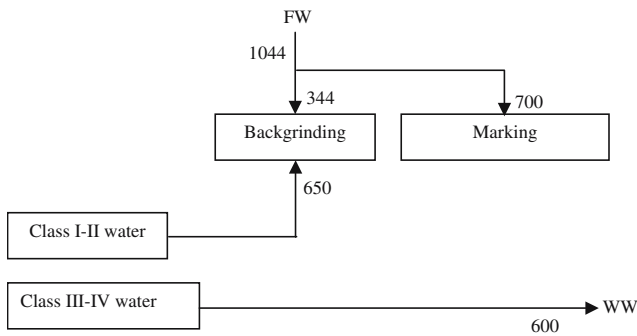


Fig. 9 Optimum network with one-limited links achieved by GA

$$N_{\text{trial}} = \frac{P!}{N!(P - N)!} \tag{11}$$

where

P $n \times m$

N number of water reuse links specified in problem.

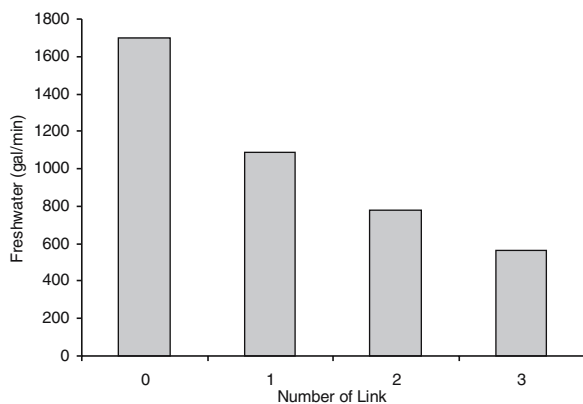


Fig. 10 Variation of freshwater consumption with different limited link: 0 link for unintegrated network; 1 and 2 links were achieved via PSO; 3 links were minimum freshwater scenario achieved via property pinch analysis (Ng et al. 2006)

Table 6 Comparison of optimum result between PSO and GA

Number of links	PSO (gal/min)	GA (gal/min)
2	782 ± 189	1,286 ± 188
1	1086 ± 47	1230 ± 213

For instance, for two sources and two sinks, there are four trials needed to solve by decomposition LP when the maximum number of water reuse link is one ($N = 1$). However, with a large problem, LP decomposition takes very long time to solve for all topologies. For example, with four sources and four sinks ($P = 16$), it requires 560 sub-problems for three water reuse links ($N = 3$). So, an automated approach that can handle this problem is much more efficient in these cases.

It is possible to improve the speed of the solution by seeding the initial population with feasible or near-feasible networks, such as the following:

- Solution found by LP or pinch analysis
- The original, unintegrated network

In seeding strategy, there is a large improvement when a feasible network is chosen as one of the initial solutions. In this case, when the correct result found by LP is chosen as an initial value for one particle among the 20 particles, the algorithm settles rapidly to the correct topology. Thus, initialization is very important in facilitating the searching efficiency of the algorithms. For a maximum number of two reuse streams, the result achieved is around 590 gal/min, which is about 65% FW reduction relative to the base line. Consequently, the WW generated is reduced about 88%. The evolution of PSO with seeding strategy of two reuse streams is given in Fig. 11. The algorithm starts to converge significantly faster, in about 2,500 iterations, than when all particles are randomly seeded; in the latter case it takes about 4,000 iterations to converge, as shown in Fig. 6. The network design is given in Fig. 4 with the errors around the constraint equations satisfied to within ± 1%.

Tests on these case studies, however, showed no major improvement resulting from seeding with the non-reuse solution. Further work can focus on evaluating the effectiveness of different seeding methods on a large number of cases.

Conclusion

Property-based water network with topology constraints has been formulated as MINLP problem and solved using a PSO code. A case study that involves

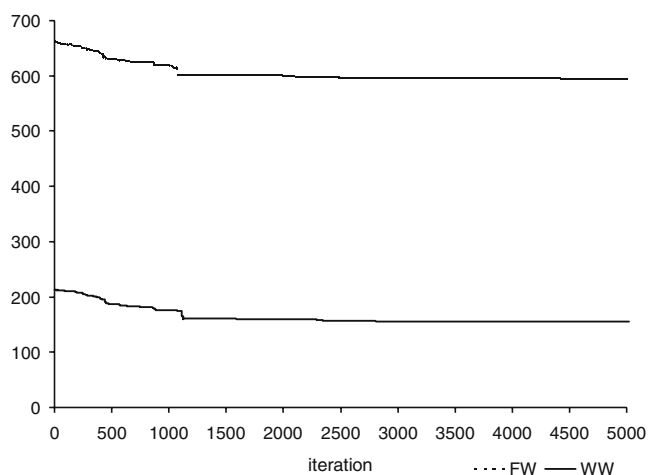


Fig. 11 Fitness evolution of PSO of two reuse streams with seeding strategy

water reuse/recycle in a semiconductor process is solved to illustrate the proposed method. This model gives the plant designer flexibility to simplify the network complexity and satisfy the trade-off between water savings and other capital investments for plant modification. Two cases were solved by two EAs. Prototype PSO software was developed using Visual Basic for Application. The use of PSO to solve the model was shown to be better than commercial GA in terms of speed and solution quality. This is the first reported work to solve a topologically constrained water reuse/recycle network using PSO model. Future work to be undertaken could include the following areas:

- Improving the performance of PSO by tuning and use of adaptive strategies
- Introducing the combined/hybrid method with other optimization algorithms to speed up the convergence behavior and the solution quality of PSO
- Extending the research to other water and/or property-based problems or to batch process
- Testing the methodology for larger networks
- Development of improved seeding or initialization methods

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