

Global Optimization for the Synthesis of Integrated Water Systems with Particle Swarm Optimization Algorithm*

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Abstract The problem of optimal synthesis of an integrated water system is addressed in this study, where water using processes and water treatment operations are combined into a single network such that the total cost of fresh water and wastewater treatment is globally minimized. A superstructure that incorporates all feasible design alternatives for wastewater treatment, reuse and recycle, is synthesized with a non-linear programming model. An evolutionary approach—an improved particle swarm optimization is proposed for optimizing such systems. Two simple examples are presented to illustrate the global optimization of integrated water networks using the proposed algorithm.

Keywords integrated water network, water minimization, particle swarm optimization

1 INTRODUCTION

Water is one of the most important natural resources being used in the process industry. Many industrial processes need water as either raw material or utility, discharging it into the environment after its use. The extremely high toxicity of effluent from the processes and the ever-tightening environmental constraints justify the need for appropriate and responsible utilization of water in the industry, and development of methodologies to minimize water use in industries has become an important area in process integration. Numerous systematic approaches including conceptual design methods [1–5], the approach in designing water networks based on the necessary conditions of optimality [6] and mathematical methods [7–10] have been published. These design concepts have been successfully applied to improve the efficiency of the water systems and reduce the aqueous emissions to the environment. In the mathematical programming approach, there is a Mixed Integer Non-Linear Programming (MINLP) model, which is decomposed into a sequence of Mixed Integer Linear Programming (MILP) problems to approximate the optimal solution. Bagajewicz *et al.* [11] proposed a method to transform the formulation of a multi-contaminant large-scale water system from a non-linear program (NLP) to a linear program (LP) and solved it to optimality. The superstructure optimization problem was further extended by Lee and Grossmann, Karupiah and Grossmann [12, 13], who formulated the decentralized wastewater treatment network as a non-convex Generalized Disjunctive Program (GDP) and solved the problem to global optimality.

Up to present, mostly methodologies presented in the published report on water minimization mainly focus on the issue of minimizing wastewater generation in water using processes, separately from the design of effluent treatment systems [14, 15]. There are very few studies on the integration of water using and treating processes into a single system. The seminal article in this area was by Takama *et al.* [16], who

solved the problem of optimal water allocation in a petroleum refinery. They generated a superstructure allowing for all water reuse and regeneration possibilities, and then mathematically optimized it. Similar study has been done by Huang *et al.* [17], who presented a theoretical model for constructing an optimal water usage and treatment network in a chemical plant. In both of the above-mentioned works, the integrated networks were modeled as non-linear programming problems and then optimized. Global optimality is not guaranteed in either of them. Karupiah and Grossmann [18] generalized the synthesis problem by proposing a superstructure, similar to that by Takama *et al.* [16] for the design of integrated water systems that combines the water using and water treating units in a single network, and proposed a new spatial branch and contract algorithm for the global optimization of such networks. All the above-mentioned works, however, assumed that the wastewater treatment technologies are described by simple linear models with constant removal ratios for each component. This is not always true in many treatment units, such as bio-oxidation, carbon bed, centrifuge separation, chemical oxidation, crystallization, evaporation, filtration and so on, for which a constant removal ratio should not be assumed. In fact, the performance of such processes will be more easily characterized in terms of fixed outlet concentration. So in this study, to overcome the above-mentioned problems, more realistic assumptions are made regarding the outlet concentrations of the treatment units. The superstructure, which incorporates all the feasible design alternatives for water treatment, reuse and recycle, is initially formulated as an NLP problem, and an improved PSO algorithm [19] for solving non-convex NLP/MINLP problems with equality constraints is proposed to optimize the integrated water systems. Two example problems are solved to demonstrate the performance of the proposed method.

2 PROBLEM STATEMENT

Given is an integrated water network that consists

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of N water using process units that generate contaminants and M treatment units that selectively remove them. For each contaminant k , the inlet and outlet concentration of each water using unit j has an upper limit $C_{j,\text{in}}^{k,\text{max}}$ and $C_{j,\text{out}}^{k,\text{max}}$, and has a fixed contaminant load L_j^k . Each water treatment unit t has an upper inlet concentration limit $C_{t,\text{in}}^{k,\text{max}}$ and a fixed outlet concentration $C_{t,\text{out}}^k$ which represents the treatment performance of the unit for each contaminant k . Furthermore, an environmental limitation concentration C_e^k must be satisfied in the discharge point which will collect any stream coming from water using or treatment unit. The problem is then to synthesize an integrated network with these water using and water treating units to minimize the total cost.

The following assumptions are adopted prior to modeling the system.

(1) The total flowrate of a stream is taken to be equal to that of pure water in that stream since the contributions of contaminants (in 10^{-6} levels) to the flows are negligible.

(2) The cost is determined by the flows of freshwater and the flows inside the treatment units. The costs of pumping and pipeline are neglected.

(3) The network is operated under isothermal and isobaric conditions.

2.1 The superstructure of the integrated water network

As seen in Fig.1, in the inlet of water using process unit j , fresh water F_j^w mixes with reused wastewater $F_{i,j}$ from other water using process i and reused wastewater $F_{t,j}$ from wastewater treatment unit t . In

the outlet of process j , the flow rate of wastewater reused by other water using process i is $F_{j,i}$, the flow rate of wastewater discharged is $F_{j,\text{out}}$, and the flow rate of wastewater treated by treatment unit t is $F_{j,t}$. In the inlet of wastewater treatment unit t (Fig. 2), wastewater $F_{j,t}$ from water using unit j mixes with wastewater $F_{l,t}$ from other water treatment unit l . In the outlet of process t , the flow rate of wastewater reused by water using process j is $F_{t,j}$, the flow rate of wastewater discharged is $F_{t,\text{out}}$, and the flow rate of wastewater treated by treatment unit l is $F_{t,l}$. The wastewater discharged from discharged point must satisfy an environment limit concentration C_e^k (Fig. 3).

2.2 The NLP model of the integrated water network

The mathematical model of the integrated water network is based upon the overall and species mass balances around each unit operation.

Objective function:

$$\text{Min} \left[\alpha \sum_j F_j^w + \sum_t \beta_t \left(\sum_j F_{j,t} + \sum_l F_{l,t} \right) \right] \quad (1)$$

Where, α and β_t are the cost parameters related relatively to the fresh water consumption and the water treatment/RMB Yuan $\text{kg}^{-1} \cdot \text{h}^{-1}$.

The constraints equations are given as:

Total mass balance for water using process j and treatment unit t :

$$F_j^w + \sum_i F_{i,j} + \sum_t F_{t,j} - \sum_i F_{j,i} - \sum_t F_{j,t} - F_{j,\text{out}} = 0 \quad (2)$$

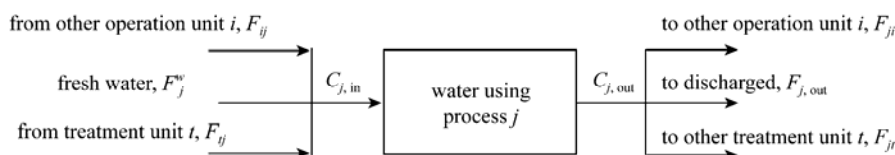


Figure 1 The superstructure model of water using network

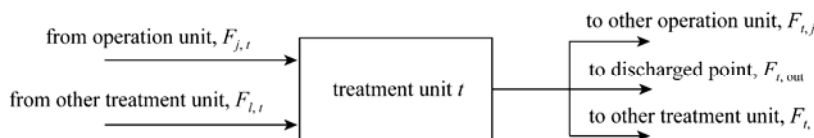


Figure 2 The superstructure model of wastewater treatment network

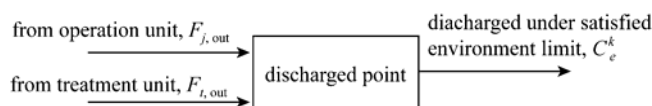


Figure 3 The superstructure model of discharged point

$$\sum_i F_{i,j} (C_{i,\text{out}}^k - C_{j,\text{out}}^k) + \sum_i F_{t,j} (C_{t,\text{out}}^k - C_{j,\text{out}}^k) - F_j^w C_{j,\text{out}}^k + L_j^k = 0 \quad (3)$$

$$\sum_j F_{j,t} + \sum_l F_{l,t} = \sum_j F_{t,j} + \sum_l F_{l,t} + F_{t,\text{out}} \quad (4)$$

Partial mass balance, for the contaminant k : at the inlet of the unit operation j and t :

$$\sum_i F_{i,j} C_{i,\text{out}}^k + \sum_t F_{t,j} C_{t,\text{out}}^k = \left(\sum_i F_{i,j} + \sum_t F_{t,j} + F_j^w \right) C_{j,\text{in}}^k \quad (5)$$

$$\sum_j F_{j,t} C_{j,\text{out}}^k + \sum_l F_{l,t} C_{l,\text{out}}^k = \left(\sum_j F_{j,t} + \sum_l F_{l,t} \right) C_{t,\text{in}}^k \quad (6)$$

Concentration limitations:

$$\begin{aligned} C_{j,\text{in}}^k &\leq C_{j,\text{in}}^{k,\text{max}} \\ C_{t,\text{in}}^k &\leq C_{t,\text{in}}^{k,\text{max}} \\ C_{j,\text{out}}^k &\leq C_{j,\text{out}}^{k,\text{max}} \end{aligned} \quad (7)$$

Outlet constraints:

$$\sum_j F_{j,\text{out}} C_{j,\text{out}}^k + \sum_t F_{t,\text{out}} C_{t,\text{out}}^k \leq \sum_j F_j^w C_e^k \quad (8)$$

3 GLOBAL OPTIMIZATION ALGORITHM FOR NON-CONVEX NLP PROBLEMS

So far, many methods have been proposed for solving NLP/MINLP problems, such as branch and bound technique, outer-approximation (OA)/equality relaxation algorithm, adaptive random-search method, branch and reduce algorithm, MINLP Simplex Simulated Annealing Algorithm (M-SIMPSA), and genetic algorithm and evolution strategies and so on. Amongst these methods, deterministic algorithms assume convexity to insure convergence to global optimum solution. As to stochastic optimization algorithms based on adaptive random search, a main difficulty to prevent a stochastic method from being effective is its weakness in handling highly constrained problems. Particle Swarm Optimization (PSO) method is a population based stochastic optimization technique developed by Kennedy and Eberhart [20]. PSO shares many similarities with evolutionary computation techniques, such as Genetic Algorithms (GA). However, an essential feature of optimization algorithms applicable to chemical engineering problems is its capability of dealing with non-linear equality constraints.

More recently, an improved PSO algorithm [19] has been proposed for solving non-convex NLP/MINLP problems with equality constraints. Through variables partitioning and tearing equality constraints, NLP/MINLP problem with non-linear equality constraints can be transformed into that with no equality constraints.

Mathematically, MINLP problem is given by:

$$(1) \text{ Minimize } f(\mathbf{x}, \mathbf{y}) \quad (9)$$

$$\text{s.t. } g(\mathbf{x}, \mathbf{y}) \leq 0 \quad (10)$$

$$h(\mathbf{x}, \mathbf{y}) = 0 \quad (11)$$

$$\mathbf{x} \in \mathbf{X}, \mathbf{y} \in \mathbf{Y} \quad (12)$$

where, vector $\mathbf{x}$ consists of n continuous real variables, and $\mathbf{y}$ consists of m integer variables. $\mathbf{X} \subset \mathbf{R}^n$ and $\mathbf{Y} \subset \mathbf{N}^m$ are the solution space of $\mathbf{x}$ and $\mathbf{y}$, respectively. $f(\mathbf{x}, \mathbf{y})$ is an objective function, $g(\mathbf{x}, \mathbf{y}) \leq 0$ and $h(\mathbf{x}, \mathbf{y}) = 0$ represent vectors of inequality and equality constraints with dimensions of p and q , respectively.

In the improved PSO method, the continuous and integer variables are decomposed as:

$$\mathbf{x} = [\mathbf{v}, \boldsymbol{\xi}]^T, \quad \mathbf{y} = [\boldsymbol{\omega}, \boldsymbol{\psi}]^T \quad (13)$$

Variables $\mathbf{v} \in \boldsymbol{\Xi} \subset \mathbf{R}^v$ and $\boldsymbol{\omega} \in \boldsymbol{\Omega} \subset \mathbf{N}^u$ are defined as the independent variables of the equality system given by Eq. (11), and then the sum of numbers of this variables $v+u$ should be the freedom degree of the system. So variable $\mathbf{v}$ and $\boldsymbol{\omega}$ are so defined that the following equality holds

$$v + u = n + m - q$$

Assuming that dependent variables $\boldsymbol{\xi}$ and $\boldsymbol{\psi}$ can be represented as $\boldsymbol{\xi} = \boldsymbol{\xi}(\mathbf{v}, \boldsymbol{\omega})$ and $\boldsymbol{\psi} = \boldsymbol{\psi}(\mathbf{v}, \boldsymbol{\omega})$ through Eq. (11), the functions in problem (1) can be represented by the independent variables:

$$\begin{aligned} f(\mathbf{x}, \mathbf{y}) &= f(\mathbf{v}, \boldsymbol{\xi}, \boldsymbol{\omega}, \boldsymbol{\psi}) \\ &= f(\mathbf{v}, \boldsymbol{\xi}(\mathbf{v}, \boldsymbol{\omega}), \boldsymbol{\omega}, \boldsymbol{\psi}(\mathbf{v}, \boldsymbol{\omega})) \equiv F(\mathbf{v}, \boldsymbol{\omega}) \end{aligned}$$

$$\begin{aligned} g(\mathbf{x}, \mathbf{y}) &= g(\mathbf{v}, \boldsymbol{\xi}, \boldsymbol{\omega}, \boldsymbol{\psi}) \\ &= g(\mathbf{v}, \boldsymbol{\xi}(\mathbf{v}, \boldsymbol{\omega}), \boldsymbol{\omega}, \boldsymbol{\psi}(\mathbf{v}, \boldsymbol{\omega})) \equiv G(\mathbf{v}, \boldsymbol{\omega}) \end{aligned}$$

and the original problem (1) can be transformed to:

$$(2) \text{ Minimize } F(\mathbf{v}, \boldsymbol{\omega}) \quad (14)$$

$$\text{s.t. } G(\mathbf{v}, \boldsymbol{\omega}) \leq 0 \quad (15)$$

$$\mathbf{v} \in \boldsymbol{\Xi} \cap \mathbf{V}, \quad \boldsymbol{\omega} \in \boldsymbol{\Omega} \cap \mathbf{V} \quad (16)$$

with $\mathbf{V} = \{(\mathbf{v}, \boldsymbol{\omega}) : h(\mathbf{v}, \boldsymbol{\xi}, \boldsymbol{\omega}, \boldsymbol{\psi}) = 0 \text{ for some } \boldsymbol{\xi} \in \mathbf{R}^{n-v} \cap \mathbf{X} \text{ and } \boldsymbol{\psi} \in \mathbf{N}^{m-u} \cap \mathbf{Y}\}$.

Problem (2) is a MINLP problem with exclusively equality constraints. Then a POS algorithm can be efficiently applied to solve the MINLP problem with the inequality constraints handled by penalty term in the objective function. Within the algorithm, the reduced variables can be solved directly through the equality constraints. If the reduced variables cannot be easily solved, multi-objective strategy could be used to handle the equality constraints, by considering the equality constraint residuals as a sub-criterion to be minimized. That is, the solution satisfying constraints are first found and the objective function is then evaluated.

In this article, this algorithm is applied to find the global optimum for the integrated networks.

4 EXAMPLES

Example 1: As a first example, a network which has 4 water using process unit and 2 treatment unit involving one contaminant is considered. Data for water using process unit and treatment unit are given in Tables 1 and 2, respectively. The environmental

Table 1 Water using unit data for Example 1

Water using unit	Mass load of contaminant/ kg·h ⁻¹	C_{in}^{max}	C_{out}^{max}
P1	2.0	0	1×10^{-4}
P2	5.0	5×10^{-5}	1×10^{-4}
P3	30.0	5×10^{-5}	8×10^{-4}
P4	4.0	4×10^{-4}	8×10^{-4}

Table 2 Treatment unit data

Treatment unit	$C_{t,in}^{max}$	$C_{t,out}$
T1	8×10^{-4}	6×10^{-5}
T2	1×10^{-4}	2×10^{-6}

discharge limit for the contaminant is taken to be 1×10^{-5} . The cost parameter α is assumed to be 0.01 RMB Yuan·kg⁻¹, and β for each of the two wastewater treatment units are 0.003 RMB Yuan·kg⁻¹ and 0.011 RMB Yuan·kg⁻¹ respectively. Table 3 shows the optimal network structure with an objective value of 1011 RMB Yuan·h⁻¹.

Table 3 Result of optimization for Example 1

Unit	Flow rate $\times 10^{-3}$ /kg·h ⁻¹		
	Recycle water	Fresh water	Discharged water
P1	0.00	20.00	0.00
P2	$F_{T1,P2} = 82.759$ $F_{T2,P2} = 17.241$	0.00	0.00
P3	$F_{T1,P3} = 33.103$ $F_{T2,P3} = 6.897$	0.00	0.00
P4	$F_{P2,P4} = 36.590$	0.00	
T1	$F_{P1,T1} = 12.734$ $F_{P2,T1} = 29.296$ $F_{P3,T1} = 40.00$ $F_{P4,T1} = 36.590$	0.00	2.759
T2	$F_{P1,T2} = 7.266$ $F_{P2,T2} = 34.113$	0.00	17.241
total cost	1011 RMB Yuan·h ⁻¹		

To depict the advantage of optimal integration of the water using and water treatment networks, the water using network and the water treatment network were optimized separately and sequentially. The freshwater is first minimized by optimizing the water using unit network without considering water treatment, and then the effluent wastewater is introduced to the treatment unit network, which is optimized by minimizing its cost. With the same data in Table 1 and the same cost parameters for the simultaneous solution, the optimal structure of water using network without considering the treatment is given in Table 4, and the optimal structure for the water treatment network is given in Table 5. The freshwater consumption for the water using network is found to be 90 t·h⁻¹ with the corresponding cost of 900 RMB Yuan·h⁻¹, total wastewater treatment cost is 985.19 RMB Yuan·h⁻¹, and then the total cost of the entire non-integrated networks is 1885.19 RMB Yuan·h⁻¹. It can be seen that either the total cost or the freshwater usage are substantially greater than those for the integrated net-

Table 4 The optimum solution for water using network

Process	Flow rate $\times 10^{-3}$ /kg·h ⁻¹		
	Recycle water	Fresh water	Discharged water
1		20.00	0.00
2		50.00	44.286
3	$F_{1,3} = 20.00$	20.00	40.00
4	$F_{2,4} = 5.714$	0.00	5.714
total cost	900 RMB Yuan·h ⁻¹		

Table 5 The optimum solution for wastewater treatment network

Treat process	Treated flow rate $\times 10^{-3}$ /kg·h ⁻¹	Discharged flow rate $\times 10^{-3}$ /kg·h ⁻¹
t1	$F_{3,t1} = 40.00$ $F_{4,t1} = 3.914$	12.414
t2	$F_{2,t2} = 44.286$ $F_{4,t2} = 1.800$ $F_{t1,t2} = 31.5$	77.586
total cost	985.19 RMB Yuan·h ⁻¹	

work (1011 RMB Yuan·h⁻¹ and 20 t·h⁻¹, respectively). This is simply because the integration of the two networks increases effectively the possibility of water reuse not only from the water using units but also from the treatment units.

Example 2: It is a 2 water using process unit and 2 treatment unit system involving two contaminants A and B, for which water using process unit and treatment unit data are given in Tables 6 and 7, respectively. The environmental discharge limit for both the contaminants (A and B) is taken to be 1×10^{-5} . Table 8

Table 6 Water using unit data for Example 2

Water using unit	Mass load of contaminant/kg·h ⁻¹		$C_{j,in}^{k,max}$		$C_{j,out}^{k,max}$	
	A	B	A	B	A	B
P1	1	1.5	0	0	2.5×10^{-5}	3.75×10^{-5}
P2	1	1	5×10^{-5}	5×10^{-5}	7×10^{-5}	7×10^{-5}

Table 7 Treatment unit data for Example 2

Treatment unit	$C_{t,in}^{max}$		$C_{t,out}$	
	A	B	A	B
T1	4×10^{-5}	—	2×10^{-6}	—
T2	—	6.25×10^{-5}	—	3.125×10^{-6}

Table 8 Result of optimization for Example 2

Unit	Flow rate $\times 10^{-3}$ /kg·h ⁻¹		
	Recycle water	Fresh water	Discharged water
P1	0.00	40.00	0.00
P2	$F_{P1,P2}=40$ $F_{T1,P2}=10$	0.00	0.00
T1	$F_{P2,T1}=41.68$	0.00	4.63
T2	$F_{P2,T2}=8.32$ $F_{T1,T2}=27.05$	0.00	35.37
total cost	914.11 RMB Yuan·h ⁻¹		

shows the optimal network structure with an objective value of 914.11 RMB Yuan·h⁻¹.

Here, the problem is solved separately as two non-integrated networks for water using and wastewater treatment. The optimal structures for the separated networks are given by Tables 9 and 10, respectively. The optimal freshwater consumption is found 50 t·h⁻¹ with a corresponding cost of 500 RMB Yuan·h⁻¹, and the optimal treatment cost is 581.62 RMB Yuan·h⁻¹. And the total cost is then 1081.62 RMB Yuan·h⁻¹. These are again substantially greater than those for the integrated solution. Therefore, the significance of the integration of the two networks is clearly justified.

Table 9 The optimum solution for water using network

Process	Flow rate×10 ⁻³ /kg·h ⁻¹		
	Recycle water	Fresh water	Discharged water
1		40.00	0.00
2	$F_{1,2} = 40.00$	10.00	50
total cost		500 RMB Yuan·h ⁻¹	

Table 10 The optimum solution for wastewater treatment network

Treat process	Treated flow rate×10 ⁻³ /kg·h ⁻¹	Discharged flow rate×10 ⁻³ /kg·h ⁻¹
t1	$F_{2,t1} = 39.47$	7.89
t2	$F_{2,t2} = 10.53$	42.11
	$F_{t1,t2} = 31.58$	
total cost	581.62 RMB Yuan·h ⁻¹	

5 CONCLUSIONS

This article presents a superstructure-based method for optimization of an integrated water system consisting of water using and water treating units, and this method and the significance of the integration of the two kinds of networks are illustrated with two examples. The integrated system is formulated as a NLP problem. An improved PSO algorithm, initially developed for solving non-convex NLP/MINLP problem with equality and/or inequality constraints, is introduced to solve the global optimization problem of such networks.

It should be noted that the validity of the proposed method in this study is limited within the cases where the kinds and the numbers of the units for water using and for wastewater treatment are known. For the water system synthesis problems, however, the selection and the number of the wastewater units should be simultaneously optimized. This will lead to MINLP problems. So, MINLP formulation and its solution methodology for the water using/treatment network optimization should be addressed in the future.

NOMENCLATURE

F_j^w flow rate of fresh water, kg·h⁻¹

$F_{j,t}$ flow rate of wastewater from water using process j to treatment unit t , kg·h⁻¹
 $F_{l,t}$ flow rate of wastewater from treatment unit l to treatment unit t , kg·h⁻¹
 α fresh water cost parameter (including the cost of discharging), RMB Yuan·kg·h⁻¹
 β_t treatment cost parameter, RMB Yuan·kg·h⁻¹

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