17. Water optimization in process industries

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17.1. Abstract

Global consumption of natural resources has been significantly increased over the last decades. Consequently, the research regarding sustainable utilisation of natural resources including water and energy has received considerable attention in academia and industry. The main goals have been to find promising solutions with reduced water and energy consumption within different sectors (i.e., domestic, agricultural, and industrial). Those solutions are also beneficial from the aspects of wastewater and emission minimisation and protection of the environment. The focus of this chapter is on optimisation of water consumption within industrial sector including process industries (i.e., chemical, food, petrochemical, pulp and paper). The chapter first briefly presents the global water consumption, and water use within the process industries. Then, a concept of process water networks involving water reuse, wastewater treatment reuse and recycle is explained followed by a brief description of systematic methods based on water pinch analysis and mathematical programming. An illustrative large-scale case study of the total water network including multiple contaminants is used to demonstrate a superstructure-based optimisation approach. The results of the optimal water network show that significant savings of freshwater consumption and wastewater generation can be obtained when compared to a conventional water network design.

17.2. Introduction

Global water consumption. Water is a valuable natural resource, which is used for different purposes in daily life and various sectors, namely, domestic, agricultural, and industrial. Average global water consumption within those sectors varies, and it depends of the development level of countries. In developed and industrialized countries (i.e., United States of America, Germany, France, and Canada) an average industrial water usage varies between

46–80%, while in developing countries (i.e., India, China, and Brazil) it is between 4–17% (Davé 2004). The predictions show that the population needs for freshwater as well as different products obtained within industrial and agricultural sectors will be increased. According to the predictions of global water consumption, the important issues that can be addressed in the future present rational utilisation of natural resources and sustainable water management within the above mentioned sectors.

Water use within the process industries. In a typical industrial process, water is used for different purposes (i.e., washing, extraction, absorption, cooling, and steam production). After using water within a process, wastewater is generated and discharged into the environment. Generally speaking, large amounts of freshwater are consumed and, consequently, large amounts of wastewater are generated within industrial processes. Accordingly, freshwater usage and wastewater generation should be minimized for achieving sustainable and more efficient processes. Some of the works focused on freshwater and wastewater minimisation considered separate networks (Wang and Smith 1994a, b, Wang and Smith 1995, Galan and Grossmann 1998, Kuo and Smith 1997, Castro, Teles, and Novais 2009), namely, process water-using network and/or wastewater treatment network. Also, an overall network consisting of process water-using and wastewater treatment networks (Takama et al. 1980, Huang et al. 1999, Gunaratnam et al. 2005, Karuppiah and Grossmann 2006, Ahmetović and Grossmann 2011, Faria and Bagajewicz 2011) was the focus of the research in order to explore additional freshwater and wastewater minimisation opportunities. In other words, in the process its overall water system has been studied for identifying process units, which consume water and/or generate wastewater. The main research challenges have been devoted to systematically exploring all water integration opportunities within the process in order to achieve solutions with a reduced water usage and wastewater generation. It is important to mention that the synthesis problem of an overall or total water network is more complex, and this problem has been addressed fewer papers compared to the synthesis problem of separate networks (water using network or wastewater network).

In order to address the synthesis problems of separate and total water networks, different tools and methods have been proposed. Over the last decades, it has been shown that both water-pinch technology and mathematical programming are very useful approaches for solving industrial water reuse and wastewater minimisation problems. These approaches can be used for analysing water-using processes before design, as well as after design in order to minimise both freshwater usage and wastewater generation. It has been demonstrated that by applying systematic approaches very promising solutions can be obtained, with the increased water reuse (18.6-37%) within different processes and very short payback times (0-10 months) (Mann and Liu 1999). Accordingly, it is worth pointing out that a significant progress has been made within this field. The reader is referred to several review papers (Bagajewicz 2000, Yoo et al. 2007, Foo 2009, Jeżowski 2010, Klemeš 2012, Grossmann, Martín, and Yang 2014, Khor, Chachuat, and Shah 2014, Ahmetović et al. 2015), and books (Mann and Liu 1999, Smith 2005, Klemeš et al. 2010, El-Halwagi 2012, Klemeš 2013, Foo 2013) for more details about water network synthesis and recent progress within this field.

17.3. Concepts of water use and water networks within an industrial process

Figure 17.1 shows typical water users and water treatment within an industrial process (Mann and Liu 1999). Raw water usually taken from lakes, rivers or wells is firstly treated in raw water treatment units in order to be purified and used within the process in water-using units, steam boiler and cooling tower (deaeration, demineralisation, deionisation, dealkalisation, and pH control, etc.). After using freshwater within process water-using units, cooling tower, and steam boiler, wastewater is generated and directed to a final wastewater treatment. The main role of the wastewater treatment is to remove contaminants from wastewater and to satisfy environmental constraints on the effluent discharged into the environment. Note that also water from wastewater treatment can be reused or recycled within the process (not shown in Figure 17.1) and that in this way freshwater consumption and wastewater generation can be significantly reduced.

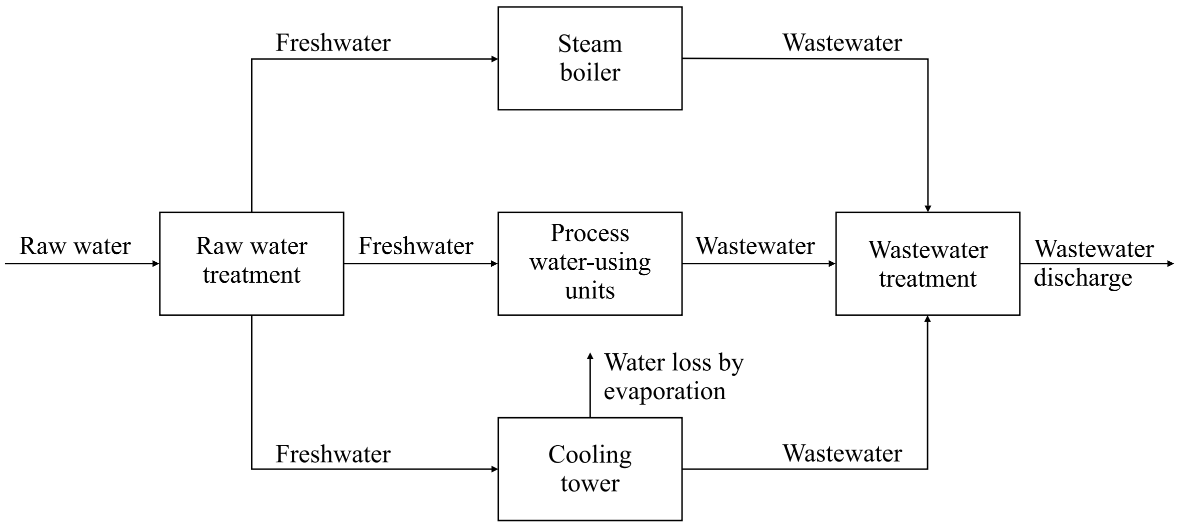

Figure 17.1. Water use and wastewater treatment within an industrial process.

Figure 17.2 shows those concepts of water networks. A water network problem is a special case of a mass exchanger network (MEN) problem (El-Halwagi and Manousiouthakis 1989). Figure 17.2a presents a process water network consisting of water-using units. Within this network mass loads of contaminants are transferred from process streams to water streams, and wastewater is generated within a process water network. Mass loads of contaminants transferred to the water streams are usually too small when compared to the water flowrate. In such cases it can be assumed that the inlet and the outlet water flows of water-using units are the same. Also it should be mentioned that wastewater can be generated by utility systems, a boiler and a cooling tower

(Figure 17.1). In those systems, a part of wastewater, namely, boiler blowdown and cooling tower blowdown, must be periodically discharged (Allegra, da Silva, and Al Goodman 2014) and make-up water introduced, in order to keep the water quality on some acceptable levels. There is loss of water within the cooling tower due to water evaporation (Figure 17.1), which cannot be reused again within a process. In the cooling tower, there is no direct contact between process and water streams. The contaminants concentration within this unit is increased due to water evaporation. Within the process water network, freshwater consumption and wastewater generation can be minimised by water reuse and local recycling of water. Figure 17.2b shows a wastewater treatment network. It consists of wastewater treatment units, which remove contaminants from wastewater. The removed mass loads of contaminants from wastewater are usually too small when compared to the wastewater flowrates, and in such cases it can be assumed that the inlet and the outlet wastewater flows of wastewater treatment units are the same. A wastewater treatment network can be a centralized or a distributed system (Galan and Grossmann 1998, Zamora and Grossmann 1998). In the centralized system, consisting of more wastewater treatment units, all wastewater streams from different processes are mixed and directed to wastewater treatment. In this case, the total flow of wastewater streams goes through each wastewater treatment unit. However, in the distributed system, consisting of more wastewater treatment units, it can happen that all flows of wastewater streams are not treated within each wastewater treatment unit. Consequently, the total cost of the distributed wastewater treatment network can be decreased compared to the centralized wastewater treatment network. It should be mentioned that different technologies can be used for removing contaminants, and in most cases wastewater treatment models are based on the fixed removal ratios of contaminants. However, note that also more realistic models (Yang, Salcedo-Diaz, and Grossmann 2014) have been recently proposed for wastewater treatment units.

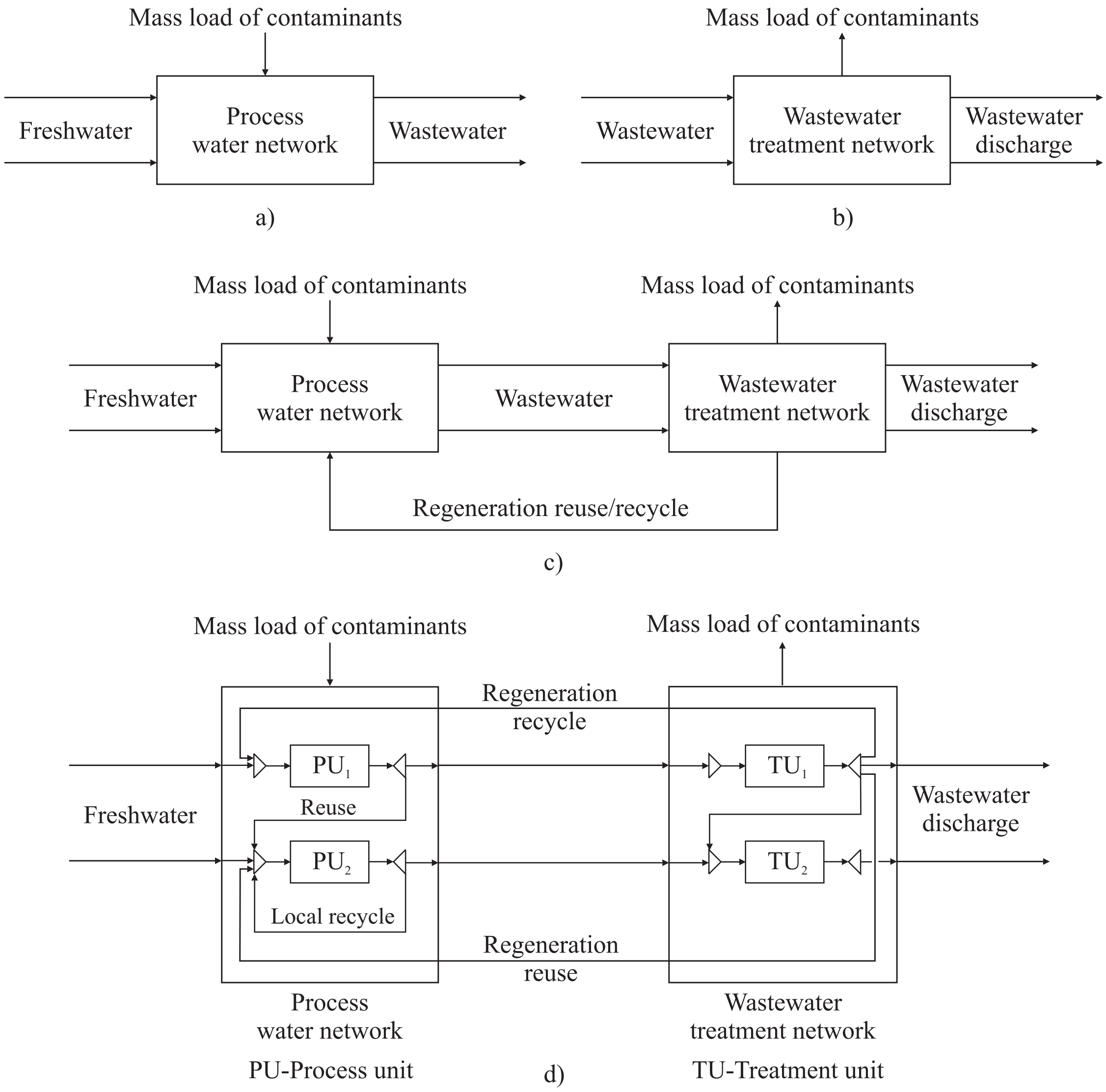

Figure 17.2. Concepts of water networks: a) process water network, b) wastewater treatment network, c) combined process water network and wastewater treatment network, d) extended case c) to show different water integration options within the combined network.

A process water network (Figure 17.2a) and a wastewater treatment network (Figure 17.2b) can be integrated producing an overall or total network (Figure 17.2c). The following water integration opportunities are enabled within this network (see Figure 17.2d), namely, water reuse (direct water reuse from process unit 1 (PU_1) to process unit 2 (PU_2)), local recycle (recycling within PU_2), wastewater regeneration reuse (wastewater from PU_1 is regenerated within wastewater treatment unit 1 (TU_1) and recycled to the same unit (PU_1), where it has previously been used) and wastewater regeneration recycle (wastewater from PU_1 is regenerated within TU_1 and reused in PU_2). Note that in the case of wastewater regeneration reuse, wastewater from TU_1 does not enter the same unit (PU_1), where it has previously been used. By solving the overall network (Figure 17.2c, d) simultaneously an improved solution can be obtained when compared to the overall network obtained by sequential solutions of networks shown in Figure 17.2a, and Figure 17.2b. This will be shown later in this chapter, as demonstrated on an illustrative case study.

17.4. Systematic methods for water network design

This section presents a brief description of systematic methods based on water pinch analysis and mathematical programming, which are used water network design. Water pinch technology/analysis (Wang and Smith 1994a, b, Wang and Smith 1995) is a graphical method, which represents an extension of pinch analysis for heat integration (Linnhoff and Hindmarsh 1983). It consists of two phases, namely, targeting and design. Assuming a single contaminant, the main goal of the targeting phase is to determine the minimum freshwater consumption (maximum water reuse) (Doyle and Smith 1997) before a water network design, while within the design phase a water network is constructed satisfying the minimum freshwater consumption. Also, water targeting models for multiple contaminants have been proposed based on mathematical programming in order to perform simultaneous flowsheet optimisation (Yang and Grossmann 2013).

The mathematical programming approach is based on a water network superstructure optimization (Takama et al. 1980). A superstructure includes all feasible alternatives from which the best is selected. The main steps within the mathematical programming approach (Biegler, Grossmann, and Westerberg 1997) are to develop a superstructure of alternative designs, develop a superstructure optimisation model, solve the model in order to extract the optimum design from the superstructure, and analysis of the obtained results. This approach can easily deal with multiple contaminant problems, different constraints (i.e., forbidden connections), and trade-offs between investment and operational costs when compared to water pinch analysis, which can have difficulties to address those issues, especially for large-scale problems. In some cases, it can be very useful to combine both approaches in order to solve the overall water network synthesis problem.

17.5. Steps of mathematical programming approach for water network design

As will be shown later, the mathematical programming approach was applied for the synthesis of water networks consisting of process water-using and wastewater treatment units. Accordingly, this section describes the main steps of mathematical programming approach for the synthesis of water networks, namely, problem formulation, superstructure development, optimisation model formulation, and solution strategies development. The reader is referred to the paper (Ahmetović and Grossmann 2011) for more details regarding the superstructure, model, and solution strategy described within this chapter. Here, only a brief description is given.

Problem formulation. The first step in the application of the mathematical programming approach for the synthesis of water networks is a problem formulation. The problem formulation of the water network synthesis problem can be stated as follows. Given is a set of water sources, a set of water-using units, and a set of wastewater treatment operations. For the set of water sources, concentrations of contaminants within water sources, and the cost of water are specified. Water-using units can operate with fixed or variable flowrates. In the case of the fixed flowrates through water-using units, for the set of process water-using units, given are the fixed flowrates, maximum concentrations of contaminants within inlet streams at process units, and mass loads of contaminants within process units. However, in the case that the flowrate of water is not fixed, given are maximum concentrations of contaminants within inlet and outlet streams of process units, and mass loads of contaminants within process units. For a set of wastewater treatment units, percentage removals (removal ratios) of each contaminant within wastewater treatment units are specified and corresponding cost relations of the investment and operation cost, which depend on flowrates of wastewater treated within treatment units. Wastewater discharged from the network has to satisfy environmental constraints specified by regulations. Accordingly, the maximum acceptable level of concentrations of contaminants within effluent is given. The problem formulation can be extended to include a set of water demand units and a set of water source units.

The main goal of the water network synthesis problem is to determine the minimum freshwater usage and wastewater generation, the interconnections, flowrates and contaminants concentrations within each stream of the water network. The objective can be formulated as the minimisation of the total annualized cost of the water network consisting of the cost of freshwater usage, the cost of wastewater treatment, the cost of piping, and the cost of pumping water through pipes. It is assumed that the water network operates under isothermal and isobaric conditions. However, those assumptions can be easily relaxed and the model extended (Ahmetović, Ibrić, and Kravanja 2014).

Superstructure development. On the basis of problem formulation, a superstructure should be synthesised including all feasible network alternatives. Figure 17.3 shows a superstructure consisting of freshwater sources, process water using units, wastewater treatment units, internal water source units and water demand units (Ahmetović and Grossmann 2011). The superstructure incorporates both the mass transfer and non-mass transfer operations. In the mass transfer process operations (process units PU_p) there is a direct contact between a contaminant-rich process stream and a contaminant-lean water stream. In this case, during the mass-transfer processes, the contaminants mass load $LPU_{p,j}$ (pollutants) is transferred from the process streams to the water. The contaminant concentration within the process stream is reduced, while the contaminant concentration increases within the water stream. In some processes there is a loss of water that cannot be re-used in water-using operations. This unit is represented by a water demand unit DU_d . Water can be produced within some operations and it can be available for re-using within other operations. This unit is represented by an internal water source unit SU_r. There is also wastewater treatment unit TU_t within the superstructure in order to remove contaminants (percentage removal $RR_{t,j}$ is specified) from wastewater stream FTU_t^{in} .

The superstructure considers all feasible connections between units including options for water integration (water reuse, regeneration reuse and regeneration recycling). The freshwater from the freshwater splitter SI_s can be directed towards process water-using units (stream $FIP_{s,p}$), wastewater treatment units ($FIT_{s,t}$) in order to enable freshwater pre-treatment if required, final wastewater mixer (stream FIF_s) and demand units ($FID_{s,d}$). Streams from other process units (stream $FP_{p',p}$) and source units ($FSP_{s,p}$) are directed to process unit mixer MPU_p, enabling water reuse options. Also water regeneration reuse and recycling is enabled by the existence of stream $FTP_{t,p}$ connecting treatment unit t with process unit p. The wastewater stream $FP_{p,p'}$ leaving process unit p (from splitter SPU_p) is directed to other process unit p', demand unit d (stream $FPD_{p,d}$), wastewater treatment unit t ($FPT_{p,t}$) for wastewater regeneration or directly discharged into the environment (FPO_p). The inlet streams to demand unit mixer (MDU_d) are those directed from external freshwater source and internal source ($FID_{s,d}$ and $FSD_{r,d}$) as well as streams leaving process and treatment units ($FPD_{p,d}$ and $FTD_{t,d}$). From the internal water source *r* water can be sent towards process unit *p* ($FSP_{r,p}$), demand unit *d* ($FSD_{r,d}$), treatment unit *t* ($FST_{r,t}$) or discharged directly into the environment (FSO_r). Streams from all the splitters within the network are directed to the treatment unit mixer MTU_t enabling freshwater pre-treatment if required ($FIT_{s,t}$) and wastewater regeneration ($FPT_{p,t}$, $FST_{r,t}$). Also, streams from other treatment units $FT_{t',t}$ are directed to mixer MTU_t.

Optimisation model formulation. For a given superstructure, an optimisation model is formulated in order to perform optimisation and extract the optimal solution embedded within the superstructure. The optimization model of water network synthesis problem consists of an objective function and constraints. The objective functions can be formulated using various economic criteria (Pintarič et al. 2014). The objective function used in this chapter represents the minimization of total annualized cost of the network consisting of the freshwater cost, the cost of wastewater treatment, the cost of piping and the operational cost of water pumping through pipes (Ahmetović and Grossmann 2011). In addition to economic nature of the objective function of water network problem, it can be also formulated as the minimization of the total freshwater consumption, or the minimisation of the total flowrate of the freshwater consumption and wastewater treated within treatment units because the cost of the wastewater treatment units depends on wastewater flowrates treated within wastewater treatment units.

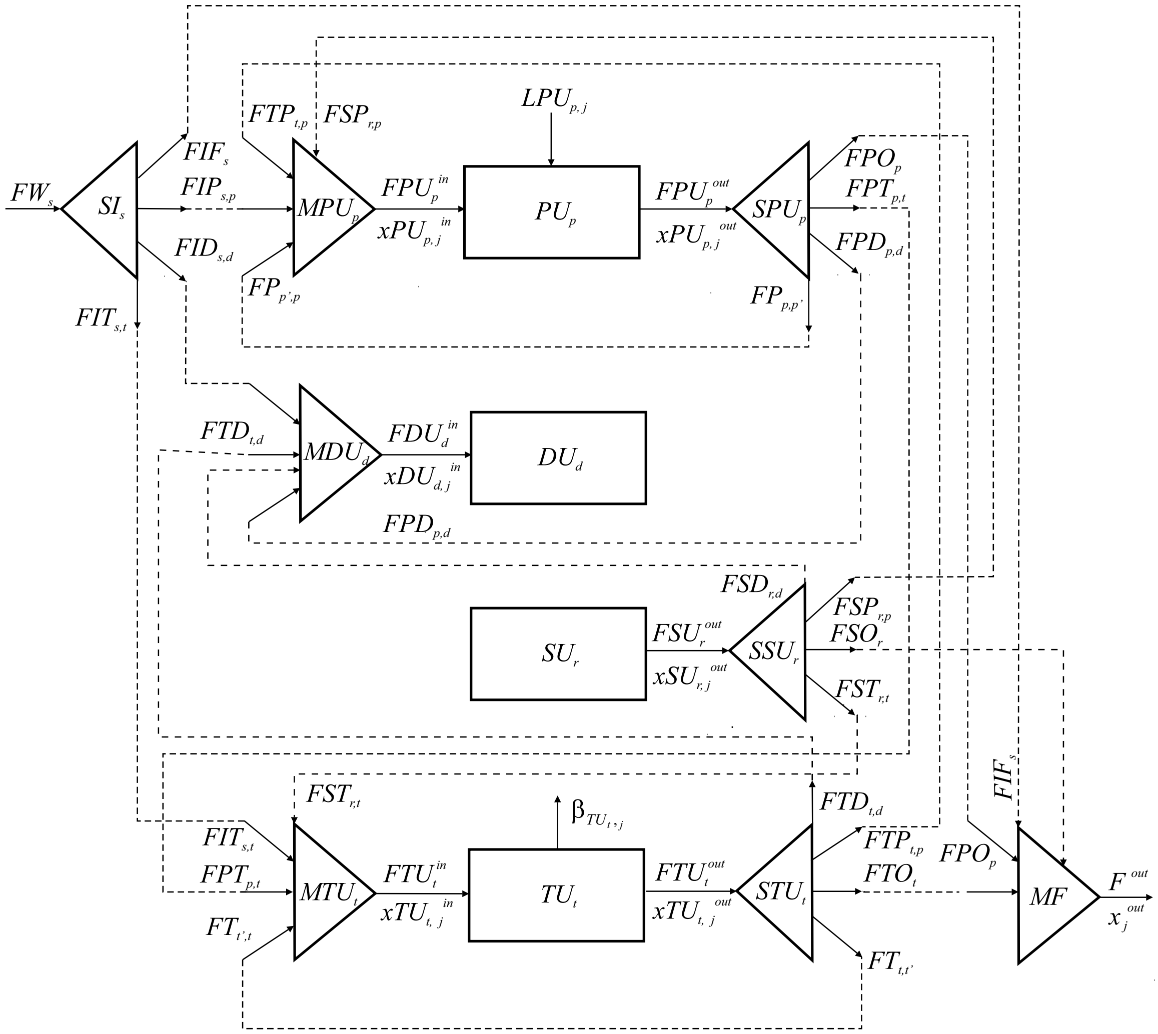

Figure 17.3. The superstructure of an integrated water network (Ahmetović and Grossmann 2011).

The model constraints can be formulated as equalities and inequalities. The equalities are, for example, the overall mass and contaminant mass balance equations, while inequalities can represent constraints on variables, for example, flowrates, contaminant concentrations, or design constraints corresponding to the existence of pipes or wastewater treatment technologies, etc. The variables within an optimization model of water network synthesis problem can be continuous and binary. Continuous variables are, for example, flowrates, contaminant concentrations, while binary variables can only have values 0 or 1 and they are used for selecting, for example, a wastewater treatment technology or a piping connection. If a binary variable has the value 1 in that case the wastewater treatment technology or the piping connection is selected and vice versa. The optimization problem can be formulated as linear programming (LP), nonlinear programming (NLP), mixed-integer linear programming (MILP) or mixed-integer nonlinear programming problem (MINLP). The last one is the most difficult to solve due to nonlinear nature of the problem and many design alternatives within the network. For the purposes of solving case study presented in this chapter, an MINLP optimisation model of water network proposed by Ahmetović and Grossmann (2011) was used. The model was implemented in General Algebraic Modeling System (GAMS) (Rosenthal 2014). It is worth mentioning that the model is generic and independent of initial data, and it can be used for solving different types of water network synthesis problems. For example, process water network or wastewater treatment network can be optimised separately (sequentially) or as an integrated network (simultaneously). Also, the proposed model can be used for the synthesis problems with fixed or variable flowrates through process water-using units, and to establish trade-offs between the network cost and network complexity. The generic nature of the model enables easy manipulation within the proposed model, for example, excluding some units from the superstructure can be done only by specifying empty set for the given units. Figure 17.4 shows different options of the water network model starting from a data input to the optimal network design solution. The following data input is required, for example, in the case that an overall network consisting of a process water network (fixed flowrates through process water-using units) and a wastewater treatment network should be synthesized:

- a number of freshwater sources, a number of contaminants and corresponding concentrations within the freshwater source stream, and the cost of freshwater;

- a number of process water-using units, mass flowrates of process units, mass loads of contaminants transferred to water streams within the process units, maximum inlet concentration of contaminants at the inlet streams to the process units;
- a number of wastewater treatment units, removal percentages of contaminants within the wastewater treatment units, operation and investment cost coefficients, cost function exponents, and an annualized factor for investment on treatment units;
- cost coefficients corresponding to existence of pipes, investment cost coefficients, cost function exponent for the investment cost of pipes, and an annualized factor for investment on pipes;
- operating cost coefficient for pumping water through pipes;
- hours of network plant operation per annum; and
- limiting concentration of contaminants within the wastewater stream discharged into the environment.

Accordingly, only the number of units has to be specified next to data input in order to solve the model using MINLP optimisation solvers, for example, BARON (Tawarmalani and Sahinidis 2005) in order to obtain the global optimum solution of the network design.

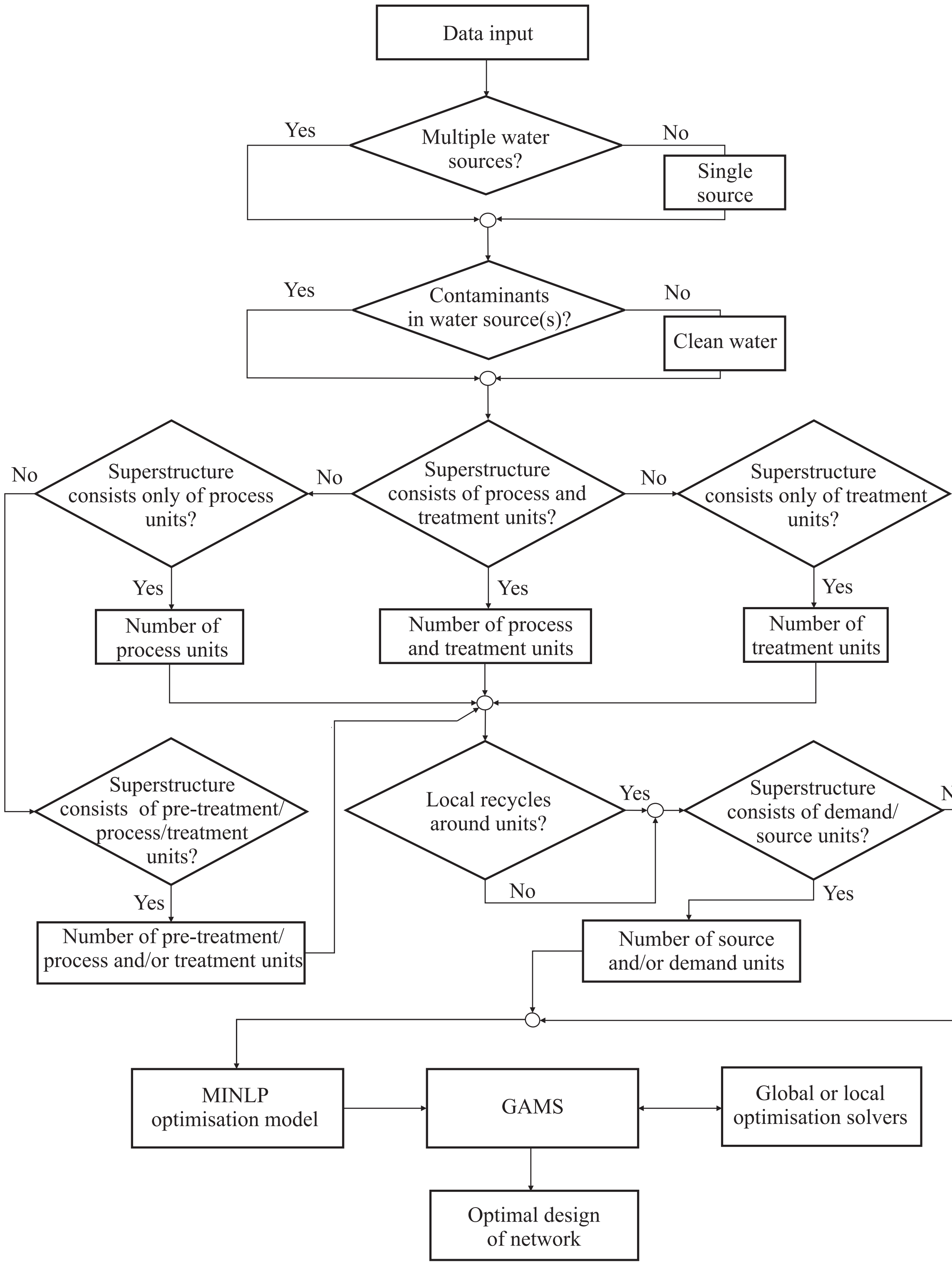

Figure 17.4. Different options of the water network model proposed by Ahmetović and Grossmann (2011).

Solution strategies development. The overall synthesis problem consisting of process water-using and wastewater treatment network can be solved sequentially and simultaneously. In a sequential approach, a process water-using network is firstly solved in order to determine the minimum freshwater usage and the water network design, followed by solving a wastewater treatment network in order to determine a wastewater network design (see Figure 17.2a and Figure 17.2b as well as Figure 17.4). On the basis of the obtained network design solutions, an overall network consisting of water-using network and wastewater treatment network can be constructed. In a simultaneous approach, process water-using and wastewater treatment networks are solved together as an overall synthesis problem (see Figure 17.2c as well as Figure 17.4) in order to extract the optimal design of integrated network from the superstructure. Water pinch technology and mathematical programming can be used for sequentially solving the overall water network synthesis problem. However, only mathematical programming approach can address the overall water network synthesis problems simultaneously. The obtained solution by the sequential strategy is sub-optimal, while the simultaneous strategy enables obtaining locally optimal as well as globally optimal solutions depending on the type of solver that is used. In the cases of using local optimisation solvers a good initialisation point should be provided as well as tights bounds for optimisation variables, while an initialisation point not needed to be provided for global optimisation solver, for example BARON. The proposed MINLP optimisation model can be solved by global optimisation solver BARON directly or by using a two-stage solution strategy. The reader is referred to works (Ahmetović and Grossmann 2010, 2011) for more details about the MINLP model and those strategies. For solving of case studies in this chapter, MINLPs were solved directly with BARON, and global optimal solutions of all case studies were found within the specified optimality tolerance (1%) and reasonable computational times. It is worth pointing out that the special redundant constraint for the overall contaminant mass balance (Karuppiah and Grossmann 2006) and good variable bounds were incorporated within the model, and this had a very big impact in improving the strength of the lower bound for the global optimum, as well as reducing the CPU time for BARON.

17.6. Case study

The case study considered in this section represents a large-scale example involving five process water–using units, three treatment units and three contaminants (A, B and C). The contaminants concentrations within the wastewater stream discharged into the environment are limited to 10 ppm. Data for the process units (flowrates, discharge load/contaminant mass load and maximum inlet concentrations of contaminants) were taken from the literature (Karuppiah and Grossmann 2006) and are given in Table 17.1. Table 17.2 shows data for the process units modified to address a case with variable flowrate through water-using units. Table 17.3 shows data for wastewater treatment units (percentage removal of contaminants, operating and investment cost coefficients, cost function exponent). Data for piping and water pumping costs were taken from the literature (Karuppiah and Grossmann 2008). The several cases are presented in this section for the same case study addressing the issues of a conventional water network, centralized and distributed wastewater treatment systems, water reuse and recycling, sequential and simultaneous synthesis of process water and wastewater treatment networks, fixed and variable flowrates through process water-using units. For all cases optimality tolerances were set to be 0.01, and MINLPs of all cases were directly solved by BARON.

Table 17.1. Data for process units (fixed flowrate problem) (Karuppiah and Grossmann 2006).

Process unit	Flowrate (t/h)	Discharge load (kg/h)			Maximum inlet concentration (ppm)		
		A	B	C	A	B	C
PU_1	40	1	1.5	1	0	0	0
PU_2	50	1	1	1	50	50	50
PU_3	60	1	1	1	50	50	50
PU_4	70	2	2	2	50	50	50
PU_5	80	1	1	0	25	25	25

Table 17.2. Data for process units (variable flowrates through the process units) (Ahmetović and Grossmann 2011).

Process unit	Discharge load (kg/h)			Maximum inlet concentration (ppm)			Maximum outlet concentration (ppm)			Limiting water flowrate (t/h)
	A	B	C	A	B	C	A	B	C	
PU_1	1	1.5	1	0	0	0	25	37.5	25	40
PU_2	1	1	1	50	50	50	70	70	70	50
PU_3	1	1	1	50	50	50	66.67	66.67	66.67	60
PU_4	2	2	2	50	50	50	78.57	78.57	78.57	70
PU_5	1	1	0	25	25	25	37.5	37.5	25	80

Table 17.3. Data for treatment units (Karuppiah and Grossmann 2006).

Treatment units	% removal of contaminant			Investment cost coefficient	Operating cost coefficient	Cost function exponent
	A	B	C			
TU_1	95	0	0	16,800	1	0.7
TU_2	0	0	95	9,500	0.04	0.7
TU_3	0	95	0	12,600	0.0067	0.7

Firstly, a conventional water network without water reuse and with centralised wastewater treatment was considered as a base case 1 (BC_1). In this case, the freshwater is used in all process units (see Figure 17.5). The freshwater consumption for this case is 300 t/h and the concentrations of contaminants (A, B and C) within the mixed wastewater stream are 20, 21.67

and 16.67 ppm. The total annual cost (TAC) of the network including freshwater, water pumping and piping cost is 2,429,964.5$/y (see BC_1 in Table 17.4). The concentrations of the contaminants in the wastewater stream exceed the limiting concentrations of 10 ppm. In order to satisfy this constraint, in the next base case 2 (BC_2), the wastewater stream is firstly treated within the centralised wastewater treatment system with the same wastewater flowrate going through all treatment units subsequently (see Figure 17.5).

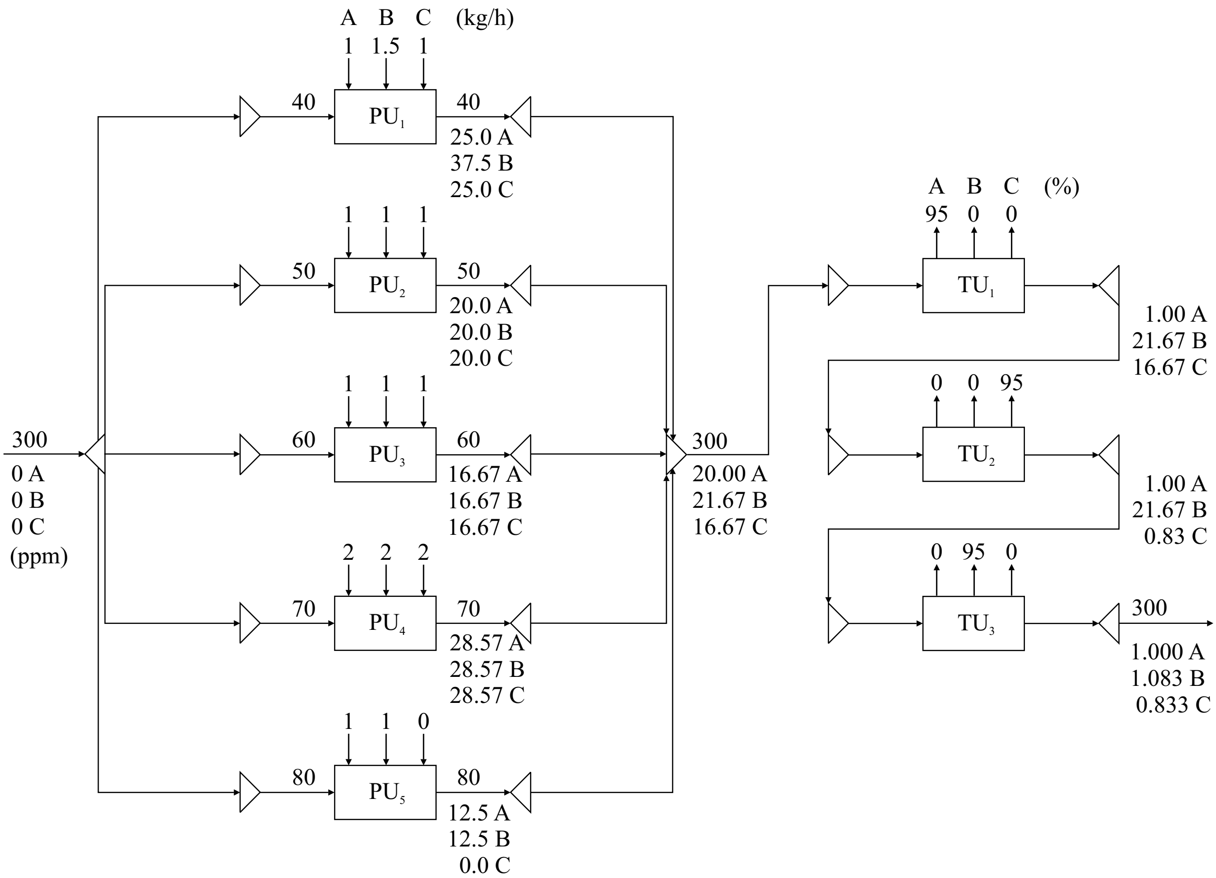

Figure 17.5. Base case of process water-using and wastewater treatment network (cases BC_1+BC_2)

The centralised wastewater treatment system is characterised with very high operating and investment cost of treatment units (see BC_2 in Table 17.4) due to maximum wastewater flowrate through all tree treatment units. The TAC of the centralised wastewater treatment for the BC_2 is

2,781,739.0 \$/y. As can be seen from Figure 17.5, the network solutions of the base cases BC_1, and BC_2 were merged representing an overall network (BC_1+BC_2) (Figure 17.5). The TAC of the merged base case networks shown in Figure 17.5 is 5,211,703.5 \$/y.

Table 17.4. Base case results of conventional networks.

	Base case networks		
	BC_1	BC_2	BC_1+BC_2
FW (t/h)	300	0.0	300
$Cost_{FW}$ (\$/y)	2,400,000.0	0.0	2,400,000.0
IC_{TU} (\$/y)	0.0	210,831.0	210,831.0
OC_{TU} (\$/y)	0.0	2,512,080.0	2,512,080.0
IC_{Pipes} (\$/y)	1,164.5	1,228.0	2,392.5
$OC_{Pumping}$ (\$/y)	28,800.0	57,600.0	86,400.0
TAC (\$/y)	2,429,964.5	2,781,739.0	5,211,703.5
CPU (s)	0.1	0.1	0.2

BC_1–Base case process water network, which uses freshwater in all process units; BC_2–Base case centralized wastewater treatment network.

In the previous base case (BC_1), water reuse options were not considered within network and consequently network required the maximum amount of freshwater (300 t/h). In order to consider water reuse options, on the basis of the general superstructure (Figure 17.3), the superstructure is constructed for 5 process units (Figure 17.6). This superstructure includes all possible connections between a freshwater source splitter, process units, and a final wastewater mixer. The objective in this case (C_1) is to find the optimal network design by minimising TAC of the network. From the initial data (Table 17.1) regarding the maximum inlet concentrations of contaminants (0 ppm for A, B, and C) within the water stream directed to the process unit 1 (PU_1) note that water reuse options from all process units to PU_1 are infeasible because the PU_1 requires only clean freshwater without contaminants (0 ppm). Accordingly, these connections can be removed from the superstructure and a simplified network can be obtained (5 connections can be removed). The optimal network design obtained by using the MINLP model (Ahmetović and Grossmann 2011) is given in Figure 17.7. The network design (case C_1) exhibits the minimum freshwater consumption of 84.286 t/h. The freshwater consumption was reduced by approximately 71.9 % (84.286 vs. 300 t/h) compared to the base case BC_1. Note that investment cost for piping (see solution C_1 in Table 17.5) are also significantly reduced compared to the base case design even though the base case design exhibits lower number of connections. The reason for this is that piping costs are directly proportional to the water flowrate which is at the maximum through all connections in the base case. The TAC of the network comparing BC_1 and C_1 designs is reduced from 2,429,964.5 $/y to 693,655.5 $/y.

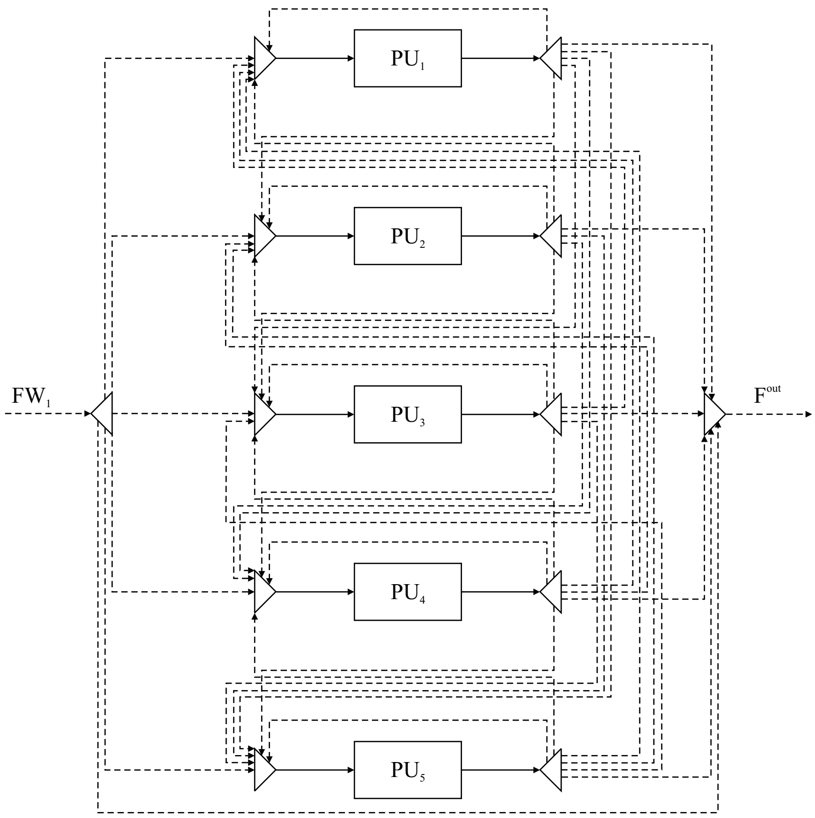

Figure 17.6. Superstructure of process water network (case C_1).

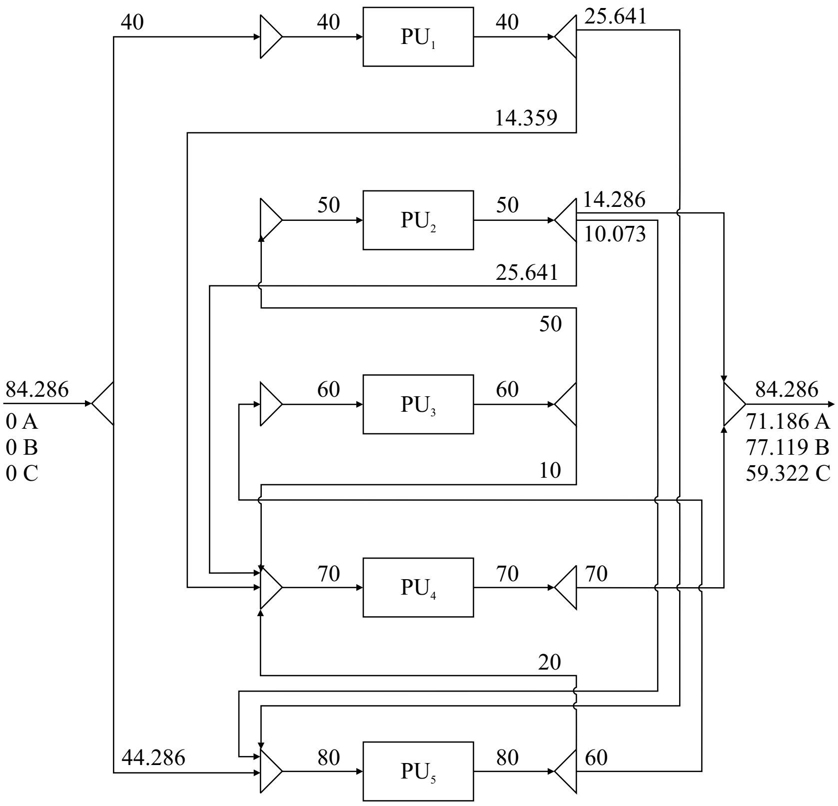

Figure 17.7. Optimal design of process water network (case C_1).

Two wastewater streams leaving process units PU_2 and PU_4 are collected and discharged as a single wastewater stream (84.286 t/h) and given contaminants concentrations as shown in Figure 17.7. As can be seen contaminants concentrations within the wastewater stream are above their maximum allowable concentrations of 10 ppm. Accordingly, the wastewater needs to be treated before it is discharged into the environment. Two cases were studied, first one (case C_2) when the wastewater stream was directed as a single stream to a wastewater treatment network and the second one (case C_{2a}) when two separate wastewater streams leaving process units PU_2 and PU_4 were directed to a wastewater treatment network. The superstructure representation of the wastewater treatment network for these two cases was given in Figure 17.8. The superstructures presented includes options of distributed wastewater treatment, where wastewater streams can be distributed amongst different treatment units in order to reduce wastewater treatment cost that depends on wastewater flowrate through the treatment units. The objective is to find the optimal wastewater treatment design by minimising the total annual cost. Figure 17.9 shows the optimal network designs obtained for two cases of single (Figure 17.9a) and two separate (Figure 17.9b) wastewater streams. As can be seen, wastewater streams were distributed within three different treatment units compared to base case design (BC_2), where a centralised wastewater treatment was used. The TACs of the wastewater treatment networks for cases C_2 and C_{2a} are 733,987.5 and 727,958.1 \$/y (see Table 17.5). An additional reduction in wastewater treatment cost for the case C_{2a} is possible due to existence of more options for distributive wastewater treatment caused by increased number of wastewater connections. Note that by not merging the wastewater streams enabled more than a half of the first wastewater stream is directed to the effluent, thereby reducing the loads of the treatment units. The wastewater treatment operating costs, for cases C_2 and C_{2a}, were 637,813.5 and 632,454.8 \$/y, respectively. The centralised wastewater system (BC_2), which treated wastewater stream generated within process units has a substantial increase in operating treatment cost (2,512,080.0 \$/y) compared to both cases of distributive wastewater treatments (C_2 and C_{2a}). The solutions presented for cases C_1 and C_2/C_{2a} are sequential solutions, where a process water network and a wastewater treatment network were synthesised separately and sequentially. This approach cannot produce the best solutions because all interactions were not considered between the process water network and the wastewater treatment network. Table 17.5 shows the operating, investment and total annual costs of the individual networks cases (cases C_1, C_2, C_{2a}) as well as merged individual networks (C_1+C_2 and C_1+C_{2a}) in order to produce overall network designs. Note that this approach could not produce best solutions because only one-way interactions were considered – those from the process water network to the wastewater treatment network. Nevertheless, the TACs of both total network designs (C_1+C_2 and C_1+C_{2a}) were decreased almost to one quarter when compared to the one of the conventional network (BC_1+BC_2).

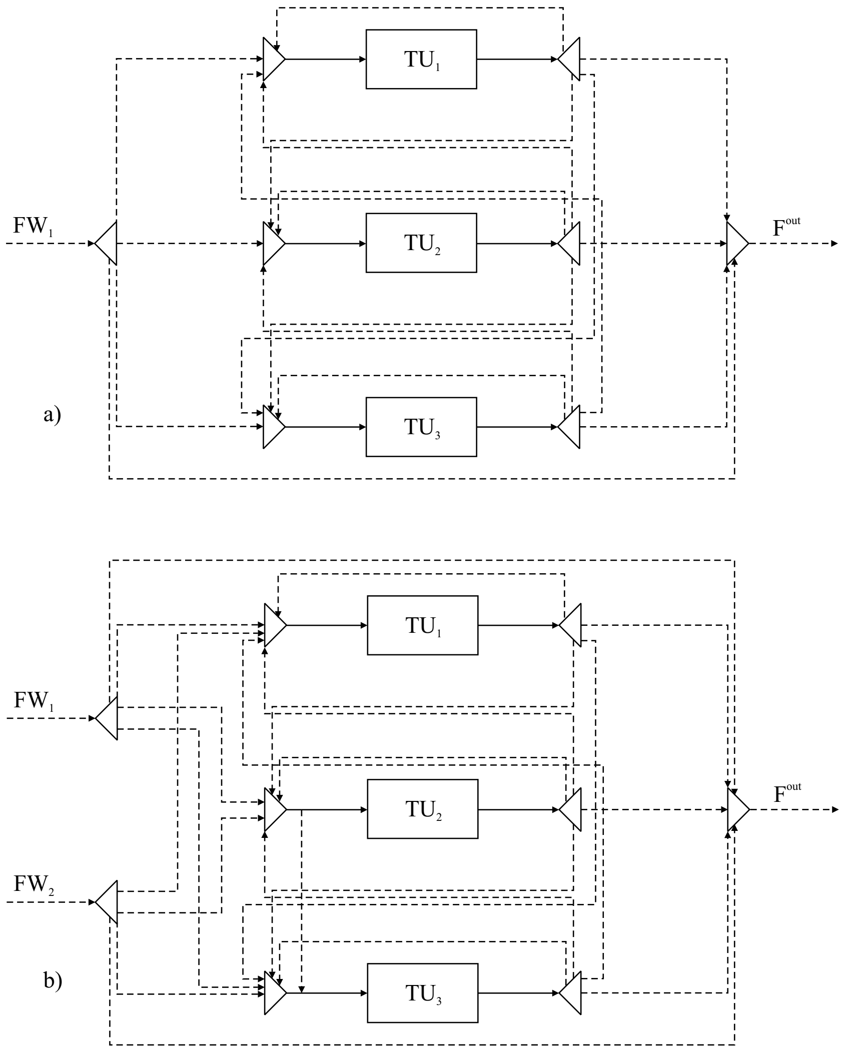

Figure 17.8. Superstructures of wastewater treatment networks a) C_2 and b) C_{2a}.

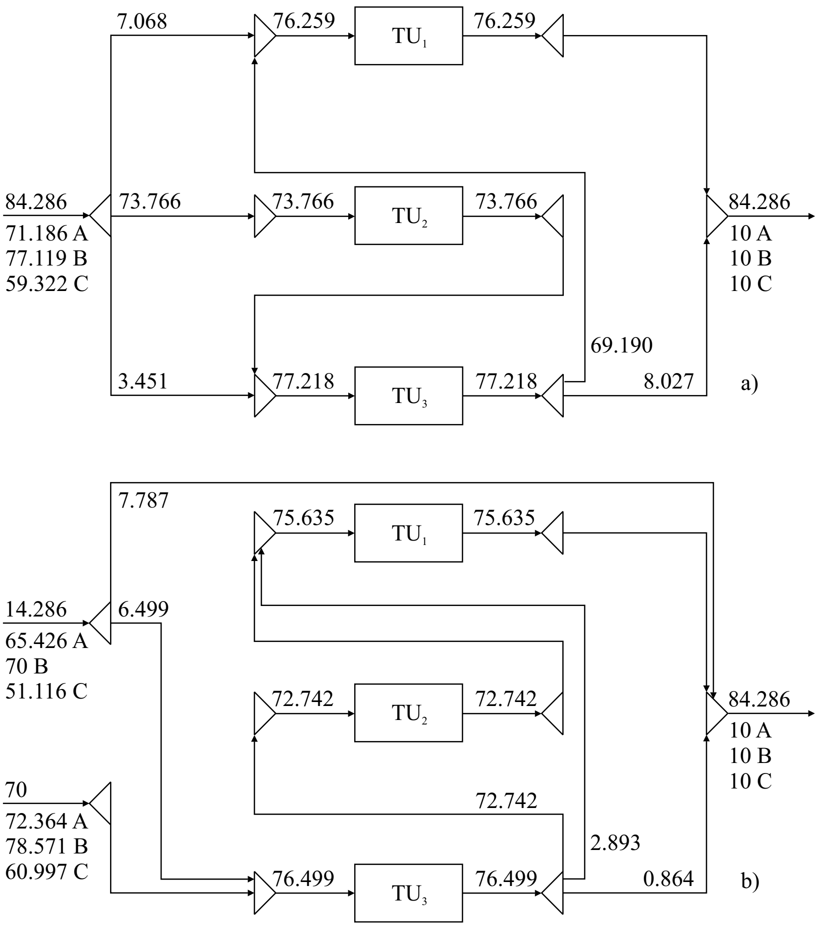

Figure 17.9. Optimal designs of wastewater treatment networks a) C_2 and b) C_{2a}.

Table 17.5. Sequential solution results of integrated water network.

	Sequential solution 1			Sequential solution 2	
	C_1	C_2	C_1+C_2	C_{2a}	C_1+C_{2a}
FW (t/h)	84.286	0	84.286	0	84.286
$Cost_{FW}$ (\$/y)	674,285.7	0.0	674,285.7	0.0	674,285.7
IC_{TU} (\$/y)	0.0	80,602.3	80,602.3	80,041.9	80,041.9
OC_{TU} (\$/y)	0.0	637,813.5	637,813.5	632,454.8	632,454.8
IC_{Pipes} (\$/y)	924.0	618.3	1,542.4	621.8	1,545.8
$OC_{Pumping}$ (\$/y)	18,445.7	14,953.4	33,399.1	14,839.7	33,285.4
TAC (\$/y)	693,655.5	733,987.5	1,427,642.9	727,958.1	1,421,613.6
CPU (s)	0.28	0.12	0.40	0.16	0.44

C_1–optimal solution of water–reuse network; C_2–optimal solution of wastewater treatment network (wastewater streams from process water units are mixed and directed to wastewater treatment network.

C_{2a}–optimal solution of wastewater treatment network (wastewater streams from process water units are distributed to wastewater treatment network.

In the next case (C_3), the superstructure of integrated water and wastewater treatment networks (Figure 17.10) was constructed in order to explore all interactions between the two different networks. Additional interactions, those directed from the wastewater treatment network to the process water network, enable additional options of wastewater reuse and recycling within the process and, hence, possible reductions in freshwater consumption and the total annualized cost of the network. Similarly, as explained earlier in this chapter, due to the specified contaminants concentrations (0 ppm A, B, and C) within the inlet water stream to PU_1, all connections from all process units (PU_1-PU_5) and all treatment units (TU_1-TU_3) to PU_1 can be excluded from the superstructure because they are infeasible in this case study. Accordingly, the superstructure given in Figure 17.10 can be simplified by 8 connections.

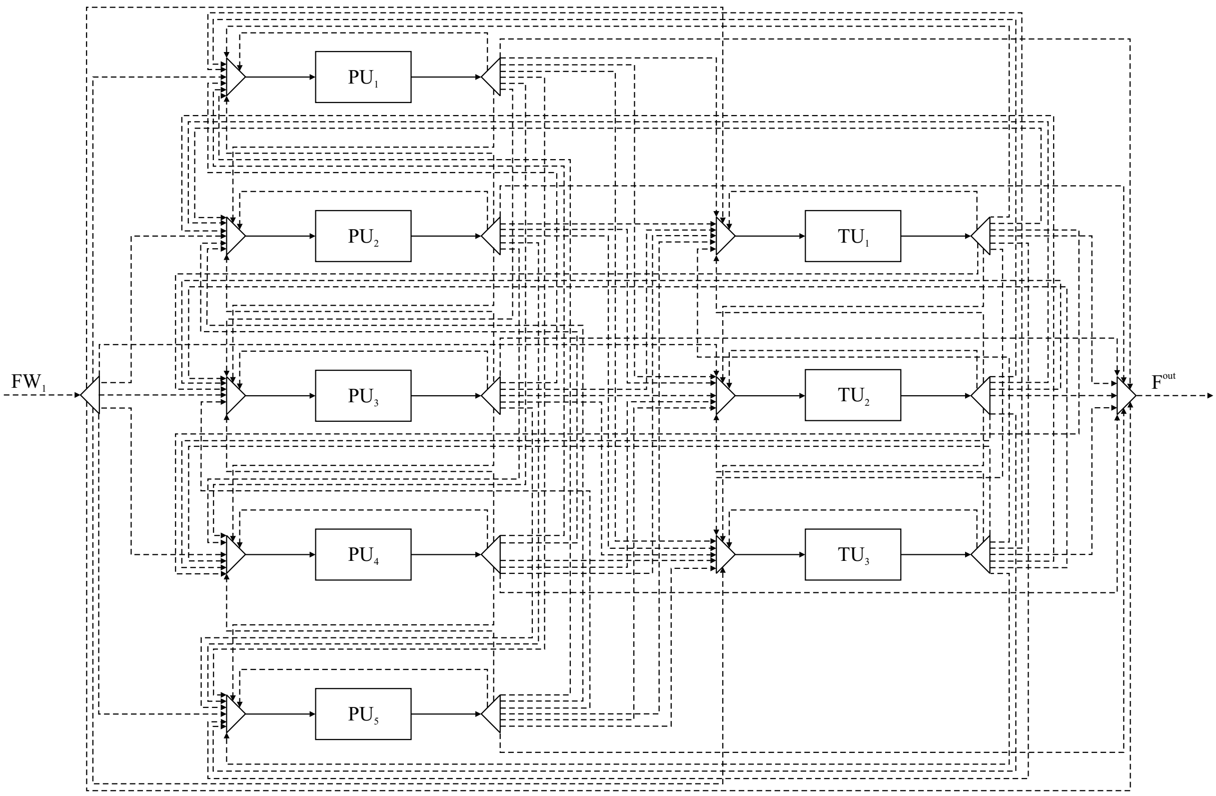

Figure 17.10. Superstructure of integrated process water and wastewater treatment networks (case C_3).

The optimal network design (Figure 17.11) exhibits the minimum freshwater consumption of 40 t/h, which is reduced by 52.5 % when compared to the solution obtained with the sequential approach. An additional reduction of freshwater consumption is enabled by the existence of treatment units in which the contaminants were removed from the wastewater streams increasing the potential for water reuse.

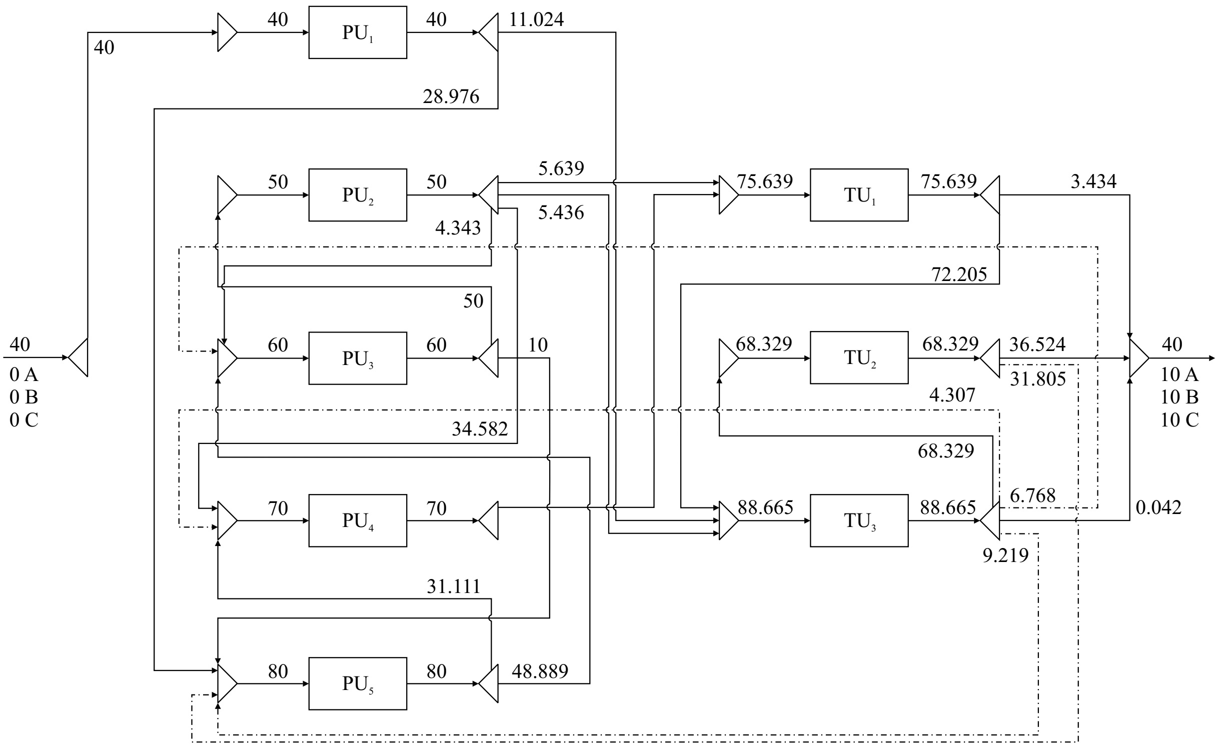

Figure 17.11. Optimal solution of integrated process water and wastewater treatment networks for fixed flowrates through water-using units (case C_3).

The dotted lines in Figure 17.11 represent regenerated wastewater streams reused in the process units. The freshwater consumption of 40 t/h is the theoretically minimum consumption determined by the existence of process unit PU_1 requiring only freshwater without contaminants (see Table 17.1). The optimal network design obtained by the simultaneous optimisation approach using the integrated superstructure exhibits lower operating cost as well as investment cost in treatment units and piping installation (see solution C_3 in Figure 17.11 and Table 17.6). The TAC is reduced by approximately by 25 % when compared to the sequential solution

(1,062,675.6 vs. 1,427,642.9 \$/y). This clearly shows that the simultaneous approach integrating process water network with wastewater treatment networks is the best approach to synthesising water networks. Note that wastewater stream (0.042 t/h), leaving wastewater treatment unit TU_3 and directed to the final wastewater mixer, is too small and could be impractical. Accordingly, the same model (C_3) was solved again when wastewater stream of 0.042 t/h was fixed to zero. As can be seen from Table 17.6 in this case (C_4) an insignificantly increase in TAC (1,062,709.2 vs. 1,062,675.6 \$/y) was obtained by excluding the impractical flowrate. In addition, the integrated model of a process water network and a wastewater treatment network was solved for the case of variable flowrates through the process units (fixed mass load problem). Figure 17.12 shows the optimal network design.

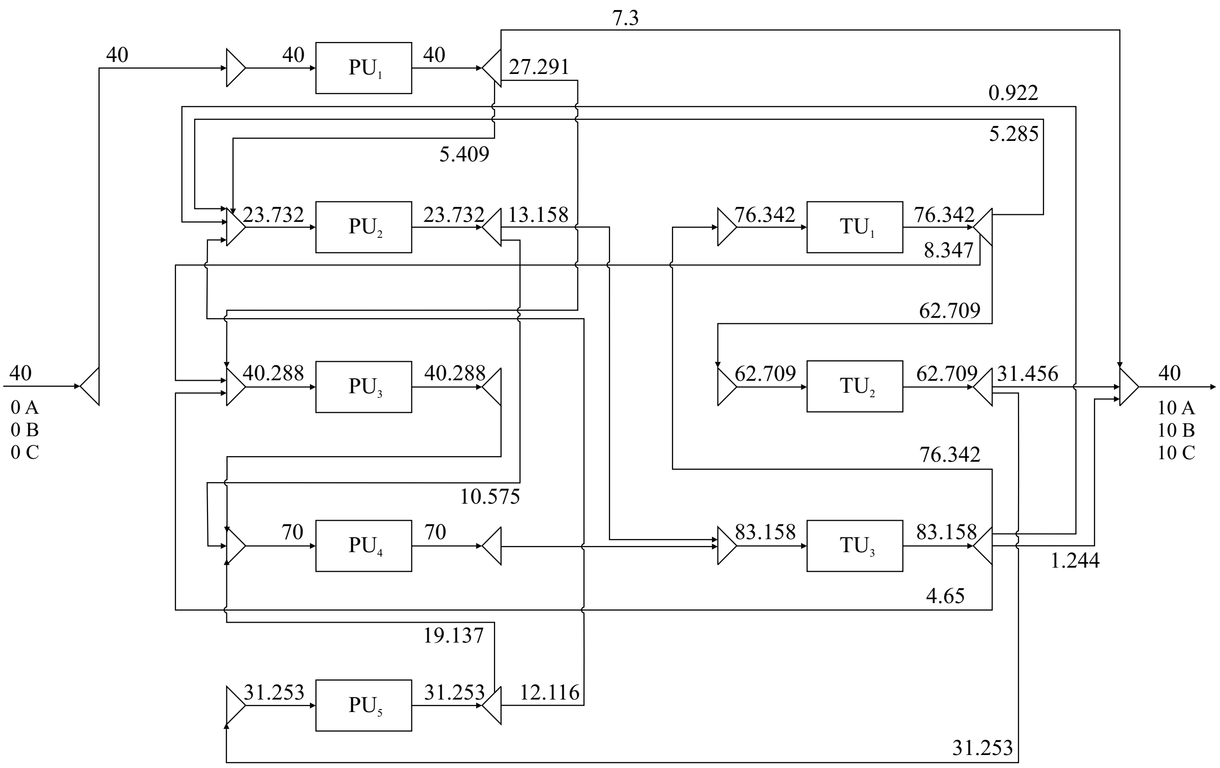

Figure 17.12. Optimal solution of integrated process water and wastewater treatment networks for variable flowrates through water-using units (case C_5).

As can be seen, water flowrates through the process units PU_2, PU_3 and PU_5 were significantly reduced when compared to the case of the fixed flowrates (see Figure 17.11 and Figure 17.12). However, this did not affect the minimum freshwater consumption of 40 t/h. On the other side, treatment units' operating and investment costs as well as pumping and piping costs were reduced due to decreased water flowrates within the network (see comparison between cases C_3 and C_5 in Table 17.6). The TAC was reduced only by about 0.4 % in this case. In the previous case studies considered, local recycles around process and treatment units were not allowed. Figure 17.13 shows the optimal network design for the integrated water network (variable flowrates through process units) when local recycles were allowed (case C_6) within the superstructure. However, local recycle options were not selected by optimisation and most of the network connections were the same as in the previous case (C_5).

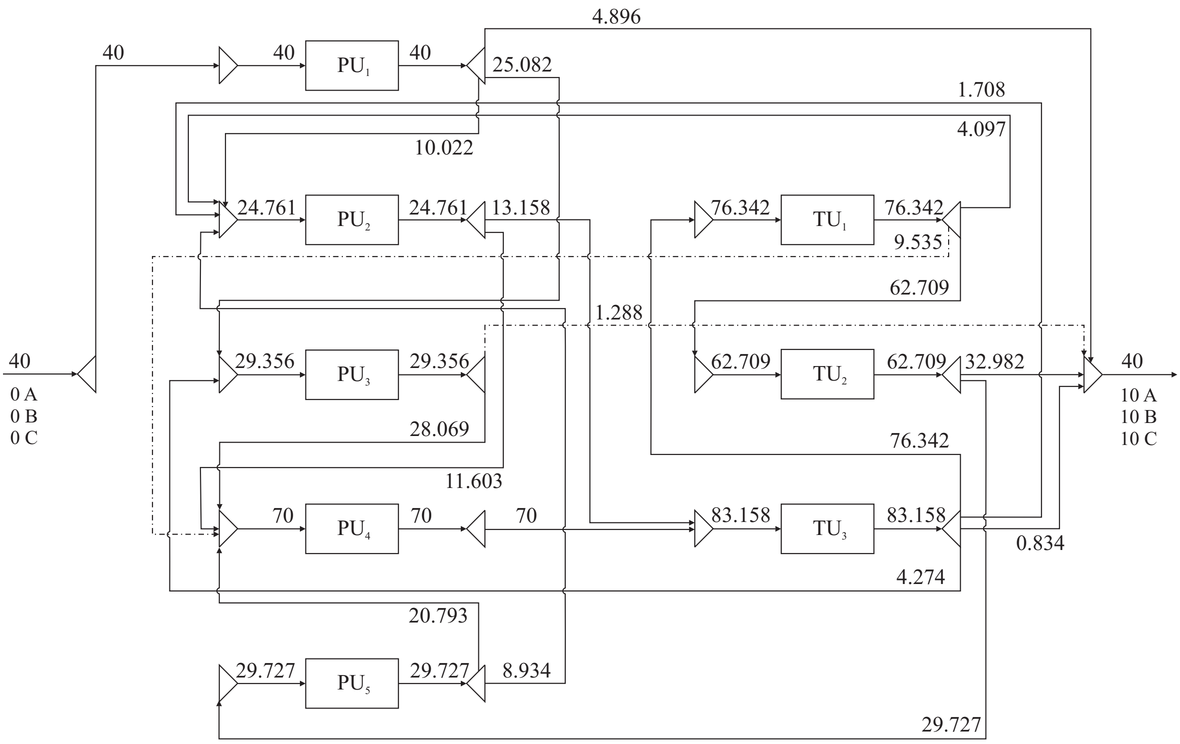

Figure 17.13. Optimal solution of integrated process water and wastewater treatment networks for variable flowrates through water-using units (local recycle allowed but not selected) (case C_6).

The dotted lines in Figure 17.13 represent connections not existing within the network design given in Figure 17.12. The TAC of the network for the case C_6 is only very slightly reduced compared to network design C_5 (1,058,273.8 vs. 1,058,828.8 \$/y). Note that both solutions are within the selected optimality tolerance of 1% when solving the model by using global optimisation solver BARON. As can be seen from Table 17.6, all simultaneous solutions were obtained within reasonable computational times.

Table 17.6. Simultaneous solutions of integrated process water and wastewater treatment network.

	Simultaneous solutions			
	C_3	C_4	C_5	C_6
FW (t/h)	40	40	40	40
$Cost_{FW}$ (\$/y)	320,000.0	320,000.0	320,000.0	320,000.0
IC_{TU} (\$/y)	82,080.5	82,088.4	79,963.0	79,963.0
OC_{TU} (\$/y)	631,730.4	631,743.9	635,257.6	635,257.6
IC_{Pipes} (\$/y)	1,378.3	1,388.4	1,169.0	1,162.6
$OC_{Pumping}$ (\$/y)	27,486.4	27,488.4	22,439.2	21,890.5
TAC (\$/y)	1,062,675.6	1,062,709.2	1,058,828.8	1,058,273.8
CPU (s)	38.5	41.1	75.5	39.0

C_3, C_4–optimal network solutions with fixed flowrates through process units; C_5, C_6–optimal network solutions with variable flowrates through process units;

Table 17.7 shows the summarized results of the various presented cases for the fixed flowrate problem. Those results clearly show significant savings in freshwater consumption (FW) and total annual cost (TAC) obtained by the simultaneous optimisation of the integrated network.

Table 17.7. The summarized results of freshwater consumption and total annual cost.

	No optimization (BC_1+BC_2)	Sequential optimization (C_1+C_{2a})	Simultaneous optimization (C_3)
FW (t/h)	300	84.286	40
TAC (\$/y)	5,211,703.5	1,421,613.6	1,062,675.6

17.7. Conclusions

This chapter has presented water optimisation in process industries as a challenging problem that should be addressed to achieve sustainable solutions with the minimum freshwater consumption and wastewater generation. It has been shown that using systematic methods and considering water integration opportunities (water reuse, regeneration reuse and regeneration recycling) a significant reduction in freshwater consumption and wastewater generation can be achieved. Different cases of a large-scale example involving total water network and multiple contaminants have been solved in order to present the development of increasingly better network solutions obtained by applying sequential and simultaneous strategies, as well as solutions of a fixed flowrate and a fixed mass load problem. The results showed that by using the simultaneous approach more than 50 % of saving in water usage and wastewater generation can be obtained when compared to the design obtained by the sequential approach, and more than 86 % when compared to the conventional network design. The obtained results in all cases correspond to global optimal solutions. The applied model is general, data independent and can be used for solving different water network problems to global optimality.

17.8. Acknowledgments

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17.9. Nomenclature

Abbreviations

BARON	Branch and Reduce Optimisation Navigator
CPU	central processing unit time
FW	freshwater
GAMS	General Algebraic Modeling System
IC_{Pipes}	investment cost for piping
IC_{TU}	investment cost for treatment units
LP	linear program
MEN	mass exchange network
MILP	mixed-integer linear program
MINLP	mixed integer nonlinear program
NLP	nonlinear program
OC_{TU}	operating cost for treatment units
$OC_{Pumping}$	pumping operating cost
PU	process unit
TU	treatment unit
TAC	total annual cost

Sets and Indices

j	contaminant
DU	set of demand units
d	demand unit
PU	set of process units

p	process unit
SU	set of source units
r	source unit
SW	set of freshwater sources
s	freshwater source
TU	set of treatment units
t	treatment unit

Parameters

FDU_d^{in}	mass flowrate of inlet water stream in demand unit d
FPU_p^{in}	mass flowrate of inlet water stream in process unit p
FSU_r^{out}	mass flowrate of outlet water stream from source unit r
$LPU_{p,j}$	mass load of contaminant j in process unit p
$RR_{t,j}$	percentage removal of contaminant j in treatment unit t
$x_j^{out,\max}$	maximum concentration of contaminant j in discharge stream to the environment
$xDU_{d.j}^{in,\max}$	maximum concentration of contaminant j in inlet stream into demand unit d
$xPU_{p.j}^{in,\max}$	maximum concentration of contaminant j in inlet stream into process unit p
$xSU_{r.j}^{out}$	concentration of contaminant j in outlet stream from source unit r
$xW_{s.j}^{in}$	concentration of contaminant j in freshwater source s

Continuous variables

F^{out}	mass flowrate of outlet wastewater stream from final mixer
$FID_{s,d}$	mass flowrate of water stream from freshwater source s to demand unit d

FIF_s mass flowrate of water stream from freshwater source *s* to final mixer

$FIP_{s,p}$ mass flowrate of water stream from freshwater source *s* to process unit *p*

$FIT_{s,t}$ mass flowrate of water stream from freshwater source *s* to treatment unit *t*

$FP_{p',p}$ mass flowrate of water stream from other process unit *p'* to process unit *p*

$FPD_{p,d}$ mass flowrate of water stream from process unit *p* to demand unit *d*

FPO_p mass flowrate of water stream from process unit *p* to final mixer

$FPT_{p,t}$ mass flowrate of water stream from process unit *p* to treatment unit *t*

FPU_p^{out} mass flowrate of outlet water stream from process unit *p*

$FSD_{r,d}$ mass flowrate of water stream from source unit *r* to demand unit *d*

FSO_r mass flowrate of water stream from source unit *r* to final mixer

$FSP_{r,p}$ mass flowrate of water stream from source unit *r* to process unit *p*

$FST_{r,t}$ mass flowrate of water stream from source unit *r* to treatment unit *t*

$FT_{t',t}$ mass flowrate of water stream from other treatment unit *t'* to treatment unit *t*

$FTD_{t,d}$ mass flowrate of water stream from treatment unit *t* to demand unit *d*

FTO_t mass flowrate of water stream from treatment unit *t* to final mixer

$FTP_{t,p}$ mass flowrate of water stream from treatment unit *t* to process unit *p*

FTU_t^{in} mass flowrate of inlet water stream in treatment unit *t*

FTU_t^{out} mass flowrate of outlet water stream from treatment unit *t*

FW_s mass flowrate of water for freshwater source *s*

x_j^{out} concentration of contaminant *j* in discharge stream to the environment

$xDU_{d,j}^{in}$	concentration of contaminant *j* in inlet stream into demand unit *d*
$xPU_{p,j}^{in}$	concentration of contaminant *j* in inlet stream into process unit *p*
$xPU_{p,j}^{out}$	concentration of contaminant *j* in outlet stream from process unit *p*
$xSPU_{t,j}^{out}$	concentration of contaminant *j* in outlet stream from splitter process unit *p*
$xSTU_{t,j}^{out}$	concentration of contaminant *j* in outlet stream from splitter treatment unit *t*
$xTU_{t,j}^{in}$	concentration of contaminant *j* in inlet stream into treatment unit *t*
$xTU_{t,j}^{out}$	concentration of contaminant *j* in outlet stream from treatment unit *t*

Subscripts/superscripts

in	inlet stream
out	outlet stream

17.10. References

Ahmetović, Elvis, and Ignacio E. Grossmann. 2010. "Strategies for the Global Optimization of Integrated Process Water Networks." In *Computer Aided Chemical Engineering*, edited by S. Pierucci and G. Buzzi Ferraris, 901-906. Elsevier.

Ahmetović, Elvis, and Ignacio E. Grossmann. 2011. "Global superstructure optimization for the design of integrated process water networks." *AIChE Journal* 57 (2):434-457. doi: http://dx.doi.org/10.1002/aic.12276.

Ahmetović, Elvis, Nidret Ibrić, and Zdravko Kravanja. 2014. "Optimal design for heat-integrated water-using and wastewater treatment networks." *Applied Energy* 135:791-808. doi: http://dx.doi.org/10.1016/j.apenergy.2014.04.063.

Ahmetović, Elvis, Nidret Ibrić, Zdravko Kravanja, and Ignacio E. Grossmann. 2015. "Water and energy integration: A comprehensive literature review of non-isothermal water network synthesis." *Computers & Chemical Engineering* 82:144-171. doi: 10.1016/j.compchemeng.2015.06.011.

Allegra, K., P. E. da Silva, and P. E Al Goodman. 2014. "Reduce water consumption through recycling." *Chemical Engineering Progress* 110 (4):29-35.

Bagajewicz, Miguel. 2000. "A review of recent design procedures for water networks in refineries and process plants." *Computers & Chemical Engineering* 24 (9-10):2093-2113. doi: 10.1016/s0098-1354(00)00579-2.

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg. 1997. *Systematic methods of chemical process design*. New Jersey: Prentice-Hall.

Castro, PedroM, JoãoP Teles, and AugustoQ Novais. 2009. "Linear program-based algorithm for the optimal design of wastewater treatment systems." *Clean Technologies and Environmental Policy* 11 (1):83-93. doi: 10.1007/s10098-008-0172-5.

Davé, B. 2004. "Water and Sustainable Development: Opportunities for the Chemical Sciences: A Workshop Report to the Chemical Sciences Roundtable. Washington (DC): National Academies Press (US). 2004. www.ncbi.nlm.nih.gov/books/NBK83724/. Accessed 29.08.2013.".

Doyle, S. J., and R. Smith. 1997. "Targeting Water Reuse with Multiple Contaminants." *Process Safety and Environmental Protection* 75 (3):181-189. doi: 10.1205/095758297529020.

El-Halwagi, Mahmoud M. . 2012. *Sustainable Design Through Process Integration, Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement*. Amsterdam, The Netherlands: Butterworth-Heinemann/Elsevier.

El-Halwagi, Mahmoud M., and Vasilios Manousiouthakis. 1989. "Synthesis of mass exchange networks." *AIChE Journal* 35 (8):1233-1244. doi: 10.1002/aic.690350802.

Faria, Débora C., and Miguel J. Bagajewicz. 2011. "Global Optimization of Water Management Problems Using Linear Relaxation and Bound Contraction Methods." *Industrial & Engineering Chemistry Research* 50 (7):3738-3753. doi: 10.1021/ie101206c.

Foo, D. C. Y. 2009. "State-of-the-Art Review of Pinch Analysis Techniques for Water Network

Synthesis." *Industrial & Engineering Chemistry Research* 48 (11):5125-5159. doi: 10.1021/ie801264c.

Foo, D. C. Y. 2013. *Process Integration for Resource Conservation*. Boca Raton, Florida, USA: CRC Press.

Galan, B., and I. E. Grossmann. 1998. "Optimal Design of Distributed Wastewater Treatment Networks." *Industrial & Engineering Chemistry Research* 37 (10):4036-4048. doi: 10.1021/ie980133h.

Grossmann, Ignacio E., Mariano Martín, and Linlin Yang. 2014. "Review of optimization models for integrated process water networks and their application to biofuel processes." *Current Opinion in Chemical Engineering* 5 (0):101-109. doi: http://dx.doi.org/10.1016/j.coche.2014.07.003.

Gunaratnam, M., A. Alva-Argáez, A. Kokossis, J. K. Kim, and R. Smith. 2005. "Automated Design of Total Water Systems." *Industrial & Engineering Chemistry Research* 44 (3):588-599. doi: 10.1021/ie040092r.

Huang, C. H., C. T. Chang, H. C. Ling, and C. C. Chang. 1999. "A mathematical programming model for water usage and treatment network design." *Industrial and Engineering Chemistry Research* 38 (7):2666-2679.

Jeżowski, Jacek. 2010. "Review of Water Network Design Methods with Literature Annotations." *Industrial & Engineering Chemistry Research* 49 (10):4475-4516. doi: 10.1021/ie901632w.

Karuppiah, Ramkumar, and Ignacio E. Grossmann. 2006. "Global optimization for the synthesis of integrated water systems in chemical processes." *Computers & Chemical Engineering* 30 (4):650-673. doi: 10.1016/j.compchemeng.2005.11.005.

Karuppiah, Ramkumar, and Ignacio E. Grossmann. 2008. "Global optimization of multiscenario mixed integer nonlinear programming models arising in the synthesis of integrated water networks under uncertainty." *Computers & Chemical Engineering* 32 (1–2):145-160. doi: http://dx.doi.org/10.1016/j.compchemeng.2007.03.007.

Khor, Cheng Seong, Benoit Chachuat, and Nilay Shah. 2014. "Optimization of Water Network Synthesis for Single-Site and Continuous Processes: Milestones, Challenges, and Future Directions."

Industrial & Engineering Chemistry Research 53 (25):10257-10275. doi: 10.1021/ie4039482.

Klemeš, J. J., ed. 2013. *Handbook of Process Integration (PI): Minimisation of energy and water use, waste and emissions*. Cambridge: Woodhead Publishing Limited.

Klemeš, Jiří , Ferenc Friedler, Igor Bulatov, and Petar Varbanov. 2010. *Sustainability in the Process Industry: Integration and Optimization*. New York, USA: McGraw-Hill.

Klemeš, Jiří Jaromír. 2012. "Industrial water recycle/reuse." *Current Opinion in Chemical Engineering* 1 (3):238-245. doi: 10.1016/j.coche.2012.03.010.

Kuo, Wen-Chu Janice, and Robin Smith. 1997. "Effluent treatment system design." *Chemical Engineering Science* 52 (23):4273-4290. doi: http://dx.doi.org/10.1016/S0009-2509(97)00186-3.

Linnhoff, B., and E. Hindmarsh. 1983. "The pinch design method for heat exchanger networks." *Chemical Engineering Science* 38 (5):745-763. doi: http://dx.doi.org/10.1016/0009-2509(83)80185-7.

Mann, J.G. , and Y.A. Liu. 1999. *Industrial water reuse and wastewater minimization*. New York: McGraw Hill.

Pintarič, Z.N., N. Ibrić, E. Ahmetović, I.E. Grossmann, and Z. Kravanja. 2014. "Designing optimal water networks for the appropriate economic criteria." *Chemical Engineering Transactions* 39:1021-1026. doi: 10.3303/CET1439171.

Rosenthal, R.E. 2014. *GAMS - A User's Guide*. Washington, DC, USA: GAMS Development Corporation.

Smith, R. 2005. *Chemical process design and integration*. Chichester, England: John Wiley & Sons Ltd.

Takama, N., T. Kuriyama, K. Shiroko, and T. Umeda. 1980. "Optimal water allocation in a petroleum refinery." *Computers & Chemical Engineering* 4 (4):251-258. doi: http://dx.doi.org/10.1016/0098-1354(80)85005-8.

Tawarmalani, Mohit, and Nikolaos V. Sahinidis. 2005. "A polyhedral branch-and-cut approach to global optimization." *Mathematical Programming* 103 (2):225-249. doi: 10.1007/s10107-005-0581-8.

Wang, Y. P., and R. Smith. 1994a. "Design of distributed effluent treatment systems." *Chemical*

Engineering Science 49 (18):3127-3145. doi: http://dx.doi.org/10.1016/0009-2509(94)E0126-B.

Wang, Y. P., and R. Smith. 1994b. "Wastewater minimisation." *Chemical Engineering Science* 49 (7):981-1006. doi: http://dx.doi.org/10.1016/0009-2509(94)80006-5.

Wang, Y.P., and R. Smith. 1995. "Wastewater minimization with flowrate constraints." *Trans. IChemE* 73 (Part A):889–904.

Yang, Linlin, and Ignacio E. Grossmann. 2013. "Water Targeting Models for Simultaneous Flowsheet Optimization." *Industrial & Engineering Chemistry Research* 52 (9):3209-3224. doi: 10.1021/ie301112r.

Yang, Linlin, Raquel Salcedo-Diaz, and Ignacio E. Grossmann. 2014. "Water Network Optimization with Wastewater Regeneration Models." *Industrial & Engineering Chemistry Research* 53 (45):17680-17695. doi: 10.1021/ie500978h.

Yoo, ChangKyoo, TaeYoung Lee, Jiyong Kim, Il Moon, JaeHak Jung, Chonghun Han, Jong-Min Oh, and In-Beum Lee. 2007. "Integrated water resource management through water reuse network design for clean production technology: State of the art." *Korean Journal of Chemical Engineering* 24 (4):567-576. doi: 10.1007/s11814-007-0004-z.

Zamora, Juan M., and Ignacio E. Grossmann. 1998. "Continuous global optimization of structured process systems models." *Computers & Chemical Engineering* 22 (12):1749-1770. doi: http://dx.doi.org/10.1016/S0098-1354(98)00244-0.

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