UNIVERSITY OF OKLAHOMA

GRADUATE COLLEGE

OPTIMAL DESIGN OF WATER UTILIZATION SYSTEMS IN REFINERIES AND PROCESS PLANTS

A Dissertation

SUBMITTED TO THE GRADUATE FACULTY

in partial fulfillment of the requirements for the

degree of

Doctor of Philosophy

By

Mariano Javier Savelski

Norman, Oklahoma

1999

UMI Number: 9940294

OPTIMAL DESIGN OF WATER UTILIZATION SYSTEMS IN REFINERIES AND PROCESS PLANTS

A Dissertation APPROVED FOR THE
DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

BY

[illegible]

John Scamehorn

Lance Lobban

Lloyd L. Lee

[illegible]

ACKNOWLEDGMENTS

I gratefully acknowledge the Environmental Protection Agency of the United States of America for funding this project. I appreciate the companionship and support of Mabel Sanchez, Margiori Rivas, and Hernán Rodera.

I would like to thank all of the Chemical Engineering Faculty and Staff at the University of Oklahoma for their friendship and helpful advice. I would especially like to thank Dr. Jeffery Harwell and Dr. Lance Lobban for given me the opportunity to serve as instructor for the Chemical Engineering Department. I gratefully acknowledge Dr. Lloyd Lee, Dr. Lance Lobban, Dr. John Scamehorn, and Dr. Theodore Trafalis for their participation on my dissertation committee. It is with enormous gratitude and appreciation that I acknowledge Dr. Miguel Bagajewicz for the countless hours of work, guidance, advice, and laughter we have shared. I will be forever grateful.

Finally, I would like to thank my wife, Marcela; my daughter, Brenda; and my son, Julian. Thank you for your support, tolerance, encouragement, and love.

TABLE OF CONTENTS

ABSTRACT

The intensive use of water in refineries and process plants was the object of several studies starting in the early eighties. All these studies have aimed at the reduction of the water consumption as well as the allocation of wastewater to treatment units. Two major problems have been proposed and solved to various degrees of detail. On one hand, the fresh water allocation wastewater reuse problem has been addressed by various researchers. The first line of work started mostly as graphical and evolved lately towards mathematical programming. On the other hand, the problem of designing wastewater treatment units has been also studied using semi-empirical as well as mathematical programming. Some connections between the two problems have also been studied. This thesis focuses on the optimal solution of the single component water/wastewater allocation-planning problem. First, a robust methodology to obtain an optimal design is presented. The method uses a concentration grid water allocation procedure to obtain preliminary optimal structures. A merging procedure provides the final structures. In addition, the use of different water allocation strategies shows that the problem has several alternative solutions. Secondly, this work shows the existence of necessary conditions of optimum for single component for the aforementioned problem. Furthermore, it is shown that using these necessary conditions in combination with some sufficient conditions, the single component problem can be efficiently solved by hand through a simple and systematic algorithm. Moreover, it is also shown that using the necessary

conditions of optimality, the water allocation-planning problem can be reduced to one single LP for the single component case. The solutions are rigorous and global, even when compulsory and forbidden connections are imposed. Finally, the intricacies of the heat integration of these systems as well as different aspects of design and retrofit of these systems are explored.

CHAPTER 1

Background

1.1 Overview

The chemical and petrochemical industries make an intensive usage of water. The spent water contains several contaminants (phenols, sulfides, ammonia, benzene, oil, etc.) which cannot be discharged directly without creating an environmental pollution problem. Water cleanup has been the object of several retrofit programs in industry, and several legislation exist that regulate and establish goals for these efforts (e.g. Clean Water Act).

Wastewater has several contaminants that make it unsuitable for discharge. For example, the total organic carbon (TOC), the biochemical oxygen demand (BOD) and the chemical oxygen demands (COD) indicate the organic matter content. Oil and grease (O&G) and total petroleum hydrocarbons (TPH) give a measure of the presence of oil, grease and other hydrocarbons. The physical characteristics of the wastewater are also adjusted before disposal. These characteristics include the total suspended solids (TSS), pH, temperature, color, and odor.

For these reasons and in compliance with the EPA Clean Water Act of 1977, wastewater must be treated before discharge (that is, end of pipe treatment). Several treatment options are taken into account depending on the sludge characterization. In other words: wastewater treatment procedures are based on the type and concentration of its contaminants.

Treatment is divided in four levels: primary treatment involves physical treatment processes, secondary treatment comprises operations where soluble matter is removed, and tertiary and quaternary treatments "polish" the effluent even more. Regardless of the treatment level, the unit operations for wastewater treatment are classified as physical, chemical, thermal, and biological.

- *Physical Treatment Processes.* Separation is obtained by taking advantage and/or manipulating physical properties of the pollutants. These processes are: gravity separation, air flotation, oil coalescing, evaporation, filtration, activated carbon adsorption, air or stream stripping, liquid-liquid extraction, and reverse osmosis. Gravity separation is a primary treatment to remove suspended solids as well as oil and grease, whereas air flotation is a secondary treatment process to enhance the oil and grease removal not attained in the gravity separation process. Oil coalescence might be used as a primary or a secondary treatment process. Evaporation is used when the concentration of contaminants is very high. It also reduces the amount of disposed sludge. The other treatments range from the secondary to the quaternary wastewater treatment processes.
- *Chemical Treatment.* These operations involve chemical changes in the constituents to facilitate the removal of pollutants or to decompose them to innocuous compounds. Chemical treatment processes typically employed in industry are chemical precipitation and coagulation, electrolytic recovery and ion exchange. Precipitation and coagulation are primary or secondary treatment processes that remove metals or other settling materials. Electrolytic recovery, ion

exchange, reverse osmosis are employed for secondary, tertiary or even quaternary treatment of wastewater. Oxidation and reduction are secondary or tertiary processes that degrade or alter the contaminant based on its specific chemistry in order to reduce its toxicity.

- *Thermal Treatment Processes*. These processes employ elevated temperatures to decompose contaminants. Metallic species are decomposed to their elemental form as ash or pure gases, while organic species are decomposed to carbon dioxide, water and halides or halogen gases.
- *Biological Treatment.* These treatments employ biological or biochemical mechanisms to change the chemical properties of certain contaminants. In this way, the organic matter susceptible to biodegradation is stabilized so that no further biological degradation occurs downstream. This is done to protect the receiving stream both from depletion of oxygen or other critical nutrients, and from the build-up of waste products.

Several procedures have been proposed to design economical wastewater treatment. With a few exceptions, these procedures rely on the application of certain rules of thumb. The current installations usually merge several waste streams and use appropriate technologies to clean them before disposal. These are therefore, *end-of-pipe* wastewater cleanup solutions. Several papers discuss these options. Belhateche (1995) offers a complete discussion of these technologies.

To attack the problem at its roots, i.e. the generation of pollutants, process simulation was proposed as a tool to perform pollution balances on processes and calculates pollution indices (Sowa, 1994; Hilaly and Sikdar, 1996). One of the main results of this line of work is the WAR algorithm developed by the EPA Risk Reduction Engineering Laboratory. However, for many processes the reduction of the generation of many pollutants is not possible. The petroleum processing industry is such an example. The major pollutants in refinery wastewater are part of the crude and are not generated in the plant. Many other pollutants are by-products that are difficult to reduce.

Finally, starting in the eighties and increasingly in the nineties water re-use started to become popular as means of reducing the total amount of water intake. This, in turn, not only saves upstream treatment but also saves wastewater treatment. Industry and the EPA in the United States is now seriously considering and discussing the advantages and disadvantages of zero-liquid discharge solutions as the ultimate goal of green chemistry.

1.2 Roadmap for Improved Process Solutions

Until a few years ago, the problem of water treatment was considered as a set of sequential treatment operations of a single wastewater stream consisting of the wastewater from all unit operations (desalters. strippers, etc.). At the same time, without the concept of wastewater re-use, processes are fed by freshwater only. Such a system is depicted for three water user processes (P_i) and three treatment units (T_i) in Figure 1-1 (a). One way of obtaining improved designs is the reuse of wastewater from one process to feed another without sending it to treatment. This reduces the cost because the overall water intake is smaller (Figure 1-1 (b)). The next step is to introduce a series/parallel designs of the wastewater treatment unit avoiding at the same time the merging of all the wastewater streams into a single feed stream (Figure 1-1 (c)). Finally, treatment can be decentralized in such a way that some pollutants are removed from wastewater of selected processes allowing the reuse of these waters (Figure 1-1 (d)).

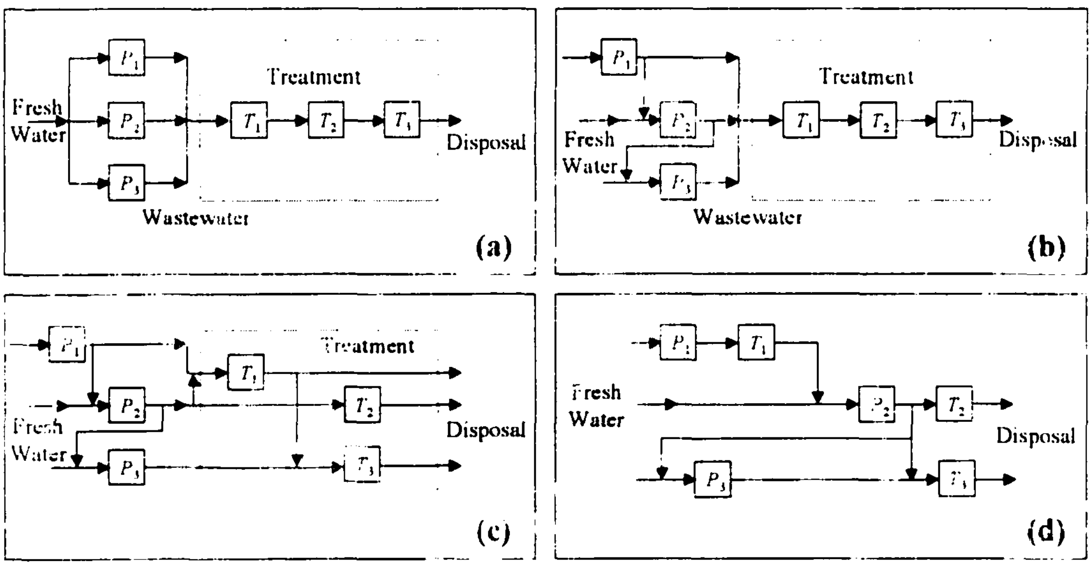


Figure 1-1
The water/wastewater allocation problem. **(a)** No wastewater reuse and centralized treatment with units in series. **(b)** Wastewater reuse and centralized treatment with units in series. **(c)** Wastewater reuse and centralized treatment. **(d)** Wastewater reuse and decentralized treatment.

The concept of zero discharge applies alternatively to the total elimination of the disposal of environmentally hazardous substances or to the concept of a closed circuit of water, such that water disposal is eliminated altogether, that is zero "liquid" discharge. Closed circuits are appealing because end-of-pipe regeneration does not have to be conducted to the full extent required for disposal as water can be reused with higher level of contaminants (Figure 1-2). Additionally, the absence of a discharge eliminates internal administrative costs associated with the enforcement of environmental protection agencies (EPA in the United States) and local limits as well as the interface with other government agencies.

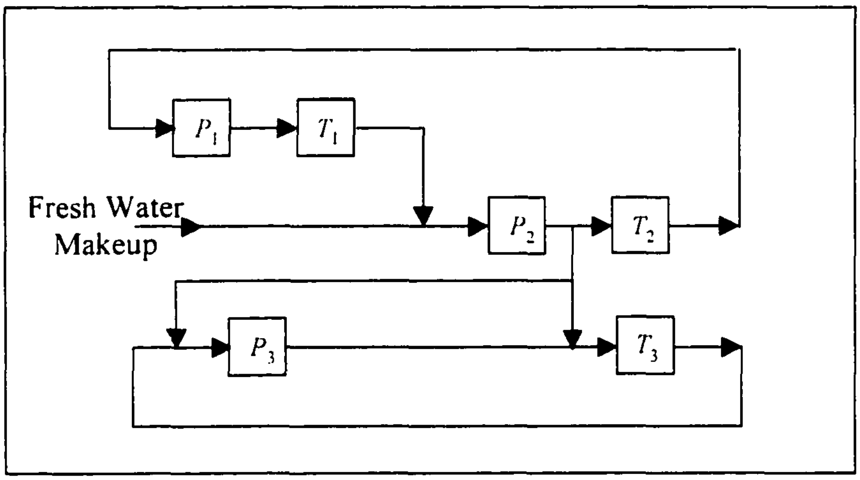


Figure 1-2
Wastewater reuse and/or treatment and recycle for a zero discharge cycle.

These zero discharge process solutions have never been attempted, neither in case studies, nor in practice. They constitute the burning challenge for both academia and practice. There are however, a few issues than can readily be pointed out. First, many units require steam, that is, pure fresh water of very good quality. Thus, in order for these zero discharge cycles to exists, wastewater cleanup should be thorough, something that could be too expensive to be realistic. Second, some water make-up and disposal should take place, as a cycle will tend to accumulate certain species not being removed normally.

The analysis made in this section suggests that in reality the problem one wishes to solve is the one depicted in Figure 1-2, which has all the previous alternatives embedded. Diepolder (1992) and Goldblatt *et al.* (1993) discussed how realistic is this concept from the practical point of view, addressing issues such as the disposal of solids, and the possible sizable revenues obtained for the selling of low grade salts and avoiding their disposal (close to a million dollar per year for a typical refinery), or the costs of disposal of groundwater solids, etc.

There have been traditionally two approaches used to obtain good designs of these systems:

- Conceptual Approach
- Mathematical Programming

It is interesting and ironic that the seminal paper of this area (Takama *et al.*, 1980) proposed a mathematical programming approach to design a structure similar to the one in Figure 1-1 (d). However, the conceptual approach that dominated the early work of the area focused mostly on structures like the one in Figure 1-1 (b) or 1-1 (c). It is only in the last few years that the conceptual design paradigm is showing limitations to address the complexity of the problem. Despite this limitation, the conceptual approach has provided a simplified description of the problem that has been of great value to build effective mathematical programming solutions. On the other hand, mathematical programming using superstructures also faces several limitations, as it cannot sometimes guarantee optimality, or simply generates mixed integer problems that are too difficult to solve. Recent work, some of it still unpublished, is proving that a synergistic combination of both approaches, that is, the use of conceptual insights to help formulating better tractable models for mathematical programming (good initial points, heuristics to help in branch an bound procedures, use of necessary conditions of optimality, etc.) is at this point in time the most effective alternative. With computer power doubling every year, with the expectation that this frequency of doubling will increase, and the amount of innovations in optimization methods being produced, it is not audacious to forecast that the mathematical programming part of the effort will increasingly dominate.

The process systems engineering community has not however addressed the problem of optimizing the structure of problem of Figure 1-1 (d) directly. It has instead focused in the solution of either the minimization of freshwater usage through re-use and proper allocation of wastewater, or the series/parallel clean-up structure. That is, it has partitioned the problem of Figure 1-1 (c) into two sub-problems. Despite some encouraging conceptual analysis of the interaction between these two parts, very little additional work has been performed lately. We now review the work performed in each of these sub-problems separately.

1.3 Optimal Water/Wastewater Allocation

The search for optimal wastewater reuse solutions was addressed by industry itself more than twenty years ago (Carnes *et al.*, 1973; Skylov and Stenzel, 1974;

Hospondarec and Thompson, 1974; Mishra *et al.*, 1975; Sane and Atkins, 1977). Takama *et al.* (1980) used mathematical programming to solve a refinery example. A superstructure of all water-using operations and cleanup processes was set up and an optimization was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. The authors made an important contribution by addressing the problem of water management as a combination of water/wastewater allocation among processes and wastewater distribution to cleanup units. *This can be considered as the seminal paper of all this area.*

After the paper by Takama *et al.* (1980), several papers followed addressing the problem as a single contaminant problem and later as a multi-contaminant or multicomponent problem. It was not until very recently when the issue of energy efficient utilization was researched.

1.3.1 Conceptual Design Procedures

Conceptual Design is a term coined in the eighties in which process insights are used to make decisions about a flowsheet. In general, the method proposes to start with some critical equipment (usually the reactor) of the flowsheet and continue building the flowsheet from the inside out going through the separation system and later through the heat recovery system. As applied to water/wastewater re-use systems the conceptual design approach was initiated by Prof. R. Smith from UMIST. In this approach, guidelines are given to obtain a good flowsheet. However, sometimes no algorithm is given to solve the problems, leaving the design to the hands of experienced professionals. Despite this limitation, this approach has produced significant advances in the solution of these problems, and has been instrumental in popularizing simplified solutions to the problem. In particular, a targeting procedure that allows the calculation of the minimum fresh water usage without the need to construct a network should be mentioned as the most important contribution. Several researchers, including Dr. Smith, have used these pioneering contributions to solve more realistic versions of the problem using mathematical programming. We describe some of these advances now.

1.3.1.1 Targeting for Fresh Water Usage

The targeting graphical method exploits the idea of plotting the cumulative exchanged mass vs. composition for a set of reach and lean streams, a concept first presented by El-Halwagi and Manousiouthakis (1989) for synthesizing Mass Exchanger Networks. Wang and Smith (1994a) proposed a methodology that can effectively pick optimal reuse solutions. Dhole *et al.* (1996) popularized this methodology calling it the "water pinch". Limiting water profiles for each operation can be obtained from plotting water maximum inlet and outlet concentrations vs. mass load (Figure 1-3 (a)). The method is based on assuming:

- Constant pollutant load picked up in each process. This is a fair simplifying assumption.
- Maximum inlet and outlet concentrations on each process. These are dictated by solubility, flowrate limitations, fouling, corrosion, etc.

By combining all these streams in one unique profile, a water limiting profile can be obtained, as it is shown in Figure 1-3 (b) for four processes. The fresh water line touches the composite curve at the pinch point and determines the overall water consumption.

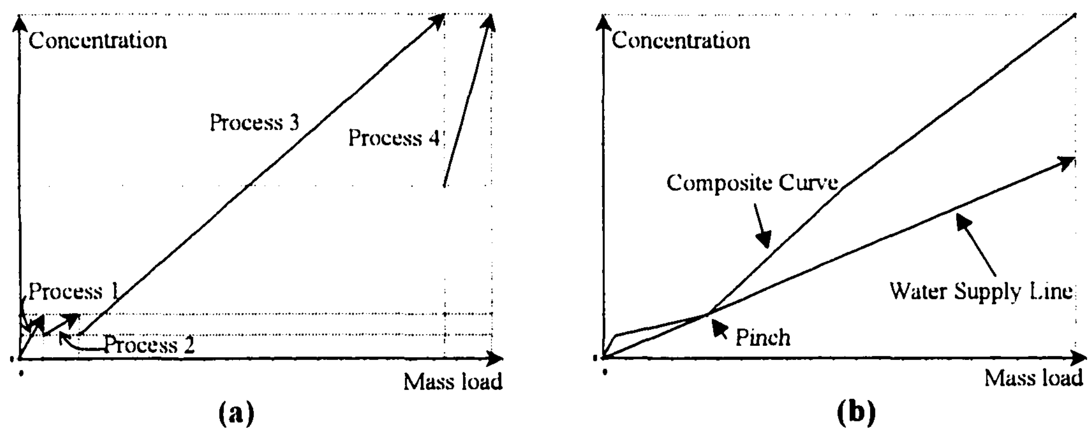


Figure 1-3
(a) Limiting profiles of four water-using units. **(b)** Composite curve of the entire water network and its pinch point.

Once the target flowrate is obtained, a preliminary network is developed using a matching procedure. The procedure is briefly illustrated next. Consider the data given in Table 1-1.

Table 1-1: Example data from Wang and Smith (1994a)

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	2.0	0	100
2	5.0	50	100
3	30.0	50	800
4	4.0	400	800

Wang and Smith (1994a) proposed two techniques: "*Maximum Driving Forces*" and "*Minimum Number of Water Sources*". The first one showed some limitations and will not be discussed further. The first step of the Minimum Number of Water Sources method is the construction of the design grid, as shown in Figure 1-4 (b) from which a network can be obtained (Figure 1-4 (c)). The basis of the procedure is rooted in the work of Linnhoff and Hindmarsh (1983) and Wood *et al.* (1985).

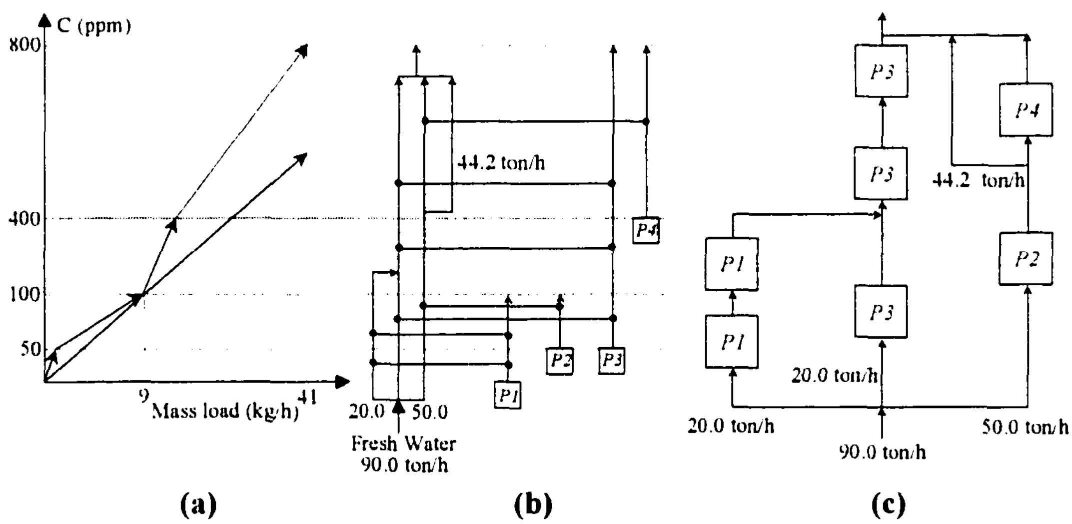


Figure 1-4
(a) Composite curve. (b) Concentrations grid diagram. (c) Preliminary design. (All diagrams were performed following the guidelines given by Wang and Smith, 1994a)

This design grid contains mixing in the middle of processes, a solution that is clearly not acceptable. To overcome this difficulty, Wang and Smith (1994a) propose a loop breaking technique, which eliminates bypassing and mixing. Figure 1-5 shows the loop and the result of the breaking procedure. We omit further explanation of this method as it is well known.

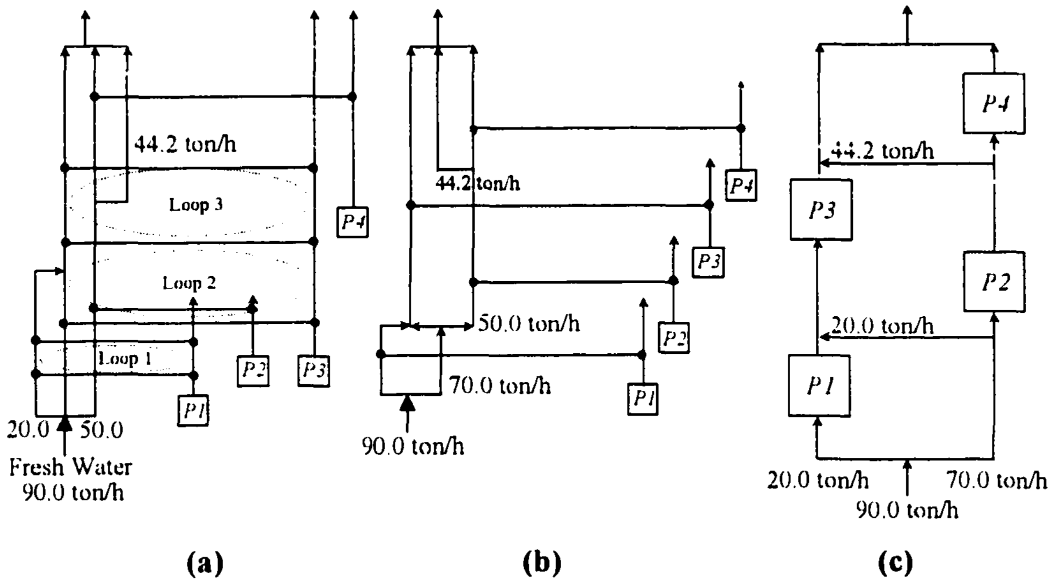


Figure 1-5

(a) Identification of loops. (b) Design grid after breaking all the loops. (c) Final realizing network. (All diagrams were performed following the guidelines given by Wang and Smith, 1994a)

In a follow-up paper, Wang and Smith (1995), showed how the above method can be adapted to consider constraints on the flowrate used for each process as well as water losses. The loop breaking proposed by Wang and Smith (1994a) was proven rather difficult, especially for large systems. The difficulty stems from the fact that there is no clear criterion to identify the loop that needs to be broken at each step.

To overcome this difficulty, Olesen and Polley (1997) proposed a simplified design procedure for single contaminant. The authors used the water pinch to obtain the minimum flowrate target and then modeled the realizing network by inspection. However, as stated by the authors, because it is based on a special ad-hoc inspection procedure, this approach cannot handle more than four or five operations.

Kuo and Smith (1998) also recognized the complexity of the evolutionary design procedure proposed earlier by Wang and Smith (1994a). In an effort to simplify the previous method, the authors introduced a new graphical approach. In addition, they addressed the optimal allocation of fresh water in combination with the distribution of quality of the wastewater that is to be treated. To illustrate their procedure, consider the problem of Table 1-2.

Table 1-2: Example from Kuo and Smith (1998)

Process Number	**Mass Load of Contaminant (kg/h)**	C_{in}^{max} **(ppm)**	C_{out}^{max} **(ppm)**
1	10.0	0	200
2	10.0	100	300
3	12.0	100	500
4	12.0	300	500

The grand composite curve of this system is shown in Figure 1-6. The method consists in identifying the pockets that can be created by successively bending the water supply line upwards. Thus, as seen in Figure 1-6, two pockets exist for this example. The first pocket always runs up to the pinch. The second pocket has an effective water flowrate of 86.7 ton/h, a little lower than the minimum freshwater intake of 90 ton/h.

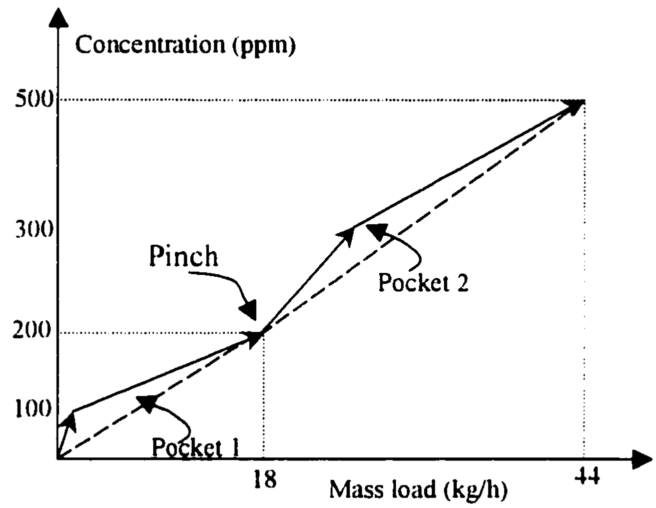


Figure 1-6
Identification of pockets of the limiting composite curve.

The next step is to create a water "main" at the end of each pocket and identify processes that should be fed by these mains. This is shown in Figure 1-7.

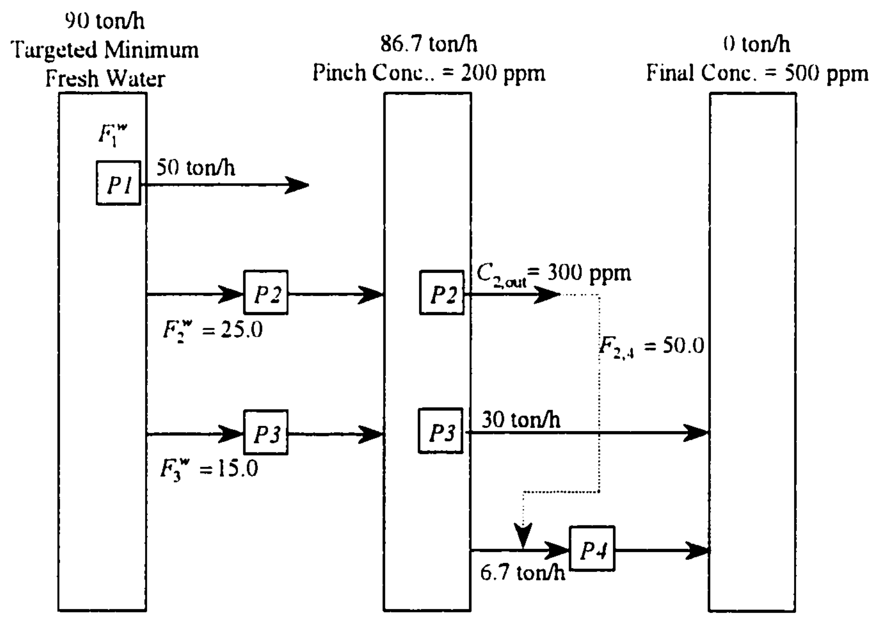


Figure 1-7
Design grid for the Water Mains procedure.

Since some processes exist in different regions, a merging needs to take place. Such merging is shown in Figure 1-8. The final network after merging is shown in Figure 1-9.

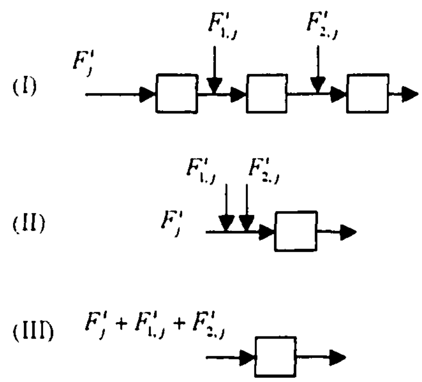


Figure 1-8
Merging.

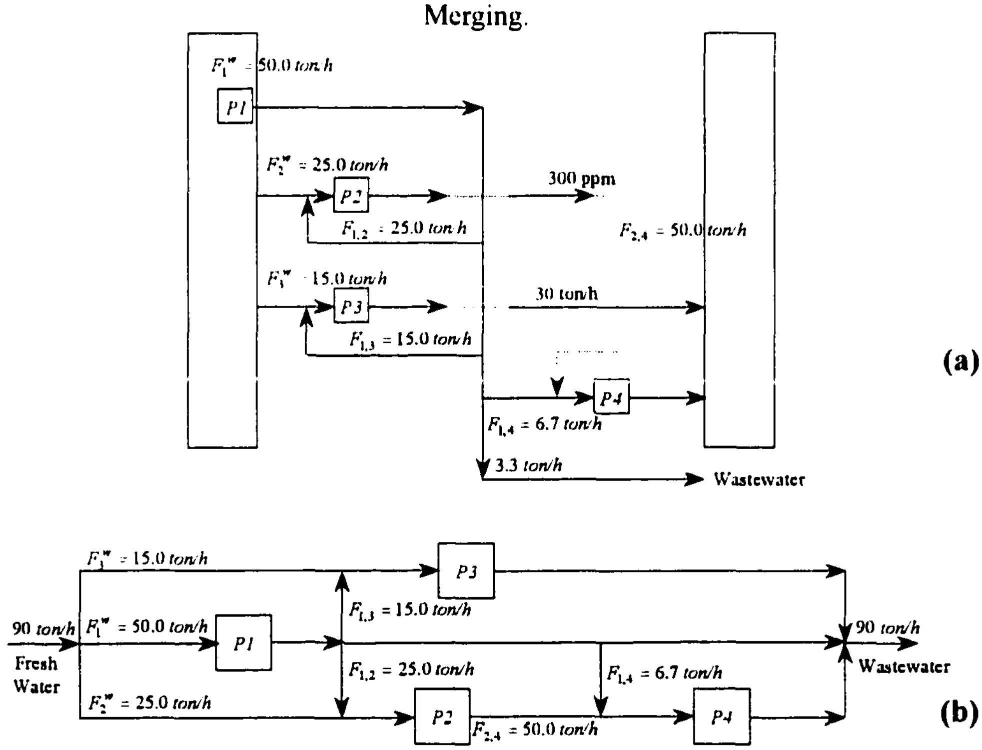


Figure 1-9
(a) The intermediate water main is removed. **(b)** Final design network.

This method has some limitations. Consider the case of several processes below the pinch, many of them with maximum inlet concentration larger than zero. In the same way as it is apparent that process 2 needs to feed process 4 (Figure 1-7), one will have to find out which process needs to be fed using fresh water first and to what process each wastewater has to be sent. This was clarified later by Savelski and Bagajewicz (1999a, b, c, and d) by introducing the concept of monotonicity in the process-to-process connections. In addition, Gómez *et al.* (1999) provided an algorithmic procedure to address this matter. Both issues are discussed in later chapters.

1.3.1.2 Multicomponent Systems

In their paper of 1994, Wang and Smith also attempt to address a targeting and network design procedure for the case of multicomponent systems. Targeting proved to be very cumbersome, as it required elaborate special shifting of streams in the concentration-load diagram. Later, Doyle and Smith (1997) presented a mathematical programming approach, which will be commented below. They also addressed the issue of partial regeneration of streams. Liu (1999) presented a few heuristic rules, some of which are incorrect. However, the solution procedure has remarkable simplicity and provides good sub-optimal (and sometimes optimal) solutions. All this work is proving the assertions stated at the beginning of this chapter regarding the natural drift towards mathematical programming methods as means of addressing the increasing complexity of these problems.

1.3.2 Mathematical Programming Procedures

After the pioneering work of Takama *et al.* (1980), we have no knowledge of any journal publication addressing a mathematical programming formulation of the problem for several years. However, Doyle *et al.* (1997) and more recently Alva-Argáez *et al.* (1998) as well as Huang *et al.* (1999) presented MINLP or NLP models. Savelski and Bagajewicz (1999e), in particular showed that the models can be linearized even for the multiple contaminant case (Savelski *et al.*, 1999). Doyle and Smith (1997) stated that one can construct a linear problem by assuming that all contaminants are at their maximum outlet concentration. This is obviously not true, so, to make the problem feasible, they proposed to relax the component balance constraints. With the solution of such LP problem, they proposed to solve the NLP multicomponent problem. To aid in the search for such solutions, they proposed to add several other constraints on maximum flows of wastewater that can go from one process to another.

Alva-Argáez *et al.* (1998) presented a solution approach for multiple contaminant systems in combination with water treatment, in which they include piping costs as well as treatment costs. One can however, solve the problem for the water allocation only. They also relaxed the component mass balances, but in this case, they solved the problem by adding a penalty function consisting of the summation of all the slack variables coming from the aforementioned relaxation. Thus, the linear problem can be solved to obtain a network of flows, which in turn can be used to obtain a new set of concentrations. These concentrations were substituted in the relaxed component mass balances again, until convergence was achieved. This is the same procedure that Takama *et al.* (1980) used. The sequence of MILP obtained is a sequence of infeasible problems. At the end, the authors claimed a) that the sequence converges, and in such case, b) that the solution is near optimal. Global optimality is, of course, not guaranteed.

Recently, Benko *et al.* (1999) modeled the example problem proposed by Takama *et al.* (1980) as a non-convex MINLP problem. The authors updated the concentration limits in the desalter to make the problem more realistic. This approach cannot guarantee optimality and numerical limitations may limit its use to small-scale problems.

1.4 Simultaneous Water Minimization and Heat Integration

The importance of simultaneous minimization of utility and fresh water usage was first addressed by Savelski *et al.* (1997). More recently, Savulescu and Smith (1998) proposed a graphical method to solve the minimization of fresh water achieving at the same time the minimum utility target. The authors' approach is limited to small-scale problems and considers direct (mixing) heat transfer but only indirect heat exchange between fresh water inlet and wastewater outlet streams. Moreover, it requires that all wastewater streams are mixed and it cannot deliver a network featuring minimum number of heat exchangers. The method is a sequential procedure in which certain heuristics are used in a first stage to obtain a network of process-to-process interconnections such that the indirect heat exchange structure might feature minimum utility. However, these rules cannot guarantee that the resulting structure will be optimal. Moreover, the notion of connecting processes close in temperature may clash with the fact that monotonicity of outlet concentrations should hold (Savelski and Bagajewicz, 1999a). Finally, in a second stage, the authors assumed that there were no process-to-process wastewater connections that require heating or cooling in a heat exchanger. This allowed them to introduce the so-called separate systems, which consist in vertically aligning portions of the hot and cold composite curves (Figure 1-10).

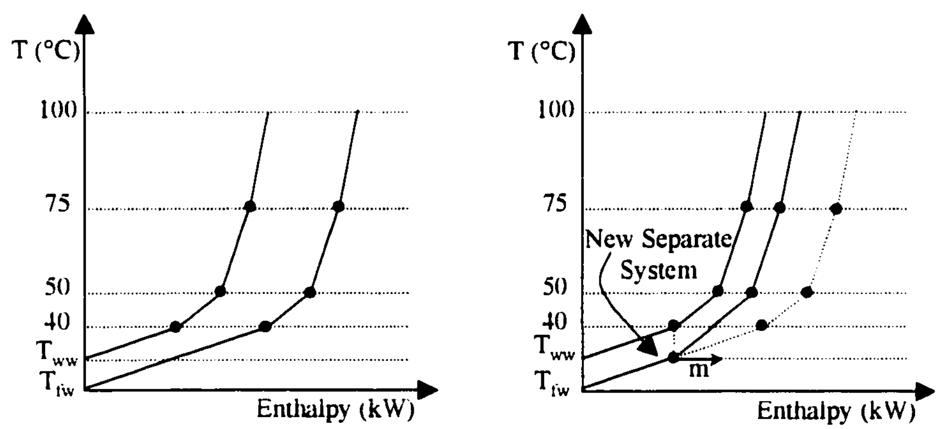


Figure 1-10
Separate System Method as presented by Savulescu and Smith (1998)

However, there are processes where indirect heating or cooling of process-to-process streams is needed. The method of separate systems proposed does not address this case. Finally, to build the heat exchanger network, it was assumed that the wastewater is merged to be sent as a unique stream to treatment. If one wants to send these streams to water treatment separately, the concept of separate systems has to be re-formulated at the least.

1.5 Optimal Wastewater Treatment Allocation

As it was outlined above, the optimal design of wastewater systems started with Takama *et al.* (1980), who solved this problem in conjunction with the water allocation problem. In this section the contributions to the design of wastewater treatment systems only is reviewed. The synergy between the two systems and the efforts to address structures such as those of Figure 1-1 (d), are discussed in the next section.

1.5.1 Conceptual Design Procedures

Wang and Smith (1994b) approached the design of distributed effluent treatment by a similar graphical procedure as presented for the water/wastewater allocation problem. The authors used the same cost functions for the effluent treatment units as those proposed by Takama *et al.* (1980). The model is based on the following assumptions:

- Several streams available for cleaning can be split and sent to different treatment operations. That is, no merging of these streams is assumed. However, this still implies end-of-pipe treatment, as in Figure 1-1 (c).
- The flowrate of water through the processes is constant.
- The treatment units have fixed pollutant removal ratio.

- Cost of treatment is assumed proportional to the flowrate of the stream to cleanup. A concentration-load diagram discussion justifies this simplifying assumption.
- Once the problem has been put in the framework of concentration-load diagrams, a composite curve representing all wastewater streams can be constructed. A minimum treatment flowrate is then obtained by assuming a fixed removal ratio. This is accomplished by rotating a treatment flowrate line around point O (Figure 1-11).

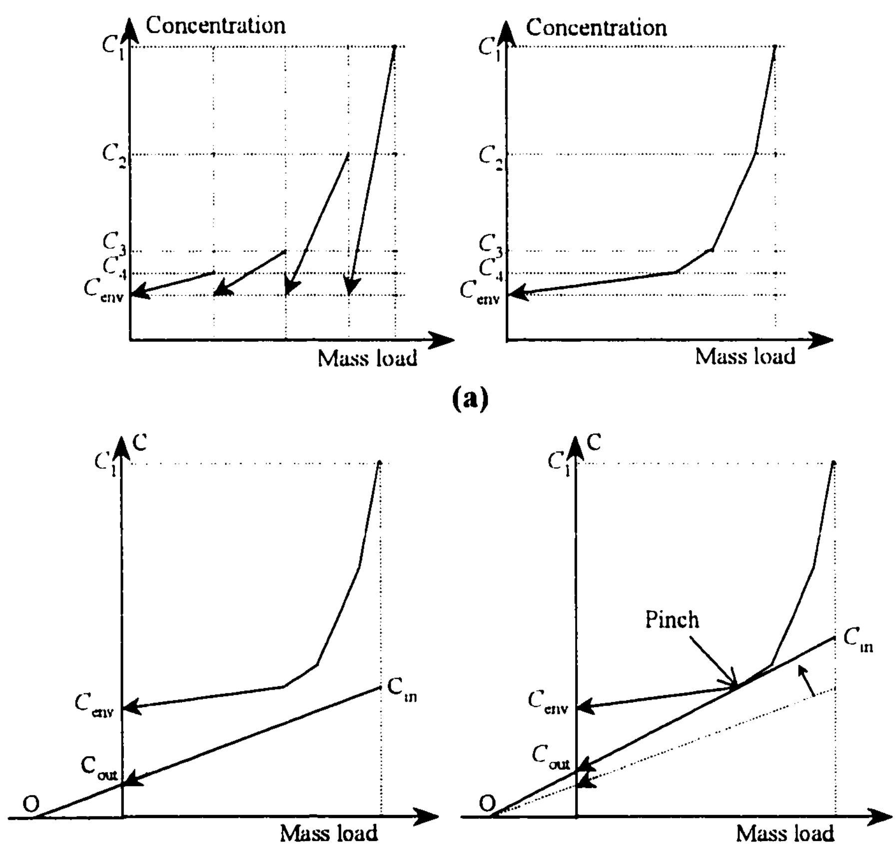


Figure 1-11
(a) Wastewater streams and their composite curve. **(b)** Minimum flowrate targeting.

When cost does not decrease with flowrate, Wang and Smith identify a feasible region within which the treatment flowrate line should lie. A classification of streams then follows and certain design rules are used to obtain the network. For the case of multiple contaminant, a network for each contaminant is designed and a merging procedure produces the final unified network. A revised version of this procedure was presented by Kuo and Smith (1997). A graphical method that utilizes the pinch concept along with what the authors referred to as the *wastewater degradation* concept. The wastewater degradation takes into account the exergy losses due to the mixing of wastewater streams of different qualities. Then, the authors explored several flowsheet alternatives and choose the network with lower exergy losses. This approach cannot be effectively applied to a system with many contaminants and many wastewater streams. Despite their value in understanding and dissecting the complexity of the problem, these insights have not been proven useful in helping mathematical programming formulations to find global optima. In view of the limitations of this approach, we do not expand on it further.

Very recently, Freitas *et al.* (1999) illustrated the use of the hierarchical design approach (Douglas, 1988) to the design of these systems. They constructed a relational database and an expert system to determine the best sequence of treatment processes. The method cannot of course, guarantee any optimality.

1.5.2 Mathematical Programming Procedures

In an effort to systematize a solution procedure of these kind of problems and moving radically away from conceptual design procedures into mathematical programming, Alva-Argáez *et al.* (1998) modeled the entire water management problem by means of a superstructure. This approach leads to a MINLP problem that includes some elements not present in previous models. The model considers the presence of water losses, it has bounds on water flowrates and it assumes constant removal ratio in the wastewater treatment units. The objective function is non-linear and the constraints contain the bilinear constraints that arise from component balances. No heat integration is included. Although the model does not guarantee optimality, the authors claim obtaining successful results on 12 processes and 3 treatment units. Galán and Grossmann (1998) also solved the effluent-treatment distribution problem using mathematical programming. Finally, Huang *et al.* (1999) proposed a similar NLP approach. Their contribution has some more realistic assumptions regarding the outlet concentrations of certain processes and treatment units. They realized that, in some cases, certain units are better modeled if outlet concentrations are considered fixed, instead of fixed loads or fixed removal ratios. Their approach is a simple extension of the one presented by Galán and Grossmann (1998) and has merit much more in the type of examples solved, rather than in the solution procedure, which is standard.

The issue of solvability of these MINLP problems is at the heart of the challenge. While Alva-Argáez *et al.* (1998) applied the same procedure outlined by Doyle and Smith (1997) to solve the multicomponent water allocation problem (see above), Galán and Grossmann (1998) used tight linear relaxations to obtain good starting point for an NLP solver. At this point, it can be said that the whole area is moving towards mathematical programming methods. A few researchers are still exploiting conceptual insights to simplify solution procedures.

It is important to note that this problem does not have minimum outlet concentrations in the outlet of the treatment process, although maximum at both inlet and outlet can be prescribed. In addition, the removal ratio is fixed not the load. Had the load been fixed, the distributed treatment problem would be an exact mirror image of the water allocation problem.

Mass Exchanger Network (MEN) technology was proposed by El-Halwagi and Manousiouthakis (1990) to solve a special case of phenol removal from refinery wastewater. This approach has not yet been used in combination with other techniques.

1.6 Simultaneous Wastewater Treatment and Water Allocation

Takama *et al.* (1980) already posed the problem as a simultaneous optimization of the overall usage of water. They proposed a superstructure of the type shown in Figure 1-1 (c). In other words, although the water treatment is distributed, it is still centralized. Wang and Smith (1994a) showed the value of decentralized treatment, by discussing in detail the benefits of partial regeneration of water in the water allocation problem. Their approach is summarized in Figure 1-12, where the slope of the target water line can be increased because regeneration takes place, releasing thus the constraint imposed by the pinch. The figure also targets what is the concentration at which regeneration has to take place.

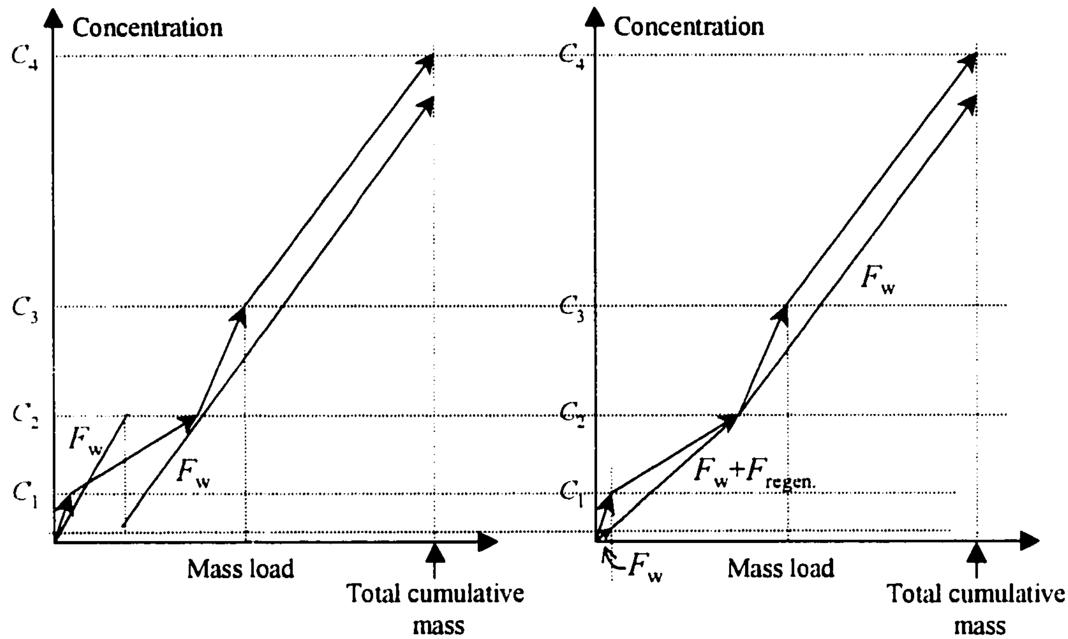


Figure 1-12
Regeneration to the pinch concentration.

Although Wang and Smith were able to identify regeneration opportunities for these systems, the conceptual design procedure for building the network has the same problems as the design without regeneration, especially for multicomponent. No attempt to address decentralized treatment was performed for a while. Kuo and Smith (1998) discussed briefly the effect of the design of the water allocation problem in the type, flowrate and quality of streams that feed the distributed treatment in system of the type of Figure 1-1 (c).

Alva-Argáez *et al.* (1998), Benko *et al.* (1999), and Huang *et al.* (1999) addressed the whole problem with an MINLP or NLP approach, depending of the case. The advantages of these formulations were discussed above. While it is not clear to what extent Alva-Argáez (1998) used superstructures of the type shown in Figure 1-1 (d), it is worth pointing out that the other two papers considered these structures in their models. For those that consider this issue of paramount importance, global optimality is not guaranteed by any of these methods, nor is it clear what is the maximum size of problems that can be solved. It appears however, that realistic sizes can be achieved by sacrificing some nonlinearities.

1.7 Objectives of Research

To investigate and develop new methodologies to optimally solve the fresh water allocation /waster reuse planning problem in refineries and process plant.

1.8 Structure of Dissertation

- Chapter 2 presents a robust design procedure that rectifies the shortcoming of previous methodologies (Wang and Smith, 1994 and 1995; Kuo and Smith, 1998).
- Chapter 3 introduces necessary conditions of optimality for water networks.

- Chapter 4 presents an algorithmic design procedure to solve the single-contaminant water-planning problem. This method is based on necessary and sufficient conditions of optimality of the water system.
- In Chapter 5, a mathematical programming formulation of the single-component water-allocation problem is developed. First, an NLP model is proposed and then it is linearized using the necessary conditions of optimality. The resulting LP problem is used for targeting. Finally, different solution alternatives are presented based on an MILP formulation.
- In Chapter 6, a model to solve the simultaneous water minimization and heat integration problem is proposed.
- Finally, Chapter 7 addresses the multicomponent water-allocation problem and some challenges.

1.9 References

1. Alva-Argáez A., A.C. Kokossis and R. Smith. *Automated Design of Industrial Water Networks.* AIChE Annual Meeting, paper 13f, Miami, 1998.
2. Belhateche D.H. *Choose Appropriate Wastewater Treatment Technologies.* Chemical Engineering Progress, August, pp. 32, 1995.
3. Benko N., E. Rev, Z. Szitkai and Z. Fonyo. *Optimal Water Use and Treatment Allocation.* Comp. & Chem. Eng., Vol. 23, Supp., pp. S589-S592, 1999.
4. Carnes, B.A., D.L. Ford and S.O. Brady. *Treatment of Refinery Wastewaters for Reuse.* Nat. Conf. Complete Water Reuse, Washington D.C., 1973.
5. Diepolder P. *Is 'Zero Discharge' Realistic?* Hydrocarbon Processing, October 1992.
6. Dhole V.R., N. Ramchandani, R.A. Tainsh and M. Wasilewski. *Make your Process Water Pay for itself.* Chemical Engineering, January, pp. 100, 1996.
7. Douglas J.M. *Conceptual Design of Chemical Processes.* McGraw-Hill. New York, 1988.

8. Doyle, S.J. and R. Smith. *Targeting Water Reuse with Multiple Contaminants.* Trans IChemE, 75, Part B, No. 3, pp. 181-189, 1997.
9. El-Halwagi M.M. and V. Manousiouthakis *Mass Exchanger Networks.* AIChE Journal, 35, 8, pp. 1233, 1989.
10. El-Halwagi M.M. and V. Manousiouthakis. *Automatic Synthesis of Mass Exchanger Networks with Single Component Targets.* CES, 45, 9, pp. 2813, 1990.
11. Freitas I.S.F., R.A.R. Boaventura and C.A.V. Costa. *Conceptual Design of Industrial Wastewater Treatment Processes: A hierarchical Approach Procedure.* Proceedings of the 2nd Conference on Process Integration, Modeling and Optimization for Energy Savings and Pollution Reduction. (PRES'99). Budapest, Hungary, June 1999.
12. Galán B. and I.E. Grossmann. *Optimal Design of Distributed Wastewater Treatment Networks.* Ind. Eng. Chem. Res., 37, pp. 4036, 1998.
13. Goldblatt M.E., K. S. Eble and J. E. Feathers. *Zero Discharge: What, Why, and How.* CEP, April. p. 22, 1993.
14. Gómez J., M. Savelski and M. Bagajewicz. *On a Systematic Design Procedure for Water Utilization Systems In Refineries and Process Plants.* Submitted to Chem. Eng. Comm., 1999.
15. Hilaly A.K. and S.K. Sikdar. *Process Simulation Tools for Pollution Prevention.* Chemical Engineering, February, pp. 98, 1996.
16. Hospondarec R.W. and S.J. Thompson. *Oil-steam System for Water Reuse.* Proceeding of the Workshop (AIChE), Vol. 7, 1974.
17. Huang C-H, C-T. Chang, H-C. Ling and C-C. Chang. *A Mathematical Programming Model for Water Usage and Treatment Network Design.* Ind. Eng. Chem. Res., 38, pp. 2666, 1999.
18. Kuo W-C. J. and R. Smith. *Effluent Treatment System Design.* CES, 52, 23, pp. 4273, 1997.
19. Kuo W-C. J. and R. Smith. *Designing for the Interactions between Water-Use and Effluent Treatment.* Trans IChemE, 76, Part A, pp.287-301, 1998.
20. Linnhoff B. and E. Hindmarsh. *The Pinch Design Method for Heat Exchanger Networks.* Chemical Engineering Science, 38, 5, pp. 745, 1983.
21. Liu Z. *Wastewater Minimization using a Heuristic Procedure.* AIChE Spring Meeting, Houston, paper 43e, 1999.
22. Mishra P.N., L.T. Fan and L.E. Erickson. *Application of Mathematical Optimization Techniques in Computer Aided Design of Wastewater Treatment Systems.* Water-1974 (II). AIChE Symp. Series, 71, 145, 1975.
23. Olesen S.G. and G.T. Polley. *A Simple Methodology for the Design of Water Networks Handling Single Contaminants.* Trans IChemE, 75, part A, pp. 420-426, 1997.
24. Sane M., U. S. Atkins. *Industrial Water Management.* Int. Chem. Eng. Symp. Series, 52, 1977.

25. Savelski M., S. Lingareddy and M. Bagajewicz. *Design and Retrofit of Water Utilization Systems and Zero Discharge Cycles in Refineries and Process Plants*. Paper 188g. AIChE Annual Meeting, Los Angeles, 1997.
26. Savelski M. and M. Bagajewicz. *A New Algorithmic Design Procedure for the Design of Water Utilization Systems in Refineries and Process Plants.* Proceedings of PRES'99 Meeting. Budapest, June 1999a.
27. Savelski M. and M. Bagajewicz. *Watersave. A New Approach To the Design of Water Utilization Systems in Refineries and Process Plant.* Proceedings of the 2nd International Conference on Refining Processes, AIChE Meeting, Houston, 1999b.
28. Savelski M. and M. Bagajewicz. *On the Necessary Conditions of Optimality of Water Utilization Systems in Refineries and Process Plants.* Submitted to Chemical Engineering Science, 1999c.
29. Savelski M. and M. Bagajewicz. *Algorithmic Procedure to Design Water Utilization Systems in Refineries and Process Plants.* Submitted to Chemical Engineering Science, 1999d.
30. Savelski M. and M. Bagajewicz. *On The Use of Linear Models for the Design of Water Utilization Systems in Refineries and Process Plants.* Annual AIChE Meeting, Dallas, (Submitted to Chemical Engineering Research and Design), 1999e.
31. Savelski M., M. Rivas and M. Bagajewicz. *A New Approach to the Design of Water Utilization Systems with Multiple Contaminants in Process Plant.* Annual AIChE Meeting, Dallas, 1999.
32. Savulescu L. E. and R. Smith. *Simultaneous Energy and Water Minimisation.* AIChE Annual Meeting, paper 41f, Miami, 1998.
33. Skylov V. and R.A. Stenzel. *Reuse of Wastewaters-Possibilities and Problems.* Proceeding of the Workshop (AIChE), Vol. 7, 1974.
34. Sowa C.J. *Explore Waste Minimization via Process Simulation.* Chemical Engineering Progress, November, pp. 40, 1994.
35. Takama N., T. Kuriyama, K. Shiroko and T. Umeda. *Optimal Water Allocation in a Petroleum Refinery.* Comp. & Chem. Eng. 4, 251-258, 1980.
36. Wang Y.P. and R. Smith. *Wastewater Minimization.* CES, 49, 7, pp. 981, 1994a.
37. Wang Y.P. and R. Smith. *Design of Distributed Effluent Treatment Systems.* CES, 49, 18, pp. 3127, 1994b.
38. Wang Y.P. and R. Smith. *Wastewater Minimization with Flowrate Constraints.* Trans IChemE, 73, Part A, pp. 889-904, 1995.
39. Wood R.M., R.J. Wilcox and I.E. Grossmann. *A Note on Minimum Number of Units Heat Exchanger Network Synthesis.* Chem. Eng. Comm., 39, pp. 371, 1985.

CHAPTER 2

On a Systematic Design Procedure for Water Utilization Systems in Refineries and Process Plants

2.1 Introduction

As mentioned in Chapter 1, several researchers have addressed the water allocation planning (WAP) problem by means of conceptual design procedures. Wang and Smith (1994,1995), Olesen and Polley (1997), and Kuo and Smith (1998) have all proposed different alternative methods for solving this problem. In all this work, the procedures are either difficult to apply or they are limited to small-scale network systems.

This chapter presents a robust methodology to obtain an optimal design of the single component water/wastewater allocation problem in process plants. The method uses the water pinch targeting method first and a concentration grid water allocation procedure to obtain preliminary optimal structures. A merging procedure provides the final structures. The use of different water allocation strategies shows that the problem has several alternative solutions. The method we present is a systematical procedure to obtain a water network that realizes the minimum water target regardless of problem size. A problem statement is presented first, followed by the design procedure and some examples.

2.2 Problem Statement

Given a set of water-using/water-disposing processes, it is desired to determine a network of interconnections of water streams among the processes so that the overall fresh water consumption is minimized, while the processes receive water of adequate quality. This is what is referred to as the Water/Wastewater Allocation Planning (WAP) problem.

A more stringent version of this problem was the one presented by Takama *et al.* (1980) and later used by Wang and Smith (1994). In this version, limits on inlet and outlet concentration of pollutant are imposed a-priori on each process and a fixed load of contaminants is used. These inlet and outlet concentrations limits account for corrosion, fouling, maximum solubility, etc.

2.3 New Design Method

The new procedure is based on the construction of a concentration grid, similar to the one proposed by Wang and Smith (1994). The first step requires obtaining the target, which can be performed using the same method proposed by Wang and Smith (1994). After the minimum fresh water is determined, the method requires that a concentration grid, based on maximum inlet and outlet concentrations be constructed. All processes are allocated within this grid such that they appear in as many intervals as their respective inlet and outlet maximum concentrations span through.

The second step requires assigning all the available fresh water to all fresh water users. The amount of water supplied is only the required to reach the outlet concentration of the first interval. In a third step, wastewater from these processes is assigned to processes in the subsequent intervals as required. Additional fresh water is used as needed. Figure 2.1 illustrates the allocation of fresh water at each interval in each of the processes.

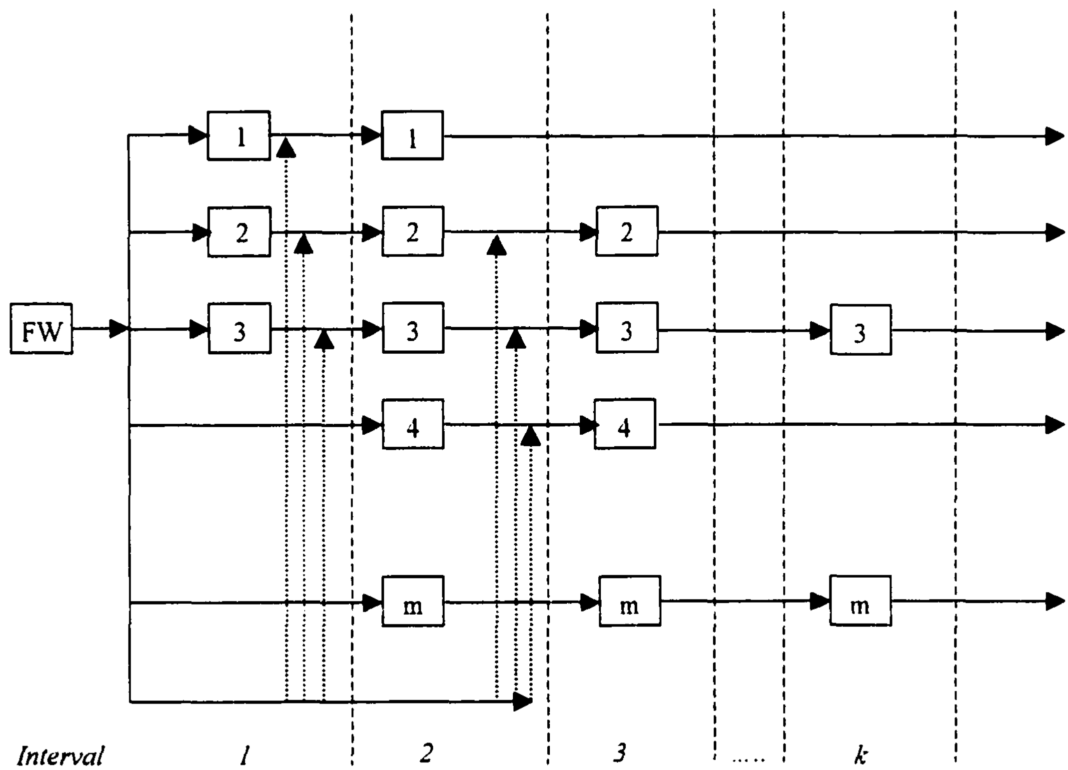


Figure 2-1
Initial Allocation of Fresh Water in the '*m*' processes involved.

To assign water from one process to another in any subsequent interval it is necessary to define all the sources available from previous intervals. These sources can be either fresh water, or some wastewater coming from other previous concentration intervals. All processes must reuse their own water.

Three different approaches to perform the wastewater allocation are discussed next.

2.3.1 Water Assignment Procedures

Consider a set of m wastewater users in interval k, and assume wastewater from m processes is available.

2.3.1.1 Mixers

In this first approach, all available wastewater sources from previous concentration intervals are mixed to convene into just one source. Then, wastewater is taken from this mixer to supply all the water requirements at the given concentration interval. Water moving between concentration intervals and going through the same operation would not be defined as a water source available so that unnecessary unit splitting is avoided. Figure 2-2 shows a schematic example where the water moves within processes 1 and 2 and a mixer is formed using the outlet streams from processes 3 through m. Water coming out from the mixer is available to feed water requirements in the next concentration interval. Operations 1 and 2 require additional water to complete the load pick-up and this water is supplied by the mixer. Process n is new in the concentration interval under study and it receives water from the mixer only. Some water in the mixer may not be required and the excess bypassed to the next concentration interval, to be reused in other downstream processes.

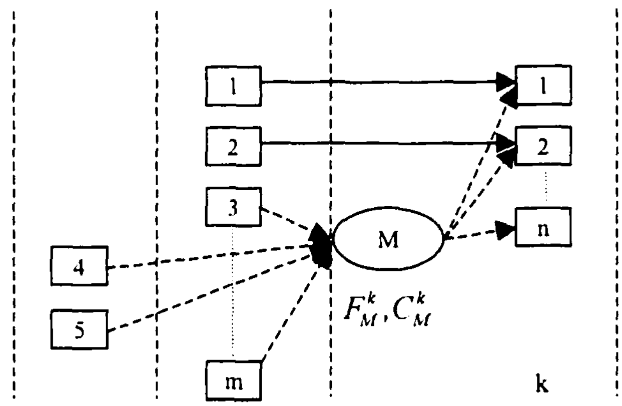


Figure 2-2
Mixing available water sources to supply water sinks.

2.3.1.2 Use of the Worst Quality Water Available First

In this approach, processes at a certain concentration interval are provided with the available wastewater at the worst possible concentration. To illustrate this approach, consider Figure 2-3 where process 3 and process 5 are the only available wastewater sources to provide processes 1, 2 and 4. Assume also that the outlet concentration of process 3 is larger than of process 5. In this approach, the most contaminated water, coming from process 3, must be used first. If needed, water from the other source, process 5, should be also used. Finally, any process can be the first one served. The required water for each operation can be calculated by a component mass balance performed at the receiving process. Any wastewater excess is also bypassed to the next concentration interval, to be used in another downstream process. Following this criterion, bypassed water will always be at the lowest possible concentration. As pointed out by Kuo and Smith (1998), this may help obtain some wastewater streams cleaner than others.

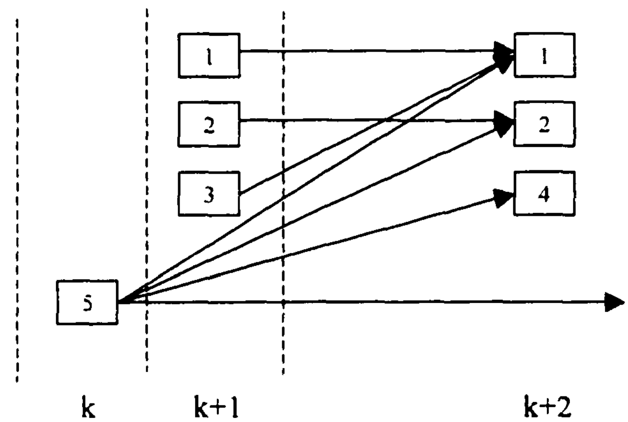


Figure 2-3
Assigning the most contaminated water first.

2.3.1.3 Use of the Cleanest Water Available First

Assigning the cleanest water first maximizes the driving force within the process. This approach helps reduce the size of the equipment and may also lower the number of interconnections among processes.

2.3.1.4 Advantages and Disadvantages

- *Mixing*: The mixing approach provides with a sole wastewater source, which could be economical from a point of view of the associated piping. This facilitates calculations when assigning water to receiving processes. It also eliminates the necessity of an assignment rule to decide how to order the precursors to be used. A particular drawback of this rule is that cleaner wastewater can be mixed with others of higher contaminant concentration degrading the quality of the less polluted wastewater.

- *Higher vs. lower polluted wastewater used first*: The water flowrate necessary to remove a given pollutant load increases as the quality of the used wastewater decreases. A large flowrate may not be possible to handle by an already existing unit or the increase in capital investment associated with the design may not be economical. In addition, operating costs for heat and/or cooling as well as pumping could increase, as the flowrate needed for the task increases. Therefore, the utilization of cleaner wastewater may in certain cases present a greater advantage. The contaminants and the type of cleanup operations available in the wastewater treatment plant are also of vital consideration when deciding the quality of wastewater to be used. For example, concentration-difference driven processes, such as liquid-liquid extraction, may not be able to remove the contaminant to its final discharge limit. Other treatments, like those having live microorganisms, can be severely damage due to toxicity of large concentrations of certain pollutants. Therefore, favoring the bypass of large amount of wastewater at high/low concentrations of contaminant need to be thoroughly analyzed before choosing a policy.

In addition, the use of the above rules of assignment of wastewater policies varies depending on whether the pinch concentration has been reached or not. This is discussed next.

2.3.1.5 Use of the Assignment Procedures Below the Pinch

To fulfill the water requirements of each process at concentrations below the pinch, the total water in use will continuously increase because fresh water is added until the target value is completely utilized. All the wastewater exits the pinch interval at pinch concentration. For these reasons, the assignment method used will not alter the discharge concentration to the subsequent intervals and to the wastewater treatment plant.

Thus, below the pinch freshwater is assigned until it is depleted. Then a mixer can be created. When the water from this first mixture is completely consumed, it is always possible to create another mixer of the sources available in that interval. This method is very useful and can always be done up to the water pinch. Alternatively, the two other policies can be used.

Occasionally, a water source is enough to feed a process close to it, therefore moving this water through a pipeline to a mixer could be unworthy. It is then possible to use a combination of the three approaches shown before in order to reduce transportation costs and simplify the water network. Figure 2-4 shows a combined approach.

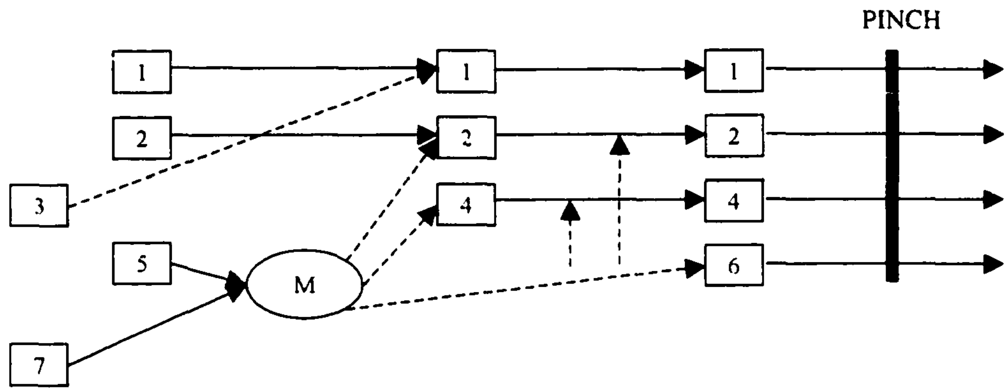


Figure 2-4
Combined design of a water network before the 'pinch'.

Sometimes large distances between processes, difficulties to build by-pass pipelines, heat transfer requirements or any other limitations, can determine the design criteria rather than a fixed design method. In order to minimize costs and simplify the water network, adding more fresh water could be considered.

2.3.1.6 Use of the Assignment Procedures Above the Pinch

After the water pinch, there will be more water available than the required amount to remove the remaining loads. In other words, a surplus of wastewater is present after crossing the pinch point. Downstream requirements at the water treatment plant should be emphasized in the decision making process.

2.3.1.7 Determination of Flowrates

A precursor of a process can be another process or a mixer. Consider a precursor of process j in an interval i as shown in Figure 2-5. The pollutant concentration of the precursor is always lower $\left(C^i_{P_j,j} \le C^{i-1}_j\right)$. This is a consequence of the grid construction. The values of m^i_j, F^{i-1}_j, C^{i-1}_j, C^i_j and $C^i_{P_j,j}$ are known. Therefore, the values of $F^i_{P_j,j}$ and F^i_j need to be determined. To do this, overall and contaminant mass balances are done. When only fresh water is available, $F^i_{P_j,j}$ becomes $F^i_{w,j}$ and $C^i_{P_j,j}$ will be equal to zero. Regardless whether a precursor is another process or a mixer the mass balances can be simultaneously solved for $F^i_{P_j,j}$ and F^i_j.

$$F^i_j = F^{i-1}_j + F^i_{P_j,j} \tag{2-1}$$

$$F^{i-1}_j C^{i-1}_j + F^i_{P_j,j} C^i_{P_j,j} + m^i_j - F^i_j C^i_j = 0 \tag{2-2}$$

$$F^i_{P_j,j} = \frac{F^{i-1}_j (C^i_j - C^{i-1}_j) - m^i_j}{C^i_{P_j,j} - C^i_j} \tag{2-3}$$

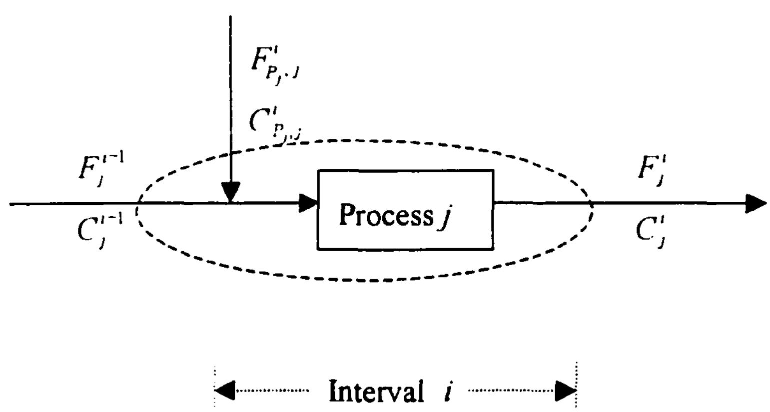


Figure 2-5
Schematic representation of process j through interval i.

If $F^i_{P_j,j} > F_{P_j}$, then another source should be added to fulfil the water requirements of the process. This procedure is repeated until the conditions of process j have been met. In general, for m precursors providing process j in interval i, (2-1) and (2-2) can be written as follows:

$$F_j^i = F_j^{i-1} + \sum_k^m F_{P_k,j} \tag{2-4}$$

$$\sum_k^m F^i_{P_k,j} C^i_{P_k,j} + F_j^{i-1} C_j^{i-1} + m_j^i - F_j^i C_j^i = 0 \tag{2-5}$$

Combining (2-4) and (2-5),

$$F^i_{P_m,j} = \frac{\sum_k^{m-1} F^i_{P_k,j}\left(C_j^i - C^i_{P_k,j}\right) + F_j^{i-1}\left(C_j^i - C_j^{i-1}\right) - m_j^i}{C^i_{P_m,j} - C_j^i} \tag{2-6}$$

The total flowrate through process j can then be calculated from (2-1) or (2-4). As a result of these steps, a preliminary grid assignment of water is obtained. This is illustrated next.

2.3.2 Examples

2.3.2.1 Example 2-1

This example is taken from Olesen and Polley (1997). It comprises six water-using processes. Table 2-1 provides the limiting data and Figure 2-6 shows the design obtained with our method.

Table 2-1: Limiting data for Example 2-1

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	2.0	25	80
2	5.0	25	100
3	4.0	25	200
4	5.0	50	100
5	30.0	50	800
6	4.0	400	800

As illustrated in Figure 2-6, in this problem fresh water is used to supply the water requirements of processes 1, 2, 3, 4, and 5 up to interval 2. In interval 3, fresh water is exhausted before process 5 requirements are completely fulfilled. The only wastewater available for reuse is from process 1. No other processes are completed in this interval hence it is not possible to create a mixer. Therefore, wastewater is sent from process 1 to process 5, the only process that needs additional water. In interval 4, process 3 still needs water. Wastewater is available from processes 2 and 4, both at 100 ppm. No real gain would be obtained from mixing because the resulting wastewater would have the same concentration. If either process 2 or 4 cannot fulfill process 3 requirement; then, mixing would reduce the number of interconnections. Using equation (2-3) the necessary flowrate at 100 ppm is calculated. Since this flowrate does not exceed the availability from process 2, no mixing is performed. Finally, wastewater from process 2 is used to feed process 6.

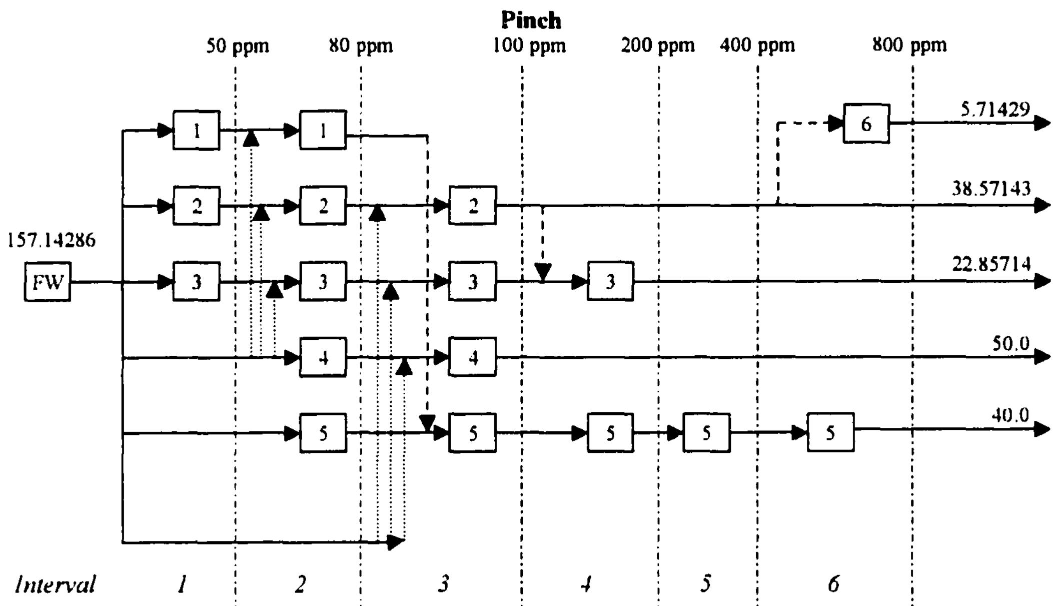


Figure 2-6
Preliminary design of the water network.

2.3.2.1.1 Merging

The operations are split at each concentration interval in the preliminary grid solution. The splitting is a consequence of having to remove a certain mass load at each concentration interval. These kinds of networks are not real solutions to the problem because unit operations can not be represented or built in reality as a collection of smaller processes. Therefore, as a final step, a network merging is done. Figure 2-7 illustrates the merging procedure. All the individual mass loads of the process are transferred upstream and a combined feed stream at the entrance of the operation is obtained. The water sources would be added and used as new feed. This merging was proposed by Kuo and Smith (1998) but a proof of its validity was not presented. Such proof is given next.

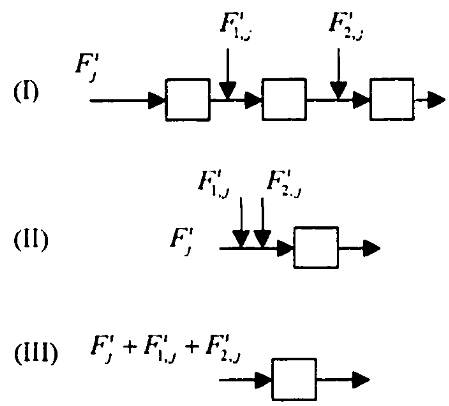


Figure 2-7
Operation merge. The breached process is recombined by adding all water sources.

Consider a process j, which has been split into n parts throughout the concentration grid. Figure 2-8 shows a schematic representation of the situation. At each concentration interval i, there is a precursor, P_j^i, providing the necessary water to remove the partial load m_j^i. The proof that follows shows that the first two intervals can always be merged into one as shown in Figure 2-9. An overall merging can then be performed by a sequential repetition of the aforementioned basic merging process.

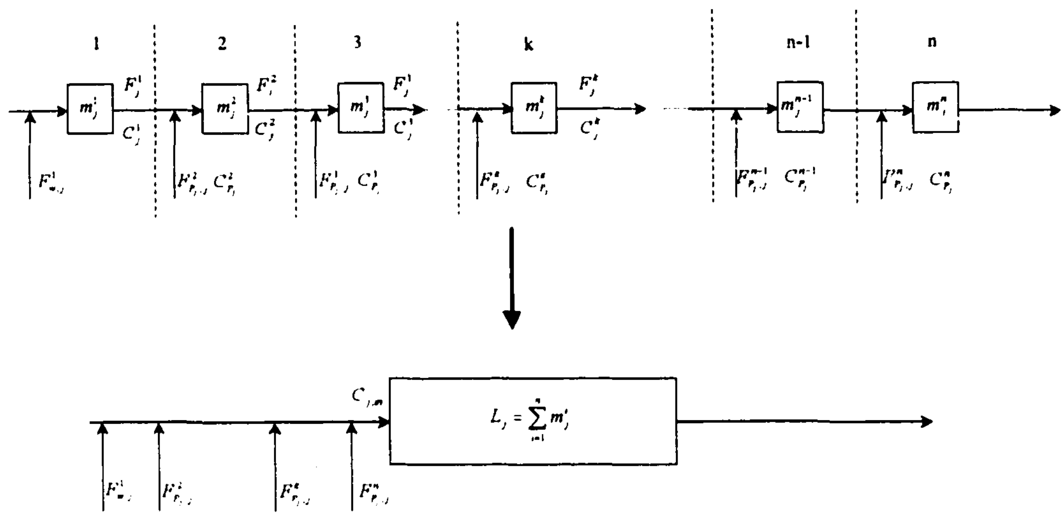
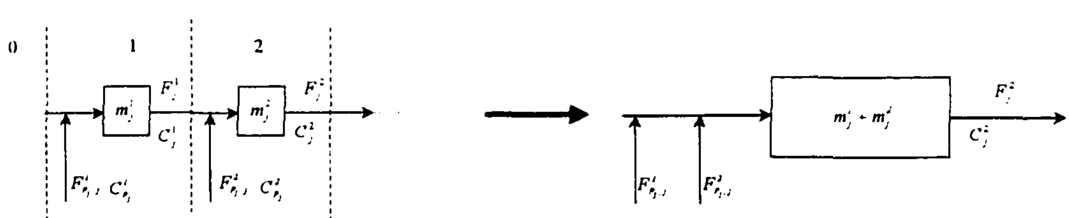


Figure 2-8
Merging of a split process.

Proof

Consider a merging of the second feed as shown in Figure 2-9. The merge is feasible if and only if

$$C_{j,in} \leq C_{j,in}^{max} \qquad (2\text{-}7)$$



(a) (b)

Figure 2-9
Merging of two segments of a process.

$C_{j,in}$ can be obtained from a component mass balance at the inlet of (b),

$$C_{j,in} = \frac{F^1_{P_j,j} C^1_{P_j,j} + F^2_{P_j,j} C^2_{P_j,j}}{F^1_{P_j,j} + F^2_{P_j,j}} \tag{2-8}$$

Rewriting (2-7) using (2-8) and rearranging, we obtain

$$F^1_{P_j,j}\left(C^1_{P_j,j} - C^{max}_{j,in}\right) + F^2_{P_j,j}\left(C^2_{P_j,j} - C^{max}_{j,in}\right) \leq 0 \tag{2-9}$$

which is what needs to be proven.

By grid construction,

$$m^1_j = L_j \frac{\left(C^1_j - C^{max}_{j,in}\right)}{\left(C^{max}_{j,out} - C^{max}_{j,in}\right)} \tag{2-10}$$

and

$$m^2_j = L_j \frac{\left(C^2_j - C^1_j\right)}{\left(C^{max}_{j,out} - C^{max}_{j,in}\right)} \tag{2-11}$$

The grid construction also requires that $C^0_j = C^{max}_{j,in}$.

Performing a component mass balance at the outlet conditions of interval 1, we get

$$F^1_{P_j,j} C^1_{P_j,j} + m^1_j = F^1_{P_j,j} C^1_j \tag{2-12}$$

Using (2-10) and (2-12) we obtain,

$$F^1_{P_j,j} = \frac{L_j}{\Delta C^{max}_j} \frac{\left(C^1_j - C^{max}_{j,in}\right)}{\left(C^1_j - C^1_{P_j,j}\right)} \tag{2-13}$$

where $\Delta C^{max}_j = C^{max}_{j,out} - C^{max}_{j,in}$

A component mass balance for the second interval is

$$F^1_{P_j,j} C^1_{P_j,j} + F^2_{P_j,j} C^2_{P_j,j} + m^1_j + m^2_j = \left(F^1_{P_j,j} + F^2_{P_j,j}\right) C^2_j \tag{2-14}$$

Replacing (2-10), (2-11) and (2-13) into (2-14), we can obtain an equation for $F^2_{P_j,j}$.

$$F^2_{P_j,j} = \frac{L_j}{\Delta C^{max}_j} \frac{\left(C^2_j - C^1_j\right)}{\left(C^2_j - C^2_{P_j,j}\right)} \frac{\left(C^{max}_{j,in} - C^1_{P_j,j}\right)}{\left(C^1_j - C^1_{P_j,j}\right)} \qquad (2\text{-}15)$$

Replacing first the formula for $F^1_{P_j,j}$ (2-13) and for $F^2_{P_j,j}$ (2-15) into the l.h.s. of (2-9) and simplifying, we obtain

$$\begin{aligned} &F^1_{P_j,j}\left(C^1_{P_j,j} - C^{max}_{j,in}\right) + F^2_{P_j,j}\left(C^2_{P_j,j} - C^{max}_{j,in}\right) = \\ &= \frac{L_j}{\Delta C^{max}_j} \frac{\left(C^2_j - C^{max}_{j,in}\right)\left(C^1_{P_j,j} - C^{max}_{j,in}\right)\left(C^1_j - C^2_{P_j,j}\right)}{\left(C^2_j - C^2_{P_j,j}\right)\left(C^1_j - C^1_{P_j,j}\right)} \end{aligned} \qquad (2\text{-}16)$$

The left-hand side of (2-16) is the same as the left hand side of (2-9). Now, by grid construction we know that,

$C^2_j - C^{max}_{j,in} > 0, C^2_j - C^2_{P_j,j} > 0, C^1_j - C^1_{P_j,j} > 0, C^1_j - C^2_{P_j,j} \geq 0$ *and* $C^1_{P_j,j} - C^{max}_{j,in} \leq 0$.

Then, since $\frac{L_j}{\Delta C^{max}_j} > 0$, (2-9) is proven correct.

2.3.2.1.2 Example 2-1 (continued)

The final design obtained after merging is the one shown in Figure 2-10. Process 6 requires 5.71 ton/h of water at 100 ppm to remove the contaminants. In this case the water has been taken from process 2, but it could has also been taken from process 4, and even from process 3. Since a lot of sources can be used to supply these non-fresh water users, decisions of this type should be mainly based on geographical (distance between processes), preexisting interconnections, equipment volume limitations or any other additional constraint in the design.

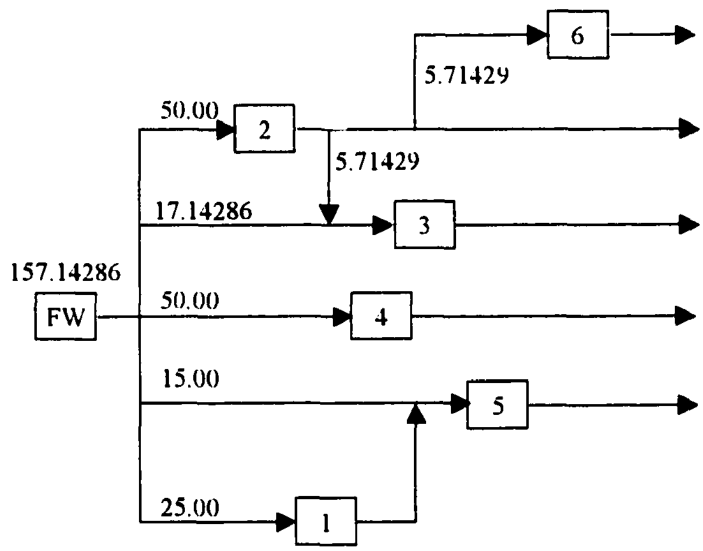


Figure 2-10
Final design of the water network for Example 2-1.

2.3.2.2 Example 2-2

A ten water-using processes system is proposed. Table 2-2 shows the corresponding limiting data for this example problem. Targeting is performed according to Wang and Smith (1994) method. The minimum fresh water target is 166.26667 ton/h.

All three water assignment policies are applied to this example, and three different solution networks are obtained. The design networks and the tables of results are presented below.

Table 2-2: Limiting data for Example 2-2

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Minimum Fresh Water Flowrate without Reuse (ton/h)
1	2.0	25	80	25.0
2	2.88	25	90	32.0
3	4.0	25	200	20.0
4	3.0	50	100	30.0
5	30.0	50	800	37.5
6	5.0	400	800	6.25
7	2.0	200	600	3.3333
8	1.0	0	100	10.0
9	20.0	75	300	66.6667
10	6.5	150	300	21.6667
		Total Minimum Flowrate (ton/h)		**252.4167**

2.3.2.2.1 CASE A: Solution obtained using mixers.

Fresh water is available to fulfill the needs of the first six intervals and is depleted before the needs of process 9 can be fulfilled in interval 7. The total number of interconnections among processes (including the mixer) is 14. Ten of those correspond to connections below the pinch. Figures 2-11 and 2-12 show the preliminary and the final design network respectively.

Table 2-3: Results of CASE A

Process Number	$F_{i,j}$ **(ton/h)**	C_{in} **(ppm)**	**Minimum Fresh Water Flowrate with Reuse (ton/h)**	**Wastewater Flowrate (ton/h)**
1	0.00000	0.00000	25.00000	0.00000
2	0.00000	0.00000	32.00000	0.00000
3	$F_{I,3} = 1.75629$	7.72845	19.04762	0.00000
4	0.00000	0.00000	30.00000	0.00000
5	$F_{I,5} = 9.59446$ $F_{II,5} = 3.73887$	50.00000	26.66667	40.00000
6	$F_{II,6} = 10.0000$	300.00000	0.00000	10.00000
7	$F_{3,7} = 5.00000$	200.00000	0.00000	5.00000
8	0.00	0.00	10.00	0.00000
9	$F_{I,9} = 62.04875$	66.35823	23.55238	0.00000
10	$F_{I,10} = 23.60049$ $F_{3,10} = 15.80392$	135.04387	0.00000	0.00000
Mixer I	$F_{1,I} = 25.00000$ $F_{2,I} = 32.00000$ $F_{4,I} = 30.00000$ $F_{8,I} = 10.00000$	91.54639	0.00000	0.00000
Mixer II	$F_{9,II} = 85.60113$ $F_{10,II} = 39.40441$	300.00000	0.00000	111.26667

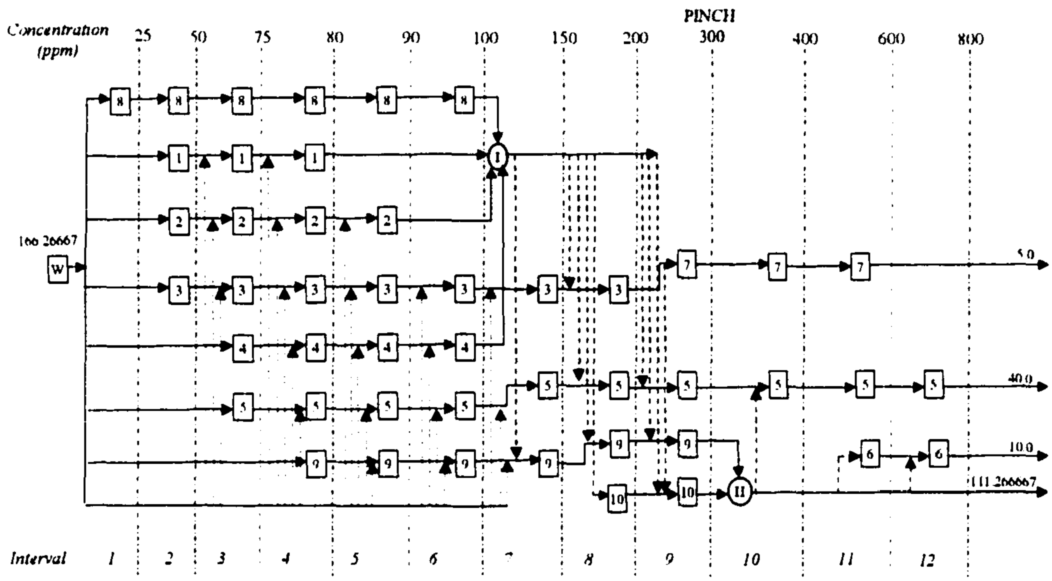


Figure 2-11
Preliminary design for Case A.

A mixer is favored in interval 7 and the water from this mixer is distributed to the rest of the processes below the pinch. A second mixer is created in interval 10 to fulfill the water needs of processes 5 and 6 above the pinch.

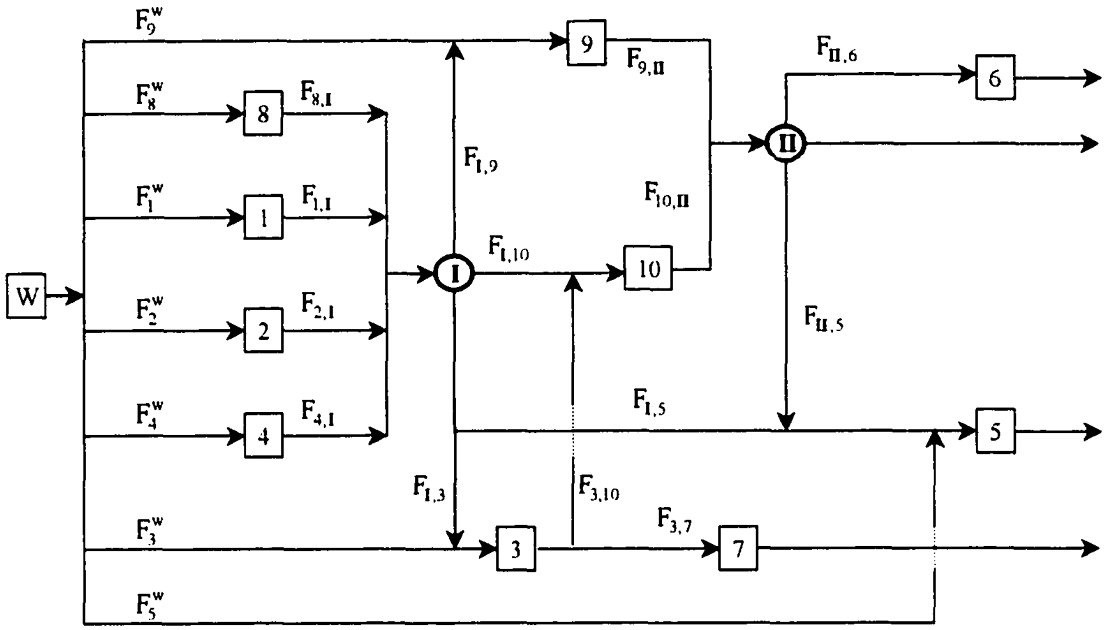


Figure 2-12
Final design for Case A.

2.3.2.2.2 CASE B: Solution obtained assigning the cleanest wastewater first

As in Case A, fresh water is depleted before process 9 can fulfill its requirements in interval 7. Consequently, it receives wastewater from processes 1 and 2 to fulfill its needs in that interval. These precursors are the ones with the lowest concentrations available in interval 7. The total number of interconnections among processes remains the same as in Case A, but the number of them below the pinch has increased in two. Figures 2-13 and 2-14 show the preliminary and the final design network respectively.

Table 2-4: Results of CASE B.

Process Number	$F_{i,j}$ (ton/h)	C_{in} (ppm)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.00000	0.00000	25.00000	0.00000
2	0.00000	0.00000	32.00000	0.00000
3	$F_{2,3} = 1.731602$	7.50000	19.04762	0.00000
4	0.00000	0.00000	30.00	0.00000
5	$F_{2,5} = 6.06061$ $F_{4,5} = 0.95556$ $F_{8,5} = 2.68081$ $F_{9,5} = 3.63636$	50.00000	26.66667	40.00000
6	$F_{9,6} = 10.0000$	300.00000	0.00000	10.00000
7	$F_{3,7} = 5.00000$	200.00000	0.00000	5.00000
8	0.00000	0.00000	10.00000	0.00000
9	$F_{1,9} = 25.00000$ $F_{2,9} = 24.20779$ $F_{4,9} = 7.37778$ $F_{8,9} = 4.37547$	63.35119	23.55238	70.87706
10	$F_{3,10} = 15.77922$ $F_{4,10} = 21.66667$ $F_{8,10} = 2.94372$	139.0675	0.00000	40.38961

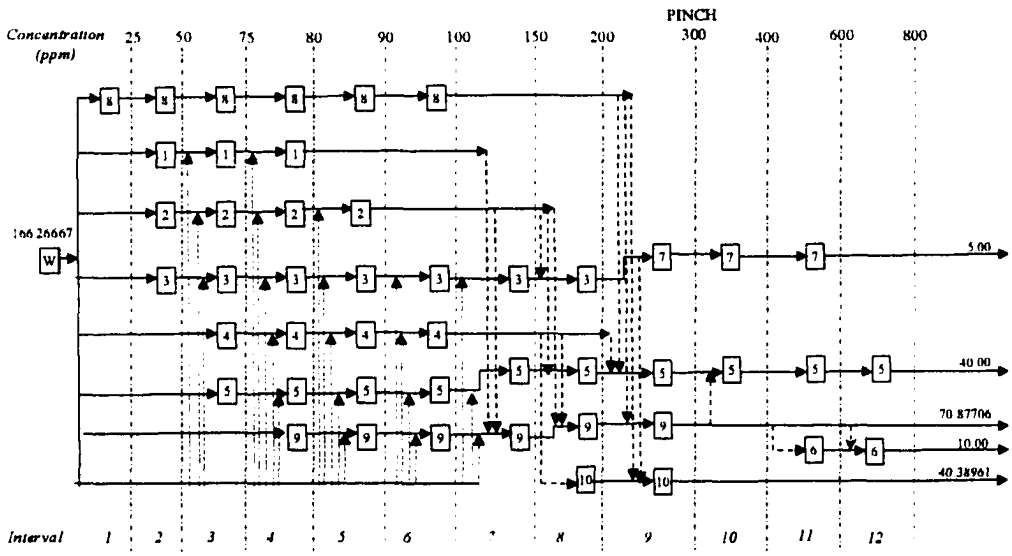


Figure 2-13
Preliminary design of Case B.

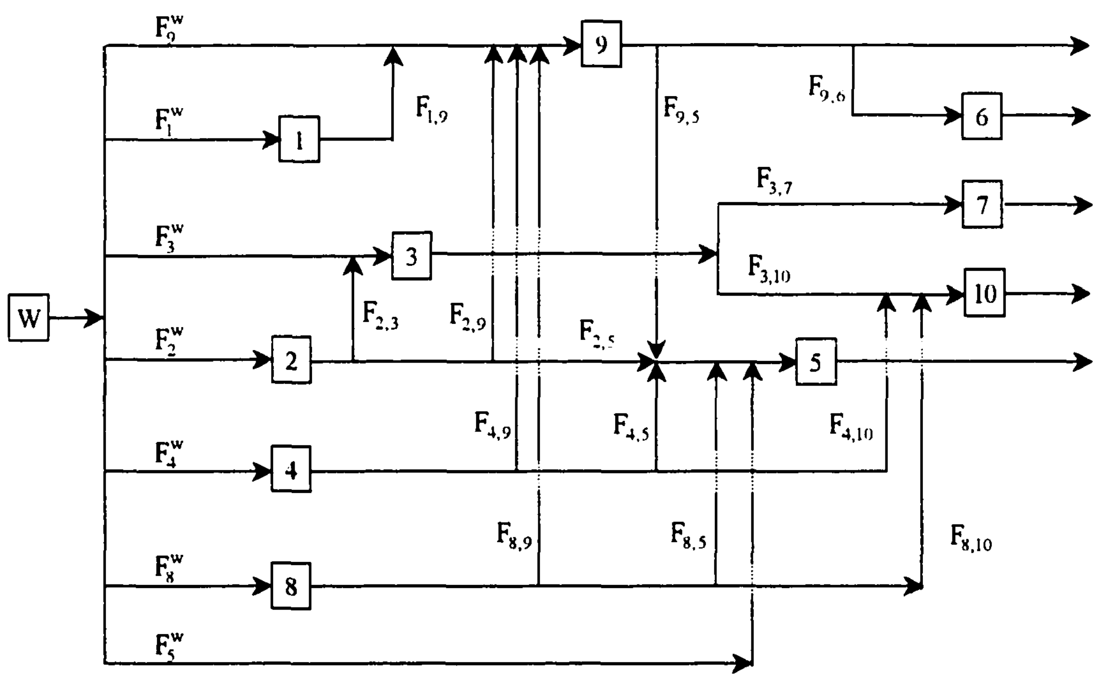


Figure 2-14
Final design for Case B.

2.3.2.2.3 **CASE C:** Reusing the most contaminated wastewater first.

Table 2-5: Results of CASE C

Process Number	$F_{i,j}$ (ton/h)	C_{in} (ppm)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.00000	0.00000	25.00000	0.00000
2	0.00000	0.00000	32.00000	0.00000
3	$F_{2,3} = 1.731602$	7.50000	19.04762	0.00000
4	0.00000	0.00000	30.00	0.00000
5	$F_{2,5} = 6.06061$ $F_{3,5} = 7.27273$	50.00000	26.66667	40.00000
6	$F_{9,6} = 10.0000$	300.00000	0.00000	10.00000
7	$F_{1,7} = 2.27273$ $F_{9,7} = 2.72727$	200.00000	0.00000	5.00000
8	0.00000	0.00000	10.00000	0.00000
9	$F_{2,9} = 21.82395$ $F_{3,9} = 3.51255$ $F_{4,9} = 30.00000$ $F_{8,9} = 10.00000$	75.00000	23.55238	76.16162
10	$F_{1,10} = 22.72727$ $F_{2,10} = 2.38384$ $F_{3,10} = 9.99394$	114.84	0.00000	35.10505

In Case C, the total number of required interconnections has decreased to 13 comparing to the previous cases. Another important observation is that the precursors of the intensive water user, processes 5, 9, and 10, have significantly changed between Cases B and C. Figures 2-15 and 2-16 show the preliminary and the final design network respectively.

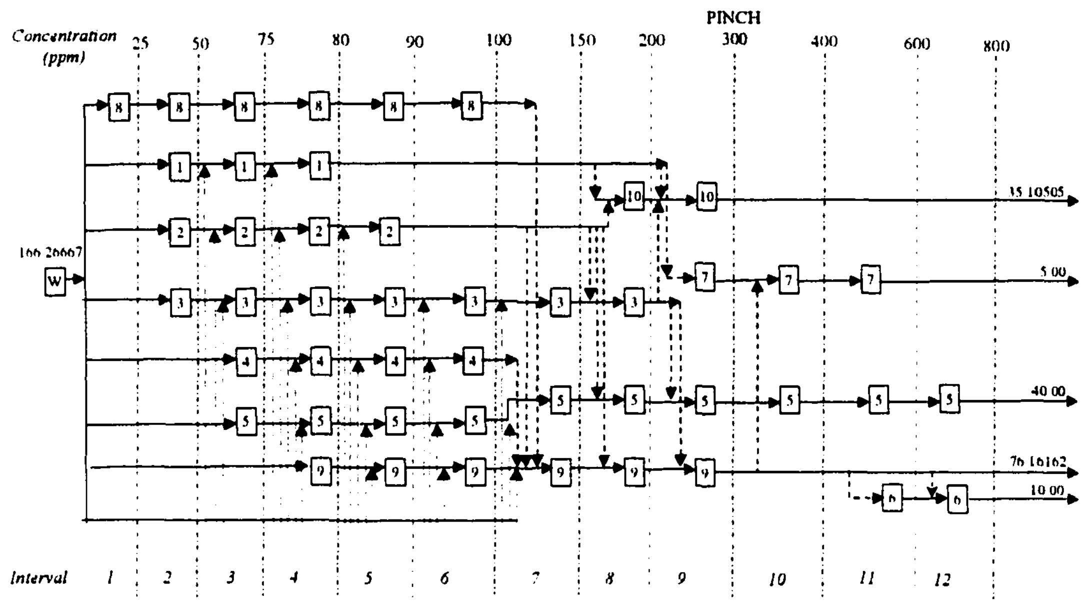


Figure 2-15
Preliminary design of Case C.

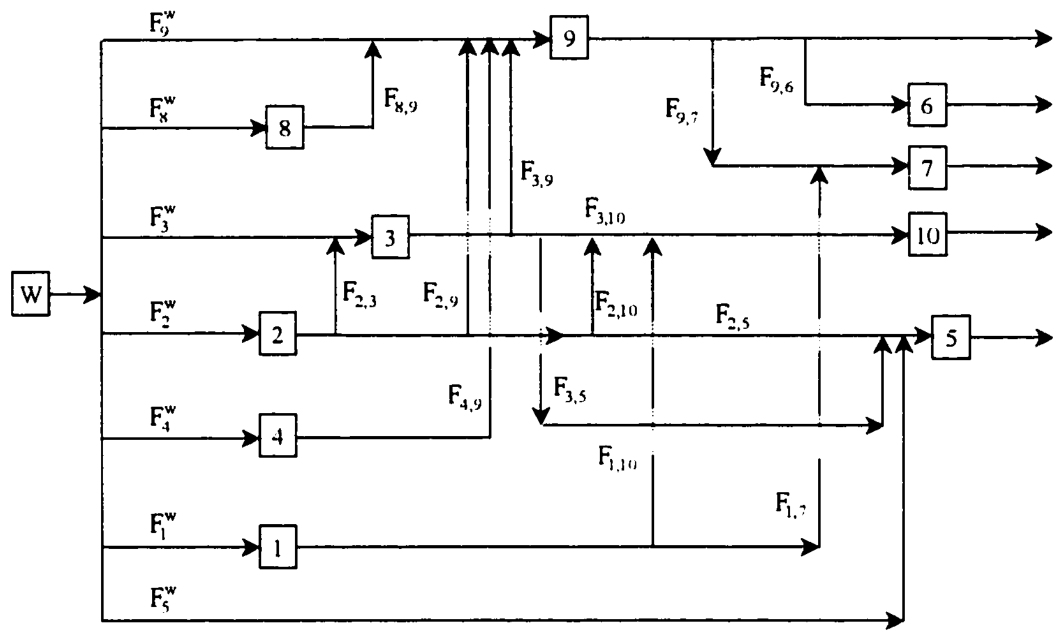


Figure 2-16
Final design for Case C.

2.4 Conclusions

A new design methodology for the solution of the single-contaminant WAP problem has been presented. Several alternatives on how to distribute water among the processes are also discussed. Finally, the application of the new procedure is illustrated through examples. The use of the different water allocation strategies shows that the problem has several alternative solutions. The existence of the above alternative solutions shows that design aspects such as distance between processes, corrosion limitations, control strategies, etc., can be taken into account within the design framework presented.

2.5 Notation

F_j^i	Outlet flowrate of process *j* in interval *i*
F_j^{i-1}	Inlet flowrate of process *j* in interval *i*
$F_{P_j,j}^i$	Water flowrate from precursors P_j of process *j* in interval *i*
$F_{w,j}^i$	Fresh water flowrate entering process *j* in interval *i*
F_j^w	Total fresh water usage of process *j*
$C_{j,in}$	Contaminant concentration in the inlet of process *j*
$C_{j,out}$	Contaminant concentration in the outlet of process *j*
$C_{j,in}^{max}$	Maximum contaminant concentration in the inlet of process *j*
$C_{j,out}^{max}$	Maximum contaminant concentration in the outlet of process *j*
C_j^i	Contaminant concentration of F_j^i
C_j^{i-1}	Contaminant concentration of F_j^{i-1}
$C_{P_j,j}^i$	Contaminant concentration of $F_{P_j,j}^i$
m_j^i	Mass of contaminant to be removed from process *j* in interval *i*
L_j	Total mass load of process *j*

2.6 References

1. Kuo W-C. J. and R. Smith. *Designing for the Interactions between Water-Use and Effluent Treatment*. Trans IChemE, 76, Part A, pp.287-301, 1998.
2. Olesen S.G. and G.T. Polley. *A Simple Methodology for the Design of Water Networks Handling Single Contaminants*. Trans IChemE, 75, part A, pp. 420-426, 1997.
3. Takama N., T. Kuriyama, K. Shiroko and T. Umeda. *Optimal Water Allocation in a Petroleum Refinery*. Comp. & Chem. Eng. 4, 251-258, 1980.
4. Wang Y. P. and R. Smith. *Wastewater Minimization*. CES, 49, 7, pp. 981-1006, 1994.
5. Wang Y.P. and R. Smith. *Wastewater Minimization with Flowrate Constraints*. Trans IChemE, 73, Part A, pp. 889-904, 1995.

CHAPTER 3

On The Necessary Conditions of Optimality of Water Utilization Systems in Refineries and Process Plants

3.1 Introduction

In this chapter, necessary conditions of optimality for the single-contaminant WAP problem are presented. The WAP problem was formally defined in Chapter 2. These conditions will be used as part of a design procedure for the WAP problem, which will be presented in Chapter 4. The necessary conditions are one by one proved in a series of theorems. Some comments are included in the text, but complete examples are analyzed out in a separate section.

Before we discuss the necessary conditions of optimality, some definitions that will be useful later are presented.

3.2 Definitions

The following types of water-using sets and processes can be defined:

***Fresh Water User Processes* (FWU):** Fresh Water User Processes are processes that require fresh water. They may also be consumers of wastewater.

***Wastewater User Processes* (WWU):** Wastewater User Processes are processes that are fed solely by wastewater.

***Head Processes* (H):** Head Process is a special case of a FWU that utilizes only fresh water.

***Intermediate Wastewater User Processes* (I):** Intermediate Wastewater User Processes are processes that are fed by wastewater from other processes and feed other processes with the wastewater they produce.

***Terminal Wastewater User Processes* (T):** Terminal Wastewater User Processes are processes that are fed by wastewater from other processes, but they discharge their wastewater to treatment.

Figure 3-1 illustrates schematically the way these processes are aligned. The set of fresh water users consists of the set **H** and subsets of sets **I** and **T**. Similarly, the set of wastewater users is formed by a subset of **I** and a subset of **T**. That is, not all intermediate and terminal processes use fresh water and/or are solely fed by wastewater.

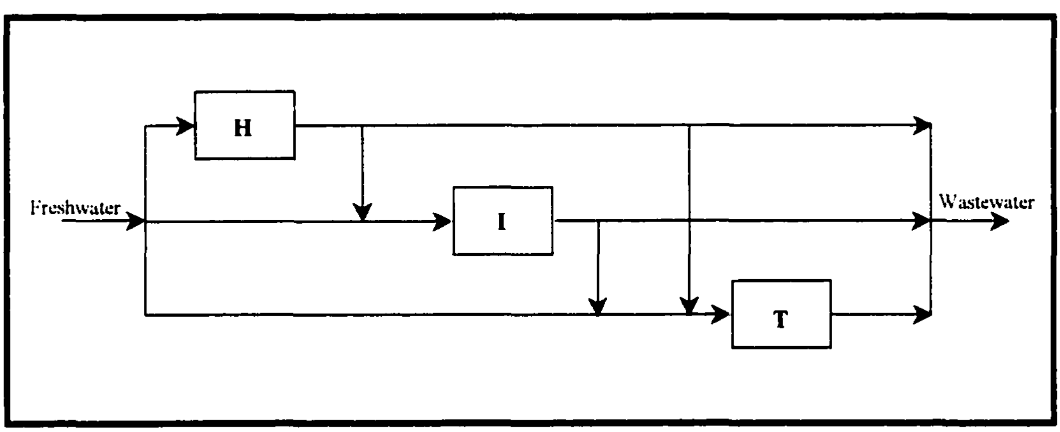


Figure 3-1
Schematic representation of a water network.

We now define the concept of a Set of Precursors and a Set of Receivers.

***Set of Precursors of a Process j* (P_j):** A set of Precursors of a process is the set of all processes that send wastewater to process j.

***Set of Receivers of Process j* (R_j):** A set of receivers of a process is the set of all processes where wastewater from process j is sent.

Finally, the following definitions will help in the presentation of the necessary conditions.

Partial Wastewater Providers (PWP): A Partial Wastewater Provider is a process whose wastewater is partially reused by other processes, that is, a portion of its wastewater is sent directly to treatment.

Total Wastewater Providers (TWP): A Total Wastewater Provider is a process whose wastewater is fully reused by other processes.

3.3 Necessary Conditions of Optimality

The necessary conditions of optimality are presented in a sequence of theorems.

3.3.1 Theorem 3-1: Necessary Condition of Concentration Monotonicity

If a solution to the WAP is optimal, then at every Partial Wastewater Provider (PWP), the outlet concentrations are not lower than the concentration of the combined wastewater stream coming from all the precursors.

In other words, given a process j that satisfies the definition of PWP, that is $F_{j,out} > 0$, then $C_{j,out} \geq C_{P_j,j}$, where $C_{P_j,j}$ is the concentration of the combined wastewater of all the precursors.

Figure 3-2 presents the set of interconnections of interest, omitting other existing that are not of relevant to this case.

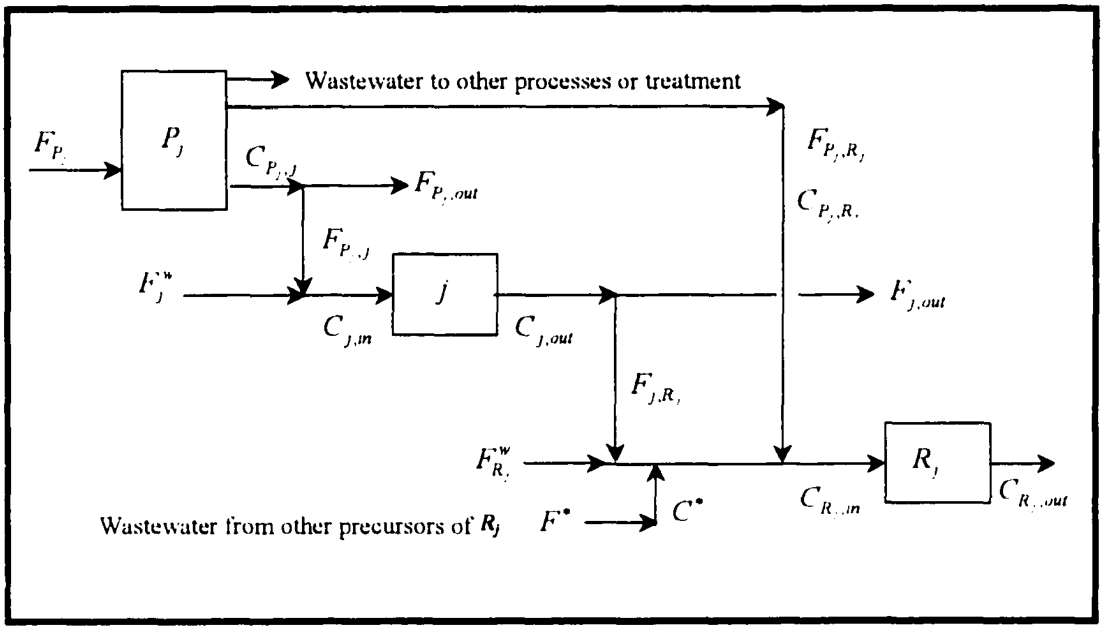


Figure 3-2
Precursors and receivers of process *j*.

Proof:

The proof is by contradiction: Assume that $C_{P_j,j} > C_{j,out}$. A component mass balance over process *j* is:

$$F_{P_j,j} C_{P_j,j} + L_j = (F_{P_j,j} + F_j^w) C_{j,out} \tag{3-1}$$

where L_j is the load of process j. Rewriting (3-1),

$$F_j^w = \frac{L_j}{C_{j,out}} + \left(\frac{C_{P_j,j}}{C_{j,out}} - 1 \right) F_{P_j,j} \tag{3-2}$$

But, by assumption

$$\left(\frac{C_{P_j,j}}{C_{j,out}} - 1 \right) > 0 \tag{3-3}$$

Thus, if $F_{P_j,j}$ (which is positive) is reduced to zero a new fresh water flowrate, $\overline{F}_j^w = \frac{L_j}{C_{j,out}} < F_j^w$ is obtained, contradicting the hypothesis that the original structure is optimal. To complete the proof one only needs to show that such reduction can be performed without altering any conditions downstream.

Two cases are possible:

(a) Process j can still supply all the necessary wastewater to the set $\boldsymbol{R}_j$, that is, $\overline{F}_j^w \geq F_{j,R_j}$. In this case, since no flowrate or concentration perturbation takes place downstream from process j, the theorem is proved.

(b) Process j cannot deliver the same amount of wastewater to the set $\boldsymbol{R}_j$, that is, $\overline{F}_j^w < F_{j,R_j}$. Thus, feasibility conditions downstream of process j need to be restored.

Since it has been proven that the fresh water consumption of process j can be reduced to its minimum by eliminating $F_{P_j,j}$, downstream feasibility may be restored by reusing part or all this available wastewater. Figure 3-3 shows the new situation.

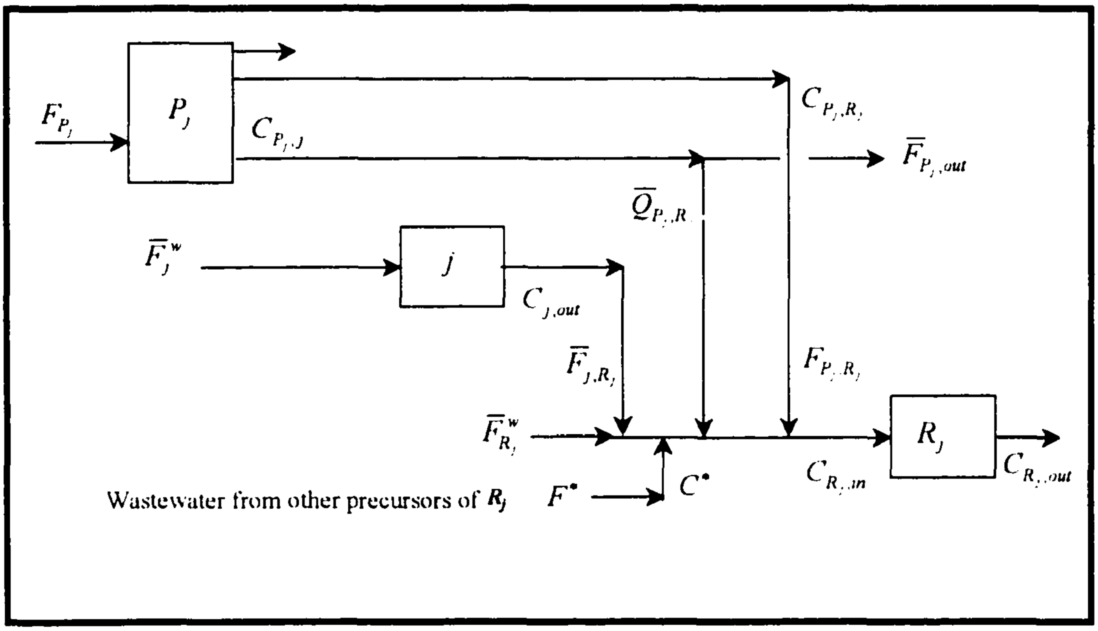


Figure 3-3
Restoring downstream feasibility.

We will now show that:

(b.1) Feasibility can be restored by reusing a flowrate $\overline{Q}_{P_j,R_j}$, which has the same concentration $C_{P_j,j}$.

(b.2) The new flowrate $\overline{Q}_{P_j,R_j}$ does not exceed the previous value used $F_{P_j,j}$. That is $\overline{Q}_{P_j,R_j} \in (0, F_{P_j,j}]$.

(b.3) In this new scheme of flowrates, the overall fresh water intake goes down ($\Delta W < 0$).

(b.1) Since $\overline{F}_j^w < F_{j,R_j}$, all the wastewater available from process j can now be sent to the set $\boldsymbol{R}_j$, resulting in

$$\overline{F}_j^w = \overline{F}_{j,R_j} \tag{3-4}$$

The conditions downstream are not altered only if $C_{R_j,in}$ and the total flowrate feeding the set $\boldsymbol{R}_j$ do not change. Since now process j cannot satisfy the demand, the precursor set $\boldsymbol{P}_j$ can be used as a source of wastewater. The amount needed should satisfy:

$$\begin{aligned} C_{R_j,in} &= \frac{F_{j,R_j} C_{j,out} + F_{P_j,R_j} C_{P_j,R_j} + F^* C^*}{F_{j,R_j} + F_{P_j,R_j} + F_{R_j}^w + F^*} = \\ &\frac{\overline{F}_{j,R_j} C_{j,out} + \overline{Q}_{P_j,R_j} C_{P_j,j} + F_{P_j,R_j} C_{P_j,R_j} + F^* C^*}{\overline{F}_{j,R_j} + \overline{Q}_{P_j,R_j} + F_{P_j,R_j} + \overline{F}_{R_j}^w + F^*} \end{aligned} \tag{3-5}$$

$$F_{j,R_j} + F_{P_j,R_j} + F_{R_j}^w + F^* = \overline{F}_{j,R_j} + \overline{Q}_{P_j,R_j} + F_{P_j,R_j} + \overline{F}_{R_j}^w + F^* \tag{3-6}$$

Using (3-6) to cancel the denominators in both sides of (3-5) and rearranging, we obtain

$$\overline{Q}_{P_j,R_j} = \frac{C_{j,out}}{C_{P_j,j}} F_{j,R_j} - \frac{C_{j,out}}{C_{P_j,j}} \overline{F}_{j,R_j} = \frac{F_{j,R_j} - \overline{F}_{j,R_j}}{\alpha} \tag{3-7}$$

where $\alpha = \dfrac{C_{P_j,j}}{C_{j,out}}$.

(b.2) We now prove that the new wastewater flowrate $\overline{Q}_{P_j,R_j}$ to the set of processes is feasible. Since we have established that downstream conditions are maintained unaltered by keeping inlet conditions at the set $\boldsymbol{R}_j$, unchanged, then the total component flow, $f_{R_j,in}$, that the set $\boldsymbol{R}_j$,is receiving before and after reducing F_j^w to $\overline{F}_j^w$ remains constant as well.

Therefore, we can write:

$$f_{R_j,in} = f_{j,R_j} + f_{P_j,R_j} + F^*C^* = \bar{f}_{j,R_j} + f_{P_j,R_j} + \overline{q}_{P_j,R_j} + F^*C^* \tag{3-8}$$

However, since $\bar{f}_{j,R_j} = L_j$, because only fresh water is now sent to process j, then, after simplifying, we get

$$f_{j,R_j} = L_j + \overline{q}_{P_j,R_j} \tag{3-9}$$

Besides,

$$f_{P_j,j} + L_j \geq f_{j,R_j} \tag{3-10}$$

because $F_{j,out} \geq 0$. Replacing (3-9) in (3-10) we get:

$$f_{P_j,j} + L_j \geq \overline{q}_{P_j,R_j} + L_j \tag{3-11}$$

After canceling L_j from both sides of (3-11) and replacing the component flows by their definitions, we obtain:

$$F_{P_j,j} C_{P_j,j} \geq \overline{Q}_{P_j,R_j}\, C_{P_j,j} \tag{3-12}$$

Consequently,

$$F_{P_j,j} \geq \overline{Q}_{P_j,R_j} \tag{3-13}$$

(b.3) We now prove that the total water intake is lower.

The change in water intake is:

$$\Delta W = \Delta F_{P_j}^{w} + \Delta F_{j}^{w} + \Delta F_{R_j}^{w} \tag{3-14}$$

where $\Delta F_i^{w} = \overline{F}_i^{w} - F_i^{w}$. Replacing $\overline{Q}_{P_j,R_j}$ obtained from (3-6) in (3-7) and rearranging,

$$\overline{F}_{R_j}^{w} - F_{R_j}^{w} = \left(1 - \frac{1}{\alpha}\right)\left(F_{j,R_j} - \overline{F}_{j,R_j}\right) \tag{3-15}$$

Thus, recalling that $\Delta F_{P_j}^{w} = 0$, and $\Delta F_j^{w} = (1-\alpha)F_{P_j,j}$, which can be obtained from (3-2), (3-14) becomes.

$$\Delta W = (1-\alpha)F_{P_j,j} - \left(1 - \frac{1}{\alpha}\right)\left(\overline{F}_{j,R_j} - F_{j,R_j}\right) \tag{3-16}$$

Rearranging

$$\Delta W = (1-\alpha)\left(F_{P_j,j} + \frac{\overline{F}_{j,R_j} - F_{j,R_j}}{\alpha}\right) \tag{3-17}$$

But

$$\overline{F}_{j,R_j} = \overline{F}_j^{w} = F_j^{w} - \Delta F_{P_j,j} = F_j^{w} - (\alpha - 1)F_{P_j,j} \tag{3-18}$$

In turn, using a balance around process j to obtain F_j^{w}, (3-18) can be rewritten as follows:

$$\overline{F}_{j,R_j} = F_{j,R_j} + F_{j,out} - \alpha F_{P_j,j} \tag{3-19}$$

Replacing (3-19) in (3-17) and in virtue that $F_{j,out} > 0$, we obtain:

$$\Delta W = (1-\alpha)\frac{F_{j,out}}{\alpha} < 0 \tag{3-20}$$

Q.E.D.

3.3.1.1 Corollary 1

If for a given process j a solution is optimal and $C_{P_j,j} = C_{j,out}$, then the solution is degenerate in the sense that any wastewater send to process j from its precursors does not alter the total water intake.

Proof:

When $C_{P_j,j} = C_{j,out}$, equation (3-2) states that $L_j = F_j^w C_{j,out}$. That is the interconnection between the set $\boldsymbol{P_j}$ and process j is of no practical use when seeking a decrease in F_j^w.

Q.E.D.

A practical consequence of this corollary is that any optimal design can have different flowrates going through process j. In particular $F_{P_j,j}$ can have any value in the interval $[0, \tilde{F}_{P_j,j}]$ where $\tilde{F}_{P_j,j}$ is the maximum flowrate that process j can admit without violating the inlet concentration constraint. This flowrate $\tilde{F}_{P_j,j}$ is such that the inlet concentration of process j reaches its maximum and can be found as follows:

Perform a component mass balance over process j at the inlet:

$$\widetilde{F}_{P_j,J} C_{P_j,J} = \left(\widetilde{F}_{P_j,J} + F_J^w\right) C_{J,in}^{\max} \quad (3\text{-}21)$$

Rearranging,

$$\widetilde{F}_{P_j,J} = \frac{F_J^w}{\left(\dfrac{C_{P_j,J}}{C_{J,in}^{\max}} - 1\right)} \quad (3\text{-}22)$$

As long as $F_{P_j} \leq \widetilde{F}_{P_j,J}$, then $C_{J,in} \leq C_{J,in}^{\max}$. Repeating (3-21) for generic inlet conditions, we get:

$$F_{P_j,J} C_{P_j,J} = \left(F_{P_j,J} + F_J^w\right) C_{J,in} \quad (3\text{-}23)$$

or after rearranging

$$F_{P_j,J} = \frac{F_J^w}{\left(\dfrac{C_{P_j,J}}{C_{J,in}} - 1\right)} \quad (3\text{-}24)$$

Since $F_{P_j} \leq \widetilde{F}_{P_j,J}$, using (3-22) and (3-24) it is easy to see that $C_{J,in} \leq C_{J,in}^{\max}$. The calculations can be repeated for any other subset of precursors.

Thus, taking a decision on whether to send wastewater through process j or not depends upon the project scope. If designing a new facility one may want to minimize the intake of a particular piece of equipment to reduce its cost if this cost is mostly based on the volume the equipment handles, i.e. a flash tank. But if the equipment size highly depends on separation efficiency, i.e. a stripping column, then a lower inlet concentration could be beneficial and overcome any extra expenditure due to volume oversizing. Another consideration is the number of interconnection and flow controls required when dealing with multiple feeds. Obviously, there exists a trade-off and an optimum situation could lie in an intermediate flowrate, $F_{P_j,j} \in [0, \tilde{F}_{P_j,j}]$. In retrofitting, possibilities may be more stringent because the equipment already exists.

3.3.1.2 Corollary 2

If a process is a TWP, there exist at least one possible optimal solution that satisfies monotonicity.

Proof:

Consider Figure 3-4 (a) where it has been assumed that process j is a TWP $(F_{j,out} = 0)$ and Figure 3-4 (b) that shows a proposed alternative solution. Basically, this alternative solution consists of eliminating the stream of wastewater that is being sent to process j from its precursors, as this is the connection that breaks monotonicity. A new connection is added where part (or all) the wastewater formerly sent to process j is now sent to its receivers.

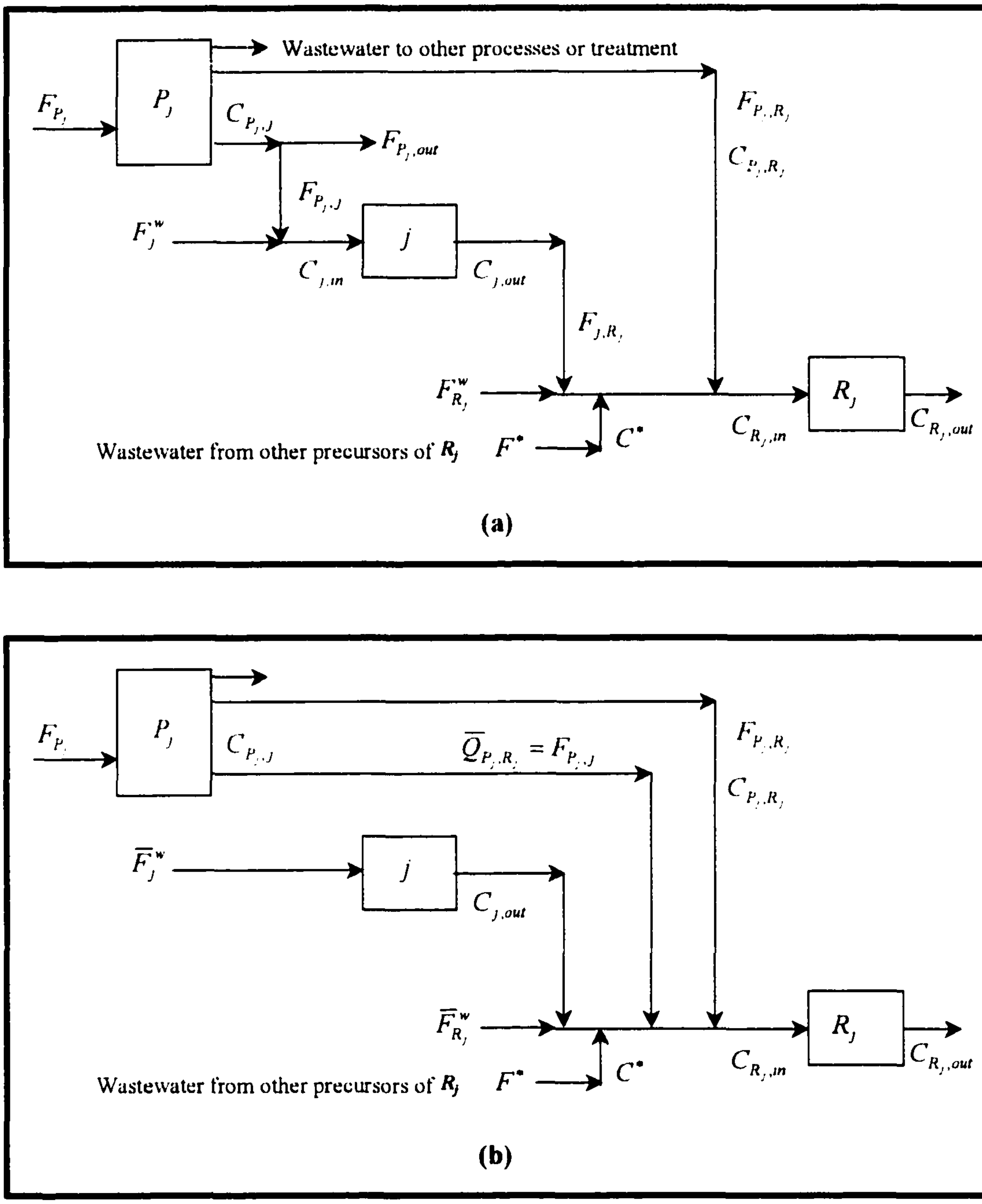


Figure 3-4
(a) Process j as a TWP. **(b)** Monotonicity restoration.

From (b.1) and (b.2) (Theorem 1) there exist a $\overline{Q}_{P_j,R_j}$ with concentration $C_{P_j,J}$ that can be sent to the set $\boldsymbol{R}_j$ while maintaining feasibility. In addition, it was proved that $\overline{Q}_{P_j,R_j} \in \left(0, F_{P_j,J}\right]$.

We now determine $\overline{Q}_{P_j,R_j}$. Since the total flowrate at the inlet of the set $\boldsymbol{R}_j$ stays constant, equate the total flowrate at inlet $\boldsymbol{R}_j$ before and after monotonicity restoration, that is:

$$F_{P_j,J} + F_J^w + F_{R_j}^w + F_{P_j,R_j} + F^* = \overline{F}_J^w + \overline{F}_{R_j}^w + F_{P_j,R_j} + F^* + \overline{Q}_{P_j,R_j} \tag{3-25}$$

After canceling common terms and rearranging, we obtain:

$$F_{P_j,J} = \left[\left(\overline{F}_J^w - F_J^w\right) + \left(\overline{F}_{R_j}^w - F_{R_j}^w\right)\right] + \overline{Q}_{P_j,R_j} \tag{3-26}$$

By definition of ΔW:

$$F_{P_j,J} = \Delta W + \overline{Q}_{P_j,R_j} \tag{3-27}$$

From (3-20), $\Delta W = 0$ then $\overline{Q}_{P_j,R_j} = F_{P_j,J}$.

In conclusion, we have proven that by making $\overline{Q}_{P_j,R_j} = F_{P_j,J}$ the alternative solution is not only optimal but also monotone.

Q.E.D.

We will now prove that if a solution of the WAP problem is optimal then all FWU processes have reached their maximum possible outlet concentration. A third possibility is that they constitute a degenerate solution for which an equivalent one with at least one concentration at its maximum exists. This will be covered in the corollaries.

Three theorems, each corresponding to a different type of FWU process, are used to prove this necessary condition.

3.3.2 Theorem 3-2: Necessary Condition of Maximum Concentration for Head Processes.

If a solution of the WAP problem is optimal, then the outlet concentration of a Partial Provider Head Process is equal to its maximum.

Proof:

We will prove the theorem by contradiction: Consider a head process h. Assume $C_{h,out} < C_{h,out}^{\max}$. Then, since the load L_h is constant we have

$$L_h = F_h^w \, C_{h,out} = \overline{F}_h^w \, C_{h,out}^{\max} \tag{3-28}$$

where $\overline{F}_h^w$ is the flowrate of water corresponding to the $C_{h,out}^{\max}$. Therefore

$$\overline{F}_h^w = \frac{C_{h,out}}{C_{h,out}^{\max}} F_h^w < F_h^w \tag{3-29}$$

Thus, the water intake can be reduced in the case where water is not reused.

In the case where the water is reused downstream, (3-29) still constitutes a proof if one is able to show that after the reduction, the conditions downstream remain feasible. Figure 3-5 shows downstream reuse of a head process wastewater outlet. For this purpose, consider the flowrate F_{h,R_h} from process h to a set of its receivers. Assume that these flowrates and the corresponding fresh water intake flowrates $F_{R_h}^w$ are changed so that the concentrations $C_{R_h,in}$ and the incoming flowrate to the set $\boldsymbol{R_h}$ remain constant.

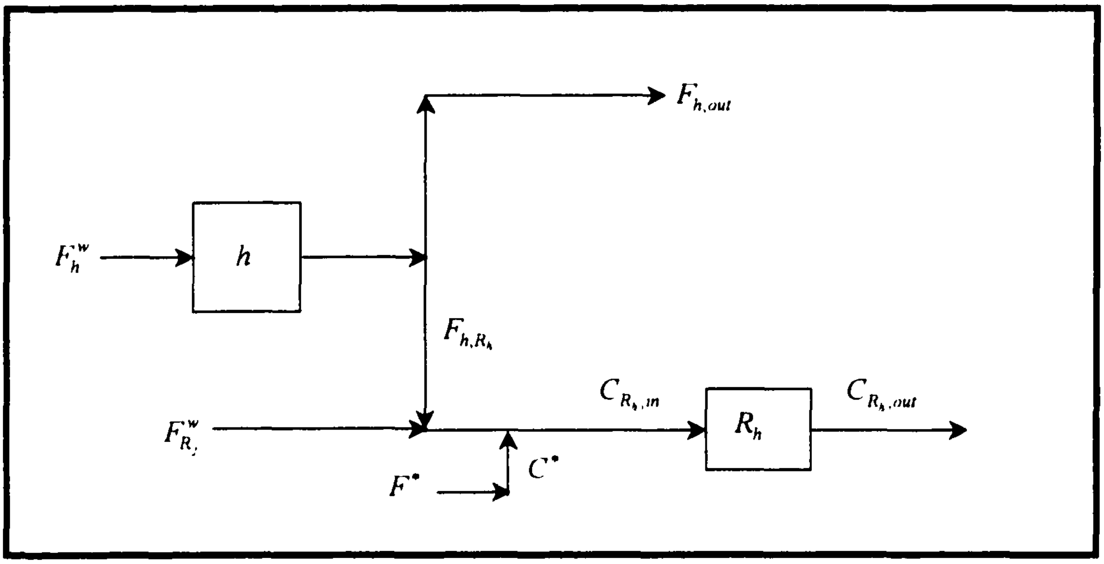


Figure 3-5
A head process and its receivers.

The original and new sets need to satisfy the following relations:

$$F_{h,R_h} C_{h,out} + F^* C^* = C_{R_h,in} (F_{h,R_h} + F_{R_h}^w + F^*) \tag{3-30}$$

$$\overline{F}_{h,R_h} C_{h,out}^{\max} + F^* C^* = C_{R_h,in} (\overline{F}_{h,R_h} + \overline{F}_{R_h}^w + F^*) \tag{3-31}$$

$$F_{h,R_h} + F_{R_h}^w + F^* = \overline{F}_{h,R_h} + \overline{F}_{R_h}^w + F^* \tag{3-32}$$

From (3-29) one obtains

$$\overline{F}_h^w - F_h^w = -(1-\beta) F_h^w \tag{3-33}$$

where $\beta = \dfrac{C_{h,out}}{C_{h,out}^{\max}}$. Dividing equation (3-31) by equation (3-30) and using (3-32) one also obtains:

$$\overline{F}_{h,R_h} = \beta\, F_{h,R_h} \tag{3-34}$$

We now substitute (3-29) and (3-31) in the definition of $\overline{F}_{h,out}$, as follows:

$$\overline{F}_{h,out} = \overline{F}_h^w - \overline{F}_{h,R_h} = \beta\,(F_h^w - F_{h,R_h}) = \beta\, F_{h,out} \tag{3-35}$$

from which we conclude that the new water consumption pattern is feasible.

Substituting (3-34) into (3-32) and rearranging,

$$\overline{F}_{R_h}^w - F_{R_h}^w = (1-\beta)\, F_{h,R_h} \tag{3-36}$$

The total difference in fresh water flowrate between the proposed solution and the new one is:

$$\Delta W = \left(\overline{F}_h^w - F_h^w\right) + \left(\overline{F}_{R_h}^w - F_{R_h}^w\right) \tag{3-37}$$

Substituting (3-33) and (3-36) into (3-37),

$$\Delta W = -(1-\beta)\, F_h^w + (1-\beta) F_{h,R_h} = (1-\beta)\left(F_{h,R_h} - F_h^w\right) \tag{3-38}$$

Since:

$$F_{h,R_h} - F_h^w = -F_{h,out} \le 0 \tag{3-39}$$

Then,

$$\Delta W = -(1-\beta)\, F_{h,out} \tag{3-40}$$

When $F_{h,out} \neq 0$, then $\Delta W < 0$ (because $\beta < 1$), which contradicts the assumption of optimality. The case $F_{h,out} = 0$ constitutes total reuse and is not covered by the theorem.

Q.E.D.

3.3.2.1 Corollary 1

If a Head Process *h* is optimal and is a Total Wastewater Provider (i.e., $F_{h,out} = 0$), then any solution having $C_{h,out} \in \left[C_{R_h,in}, C_{h,out}^{\max}\right]$ is also optimal with the same fresh water intake.

Proof:

When $F_{h,out} = 0$, by (3-40) we have $\Delta W = 0$. This means that a degenerate solution has been found. When the set of receivers is a unique process then any fresh water intake leading to an outlet concentration $C_{in,R_h} \leq C_{h,out} \leq C_{h,out}^{\max}$ changes the wastewater sent to the receivers. Conditions downstream are such that the water intake of the receivers maintains the total water intake constant.

Remark: Although it may look apparent that values of $C_{h,out} < C_{R_h,in}$ could be used, this cannot be done because that would require a change in the downstream feasibility conditions and therefore in the theorem proof.

Q.E.D.

3.3.3 Theorem 3-3: Necessary Condition of Maximum Concentration for Intermediate Processes.

If the solution of the WAP problem is optimal then the outlet concentration of an Intermediate Process reaches its maximum.

Proof:

Assume that neither $C_{j,in}$ nor $C_{j,out}$ are at their maximum possible values, that is $C_{j,in} < C_{j,in}^{\max}$ and $C_{j,out} < C_{j,out}^{\max}$.

Consider the set of processes $\boldsymbol{P_j}$. These processes are precursors of j, but they are also precursors of $\boldsymbol{R_j}$ and other processes. We define $\hat{F}_{P_j}$ as the sum of the water sent to j; in addition, the portion sent to treatment, that is $\hat{F}_{P_j} = F_{P_j,out} + F_{P_j,j}$.

Consider using thus total flowrate as feed to process j. Consider at the same time an adjustment of the fresh water sent to process j so that the outlet concentration remains the same. To do this, assume a new inlet concentration for process j. Then, the following holds:

$$\hat{C}_{j,in} = \frac{\hat{F}_{P_j} C_{P_j,j}}{\hat{F}_{P_j} + \hat{F}_j^w} \tag{3-41}$$

$$L_j = (\hat{F}_{P_j} + \hat{F}_j^w)(C_{j,out} - \hat{C}_{j,in}) \tag{3-42}$$

We recognize two conditions:

CASE I: $\hat{C}_{j,in} \geq C_{j,in}^{\max}$. In this case, we will prove the theorem by first proving that the inlet concentration of process j can be made equal to its maximum, with a reduction of the water intake of process j. Finally we will show that the total fresh water intake of the system can be lowered by maximizing the outlet concentration of process j.

CASE II: $\hat{C}_{j,in} < C_{j,in}^{\max}$. In this case, we will prove that the outlet concentration of process j can be made equal to its maximum, with a reduction of the total water intake.

3.3.3.1 CASE I: Inlet Concentration Binding Condition.

In this case, starting from (3-42)

$$\begin{aligned} L_j &= (\hat{F}_{P_i} + \hat{F}_j^{w})(C_{j,out} - \hat{C}_{j,in}) \leq (\hat{F}_{P_i,j} + \hat{F}_j^{w})(C_{j,out} - C_{j,in}^{\max}) = \\ &= \frac{\hat{F}_{P_i,j}\, C_{P_i,j}}{\hat{C}_{j,in}}(C_{j,out} - C_{j,in}^{\max}) \leq \frac{\hat{F}_{P_i,j}\, C_{P_i,j}}{C_{j,in}^{\max}}(C_{j,out} - C_{j,in}^{\max}) \end{aligned} \tag{3-43}$$

Therefore,

$$\left(\frac{C_{j,out}}{C_{j,in}^{\max}} - 1\right) \geq \frac{L_j}{\hat{F}_{P_i} C_{P_i,j}} \tag{3-44}$$

which is an inequality that will be useful later.

We will prove that the water consumption can be reduced by increasing $F_{P_i,j}$ until the maximum inlet concentration is reached, while maintaining $C_{j,out}$ constant.

Since $$C_{j,in} < C_{j,in}^{\max} \tag{3-45}$$

then an increase in $F_{P_j,j}$ will increase $C_{j,in}$.

Now $F_{P_j,out} > 0$, otherwise, by (3-44) the inlet concentration to process j would be violating the constraint. Therefore, the increase in $F_{P_j,j}$ is feasible. Let the new flowrates be $\overline{F}_{P_j,j}$ and $\overline{F}_j^w$.

From a balance in the inlet node, we obtain:

$$C_{j,in}^{\max} = \frac{\overline{F}_{P_j,j}\, C_{P_j,j}}{\overline{F}_{P_j,j} + \overline{F}_j^w} \tag{3-46}$$

In addition a component balance on process j gives:

$$C_{j,out} = \frac{\overline{F}_{P_j,j}\, C_{P_j,j} + L_j}{\overline{F}_{P_j,j} + \overline{F}_j^w} \tag{3-47}$$

Divide (3-47) by (3-46)

$$\frac{C_{j,out}}{C_{j,in}^{\max}} = \frac{\overline{F}_{P_j,j}\, C_{P_j,j} + L_j}{\overline{F}_{P_j,j}\, C_{P_j,j}} = \left(1 + \frac{L_j}{\overline{F}_{P_j,j}\, C_{P_j,j}}\right) \tag{3-48}$$

Rearranging:

$$\overline{F}_{P_j,j} = \frac{L_j}{C_{P_j,j}} \frac{1}{\left(\dfrac{C_{j,out}}{C_{j,in}^{\max}} - 1\right)} \tag{3-49}$$

Repeating the same procedure for the original conditions one obtains:

$$F_{P_j J} = \frac{L_J}{C_{P_j,J}} \frac{1}{\left(\frac{C_{J,out}}{C_{J,in}} - 1\right)} \tag{3-50}$$

and since $C_{J,in} < C_{J,in}^{\max}$, we obtain

$$F_{P_j J} < \overline{F}_{P_j J} \tag{3-51}$$

Also, rearranging (3-47)

$$\overline{F}_J^w = \overline{F}_{P_j J} \left(\frac{C_{P_j,J}}{C_{J,in}^{\max}} - 1\right) \tag{3-52}$$

Similarly,

$$F_J^w = F_{P_j J} \left(\frac{C_{P_j,J}}{C_{J,in}} - 1\right) \tag{3-53}$$

Finally, substituting (3-49) into (3-52) we obtain

$$\overline{F}_J^w = \frac{L_J}{C_{P_j,J}} \frac{\left(\frac{C_{P_j,J}}{C_{J,in}^{\max}} - 1\right)}{\left(\frac{C_{J,out}}{C_{J,in}^{\max}} - 1\right)} \tag{3-54}$$

Similarly, using a set of balances for the assumed optimal condition the following is obtained

$$F_J^w = \frac{L_J}{C_{P_j,J}} \frac{\left(\frac{C_{P_j,J}}{C_{J,in}} - 1\right)}{\left(\frac{C_{J,out}}{C_{J,in}} - 1\right)} \tag{3-55}$$

We will now prove that $\bar{F}_j^w < F_j^w$ by analyzing the r.h.s. of (3-54) and (3-55).

Multiply both sides of $C_{j,in} < C_{j,in}^{\max}$ by $\left(C_{P_j,j} - C_{j,out}\right)$,

$$(C_{P_j,j} - C_{j,out})C_{j,in} > (C_{P_j,j} - C_{j,out})C_{j,in}^{\max} \tag{3-56}$$

The sign of the inequality changed as $\left(C_{P_j,j} - C_{j,out}\right) < 0$ by the necessary condition of monotonicity. Rearranging

$$C_{P_j,j}C_{j,in} + C_{j,out}C_{j,in}^{\max} > C_{P_j,j}C_{j,in}^{\max} + C_{j,out}C_{j,in} \tag{3-57}$$

Change signs and add $C_{P_j,j}C_{j,out} + C_{j,in}C_{j,in}^{\max}$ to both sides to obtain

$$\begin{aligned} &C_{P_j,j}C_{j,out} - C_{P_j,j}C_{j,in} - C_{j,out}C_{j,in}^{\max} + C_{j,in}C_{j,in}^{\max} < \\ &< C_{P_j,j}C_{j,out} - C_{P_j,j}C_{j,in}^{\max} - C_{j,out}C_{j,in} + C_{j,in}C_{j,in}^{\max} \end{aligned} \tag{3-58}$$

Further manipulation gives:

$$(C_{P_j,j} - C_{j,in}^{\max})(C_{j,out} - C_{j,in}) < (C_{P_j,j} - C_{j,in})(C_{j,out} - C_{j,in}^{\max}) \tag{3-59}$$

However $\left(C_{j,out} - C_{j,in}^{\max}\right)$ is positive because of (3-44). Then we obtain:

$$\frac{(C_{P_j,j} - C_{j,in}^{\max})}{(C_{j,out} - C_{j,in}^{\max})} < \frac{(C_{P_j,j} - C_{j,in})}{(C_{j,out} - C_{j,in})} \tag{3-60}$$

or

$$\frac{\left(\dfrac{C_{P_j,j}}{C_{j,in}^{\max}} - 1\right)}{\left(\dfrac{C_{j,out}}{C_{j,in}^{\max}} - 1\right)} < \frac{\left(\dfrac{C_{P_j,j}}{C_{j,in}} - 1\right)}{\left(\dfrac{C_{j,out}}{C_{j,in}} - 1\right)} \tag{3-61}$$

Using (3-61) one can compare (3-54) and (3-55) and conclude that $\bar{F}_j^w < F_j^w$.

To complete the proof it is necessary to prove that:

a) $\overline{F}_{P_j,out} \geq 0$, which is part of the assumption made at the beginning of the proof.

b) $\overline{F}_{j,R_j} = F_{j,R_j}$ is feasible, that is, the conditions downstream do not need to change. In other words, a reduction in fresh water to process j, does not reduce the outlet of this process below what it was sent to its receivers.

<u>Part a</u>: $\overline{F}_{P_j,out} \geq 0$

From (3-49)

$$\frac{L_j}{C_{P_j,j}} = \overline{F}_{P_j,j}\left(\frac{C_{j,out}}{C_{j,in}^{\max}} - 1\right) \tag{3-62}$$

Substituting in (3-44)

$$\frac{\overline{F}_{P_j,j}}{\hat{F}_{P_j}} \leq 1 \tag{3-63}$$

which completes the proof.

<u>Part b</u>: $\overline{F}_{j,R_j} = F_{j,R_j}$ is feasible.

A component mass balance over process j reads:

$$F_j\, C_{j,out} = L_j + F_{P_j,j} C_{P_j,j} \tag{3-64}$$

$$\overline{F}_j\, C_{j,out} = L_j + \overline{F}_{P_j,j} C_{P_j,j} \tag{3-65}$$

Subtracting equation (3-64) from equation (3-65) and dividing by $C_{j,out}$

$$\left(\overline{F}_j - F_j\right) = \left(\overline{F}_{P_j,j} - F_{P_j,j}\right)\frac{C_{P_j,j}}{C_{j,out}} \tag{3-66}$$

Since $\left(\overline{F}_{P_j,j} - F_{P_j,j}\right) > 0$, then $\left(\overline{F}_j - F_j\right) > 0$. Therefore, F_{j,R_j} can be always kept constant by increasing $F_{j,out}$.

To complete the proof we need to show that the maximum outlet concentration of process j can be reached and that this will produce a fresh water intake reduction.

The increase in outlet concentration need to be accompanied by new conditions to maintain feasibility downstream at the inlet of the receivers from process j. This can be obtained by keeping both $C_{R_j,in}$ and F_{R_j} constant while proving that there will be sufficient wastewater for reuse, that is $\overline{\overline{F}}_j^w + \overline{\overline{F}}_{P_j,j} \geq \overline{\overline{F}}_{j,R_j}$. The fresh water decrease can be achieved by reducing $\overline{F}_{P_j,j}$ and $\overline{F}_j^w$ simultaneously. To guarantee that the overall fresh water consumption will be reduced the excess availability at process j, defined as $\left(\overline{F}_{P_j,j} - \overline{\overline{F}}_{P_j,j}\right)$, will be bypassed to the set $\boldsymbol{R}_j$ The new situation is shown in Figure 3-6.

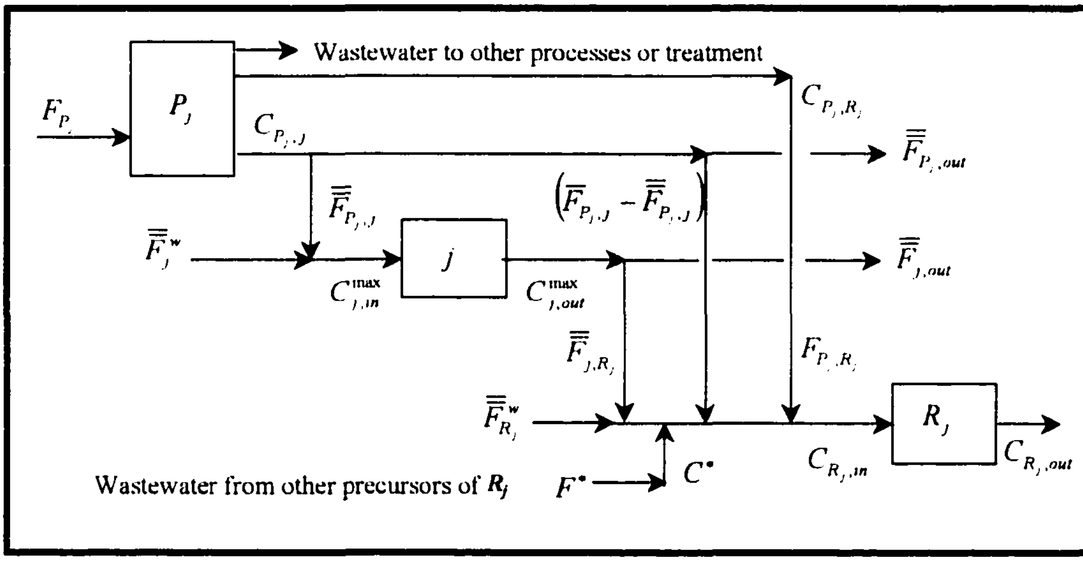


Figure 3-6
Optimal water allocation structure.

Now, from (3-49) we can write,

$$\bar{\bar{F}}_{P_j,j} = \frac{L_j}{C_{P_j,j}} \frac{1}{\left(\dfrac{C_{j\,out}^{max}}{C_{j,in}^{max}} - 1\right)} \tag{3-67}$$

Comparing (3-49) and (3-67) it clearly turns out that $\bar{\bar{F}}_{P_j,j} < \bar{F}_{P_j,j}$.

The new fresh water supply to process j, $\bar{\bar{F}}_j^w$, can be calculated using equation (3-52), that is:

$$\bar{\bar{F}}_j^w = \bar{\bar{F}}_{P_j,j}\left(\frac{C_{P_j j}}{C_{j,in}^{max}} - 1\right) < \bar{F}_j^w \tag{3-68}$$

All we need to show now is that these fresh water savings are not overcome by any necessary increased in $F_{R_j}^w$.

Consider a component mass balance of process j at outlet conditions before and after the fresh water reduction.

$$C_{j,out}\left(\bar{F}_{P_j,j} + \bar{F}_j^{w}\right) = \bar{F}_{P_j,j} C_{P_j,j} + L_j \tag{3-69}$$

$$C_{j,out}^{\max}\left(\bar{\bar{F}}_{P_j,j} + \bar{\bar{F}}_j^{w}\right) = \bar{\bar{F}}_{P_j,j} C_{P_j,j} + L_j \tag{3-70}$$

Equating (3-69) and (3-70) by L_j and rearranging, we obtain:

$$\bar{\bar{F}}_j^{w} = \alpha\, \bar{F}_{P_j,j} + \alpha\, \bar{F}_j^{w} - \bar{\bar{F}}_{P_j,j} - \beta\left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right) \tag{3-71}$$

where $\alpha = \dfrac{C_{j,out}}{C_{j,out}^{\max}}$ and $\beta = \dfrac{C_{P_j,j}}{C_{j,out}^{\max}}$.

Then,

$$\Delta F_j^{w} = \bar{\bar{F}}_j^{w} - \bar{F}_j^{w} = \alpha\, \bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j} - \beta\left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right) - (1-\alpha)\bar{F}_j^{w} \tag{3-72}$$

Downstream feasibility is maintained by:

$$C_{R_j,in} = \frac{\bar{F}_{j,R_j} C_{j,out} + F_{P_j,R_j} C_{P_j,R_j} + F^{*}C^{*}}{\bar{F}_{j,R_j} + F_{P_j,R_j} + F^{*} + \bar{F}_{R_j}^{w}} =$$

$$= \frac{\bar{\bar{F}}_{j,R_j} C_{j,out}^{\max} + F_{P_j,R_j} C_{P_j,R_j} + F^{*}C^{*} + \left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right) C_{P_j,j}}{\bar{\bar{F}}_{j,R_j} + F_{P_j,R_j} + F^{*} + \bar{\bar{F}}_{R_j}^{w} + \left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right)} \tag{3-73}$$

and

$$\bar{F}_{j,R_j} + F_{P_j,R_j} + F^{*} + \bar{F}_{R_j}^{w} = \bar{\bar{F}}_{j,R_j} + F_{P_j,R_j} + F^{*} + \bar{\bar{F}}_{R_j}^{w} + \left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right) \tag{3-74}$$

Simplifying common terms on both sides of (3-74), we get

$$\bar{F}_{j,R_j} + \bar{F}_{R_j}^{w} = \bar{\bar{F}}_{j,R_j} + \bar{\bar{F}}_{R_j}^{w} + \left(\bar{F}_{P_j,j} - \bar{\bar{F}}_{P_j,j}\right) \tag{3-75}$$

Using (3-74) in (3-73) and simplifying, we obtain

$$\overline{\overline{F}}_{J,R_j} = \alpha\,\overline{F}_{J,R_j} - \beta\left(\overline{F}_{P_j,J} - \overline{\overline{F}}_{P_j,J}\right) \tag{3-76}$$

Using (3-75) and (3-76) we can write:

$$\Delta F_{R_j}^{w} = \overline{\overline{F}}_{R_j}^{w} - \overline{F}_{R_j}^{w} = (1-\alpha)\overline{F}_{J,R_j} - (1-\beta)\left(\overline{F}_{P_j,J} - \overline{\overline{F}}_{P_j,J}\right) \tag{3-77}$$

Finally, combining (3-72) and (3-77), we obtain

$$\Delta W = \Delta F_J^{w} + \Delta F_{R_j}^{w} = (1-\alpha)\left(\overline{F}_{J,R_j} - \overline{F}_J^{w} - \overline{F}_{P_j,J}\right) \le 0 \tag{3-78}$$

To finish the proof we need to show that under the new conditions there is enough wastewater to send from process j to the set of processes $\boldsymbol{R}_j$. That is, $\overline{\overline{F}}_J^{w} + \overline{\overline{F}}_{P_j,J} \ge \overline{\overline{F}}_{J,R_j}$.

A total mass balance on process j reads:

$$\overline{F}_J^{w} + \overline{F}_{P_j,J} = \overline{F}_{J,R_j} + \overline{F}_{J,out} \tag{3-79}$$

Then, we can write that

$$\overline{F}_J^{w} + \overline{F}_{P_j,J} \ge \overline{F}_{J,R_j} \tag{3-80}$$

Adding $\overline{\overline{F}}_{P_j,J}$ to both sides of (3-71) and rearranging, we obtain

$$\overline{\overline{F}}_J^{w} + \overline{\overline{F}}_{P_j,J} + \beta\left(\overline{F}_{P_j,J} - \overline{\overline{F}}_{P_j,J}\right) = \alpha\left(\overline{F}_{P_j,J} + \overline{F}_J^{w}\right) \tag{3-81}$$

Multiplying both sides of equation (3-80) by α and comparing with (3-81), we can write

$$\overline{\overline{F}}_J^{w} + \overline{\overline{F}}_{P_j,J} + \beta\left(\overline{F}_{P_j,J} - \overline{\overline{F}}_{P_j,J}\right) \ge \alpha\,\overline{F}_{J,R_j} \tag{3-82}$$

Finally, by (3-76) we obtain $$\overline{\overline{F}}_j^{\,w} + \overline{\overline{F}}_{P_j,j} \geq \overline{\overline{F}}_{j,R_j} \tag{3-83}$$

Q.E.D.

3.3.3.1.1 Corollary 1

If an Intermediate Process j is a Total Wastewater Provider, then any solution having $C_{j,out} \in \left[C_{R_j,in}, C_{j,out}^{\max}\right]$ is also optimal with the same fresh water intake.

Proof:

When process j is a TWP then $\overline{F}_{j,out} = 0$, by (3-78) we have $\Delta W = 0$. This means that a degenerate solution has been found.

Q.E.D.

3.3.3.1.2 Corollary 2

In CASE I, it is also a necessary condition of optimality that the Intermediate Process j reaches its inlet maximum concentration.

Proof:

Assume the starting solution is such that the outlet concentration of process j is already at its maximum. Then, following exactly the same proof as depicted by (3-45) through (3-61) but replacing $C_{j,out}^{\max}$ by $C_{j,out}$, $C_{j,in}^{\max}$ can be reached without altering $C_{j,out}^{\max}$. The latter added to the fact that F_{j,R_j} can be kept constant (as shown in part b) guarantees downstream feasibility.

Q.E.D.

3.3.3.2 CASE II: Outlet Concentration Binding Condition

$$\left(\frac{C_{j,out}}{C_{j,in}^{\max}}-1\right)<\frac{L_j}{\hat{F}_{P_j}C_{P_j,j}} \tag{3-84}$$

In this case, an increase in $F_{P_j,j}$ to increase $C_{j,in}$ to its maximum is not possible without violating feasibility.

Assume that $F_{P_j,j}$ is increased to its possible maximum value of $F_{P_j,j}^{\oplus}$ corresponding to $F_{P_j,out}=0$. The new situation is shown in Figure 3-7. The new inlet concentration in process j is $C_{j,in}^{\oplus}>C_{j,in}$.

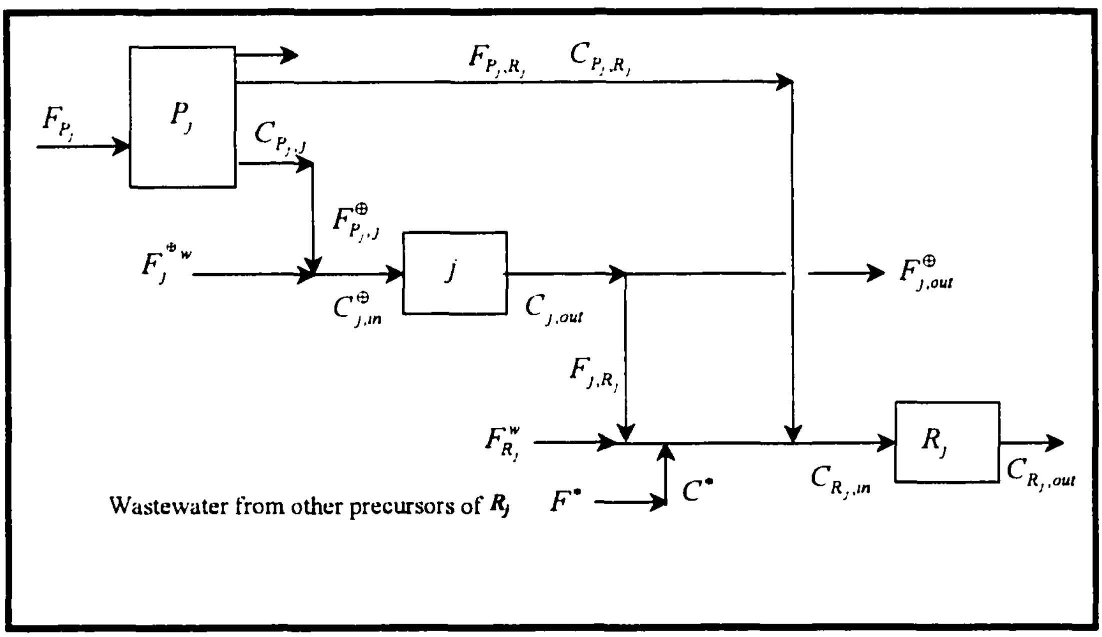


Figure 3-7
Outlet concentration biding condition for Intermediate Processes.

We will now prove that it is possible to further reduce water consumption by reducing $F_j^{\oplus w}$. As a result either maximum inlet or outlet concentration will be reached first and no further water reduction will be possible. This increase needs to be accompanied by conditions to maintain feasibility downstream at the inlet of the receivers from process j. As it was done in CASE I, feasibility can be obtained by keeping both $C_{R_j,in}$ and F_{R_j} constant while proving that there will be sufficient wastewater for reuse, that is $\overline{F}_j^{\oplus w} + \hat{F}_{P_j} \geq \overline{F}_{j,R_j}$.

We will have then two different possibilities:

(a) A reduction of the fresh water flowrate, $F_j^{\oplus w}$, will make the outlet concentration reach its maximum before the inlet does. $\overline{C}_{j,out} = C_{j,out}^{\max}$ and $\overline{C}_{j,in} < C_{j,in}^{\max}$.

(b) The inlet maximum is reached first.

The change in total water intake for both cases is

$$\Delta W = \left(\overline{F}_{R_j}^{w} - F_{R_j}^{w}\right) + \left(\overline{F}_j^{\oplus w} - F_j^{\oplus w}\right) \tag{3-85}$$

(a) $\overline{C}_{j,out} = C_{j,out}^{\max}$ and $\overline{C}_{j,in} < C_{j,in}^{\max}$

Performing mass balances on the component before and after the fresh water flow reduction, we obtain:

$$F_{P_j,j}^{\oplus} C_{P_j,j} + L_j = \left(F_{P_j,j}^{\oplus} + F_j^{\oplus w}\right) C_{j,out} \tag{3-86}$$

$$F_{P_j,j}^{\oplus} C_{P_j,j} + L_j = \left(F_{P_j,j}^{\oplus} + \overline{F}_j^{\oplus w}\right) C_{j,out}^{max} \tag{3-87}$$

Equating the r.h.s. of these balances and using the fact that $F_{P_j,out} = 0$, i.e., $F^{\oplus}_{P_j,J} = \hat{F}_{P_j}$

$$\overline{F}_J^{\oplus w} = \left(\frac{C_{J,out}}{C_{J,out}^{max}}\right) F_J^{\oplus w} - \left(1 - \frac{C_{J,out}}{C_{J,out}^{max}}\right) \hat{F}_{P_j} = \alpha\, F_J^{\oplus w} - (1-\alpha)\hat{F}_{P_j},\ 0 < \alpha < 1 \quad (3\text{-}88)$$

where $\alpha = \dfrac{C_{J,out}}{C_{J,out}^{\max}}$.

From (3-88) we write

$$\overline{F}_J^{\oplus w} - F_J^{\oplus w} = -(1-\alpha)\left(F_J^{\oplus w} + \hat{F}_{P_j}\right) \quad (3\text{-}89)$$

We now calculate $\left(\overline{F}_{R_j}^{w} - F_{R_j}^{w}\right)$.

Recalling that $C_{R_j,in}$ and F_{R_j} remain constant, we can write:

$$F_{R_j}^{w} + F_{J,R_j} + F_{P_j,R_j} + F^{\bullet} = \overline{F}_{R_j}^{w} + \overline{F}_{J,R_j} + F_{P_j,R_j} + F^{\bullet} \quad (3\text{-}90)$$

$$C_{R_j,in} = \frac{F_{J,R_j} C_{J,out} + F_{P_j,R_j} C_{P_j,R_j} + F^{\bullet} C^{\bullet}}{F_{R_j}^{w} + F_{J,R_j} + F_{P_j,R_j} + F^{\bullet}} = \frac{\overline{F}_{J,R_j} C_{J,out}^{\max} + F_{P_j,R_j} C_{P_j,R_j} + F^{\bullet} C^{\bullet}}{\overline{F}_{R_j}^{w} + \overline{F}_{J,R_j} + F_{P_j,R_j} + F^{\bullet}} \quad (3\text{-}91)$$

Rearranging (3-91) and using (3-90) we obtain:

$$\overline{F}_{J,R_j} = \frac{C_{J,out}}{C_{J,out}^{\max}} F_{J,R_j} = \alpha\, F_{J,R_j} \quad (3\text{-}92)$$

Substituting in (3-90) and rearranging we get:

$$\overline{F}_{R_j}^{w} - F_{R_j}^{w} = F_{J,R_j}(1-\alpha) \quad (3\text{-}93)$$

and therefore:

$$\Delta W = \left(\overline{F}_{R_j}^{w} - F_{R_j}^{w}\right) + \left(\overline{F}_J^{\oplus w} - F_J^{\oplus w}\right) = (1-\alpha)\left(F_{J,R_j} - F_J^{\oplus w} - F_{P_j,J}^{\oplus}\right) \le 0 \quad (3\text{-}94)$$

To finish the proof we need to show that under the new conditions there is enough wastewater to send from process j to the set of processes $\boldsymbol{R}_j$. That is: $\overline{F}_j^{\oplus w} + \hat{F}_{P_j} \geq \overline{F}_{j,R_j}$.

Add $\hat{F}_{P_j}$ to both sides of (3-88) to obtain:

$$\overline{F}_j^{\oplus w} + \hat{F}_{P_j} = \alpha \left(F_j^{\oplus w} + \hat{F}_{P_j}\right) \tag{3-95}$$

But

$$F_j^{\oplus w} + \hat{F}_{P_j} = F_{j,R_j} + F_{j,out}^{\oplus} \tag{3-96}$$

Thus, since

$$F_{j,out}^{\oplus} \geq 0 \tag{3-97}$$

We have

$$F_j^{\oplus w} + \hat{F}_{P_j} \geq F_{j,R_j} \tag{3-98}$$

And therefore,

$$\overline{F}_j^{\oplus w} + \hat{F}_{P_j} = \alpha \left(F_j^{\oplus w} + \hat{F}_{P_j}\right) \geq \alpha\, F_{j,R_j} \tag{3-99}$$

In addition, by (3-92) we obtain

$$\overline{F}_j^{\oplus w} + \hat{F}_{P_j} \geq \overline{F}_{j,R_j} \tag{3-100}$$

Q.E.D.

(b) $C_{j,out} < C_{j,out}^{\max}$ and $C_{j,in} = C_{j,in}^{\max}$

Since reducing only the fresh water intake of process j cannot render the maximum outlet concentration without violating feasibility, we need to proceed exactly the same way we did in CASE I and reduce both, $F_j^{\oplus w}$ and $F_{P_j,j}^{\oplus}$. The proof is not different from the one in CASE I, the same group of equations (3-67) through (3-78) are used to prove the theorem and then (3-79) through (3-83) are used to complete the feasibility proof. Thus $\Delta W \leq 0$.

Q.E.D.

3.3.3.2.1 Corollary 1

If an Intermediate Process j is a Total Wastewater Provider, then any solution having $C_{j,out} \in \left[C_{R_j,in}, C_{j,out}^{\max}\right]$ is also optimal with the same fresh water intake.

Proof:

When process j is a TWP then $F_{j,out}^{\oplus} = 0$, by (3-94) we have $\Delta W = 0$. This means that a degenerate solution has been found.

Q.E.D.

3.3.4 Theorem 3-4: Necessary Condition of Maximum Concentration for Terminal Processes.

If the solution of the WAP problem is optimal then the outlet concentration of a Terminal Fresh Water user Process reaches its possible maximum.

Proof:

We will prove by contradiction that if the outlet concentration is not maximum, the maximum outlet concentration can be always reached by reducing the freshwater intake, while maintaining the inlet concentration $C_{t,in}$ constant.

Thus, assume $C_{t,out} < C_{t,out}^{\max}$. A new set of flowrates $\overline{F}_t$ and $\overline{F}_t^{w}$ satisfies:

$$C_{t,in} = \frac{F_{P_t,t} C_{P_t,t}}{F_t^{w} + F_{P_t,t}} = \frac{\overline{F}_{P_t,t} C_{P_t,t}}{\overline{F}_t^{w} + \overline{F}_{P_t,t}} \tag{3-101}$$

Simplifying we obtain

$$\frac{F_{P_t,t}}{F_t^{w} + F_{P_t,t}} = \frac{\overline{F}_{P_t,t}}{\overline{F}_t^{w} + \overline{F}_{P_t,t}} \tag{3-102}$$

Rearranging,

$$\frac{\overline{F}_t}{F_t} = \frac{\overline{F}_{P_t,t}}{F_{P_t,t}} \tag{3-103}$$

However, from (3-102)

$$F_{P_j,t}\left(\overline{F}_t^{w} + \overline{F}_{P_j,t}\right) = \overline{F}_{P_j,t}\left(F_t^{w} + F_{P_j,t}\right) \tag{3-104}$$

Multiplying term by term and reducing, we get

$$F_{P_i,t}\overline{F}_t^{w} = \overline{F}_{P_i,t}F_t^{w} \tag{3-105}$$

or

$$\frac{\overline{F}_{P_i,t}}{F_{P_i,t}} = \frac{\overline{F}_t^{w}}{F_t^{w}} \tag{3-106}$$

However, by assumption,

$$\frac{F_{P_i,t}C_{P_i,t} + L_t}{F_t} = C_{T,out} < C_{T,out}^{\max} = \frac{\overline{F}_{P_i,t}C_{P_i,t} + L_t}{\overline{F}_t} \tag{3-107}$$

which can be rearranged to give

$$\frac{\overline{F}_t}{F_t}\left(F_{P_i,t}C_{P_i,t} + L_t\right) < \overline{F}_{P_i,t}C_{P_i,t} + L_t \tag{3-108}$$

Now using (3-103) we get,

$$\frac{\overline{F}_{P_i,t}}{F_{P_i,t}}\left(F_{P_i,t}C_{P_i,t} + L_t\right) < \overline{F}_{P_i,t}C_{P_i,t} + L_t \tag{3-109}$$

or simplifying

$$\frac{\overline{F}_{P_i,t}}{F_{P_i,t}}L_t < L_t \tag{3-110}$$

which gives

$$\overline{F}_{P_i,t} < F_{P_i,t} \Rightarrow \frac{\overline{F}_{P_i,t}}{F_{P_i,t}} < 1 \tag{3-111}$$

Therefore, using (3-106) we get:

$$\frac{\overline{F}_t^w}{F_t^w} < 1 \qquad (3\text{-}112)$$

Q.E.D.

3.4 Examples

We now show some examples from the literature and some additional ones solved using the water pinch when all these conditions are met. We also illustrate the degeneracies covered by the corollaries of the theorems.

3.4.1 Example 3-1

This example is taken from Wang and Smith (1994). The system involves four processes and their corresponding data is given in Table 3-1.

Table 3-1: Example from Wang and Smith (1994)

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	2.0	0	100
2	5.0	50	100
3	30.0	50	800
4	4.0	400	800

The minimum flowrate reported is 90.0 ton/h and two realizing networks are presented in Wang and Smith (1994). Each network was obtained using a different method. The first method maximizes the concentration driving forces and the second one minimizes the number of water sources. It can be observed that, even after breaking the loops, the final designs may be of no practical use. The first method, for instance, proposed a splitting of process three. If process three were an indivisible unit, such as a desalter or a reflux drum, the network would have no real meaning. However, the second method provides, after several simplifications, a realistic realizing network. It is also worth noting that before the aforementioned simplifications the flowsheet obtained was rather complex and also introduced several process splittings. Figure 3-8 shows the final network obtained using method two (Wang and Smith, 1994).

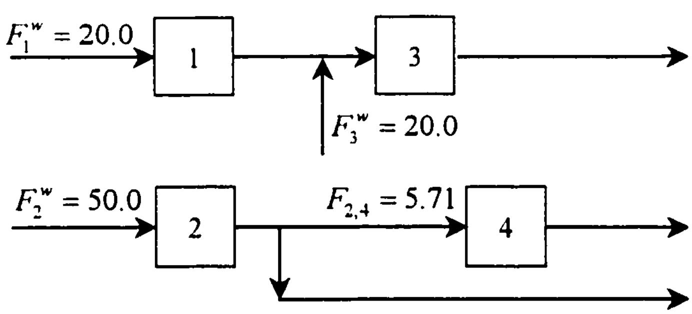


Figure 3-8
Final water network for example 3-1.

According to our definitions, Process 1, 2 and 3 are FWU processes while process 4 is a WWU process. Processes 1 and 2 are head processes and process 3 is a terminal process. There are no intermediate processes in this network. Table 3-2 summarizes all flowrates and final inlet and outlet concentrations of each process.

Table 3-2: Final Solution to Example 3-1

Process Number	**Type of Process**	**Fresh Water Intake (ton/h)**	**Wastewater Reuse (ton/h)**	C_{in} **(ppm)**	C_{out} **(ppm)**
1	H	20.0	0.0	0.0	100.0
2	H	50.0	0.0	0.0	100.0
3	T	20.0	20.0	50.0	800.0
4	WWU	0.0	5.71	100.0	800.0

We now check if the proposed flowsheet satisfies all applicable necessary conditions of optimality.

- *Monotonicity*

  Process 3 and 4 receive reusable wastewater.

  1- Process 1 delivers wastewater at 100 ppm which it is fed to process 3. Process 3 has an outlet concentration of 800 ppm, therefore monotonicity is satisfied.

  2- Process 2 delivers wastewater at 100 ppm to process 4. Process 4 has an outlet concentration of 800 ppm, thus monotonicity is satisfied.

- *Maximum Concentration for Head Processes*

  Process 1 and 2 are Head Processes.

Both process 1 and 2 have outlet concentrations equal to their possible maximum. Therefore, this condition is satisfied.

- *Maximum Concentration for Terminal Processes*

  Process 3 is a Terminal Process and its outlet concentration is at its possible maximum hence the theorem is fulfilled as well.

Consider now a different realizing network as shown in Figure 3-9 (Olesen and Polley, 1997). The total fresh water intake, 90.0 ton/h, remains unchanged. This alternative network realizes the minimum flowrate target but constitutes a degenerate solution to this example problem. This case is heeded by the Corollary of Degeneracy for Head Process. $F_{1,out} = 0$, therefore ΔW =0 and the 90.0 ton/h is an optimal solution.

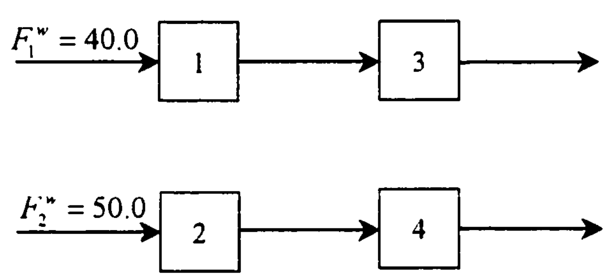


Figure 3-9
Network solution for example 3-1 as reported by Olesen and Polley (1997).

Observation: Process 4 is receiving all the wastewater generated in process 2 when in reality it only needs 5.71 ton/h to complete its load removal. It does not contradict theorem 4, as it is not a fresh water user.

3.4.2 Example 3-2

This example is taken from Olesen and Polley (1997). The system involves six processes and their corresponding data is given in Table 3-3.

Table 3-3: Example data from Olesen and Polley (1997)

Process Number	**Mass Load of Contaminant (kg/h)**	C_{in}^{max} **(ppm)**	C_{out}^{max} **(ppm)**
1	2.0	25	80
2	5.0	25	100
3	4.0	25	200
4	5.0	50	100
5	30.0	50	800
6	4.0	400	800

The minimum flowrate reported is 157.14 ton/h. Olesen and Polley (1997) obtained a realizing network by methods of inspection. Figure 3-10 shows such network.

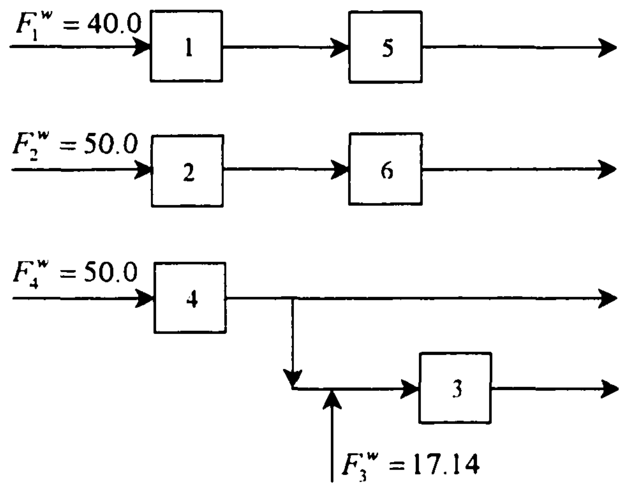


Figure 3-10
Network solution for example 3-2 as reported by Olesen and Polley (1997).

Table 3-4 summarizes the results of this example problem for the network obtained by Olesen and Polley (1997). The target is met, so the solution is optimal but constitutes a degeneracy of the solution network depicted in Figure 3-11. The flowsheet shown in Figure 3-11 satisfies all necessary conditions of optimality and meets the 157.14 ton/h target.

Table 3-4: Degenerate solution of Example 2

Process Number	Type of Process	Fresh Water Intake (ton/h)	Wastewater Reuse (ton/h)	C_{in} (ppm)	C_{out} (ppm)
1	H	40.0	0.0	0	50
2	H	50.0	0.0	0	100
3	T	17.14	$F_{4,3} = 5.714$	25	200
4	H	50.0	0.0	0	100
5	WWU	0.0	$F_{1,5} = 40.0$	50	800
6	WWU	0.0	$F_{2,6} = 50.0$	100	180
Total Flowrate (ton/h)		**157.14**	**95.714**		

We now analyze each process. Process 1 is a Head Process in this network and its outlet concentration is not at its possible maximum but its wastewater is completely reused at process 5, therefore the Degeneracy Condition for Head Processes is satisfied. Process 2 and 4 are also Head Processes and theorem 2 holds in both cases. Process 3 is the only Terminal Process in this network and satisfies theorem 4. Besides monotonicity is also met because process 3 receives wastewater at 100 ppm while its maximum outlet is 200 ppm.

In conclusion, the only degeneracy found in this solution is that of process 1. In addition, when process 1 meets the conditions of theorem 2, process 5 becomes a Terminal Process that satisfies the necessary condition of optimality.

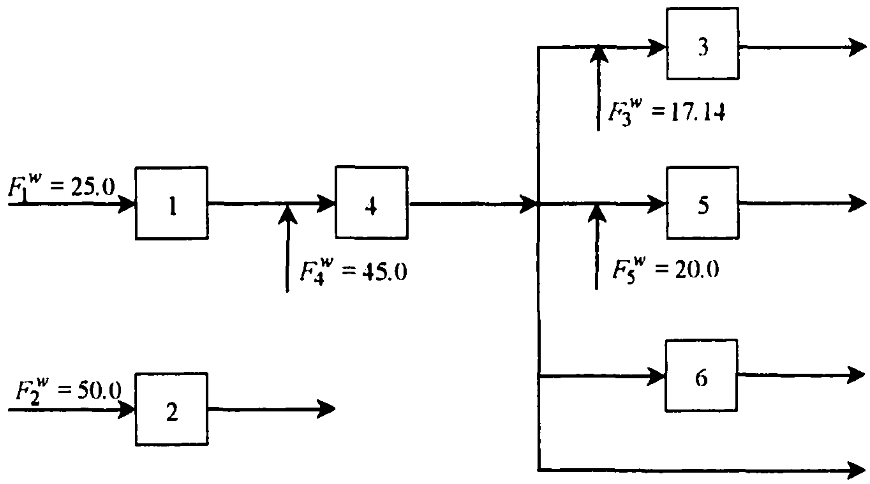


Figure 3-11
Alternative solution network for example 3-2.

Table 3-5 shows the results for the network depicted in Figure 3-11. In this flowsheet all processes have reached both maximum inlet and outlet concentration through maximum reuse. All the necessary conditions of optimality are satisfied by this alternative solution.

Table 3-5: Results for the network of Figure 3-11

Process Number	Type of Process	Fresh Water Intake (ton/h)	Wastewater Reuse (ton/h)	C_{in} (ppm)	C_{out} (ppm)
1	H	25.0	0.0	0	80
2	H	50.0	0.0	0	100
3	T	17.14	$F_{4,3} = 5.714$	25	200
4	I	45.0	$F_{1,4} = 25.0$	28.57	100
5	T	20.0	$F_{4,5} = 20.0$	50	800
6	WWU	0.0	$F_{4,6} = 5.714$	100	800
Total Flowrate (ton/h)		**157.14**	**56.428**		

3.5 Conclusions

Necessary conditions of optimality in water allocation problems have been presented. These conditions state that optimal structures satisfy monotonicity of the outlet concentrations when one process sends its wastewater to another. In addition, conditions under which the inlet or the outlet concentrations reach their maximum have been discussed. Chapter 4 builds on these conditions to develop a procedure to design these systems without the drawbacks of existing alternatives.

3.6 Notation

C concentration of contaminant, ppm

$\hat{C}$ resulting concentration of contaminant if all precursor wastewater is used, ppm.

$\overline{C}$ resulting concentration of contaminant after decreasing fresh water consumption, ppm.

f component flowrate, g/h

F water flowrate, ton/h

$\hat{F}$ total wastewater flowrate from precursors, ton/h

$\overline{F}$ water flowrate after fresh water consumption reductions, ton/h

Subscripts:

in at inlet

out at outlet

i,j connection going from process *i* to process *j*

j process *j*

Superscripts:

min minimum

max maximum

* additional sources

w fresh water

3.7 References

1. Olesen S.G. and G.T. Polley. *A Simple Methodology for the Design of Water Networks Handling Single Contaminants.* Trans IChemE, 75, part A, pp. 420-426, 1997.
2. Wang Y. P. and R. Smith. *Wastewater Minimization.* CES, 49, 7, pp. 981, 1994.

CHAPTER 4

Algorithmic Procedure to Design Water Utilization Systems in Refineries and Process Plants

4.1 Introduction

This chapter introduces a non-iterative algorithmic procedure to solve the single-contaminant WAP problem. The WAP problem was formally defined in Chapter 2. The procedure targets the water allocation problem while providing at the same time a realizing network. The new approach is based on previously discussed necessary conditions of optimality (Chapter 3) and sufficient conditions of optimality that allow the construction of a global optimal solution without the need of a targeting procedure. In addition, the steps of this procedure are such that it can be implemented by hand and have no limitations on the problem size.

The chapter is organized as follows: Conditions of maximum reuse of wastewater will be presented. These conditions are later used as a basis of the design procedure. Once this design procedure is presented, a proof of optimality is given. Finally, examples are worked out.

4.2 Conditions of Maximum Reuse

We now derive a series of rules to calculate the amount of wastewater that a process can receive from its precursors in such a way that the amount of fresh water is minimized.

Consider a set of (n-1) precursors of process n (Figure 4-1). We assume that process n has a maximum outlet concentration that is larger than that of all its precursors (monotonicity). In Figure 4-1, all possible connections from the precursors of process n are indicated. We now proceed to determine the optimal policy of water allocation, such that the fresh water usage of process n is minimum. Next, for the case when the fresh water usage is zero, we develop an allocation policy for wastewater users. Later, we will prove that the use of these policies guarantees optimality.

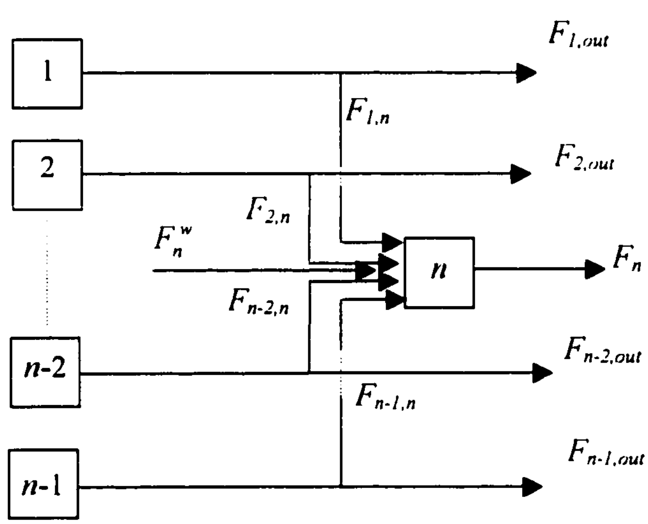


Figure 4-1
Precursors of process n.

4.2.1 Maximum Reuse for Fresh Water Users

Without loss of generality, assume that the outlet concentrations of all these processes are ordered monotonically.

$$C_{1,out}^{\max} \leq C_{2,out}^{\max} \leq \ldots\ldots \leq C_{n-1,out}^{\max} \leq C_{n,out}^{\max} \tag{4-1}$$

The last inequality is a reflection of the necessary condition of monotonicity. Consider now the following optimization problem:

$$\left.\begin{array}{l} Min\ F_n^w \\ s.t. \\ F_{i,n} \leq F_i \\ C_{n,in}\left(F_{i,n}, C_{i,out}, F_n^w\right) \leq C_{n,in}^{\max} \\ C_{n,out}\left(F_{i,n}, C_{i,out}, F_n^w, L_n\right) \leq C_{n,out}^{\max} \\ F_{i,n} \geq 0 \end{array}\right\} \tag{4-2}$$

which aims at the best reuse policy, the one that minimizes fresh water usage. We now convert this problem into a linear problem.

Note first that by Theorem 3-2 of the necessary conditions the outlet concentration is at its maximum value $\left(C_{n,out} = C_{n,out}^{\max}\right)$. Thus, in an optimal structure a component mass balance over process n is:

$$\sum_{i=1}^{n-1} F_{i,n} C_{i,out}^{\max} + L_n = \left(F_n^w + \sum_{i=1}^{n-1} F_{i,n}\right) C_{n,out}^{\max} \tag{4-3}$$

where L_n is the load of process n. This linear relation can be rewritten as follows:

$$F_n^w = K_n - \sum_{i=1}^{n-1} F_{i,n} \alpha_{i,n} \tag{4-4}$$

where $\alpha_{i,n} = \left(1 - \frac{C_{i,out}^{\max}}{C_{n,out}^{\max}}\right)$ and $K_n = \frac{L_n}{C_{n,out}^{\max}}$. Consider now the component mass balance at the inlet of process n.

$$\left(\sum_{i=1}^{n-1} F_{i,n} + F_n^w\right) C_{n,in} = \sum_{i=1}^{n-1} F_{i,n} C_{i,out}^{max} \tag{4-5}$$

Replacing (4-4) into (4-5) and rearranging, one obtains:

$$C_{n,in} = \frac{\sum_{i=1}^{n-1} F_{i,n} C_{i,out}^{\max}}{K_n + \sum_{i=1}^{n-1} F_{i,n}\left(1 - \alpha_{i,n}\right)} \tag{4-6}$$

Therefore, replacing (4-6) in $C_{n,in} \le C_{n,in}^{\max}$ one obtains:

$$\sum_{i=1}^{n-1} F_{i,n} r_{i,n} \le T_n \tag{4-7}$$

where

$$r_{i,n} = C_{i,out}^{\max} - C_{n,in}^{\max}(1 - \alpha_{i,n}) \tag{4-8}$$

$$T_n = K_n C_{n,in}^{\max} \tag{4-9}$$

We now replace (4-7) and (4-4) into (4-2) to obtain:

$$
\left.\begin{array}{l}
\text{Max} \sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} \\
s.t. \\
F_{i,n} \le F_i \\
\sum_{i=1}^{n-1} F_{i,n} r_{i,n} \le T_n \\
\sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} \le K_n \\
F_{i,n} \ge 0
\end{array}\right\} \tag{4-10}
$$

which is a linear program. The last constraint ensures that $F_n^w \ge 0$. We will now show that the solution of (4-10) can be obtained analytically. First note that (4-8) can be rewritten as follows:

$$
r_{i,n} = C_{i,out}^{\max} - C_{n,in}^{\max}(1-\alpha_{i,n}) = C_{i,out}^{\max} - C_{n,in}^{\max}\left(\frac{C_{i,out}^{\max}}{C_{n,out}^{\max}}\right) = C_{i,out}^{\max}\left(1 - \frac{C_{n,in}^{\max}}{C_{n,out}^{\max}}\right) \tag{4-11}
$$

from which we can conclude that,

$$
r_{i,n} \ge 0 \qquad \forall i = 1,\ldots,(n-1). \tag{4-12}
$$

In addition, because of (4-1), we have

$$
r_{1,n} \le r_{2,n} \le \ldots \le r_{i,n-1} \tag{4-13}
$$

$$
\alpha_{1,n} \ge \alpha_{2,n} \ge \ldots \ge \alpha_{i,n-1} \tag{4-14}
$$

We now analyze the possible solutions of this optimization problem. Consider the following two cases: (a) The inlet concentration of process n does not reach its maximum, and b) otherwise. Since this analysis is for fresh water users, in both cases, the fresh water usage is positive, that is, (4-2) has a strictly positive solution.

a) $C_{n,in} < C_{n,in}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} < T_n$. In this case, it is easy to prove that the solution of (4-10) must be $F_{i,n} = F_i, \forall i$. Indeed, if $F_{i,n} < F_i$ for any i, then $F_{i,n}$ can be increased without violating the constraints of (4-10), thus increasing the objective function.

b) $C_{n,in} = C_{n,in}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} = T_n$. In this case, the solution has the following form:

$$\left.\begin{array}{l} F_{1,n} = F_1 \\ F_{2,n} = F_2 \\ \vdots \\ F_{s,n} \leq F_s \\ F_{s+1,n} = 0 \\ \vdots \\ F_{n-1,n} = 0 \end{array}\right\} \tag{4-15}$$

with

$$\left.\begin{array}{ll} F_{s,n} = \dfrac{K_n C_{n,in}^{\max}}{C_{s,out}^{\max} - (1-\alpha_{s,n}) C_{n,in}^{\max}} & \text{if } s = 1 \\ F_{s,n} = \dfrac{K_n C_{n,in}^{\max} - \sum_{i=1}^{s-1} F_i [C_{i,out}^{\max} - (1-\alpha_{i,n}) C_{n,in}^{\max}]}{C_{s,out}^{\max} - (1-\alpha_{s,n}) C_{n,in}^{\max}} & \text{for } s > 1 \end{array}\right\} \tag{4-16}$$

which is obtained from (4-6) assuming that $C_{n,in} = C_{n,in}^{\max}$. Process, 1 through s-1 are total wastewater providers of process n, whereas process s is a partial wastewater provider of process n. A formal procedure to determine s will be presented later.

Proof: Consider a feasible perturbation of (4-15). We will show that such perturbation leads to an increase in fresh water intake. Assume $F_{k,n} = F_k - \delta_k$ for some $k < s$. Rewrite the second constraint of (4-10) as follows:

$$\left(F_k - \delta_k\right) r_{k,n} + \sum_{i=1, i \neq k}^{s-1} F_i \, r_{i,n} + F_{s,n} r_{s,n} + F_{t,n} r_{t,n} = T_n \tag{4-17}$$

where we have assumed that some flowrate $F_{t,n}\,(t > s)$ is not zero. From (4-17), we obtain the following relationship between $F_{t,n}$ and δ_k:

$$F_{t,n} = \frac{T_n - \left(F_k - \delta_k\right) r_{k,n} - \sum_{i=1, i \neq k}^{s-1} F_i \, r_{i,n} - F_{s,n} r_{s,n}}{r_{t,n}} \tag{4-18}$$

In turn, the change in objective function is:

$$\Delta of = -\delta_k \alpha_{k,n} + F_{t,n} \alpha_{t,n} \tag{4-19}$$

Thus, substituting (4-18) into (4-19) and rearranging:

$$\Delta of = \delta_k \left(\frac{r_{k,n}}{r_{t,n}} \alpha_{t,n} - \alpha_{k,n} \right) \tag{4-20}$$

Using (4-12), (4-13) and (4-14) one can find that (4-20) is negative except when all outlet concentrations in (4-1) are equal. In such case, (4-20) is zero. In such case, it does not make a difference what wastewater is used. This concludes the proof.

Q.E.D.

4.2.2 Maximum Reuse for Wastewater Users

Without loss of generality, we assume the monotonicity given by (4-1). If a WWU has more than one candidate precursor then there may exist infinitely many feasible solutions to the water assignment problem of such a process.

When all precursors have concentrations lower than the maximum inlet concentration of process n $\left(C_{j,out}^{\max} \leq C_{n,in}^{\max}\ \forall j\right)$, all linear combinations of wastewater flowrates from the precursors of n can be formed. These linear combinations are only constrained by a component mass balance and the maximum outlet concentration necessary condition. When some precursors have outlet concentrations higher than the maximum inlet concentration of process n $\left(C_{j,out}^{\max} \leq C_{n,in}^{\max}\ j = 1,\ldots k\right.$ and $\left.C_{j,out}^{\max} > C_{n,in}^{\max}\ j \geq k+1,\ldots n-1\right)$, then, linear combinations of available wastewaters of concentration higher and lower than $C_{n,in}^{\max}$ can be formed. The precursors with $C_{i,out} \leq C_{n,in}^{\max}$ can be seen as pseudo-fresh water sources each one with a certain cost associated, the better the quality the higher the cost. The precursors with $C_{i,out} > C_{n,in}^{\max}$ can then be considered as the actual reusable wastewater sources. Thus, the first k wastewaters can be considered as "good quality" precursors because they can be used to dilute the rest, which could not otherwise be used. If the WWU under consideration were the last process to be analyzed, then the assignment of water would not really affect the total water intake. However, when some receivers downstream of process n

are FWUs, the quality of the wastewater available needs to be preserved so that these other fresh water receivers downstream receive the cleanest wastewater possible. As we shall see later, this heuristic can be proven to be always true. Thus, the problem of assigning water to a WWU is analogous to that of the FWU.

To preserve the cleanest pseudo-fresh waters, we set up the following optimization problem.

$$\left.\begin{aligned} & Min \sum_{i=1}^{k} \mu_{i,n} F_{i,n} \\ & s.t. \\ & C_{n,in} \leq C_{n,in}^{\max} \\ & C_{n,out} \leq C_{n,out}^{\max} \\ & 0 \leq F_{i,n} \leq F_i \qquad\qquad \forall i \in \mathbf{P}_n \end{aligned}\right\} \tag{4-21}$$

where $\mu_{i,n} = \left(C_{n,in}^{\max} - C_{i,out}^{\max}\right)$, a positive number except when $\left(C_{n,in}^{\max} = C_{i,out}^{\max}\right)$. This objective function aims at minimizing the consumption of water of the lowest concentration that is preserving the best quality wastewater for possible downstream FWUs.

We will now convert problem (4-21) into a linear problem as it was done with (4-2).

By Theorem 3-2 of the necessary conditions of optimality, the outlet concentration is at its maximum value $\left(C_{n,out} = C_{n,out}^{\max}\right)$. Thus, using a component mass balance over process n, and since $F_n^w = 0$, we have that (4-4) becomes:

$$\sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} = K_n \tag{4-22}$$

Now, the component mass at the inlet of process n is given by (4-7).

We now replace (4-7) and (4-22) into (4-21) to obtain:

$$\left.\begin{array}{l} Min \sum_{i=1}^{k} \mu_{i,n} F_{i,n} \\ s.t. \\ \sum_{i=1}^{n-1} F_{i,n} r_{i,n} \le T_n \\ \sum_{i=1}^{n-1} F_{i,n}\alpha_{i,n} = K_n \\ 0 \le F_{i,n} \le F_i \qquad \forall i \in \mathbf{P}_n \end{array}\right\} \tag{4-23}$$

which is a linear problem.

We now analyze the two aforementioned cases.

4.2.2.1 CASE I: All Precursors are Pseudo-Fresh Water Sources.

$$C_{n-1,out}^{\max} < C_{n,in}^{\max}$$

In this case, we use the dirtiest water first and, if it is not enough, we continue using water of the next highest concentration until all requirements are fulfilled. The following set of formulas corresponds to the maximum reuse allocation.

$$\left.\begin{array}{l} F_{j,n} = 0 \quad \forall j < p \\ F_{j,n} = F_j \ \forall j > p \end{array}\right\} \tag{4-24}$$

$$
\left.\begin{aligned}
F_{p,n} &= \frac{L_n}{C^{\max}_{n,out} - C^{\max}_{p,out}} && if\ p = 1 \\
F_{p,n} &= \frac{L_n - \sum_{i=p+1}^{n-1} F_i \left(C^{\max}_{n,out} - C^{\max}_{i,out}\right)}{C^{\max}_{n,out} - C^{\max}_{p,out}} && if\ p > 1
\end{aligned}\right\} \qquad (4\text{-}25)
$$

An algorithm procedure will be presented later to establish the partial wastewater provider p. The proof to show that this policy preserves the cleanest wastewater possible is straightforward.

4.2.2.2 CASE II: Only Some Precursors are Pseudo-Fresh Water Sources

For instance:

$$
\left.\begin{aligned}
C^{\max}_{i,out} &\le C^{\max}_{n,in} && \forall i \le k \\
C^{\max}_{i,out} &> C^{\max}_{n,in} && \forall i > k
\end{aligned}\right\} \qquad (4\text{-}26)
$$

We now prove that the optimal solution of (4-23) is given a combination of the dirtiest set of pseudo-fresh water precursors possible and the cleanest set of wastewater available. The former policy is driven directly by the objective function of (4-23). The latter is indirectly driven by the same objective function. Indeed, as less polluted water is used, the usage of pseudo-fresh water is smaller. Figure 4-2 illustrates one such generic combination.

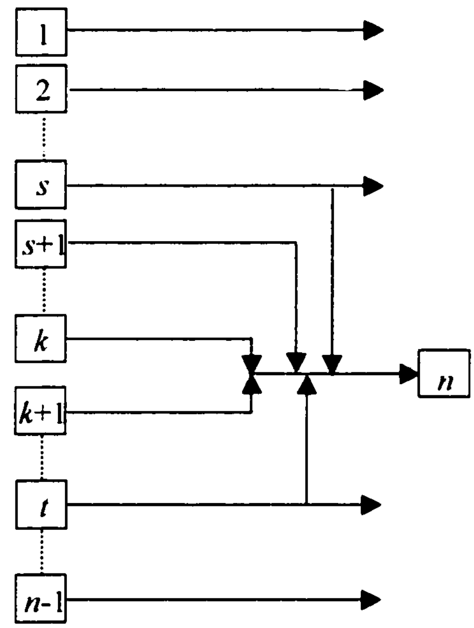


Figure 4-2
Pseudo-fresh water precursors of a WWU.

Consider the following two cases: (a) The inlet concentration of process n does not reach its maximum, and (b) otherwise.

(a) $C_{n,in} < C_{n,in}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} < T_n$. In this case, the solution of (4-23) is given by a complete use of wastewater and a partial use of pseudo-fresh waters, that is: $F_{i,n} = F_i \ \forall i \in [k+1, n-1]$, $F_{j,n} = F_j \ \forall j \in [s+1, k]$ and $F_{j,s} < F_s$ for some s. The identification of the partial wastewater provider s will be presented later. The proof is simple: If the allocation of a wastewater is not total, that is, $F_{t,n} < F_t \ (t > k)$, then $F_{t,n}$ can be increased because the inlet concentration of process n has not reached its maximum. Consequently, one or more of the pseudo-fresh waters

$F_{j,n}\,(j \le k)$ has to be decreased to maintain the component balance $\left(\sum_{i} F_{i,n}\alpha_{i,n} = K_n\right)$. It is easy to see that these two changes lead to a decrease of the objective function.

(b) $C_{n,in} = C_{n,in}^{\max}$. This is equivalent to $\sum_{i=1}^{n-1} F_{i,n} r_{i,n} = T_n$.

In this scheme, pseudo-fresh waters from process s $(s < k)$ to process k are used to dilute wastewaters from process $(k+1)$ to process t $(t > k)$. Once the partial wastewater providers s and t are identified, the following flowrates are obtained.

$$\left.\begin{array}{ll} F_{j,n} = F_j & \forall j = (s+1),\ldots,(t-1) \\ F_{s,n} < F_s & \\ F_{t,n} < F_t & \end{array}\right\} \tag{4-27}$$

where $F_{s,n}$ and $F_{t,n}$ can be obtained from the following set of equations:

$$\left.\begin{array}{l} F_{s,n} r_{s,n} + F_{t,n} r_{t,n} = T_n - \sum_{p=s+1}^{t-1} F_p r_{p,n} \\ F_{s,n}\alpha_{s,n} + F_{t,n}\alpha_{t,n} = K_n - \sum_{p=s+1}^{t-1} F_p \alpha_{p,n} \end{array}\right\} \tag{4-28}$$

We now prove that (4-27) and (4-28) give the optimal solutions of (4-26).

Consider a feasible perturbation of (4-27). We will show that such perturbation leads to an increase in the value of the objective function. Assume we increase the flowrate of a process j $(j < k)$, thus decreasing the flowrate of a process $p\,(p > k)$. Therefore, we can write the perturbation of (4-27) as follows:

$$\left.\begin{array}{ll}\overline{F}_{j,n} = F_{j,n} + \delta_j & j \le s \\ \overline{F}_{p,n} = F_{p,n} - \delta_p & s < p \le k \\ \overline{F}_{i,n} = F_{i,n} & \forall i \ne p, \forall i \ne j \\ \delta_j, \delta_p > 0 & \end{array}\right\} \qquad (4\text{-}29)$$

The change in the objective function is given by:

$$\Delta o.f. = \mu_j \delta_j - \mu_p \delta_p \qquad (4\text{-}30)$$

Replacing (4-29) in the second equation of (4-28) and rearranging, we obtain:

$$\frac{\delta_p}{\delta_j} = \frac{\alpha_{j,n}}{\alpha_{p,n}} \qquad (4\text{-}31)$$

Replacing (4-31) into (4-30), one obtains:

$$\Delta o.f. = \delta_j \left(\mu_{j,n} - \frac{\alpha_{j,n}}{\alpha_{p,n}} \mu_{p,n} \right) \qquad (4\text{-}32)$$

Using the definitions of α, μ and doing some algebraic manipulations, we obtain:

$$\Delta o.f. = \delta_j \left(\frac{\left(C_{p,out}^{\max} - C_{j,out}^{\max}\right)\left(C_{n,out}^{\max} - C_{n,in}^{\max}\right)}{\left(C_{n,out}^{\max} - C_{p,out}^{\max}\right)} \right) \qquad (4\text{-}33)$$

One can easily verify that (4-33) is strictly positive unless $C_{p,out} = C_{j,out}$ in which case it is zero.

Q.E.D.

We now present the maximum reuse algorithm, which systematically implements of the above presented wastewater allocation process. Consider the following definition first:

Definition: A maximum reuse structure is a flowsheet that satisfies the property that all inlet wastewater flows to any unit are obtained using the maximum reuse algorithm.

4.3 Maximum Reuse Algorithm

Given wastewater available from n-1 processes the maximum reuse allocation of wastewater to process n is given by the application of the algorithm below. The algorithm is based on the assumption that process n is a WWU. If no precursor has a concentration lower than the maximum inlet concentration of process n or a contradiction is found, then it is solved as a FWU.

4.3.1 Algorithm

1. Assume process n is a WWU. Then, there are two alternatives. Either all the pseudo-fresh water precursors have concentrations lower than the maximum inlet concentration of process n (Case I) or only some of its precursors satisfy this inequality (CaseII).

2. Case I: Assume $p = n - 1$. Calculate $F_{p,n}$ using (4-24) and (4-25). If the value of $F_{p,n}$ calculated is larger than F_p, then make $F_{p,n} = F_p$ update $p(p = p - 1)$ and repeat the procedure. If the water from all precursors is exhausted and the water requirements are still unfulfilled, then process n is not a WWU but a FWU. In such case, go to 6. Otherwise, stop.

3. Case II: Assume the partial wastewater providers to be $s = k$ and $t = k + 1$. Apply (4-27) and (4-28).

4. If, $F_{k,n} \leq F_k$ and $F_{k+1,n} \leq F_{k+1}$ then stop. Otherwise, go to 5.

5. If either flowrate results larger than its corresponding available flowrate, then this implies that all the available wastewater from the precursor must be used and that another set of precursors is needed. Therefore, if $F_{s,n} > F_s$, make $F_{s,n} = F_s$ update $s\left(s = s - 1\right)$, and/or if $F_{t,n} > F_t$ make $F_{t,n} = F_t$ update $t\left(t = t + 1\right)$ and return to 3. If all pseudo-fresh water precursors are exhausted and the water requirements are still unfulfilled, then process n is not a WWU but a FWU. In such case, go to 6.

6. The process has been determined to be a FWU. Assume the partial wastewater provider to be $s = 1$. Calculate $F_{1,n} \ldots F_{s,n}$ and F_n^w using (4-15), (4-16) and (4-4). If $F_{s,n} > F_s$, then make $F_{s,n} = F_s$, update $s\left(s = s + 1\right)$ and repeat the process. Otherwise, if $F_{s,n} \leq F_s$ stop.

4.4 Design Procedure

The following design procedure is proposed:

1. Feed fresh water to all processes that have zero inlet maximum concentration (Head Processes). To calculate the required flowrate use the following:

$$F_h^w = \frac{L_h}{C_{h,out}^{\max}} \tag{4-34}$$

If no process has zero inlet maximum concentration take the process with the lowest maximum outlet concentration.

2. Order the rest of processes in increasing order of maximum outlet concentration.

3. Take the first process of the list and apply the maximum reuse algorithm. Exclude from the list of sources those that violate monotonicity.

4. Keep applying the maximum reuse rule in this fashion for all the rest of the processes.

The above procedure satisfies all necessary conditions of optimum (monotonicity in the outlet concentrations and outlet concentrations at their maximum values). We now prove that the maximum reuse algorithm leads to an optimal structure.

4.5 Proof of Optimality

4.5.1 Theorem: The Maximum Reuse Structure is Optimal

Proof:

The proof is by mathematical induction. By construction, it is true for two processes. Now we assume it is true for n-1 processes and we will prove it is true for

n processes. Consider first a structure with n-1 processes. By the optimality condition of monotonicity we know that process n is not a precursor of any of the n-1 first processes. Consider first an overall balance on a structure that contains all n processes.

$$W = \sum_{i=1}^{n-1} F_i^w + F_n^w = \sum_{i=1}^{n-1} F_{i,out} + F_n \qquad (4\text{-}35)$$

$$L = \sum_{i=1}^{n} L_i = \sum_{i=1}^{n-1} F_{i,out} C_{i,out}^{\max} + F_n C_{n,out}^{\max} \qquad (4\text{-}36)$$

Eliminating F_n, one obtains:

$$W = Z_n + \sum_{i=1}^{n-1} F_{i,out} \alpha_{i,n} \qquad (4\text{-}37)$$

where $Z_n = \dfrac{L}{C_{n,out}^{\max}}$. The optimal water allocation policy for the system with n units is either,

a) a system where the water allocation for the first n-1 units is a maximum reuse structure, or

b) the water allocation in the first n-1 processes is such that the fresh water consumption of these first n-1 processes is larger than the optimum assumed for these n-1 processes, but leads to an overall smaller fresh water consumption.

We now explore the two options:

a) In this case, the theorem is readily proved, as the only water allocation policy that will minimize F_n^w is the one obtained applying the maximum reuse algorithm to process n.

b) Assume that the fresh water consumption of process s is increased,

$$\overline{F}_s^w = F_s^w + \delta_s^w \tag{4-38}$$

However, if the overall structure is to be optimal, the concentration at the outlet of process s should be maintained at its maximum. To achieve this, a smaller amount of wastewater from its precursors has to be used. Thus, the only effect of the perturbation is to lower the inlet concentration $C_{s,in}$ and to decrease the flowrate through process s (F_s). However, in a maximum reuse structure there is at the most only one precursor (k) that has wastewater sending to process s for which $F_{k,s} < F_k$. The rest are either $F_{j,s} = F_j$ or zero.

Therefore, to achieve the maximum concentration in process s the following feasible perturbation must accompany (4-38).

$$\overline{F}_{k,s} = F_{k,s} - \delta_k \tag{4-39}$$

Accordingly,

$$\overline{F}_{k,out} = F_{k,out} + \delta_k \tag{4-40}$$

for some precursor k of process s. Figure 4-3 illustrates the section of the flowsheet under study.

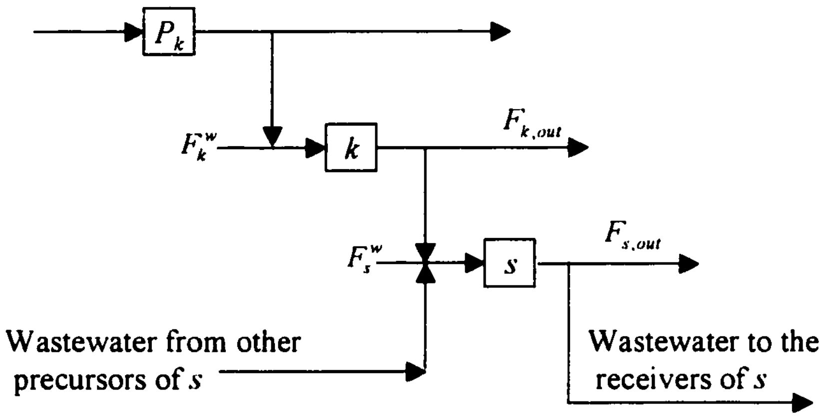


Figure 4-3
Maximum reuse structure.

We notice again that the perturbation of these two processes (s and k) is feasible only if the precursor has wastewater that has not been reused $(F_{k,out} > 0)$. The other possibility is to reduce the total water flowrate of process k. If process k is a head process, the fresh water intake is already at it minimum, so the perturbation is also infeasible. Otherwise, to reduce the total flowrate through process k, the fresh water intake of some precursor of this process has to be also reduced. This stems from the fact that a reduction of F_k^w (if there is any) would violate the maximum concentration at its outlet. As shown above, this needs to be accompanied by an increase in fresh water intake which leads to the same situation over and over, until one finds a head process or a precursor for which some of its wastewater is not reused. We call this, a chain of precursors. Therefore, the perturbation of fresh water intake is infeasible if no process in the chain of precursors has wastewater that is not being reused.

Notice that

$$\delta_k = \frac{\delta_s^w}{\alpha_{k,s}} \qquad (4\text{-}41)$$

which can be obtained using a component balance over process s. Thus,

$$\overline{F}_s = F_s - \delta_k + \delta_s^w = F_s - \delta_s^w\left(\frac{1-\alpha_{k,s}}{\alpha_{k,s}}\right) \qquad (4\text{-}42)$$

which confirms that F_s also decreases. It also shows that the perturbation is feasible if and only if $F_{s,out} \geq \delta_s^w\left(\frac{1-\alpha_{k,s}}{\alpha_{k,s}}\right)$.

Because of this perturbation, $F_{s,out}$ decreases, and the rest of the structure downstream remains unaltered. This statement stems from the fact that a perturbation of $F_{s,r}$, process r being a receiver of process s, leads to an increase in F_r^w, perturbation we do not want to make because it leads to the same analysis for process r, as the one we are making for process s.

Thus, the change in fresh water intake is given by:

$$\Delta W = \overline{W} - W = \sum_{i=1}^{n-1} \alpha_{i,n}(\overline{F}_{i,out} - F_{i,out}) = \alpha_{k,n}\delta_k + \alpha_{s,n}\left(\delta_s^w - \delta_k\right) \qquad (4\text{-}43)$$

Replacing (4-41) into (4-43) and applying the definition of α, one obtains:

$$\Delta W = \delta_s^w \qquad (4\text{-}44)$$

which is positive by definition. This concludes the proof that a perturbation in one FWU leads to an overall increase in water consumption.

Consider now that $F_{k,out} = 0$, and therefore there is a chain of precursors $D = \{k_1, k_2, \cdots, k_t\}$ such that the wastewater of some process k_1 is not completely reused that is $F_{k_1,out} > 0$ (Figure 4-4).

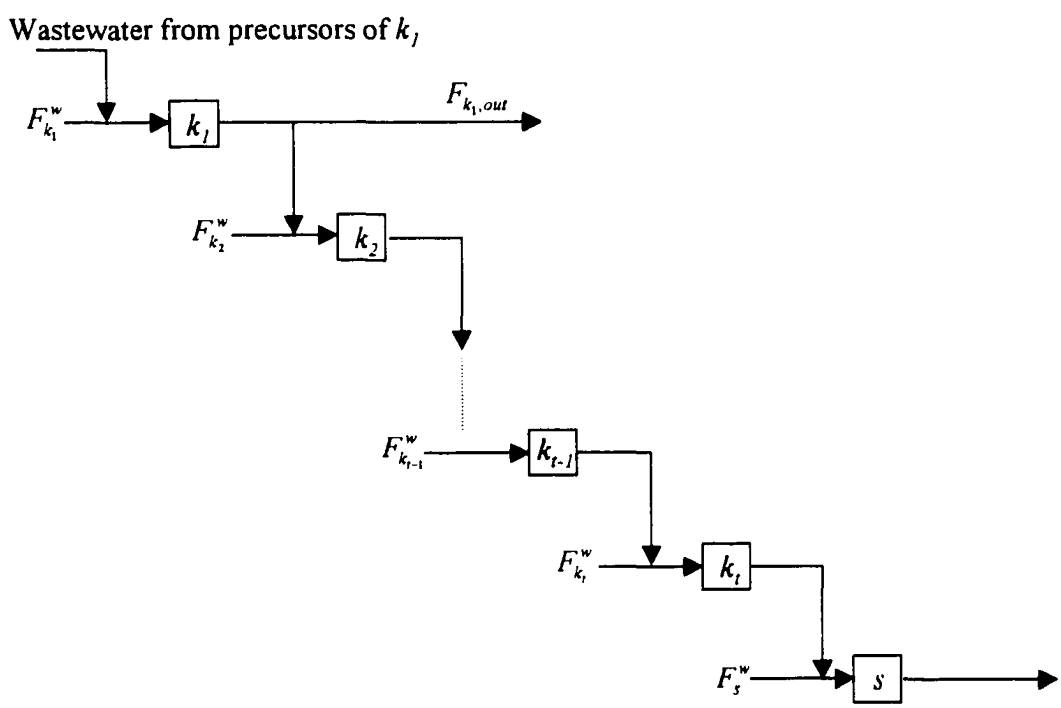


Figure 4-4
Chain of precursors of process s.

For this chain, we have:

$$\bar{F}^w_{k_i} = F^w_{k_i} + \delta^w_{k_i} \qquad k_i = k_2, k_3, \ldots, k_t \qquad (4\text{-}45)$$

In addition, since $F_{k_i,out} = 0$, then

$$\overline{F}_{k_i,k_{i+1}} = \overline{F}_{k_i} \qquad k_i = k_1, k_2, \ldots, k_t \tag{4-46}$$

and

$$\overline{F}_{k_i} = F_{k_i} - \delta_{k_i} \qquad k_i = k_2, k_3, \ldots, k_t \tag{4-47}$$

Relation (4-41) holds for δ_{k_i-1}, that is

$$\delta_{k_i-1} = \frac{\delta_{k_i}^w}{\alpha_{k_i-1,k_i}} \tag{4-48}$$

Now, similarly to (4-42), the process through process k_i is:

$$\overline{F}_{k_i} = F_{k_i} - \delta_{k_i-1} + \delta_{k_i}^w = F_{k_i} - \delta_{k_i}^w\left(\frac{1-\alpha_{k_i-1,k_i}}{\alpha_{k_i-1,k_i}}\right) \tag{4-49}$$

Using (4-47), (4-48) and (4-49)

$$\delta_{k_i} = \delta_{k_i-1}\left(1-\alpha_{k_i-1,k_i}\right) \tag{4-50}$$

Applying (4-50) recursively and using (41), one obtains:

$$\delta_{k_i} = \frac{\delta_{k_t}}{\prod_{m=k_i}^{k_t-1}\left(1-\alpha_{m,m+1}\right)} = \frac{\delta_s^w}{\alpha_{k_t,s}\prod_{m=k_i}^{k_t-1}\left(1-\alpha_{m,m+1}\right)} \tag{4-51}$$

which is positive. Thus, using (4-37)

$$\Delta W = \delta_{k_1}\alpha_{k_1,n} + \Delta F_s \alpha_{s,n} \tag{4-52}$$

Then, from (4-42)

$$\Delta W = \delta_{k_1}\alpha_{k_1,n} - \delta_s^w\left(\frac{1-\alpha_{k_t,s}}{\alpha_{k_t,s}}\right)\alpha_{s,n} \tag{4-53}$$

Using (4-51) and the fact that $\alpha_{k_1,n} > \alpha_{s,n}$, one obtains:

$$\begin{aligned} \Delta W &= \delta_{k_1}\left[\alpha_{k_1,n} - \left(1-\alpha_{k_t,s}\right)\alpha_{s,n}\prod_{m=k_1}^{k_t-1}\left(1-\alpha_{m,m+1}\right)\right] \\ &\geq \delta_{k_1}\alpha_{s,n}\left[1-\left(1-\alpha_{k_t,s}\right)\prod_{m=k_1}^{k_t-1}\left(1-\alpha_{m,m+1}\right)\right] \end{aligned} \tag{4-54}$$

The last term is positive. Consequently, we have shown that any feasible perturbation of the proposed fresh water intake of the optimum given by a maximum reused structure leads to an increase of overall fresh water intake.

To finalize the proof, we now show that the reuse structure of WWUs is optimal. Consider, without loss of generality that process n-1 is a WWU. Assume also, that process n is a FWU. Otherwise, if process n is a WWU, then any allocation policy does not alter the overall water usage. Consider a perturbation of the wastewater allocation to process $(n-1)$.

We will show that the perturbation leads to an increase of the fresh water usage of process n. Figure 4-5 illustrates one generic result of the maximum reuse rule applied to process n.

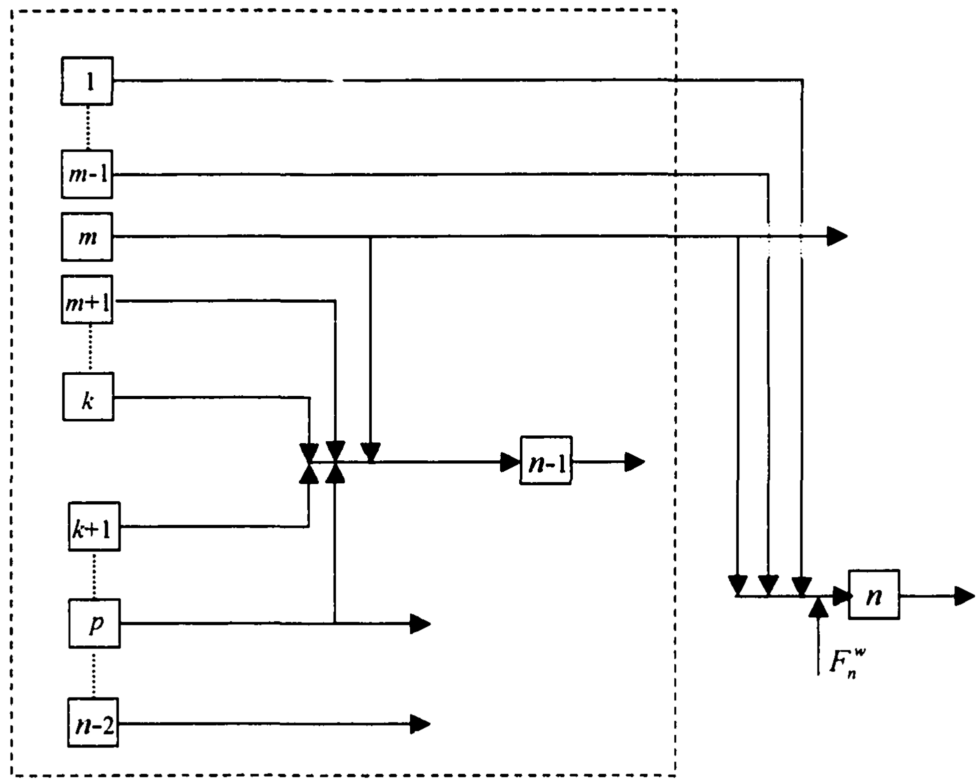


Figure 4-5
Maximum reuse generic structure for a WWU.

According to the maximum reuse rule, $F_{m,n-1} < F_m$, $F_{i,n-1} = F_i \ \forall i\,[m+1,\ldots,p-1]$, $F_{p,n-1} < F_p$ and $F_{j,n-1} = 0 \ \forall j \in [p+1,\ldots,n-2]$.

Consider now that a feasible perturbation is introduced:

$$\left.\begin{array}{l} \overline{F}_{p,n} = F_{p,n} - \delta_p \\ \overline{F}_{p+1,n} = \delta_{p+1} \\ \delta > 0 \end{array}\right\} \qquad (4\text{-}55)$$

We will first prove that increasing the flowrate of a wastewater precursor of higher concentration (δ_{p+1}) leads to an increase in the flowrate of a pseudo-fresh water precursor. That is $\delta_m > 0$.

Writing (4-28) before and after the perturbation and subtracting, one obtains:

$$\delta_m r_{m,n-1} - \delta_p r_{p,n-1} + \delta_{p+1} r_{p+1,n-1} = 0 \tag{4-56}$$

$$\delta_m \alpha_{m,n-1} - \delta_p \alpha_{p,n-1} + \delta_{p+1} \alpha_{p+1,n-1} = 0 \tag{4-57}$$

Solving for δ_m as a function of δ_{p+1}, we get:

$$\delta_m = \delta_{p+1} \frac{\left(\alpha_{p+1,n-1} r_{p,n-1} - \alpha_{p,n-1} r_{p+1,n-1}\right)}{\left(\alpha_{p,n-1} r_{m,n-1} - \alpha_{m,n} r_{p,n-1}\right)} \tag{4-58}$$

Using the definition of α and r, one obtains:

$$\delta_m = \delta_{p+1} \frac{\left(C_{p+1,out}^{\max} - C_{p,out}^{\max}\right)}{\left(C_{p,out}^{\max} - C_{m,out}^{\max}\right)} \tag{4-59}$$

Therefore, in virtue of the monotonicity of the outlet concentrations of the precursors, $\delta_m > 0$. By substituting in (4-56), one can verify that $\delta_p > 0$.

By construction, the above perturbations would not alter the total fresh water intake of the network system that includes process n-1. However, if process n is a FWU and consumes wastewater from process m, then a reduction of available wastewater of low concentration will in itself increase F_n^w. This is straightforward from (4-15), (4-16) and (4-4).

Q.E.D.

Remark: The above proof only shows that the algorithmic procedure provides one optimal solution. There are, however, many other solutions of the same overall fresh water consumption that can be constructed (Chapter 5). This result stems from the fact that the maximum reuse policy is a sufficient condition of optimum, not a necessary one. For example, in the optimality proof we showed that departing from the maximum reuse policy for WWUs does not always lead to an increase in fresh water usage.

4.6 Examples

We now show some examples form the literature where the network obtained using the algorithmic procedure is compared to the reported one.

4.6.1 Example 4-1

This example is taken from Wang and Smith (1994). The system involves four processes and their corresponding data is given in Table 3-1 from Chapter 3.

We now show how the new design methodology is applied to this problem.

Step 1: **Identify Head Processes**

Process 1 is the only process with maximum inlet concentration equal to zero. Using (4-34), one obtains:

$$F_1^w = \frac{L_1}{C_{1,out}^{\max}} = \frac{2{,}000\ g/h}{100\ ppm} = 20.0\ ton/h.$$

Step 2: **Maximum outlet concentration ordering**

There are three processes left to order. Those are shown below in Table 4-1.

Table 4-1: Ordering of processes by C_{out}^{max}

Process Number	C_{out}^{max}
2	100
3	800
4	800

Since processes 3 and 4 has the same outlet maximum concentration, either one could be listed first.

Step 3: **Apply the Maximum Reuse Rules**

3.1. We take the first process of the list (process 2) and apply the rule. We realize that due to the necessary condition of monotonicity, there are no possible precursors for this process. Therefore, fresh water is fed to process 2. Calculating the necessary fresh water intake, we obtain:

$F_2^w = 50.0\ ton/h$

3.2. We take process 3 and apply the rules. The maximum outlet concentration of this process allows us to supply it with wastewater from either process 1 or 2. Using (4-16), we can write:

$$F_{1,3} = \frac{K_3 C_{3,in}^{max}}{C_{1,out}^{max} - (1-\alpha_{1,3})C_{3,in}^{max}} = \frac{37.5 \cdot 50}{100-(1-0.875)\cdot 50} = 20.0\ ton/h$$

$F_{1,3} = 20.0 = F_1$.

Consequently, we can fulfill process 3 water intake by using process 1 only. We now calculate the necessary fresh water intake using (4-4).

$$F_3^w = K_3 - F_{1,3}\alpha_{1,3} = 37.5 - 20.0 \cdot 0.875 = 20.0\ ton/h$$

3.3. Finally, we consider process 4. This process has only one monotone precursor, which is process 2. Process 3 has wastewater of the same concentration as the maximum outlet process 4. Therefore, it cannot be used as a wastewater provider. The outlet concentration of process 2 is lower than the maximum inlet concentration of process 4, therefore the latter is a WWU candidate (Case I). Using (4-25), one obtains:

$$F_{2,4} = \frac{L_4}{\left(C_{4,out}^{\max} - C_{2,out}^{\max}\right)} = \frac{4{,}000}{(800 - 100)} = 5.7143\ ton/h < F_2$$

Since $F_{2,4} < F_2$, process 4 does not require any other water intake to fulfill its requirements. Consequently, it is a true WWU and the problem is solved.

Finally, we calculated the total fresh water intake that the network requires, that is:

$$W = F_1^w + F_2^w + F_3^w = 20.0 + 50.0 + 20.0 = 90.0\ ton/h.$$

Both, the water consumption and the network design coincide with those reported by Wang and Smith (1994). The flowrates and the network obtained are as those shown in Table 3-1 and Figure 3-8, respectively.

4.6.2 Example 4-2

The six-process WAP problem proposed by Olesen and Polley (1997) (Example 3-2) is solved using the Maximum Reuse Algorithm. The obtained water network system is shown in Figure 3-11. In this flowsheet, all processes have reached maximum outlet concentration through maximum reuse. All the necessary conditions of optimality are also satisfied by the solution. The network system obtained by Olesen and Polley (Figure 3-10) constitutes a degenerate solution.

It is important to point out that, although degenerate solutions provide the same overall fresh water consumption, they feature larger flowrate through some processes. The total flowrate through the degenerate solution is 252.857 ton/h compared to 213.571 ton/h of the maximum reuse structure solution. This represents an 18.4 % larger total flowrate through the degenerate solution. This situation may lead to larger equipment.

4.6.3 Example 4-3

Example 4-3 comprises a system of ten processes. This example is not taken from the literature. Table 4-2 shows the data for this example including all the minimum fresh water requirements of these processes without wastewater reuse.

Table 4-2: Data for Example 4-3

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Minimum Fresh Water Flowrate without Reuse (ton/h)
1	2.0	25	80	25.0
2	2.88	25	90	32.0
3	4.0	25	200	20.0
4	3.0	50	100	30.0
5	30.0	50	800	37.5
6	5.0	400	800	6.25
7	2.0	200	600	3.3333
8	1.0	0	100	10.0
9	20.0	50	300	66.6667
10	6.5	150	300	21.6667
		Total Minimum Flowrate (ton/h)		**252.4167**

Figure 4-6 shows a solution network obtained using the algorithmic procedure. Table 4-3 shows all the resulting flowrates and final concentrations of the processes.

Table 4-3: Solution of Example 4-3

Process Number	Type of Process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum Fresh Water Flowrate with Reuse (ton/h)
1	H	0.0	0	80	25.0
2	I	$F_{1,2} = 13.8462$	25	90	30.4615
3	I	$F_{2,3} = 6.3492$	25	200	16.5079
4	I	$F_{1,4} = 11.1538$ $F_{2,4} = 23.4188$	50	100	25.4273
5	T	$F_{4,5} = 9.51428$ $F_{8,5} = 10.0$ $F_{9,5} = 0.16191$	50	800	20.3238
6	WWU	$F_{9,6} = 16.6667$	300	800	0.0
7	WWU	$F_{3,7} = 1.19047$ $F_{4,7} = 1.90476$ $F_{9,7} = 1.90476$	200	600	0.0
8	H	0.0	0	100	10.0
9	T	$F_{2,9} = 14.5397$ $F_{4,9} = 26.9143$	50	300	38.5460
10	WWU	$F_{3,10} = 21.6667$ $F_{4,10} = 21.6667$	150	300	0.0
		Total minimum fresh water flowrate (ton/h)			**166.2665**

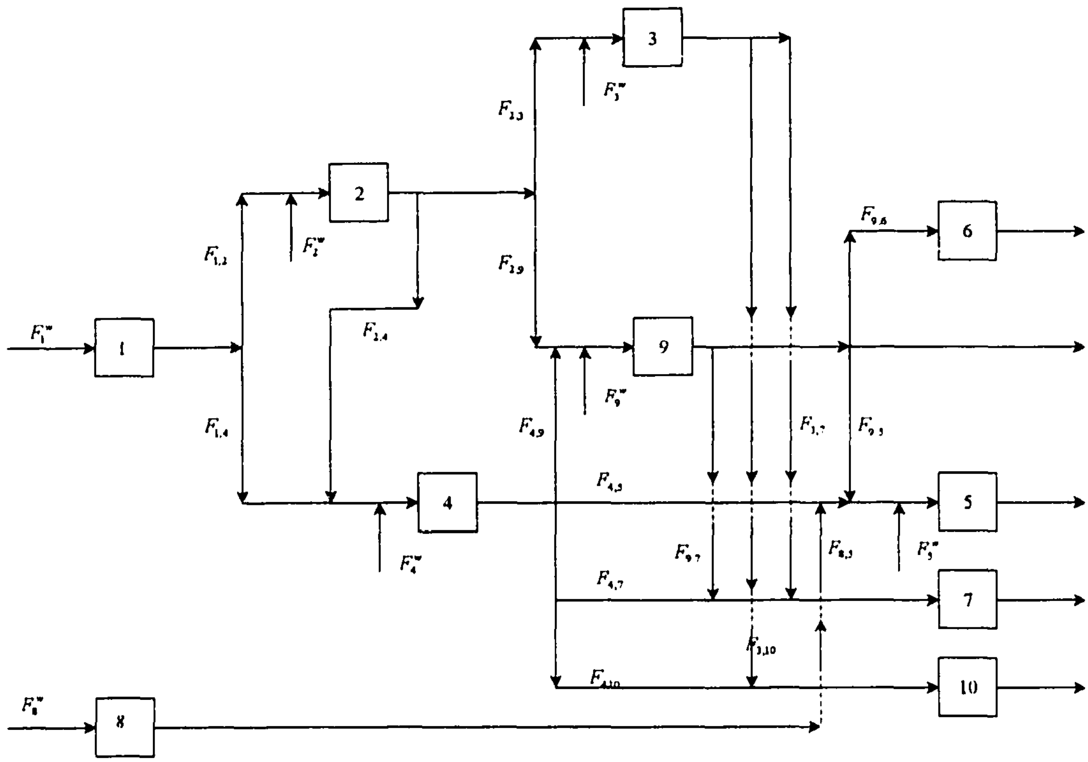


Figure 4-6
Maximum Reuse Network solution for Example 4-3.

4.6.4 Example 4-4

Example 4-4 presents a large-scale problem, which contains twenty processes. Table 4-4 shows the data for this example including all the minimum fresh water requirements of these processes without wastewater reuse. Figure 4-7 shows the network system obtained using the algorithmic procedure. Tables 4-5A and 4-5B contain the network flowrates and concentrations.

Table 4-4: Data for Example 4-4

Process Number	**Mass Load of Contaminant (kg/h)**	C_{in}^{max} **(ppm)**	C_{out}^{max} **(ppm)**	**Minimum Fresh Water Flowrate without Reuse (ton/h)**
1	1.0	0	80	12.5
2	2.0	0	100	20.0
3	2.0	0	120	16.6667
4	2.0	25	80	25.0
5	2.880	25	90	32.0
6	1.5	40	90	16.6667
7	3.0	50	100	30.0
8	4.0	75	120	33.3333
9	4.0	25	200	20.0
10	10.0	75	150	66.6667
11	8.0	120	200	40.0
12	1.8	200	300	6.0
13	20.0	75	300	66.6667
14	6.5	150	300	21.6667
15	2.0	200	600	3.3333
16	30.0	50	800	37.5
17	5.0	400	800	6.25
18	7.0	400	500	14.0
19	2.550	600	850	3.0
20	0.6	800	950	0.63158

The total fresh water that would be required if no reuse were done is 471.88158 ton/h. The minimum fresh water target found through the algorithmic procedure is 299.35873 ton/h, which means 36.6 % water savings.

Table 4-5A: Processes 1 through 10 of Example 4-4

Process Number	Type of Process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum Fresh Water Flowrate with Reuse (ton/h)
1	H	0.0	0	80	12.5
2	H	0.0	0	100	20.0
3	H	0.0	0	120	16.667
4	H	0.0	0	80	25.0
5	I	$F_{4,5} = 13.846$	25	90	30.462
6	I	$F_{1,6} = 12.5$ $F_{4,6} = 2.5$	40	90	15.0
7	I	$F_{4,7} = 8.654$ $F_{5,7} = 25.641$	50	100	25.705
8	I	$F_{5,8} = 18.667$ $F_{6,8} = 30.0$ $F_{7,8} = 22.867$	75	120	17.356
9	I	$F_{8,9} = 4.762$	25	200	18.095
10	I	$F_{2,10} = 20.0$ $F_{7,10} = 37.133$ $F_{8,10} = 35.722$	75	150	40.478

Table 4-5B: Processes 11 through 20 of Example 4-4

Process Number	Type of Process	$F_{i,j}$ (ton/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum Fresh Water Flowrate with Reuse (ton/h)
11	I	$F_{3,11} = 16.667$ $F_{8,11} = 48.405$ $F_{10,11} = 27.943$	120	200	6.986
12	I / WWU	$F_{11,12} = 18.0$	200	300	0.0
13	I	$F_{10,13} = 44.444$	75	300	44.444
14	T/ WWU	$F_{10,14} = 43.333$	150	300	0.0
15	I / WWU	$F_{9,15} = 5.0$	200	600	0.0
16	I	$F_{10,16} = 13.333$	50	800	26.667
17	I / WWU	$F_{12,17} = 6.250$ $F_{18,17} = 6.250$	400	800	0.0
18	I / WWU	$F_{13,18} = 35.0$	300	500	0.0
19	T / WWU	$F_{15,19} = 5.0$ $F_{16,19} = 1.733$ $F_{18,19} = 3.467$	600	850	0.0
20	T / WWU	$F_{17,20} = 4.0$	800	950	0.0

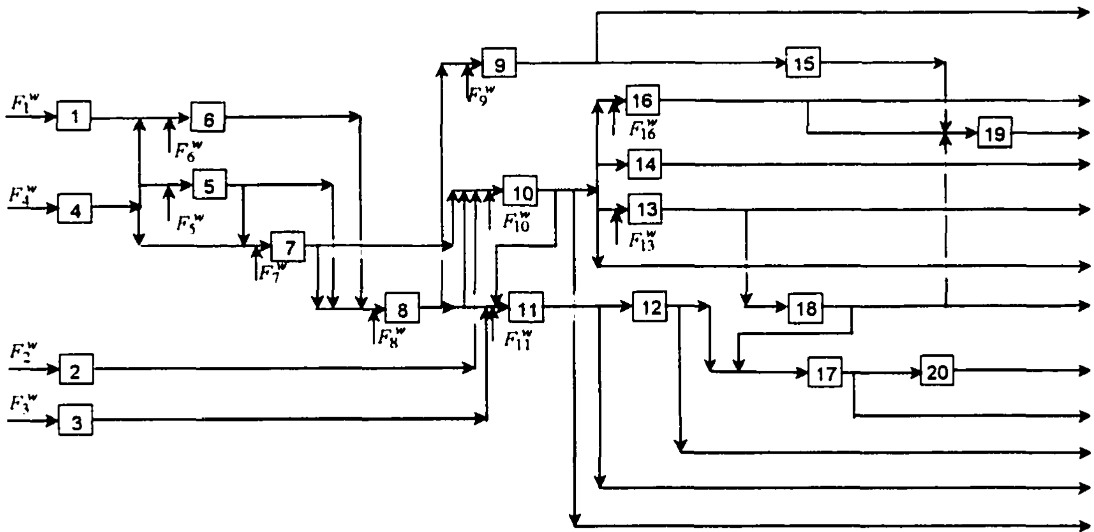


Figure 4-7
Maximum Reuse Network solution for Example 4-4.

4.7 Conclusions

A new method to solve the water allocation problem in refineries and process plants has been presented. It has been shown through multiple examples that the procedure always provides the minimum fresh water target and a realizing network. The design can be performed totally by hand even for large-scale problems.

4.8 Notation

C concentration of contaminant, ppm
F water flowrate, ton/h
$\overline{F}$ water flowrate after a perturbation, ton/h

Subscripts:

in	at inlet
out	at outlet
j	process *j*
P_j	precursors of *j*
R_j	receivers of *j*

Superscripts:

min	minimum
max	maximum
*	additional sources
w	fresh water

4.9 References

1. Olesen S.G. and G.T. Polley. *A Simple Methodology for the Design of Water Networks Handling Single Contaminants*. Trans IChemE, 75, part A, pp. 420-426, 1997.
2. Wang Y. P. and R. Smith. *Wastewater Minimization*. CES, 49, 7, pp. 981, 1994.

CHAPTER 5

On the Use of Linear Models for the Design of Water Utilization Systems in Refineries and Process Plants

5.1 Introduction

This chapter addresses the optimum design of single-contaminant water utilization systems (WAP problem) by means of mathematical programming. The WAP problem was formally defined in Chapter 2.

As mentioned in Chapter 1, Takama *et al.* (1980) used mathematical programming to solve a WAP problem for the first time. A superstructure of all water using operations and cleanup processes was set up and an optimization was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. The authors transformed the model into a series of problems without inequality constraints by using a penalty function and finally solving it using the Complex method.

Doyle and Smith (1997) presented a superstructure optimization where two cases were analyzed. In the first case, a nonlinear problem is proposed where the contaminant pickup loads for each water-using operation are fixed. Similarly, a linear problem is proposed by fixing the outlet concentrations at their maximum allowed values. The linear optimization problem is only solved to provide the nonlinear formulation with a feasible starting point.

Alva-Argáez *et al.* (1998) presented a solution approach for multicomponent systems based on mathematical programming. The problem is modeled as a nonconvex MINLP and then solved using a two-phase strategy. This approach cannot guarantee optimality.

All the above work constitutes important attempts to solve the single and multiple contaminant WAP problem. However, each of these methods has either numerical or some other problems that prevent them from being robust.

The Water Allocation Planning (WAP) problem is usually modeled as a nonconvex nonlinear optimization problem. In this chapter, we propose an LP formulation for the optimal solution of the single contaminant WAP problem and a series of MILP problems to design different network alternatives. The new approach is based on previously developed necessary conditions of optimality (Chapter 3). Several examples are presented to illustrate the proposed methodology.

5.2 Targeting

The Water Allocation Planning problem can be modeled as an NLP problem. We will assume that each water-using unit is characterized by a contaminant load that needs to be entirely removed and by inlet and outlet maximum concentration constraints. The formulation of the NLP is as follows:

$$\mathbf{M1} = Min \sum_j F_j^w$$

$s.t.$

$$F_j^w + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,out} = 0 \qquad \forall j \in \boldsymbol{N}, i \in \boldsymbol{P}_j, k \in \boldsymbol{R}_j \tag{5-1}$$

$$F_h^w - \frac{L_h}{C_{h,out}^{\max}} = 0 \qquad \forall h \in \boldsymbol{H} \tag{5-2}$$

$$\sum_i F_{i,j}\left(C_{i,out} - C_{j,in}\right) - F_j^w C_{j,in} = 0 \qquad \forall j \in \overline{\boldsymbol{H}}, i \in \boldsymbol{P}_j \tag{5-3}$$

$$\sum_i F_{i,j}\left(C_{i,out} - C_{j,out}\right) - F_j^w C_{j,out} + L_j = 0 \qquad \forall j \in \overline{\boldsymbol{H}}, i \in \boldsymbol{P}_j \tag{5-4}$$

$$C_{j,in} \le C_{j,in}^{\max} \qquad \forall j \in \overline{\boldsymbol{H}} \tag{5-5}$$

$$C_{i,out} \le C_{i,out}^{\max} \qquad \forall\, i \in \overline{\boldsymbol{H}} \tag{5-6}$$

$$F_j^w, F_{i,j}, F_{j,out} \ge 0 \qquad \forall j \in \boldsymbol{N} \tag{5-7}$$

The problem has bilinear terms in those equality constraints where flowrate and concentration are simultaneously present. However, these bilinearities can be eliminated using the necessary condition of maximum outlet concentrations, that is, setting outlet concentrations to their maximum values.

The constraints can now be combined as follows:

$$\left.\begin{array}{l} \sum_i F_{i,j}\left(C_{i,out}^{\max} - C_{j,in}\right) - F_j^w C_{j,in} = 0 \\ C_{j,in} \le C_{j,in}^{\max} \end{array}\right\} \Leftrightarrow$$

$$\sum_i F_{i,j}\left(C_{i,out}^{\max} - C_{j,in}^{\max}\right) - F_j^w C_{j,in}^{\max} \le 0 \qquad \forall j \in \overline{\boldsymbol{H}}, i \in \boldsymbol{P}_j \tag{5-8}$$

$$\left.\begin{array}{l}\sum_i F_{i,j}\left(C_{i,out}-C_{j,out}\right)-F_j^w C_{j,out}+L_j=0\\ C_{i,out}=C_{i,out}^{\max}\end{array}\right\}\Leftrightarrow$$

$$\sum_i F_{i,j}\left(C_{i,out}^{\max}-C_{j,out}^{\max}\right)-F_j^w C_{j,out}^{\max}+L_j=0 \qquad \forall j\in\overline{\boldsymbol{H}}, i\in \boldsymbol{P}_j \tag{5-9}$$

The resulting problem is:

$$\mathbf{M2}=Min\sum_j F_j^w$$

$s.t.$

$$F_j^w+\sum_i F_{i,j}-\sum_k F_{j,k}-F_{j,out}=0 \qquad \forall j\in \boldsymbol{N}, i\in \boldsymbol{P}_j, k\in \boldsymbol{R}_j \tag{5-10}$$

$$F_h^w-\frac{L_h}{C_{h,out}^{\max}}=0 \qquad \forall h\in \boldsymbol{H} \tag{5-11}$$

$$\sum_i F_{i,j}\left(C_{i,out}^{\max}-C_{j,in}^{\max}\right)-F_j^w C_{j,in}^{\max}\leq 0 \qquad \forall j\in\overline{\boldsymbol{H}}, i\in \boldsymbol{P}_j \tag{5-12}$$

$$\sum_i F_{i,j}\left(C_{i,out}^{\max}-C_{j,out}^{\max}\right)-F_j^w C_{j,out}^{\max}+L_j=0 \qquad \forall j\in\overline{\boldsymbol{H}}, i\in \boldsymbol{P}_j \tag{5-13}$$

$$F_j^w, F_{i,j}, F_{j,out}\geq 0 \qquad \forall j\in \boldsymbol{N} \tag{5-14}$$

This problem is linear. Consequently, the optimal water flowrate and a feasible realizing network are both simultaneously obtained. Furthermore, when setting up the problem, the number of variables can be reduced by not including non-monotone connections as suggested by the monotonicity necessary condition.

5.2.1 Example 5-1: Targeting the Fresh Water Usage

To illustrate this, consider the following problem, which involves ten water-using processes. Table 5-1 shows the limiting data.

Table 5-1: Limiting data for Example on Targeting

Process Number	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Minimum Fresh Water Flowrate without Reuse (ton/h)
1	2.0	25	80	25.0
2	2.88	25	90	32.0
3	4.0	25	200	20.0
4	3.0	50	100	30.0
5	30.0	50	800	37.5
6	5.0	400	800	6.25
7	2.0	400	600	3.3333
8	1.0	0	100	10.0
9	20.0	50	300	66.6667
10	6.5	150	300	21.6667
		Total Minimum Flowrate (ton/h)		**252.4167**

In this problem, after monotonicity is applied, the number of possible interconnections reduces from 72 to 40. Table 5-2 shows the results obtained using LINDO and Figure 5-1 shows the resulting realizing network. The fresh water savings are over 34 %.

Table 5-2: Solution of Targeting Example

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{1,3} = 7.14286$	15.7143	0.0
4	$F_{1,4} = 17.8571$	26.4286	0.0
5	$F_{4,5} = 20.0$	20.0	40.0
6	$F_{7,6} = 4.16667$ $F_{10,6} = 8.33333$	0.0	12.5
7	$F_{3,7} = 4.02857$ $F_{9,7} = 1.29524$	0.0	1.15714
8	0.0	10.0	0.0
9	$F_{2,9} = 32.0$ $F_{4,9} = 11.20$	36.80	78.7048
10	$F_{3,10} = 18.8286$ $F_{4,10} = 13.0857$ $F_{8,10} = 10.0$	0.0	33.5710
Total Minimum Freshwater Usage (ton/h)		**165.9424**	

It is worth noting that the optimization may render a network that, although feasible, could require too many interconnections. Moreover, some of them may be even impractical. For example, the flowrate from process 9 to 7 is only 1.2952 ton/h, which requires a 15-mm ID pipe, if an economical velocity of 2.0 m/s is assumed. In this example, there are a total of 12 interconnections among processes and 24 when counting connections from the fresh water source to the processes and connections from the units to the wastewater treatment plant.

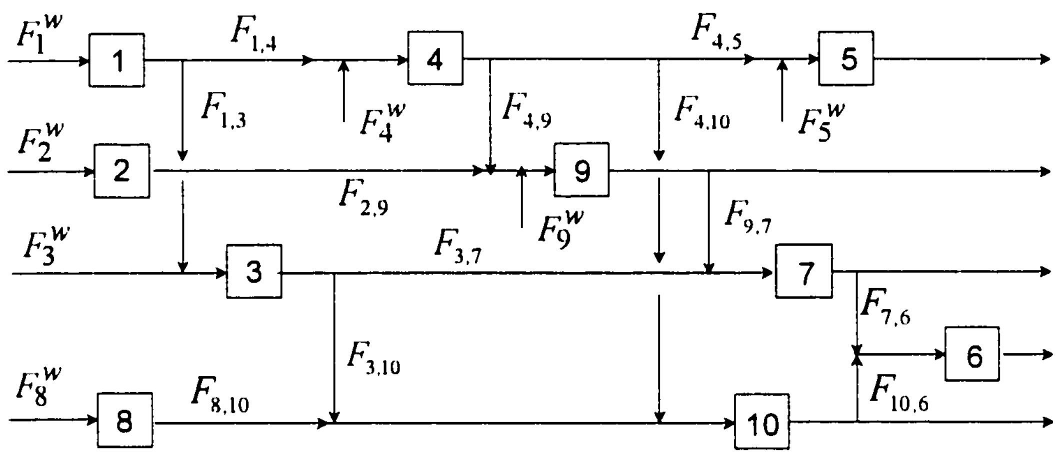


Figure 5-1
Solution network for LP formulation of Targeting Example.

5.3 Alternative Solutions

Once the target is obtained, different network alternatives can be sought. To do that, different objective functions are proposed and the minimum fresh water usage is added as a constraint. We now consider these different cases.

5.3.1 CASE 1: Minimum Number of Interconnections

The flowsheet obtained in Example 5-1 has 12 interconnections ($F_{i,j}$), 7 connections from the fresh water source to the FWU (F_j^w) and 5 connections between terminal processes and the wastewater treatment plant ($F_{j,out}$).

In a grassroots design, it would be desirable to minimize the number of interconnections as a means of reducing piping costs as well as instrumentation.

Therefore, a new model can be proposed where the objective function is no longer the fresh water consumption but the summation of the number of possible connections among processes.

The definitions of head process, monotonicity and maximum outlet concentrations are also applied to reduce the number of variables. The formulation of the problem follows:

$$\mathbf{M3} = Min\left(\sum_{i,j} Y_{i,j} + \sum_{w,j} Y_{w,j} + \sum_{j,o} Y_{j,o}\right)$$

$s.t.$

$$F_j^w + \sum_i F_{i,j} + \sum_k F_{j,k} - F_{j,out} = 0 \qquad \forall j \in \boldsymbol{N}, i \in \boldsymbol{P}_j, k \in \boldsymbol{R}_j \qquad (5\text{-}15)$$

$$\sum_j F_j^w = \alpha \qquad \textit{where } \alpha \textit{ is the targeted fresh water} \qquad (5\text{-}16)$$

$$F_h^w - \frac{L_h}{C_{h,out}^{max}} = 0 \qquad (5\text{-}17)$$

$$\sum_i \boldsymbol{F}_{i,j}\left(C_{i,out}^{max} - C_{j,in}^{max}\right) - F_j^w C_{j,in}^{max} \le 0 \qquad \forall j \in \overline{\boldsymbol{H}}, i \in \boldsymbol{P}_j \qquad (5\text{-}18)$$

$$\sum_i F_{i,j}\left(C^{max}_{i,out} - C^{max}_{j,out}\right) - F^w_j C^{max}_{j,out} + L_j = 0 \qquad \forall j \in \overline{H}, i \in P_j \qquad (5\text{-}19)$$

$$F_{i,j} - U\,Y_{i,j} \leq 0 \qquad \forall j \in \overline{H}, i \in P_j \qquad (5\text{-}20)$$

$$F^w_j - U\,Y_{w,j} \leq 0 \qquad \forall j \in \overline{H} \qquad (5\text{-}21)$$

$$F_{j,out} - U\,Y_{j,o} \leq 0 \qquad \forall j \in N \qquad (5\text{-}22)$$

$$F^w_j, F_{i,j}, F_{j,out} \geq 0 \qquad \forall i, j \in N \qquad (5\text{-}23)$$

$$Y_{i,j}; Y_{w,j}; Y_{j,o} = 0, 1 \qquad \forall i, j \in N \qquad (5\text{-}24)$$

Two new constraints have been added to the problem,

$$\sum_j F^w_j = \alpha \qquad (5\text{-}25)$$

where α is the optimal fresh water flowrate obtained solving the targeting problem, and

$$F_{i,j} - U\,Y_{i,j} \leq 0 \qquad \forall j \in \overline{H}, i \in P_j \qquad (5\text{-}26)$$

which relate the inter-processes flowrates with the integer variables. In these constraints, number larger than any feasible value of $F_{i,j}$ $(\forall i, j)$. For this problem, the value of U was chosen to be larger than the targeted fresh water flowrate, α.

Using this model, three different examples were run. The first one minimizes the number interconnections among processes, $F_{i,j}$; the second minimizes the connections between the fresh water source and the processes. Finally, all type of connections including those between the processes and the wastewater treatment plant is minimized.

5.3.1.1 Example 5-2: Minimization of the Number of Interconnections Among Processes

Consider the same limiting data as in Example 5-1 and its corresponding target value $\alpha = 165.9424$ ton/h. The problem formulation contains only the integer variables $Y_{i,j}$. The solution yields 9 interconnections instead of the 12 previously obtained for Example 5-1. Since the minimum fresh water usage is the same, this solution network constitutes a better alternative than the one of Example 5-1. Figure 5-2 and Table 5-3 show the new design network and the results, respectively. The solution was obtained using LINDO/CIPLEX.

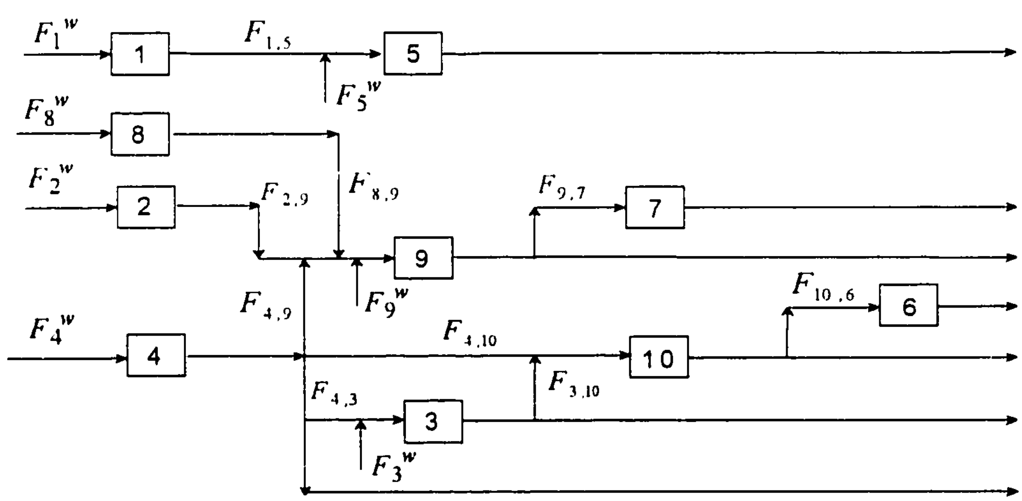


Figure 5-2
Minimum number of interconnections.

Table 5-3: Solution of Example 5-2

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{4,3} = 5.7143$	17.1429	1.1905
4	0.0	30.0	1.4190
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{10,6} = 10.0$	0.0	10.0
7	$F_{9,7} = 6.6667$	0.0	6.6667
8	0.0	10.0	0.0
9	$F_{2,9} = 32.0$ $F_{4,9} = 1.20$ $F_{8,9} = 10.0$	36.80	73.3333
10	$F_{3,10} = 21.6667$ $F_{4,10} = 21.6667$	0.0	33.3333
CONNECTIONS	**9**	**7**	**7**

5.3.1.2 Example 5-3: Minimization of the Number of Interconnections Among Processes and the Connections Between the Fresh Water Source and the FWU

In this example, we have included the connections from the water source. That is, the integer variables $Y_{w,j}$ have been added to the problem formulation. The resulting number of connections is 16, 7 of those corresponds to fresh water connections and 9 to interconnections among units. The flowsheet obtained, Figure 5-3, and is slightly different to that of Figure 5-2. The solution was also obtained using LINDO/CIPLEX.

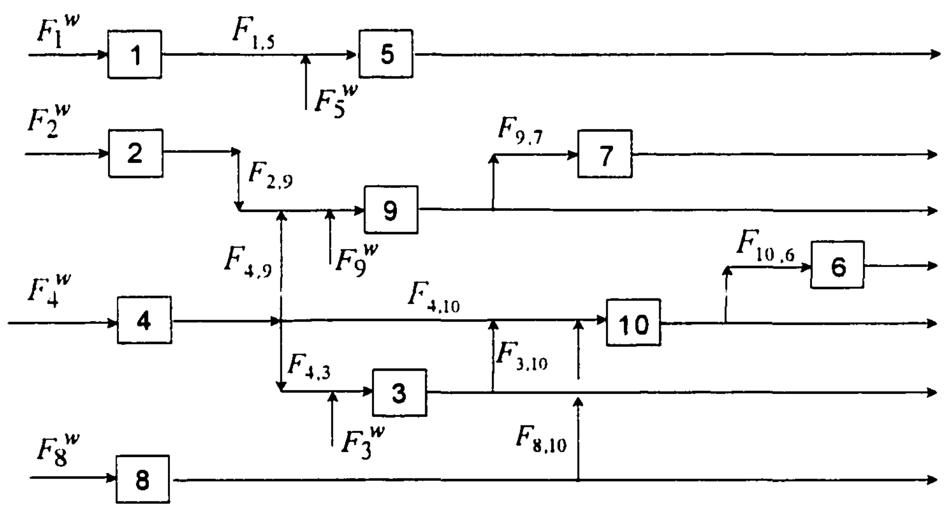


Figure 5-3
Minimum number of fresh water and inter-processes connections.

Table 5-4: Solution of Example 5-3

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{4,3} = 5.7143$	17.1428	1.190
4	0.0	30.0	0.0
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{10,6} = 10.0$	0.0	10.0
7	$F_{9,7} = 6.6667$	0.0	6.667
8	0.0	10.0	1.419
9	$F_{2,9} = 32.0$ $F_{4,9} = 11.20$	36.80	73.333
10	$F_{3,10} = 21.667$ $F_{4,10} = 13.086$ $F_{8,10} = 8.5810$	0.0	33.333
CONNECTIONS	**9**	**7**	**7**

5.3.1.3 Example 5-4: Minimization of the Total Number of Connections

In this case, all three types of connections are considered. The minimum number of connections, for the given minimum fresh water target, is 22. Table 5-5 shows that, upon optimization, the number of total interconnections was reduced by one. Figure 5-4 shows the final network for this case.

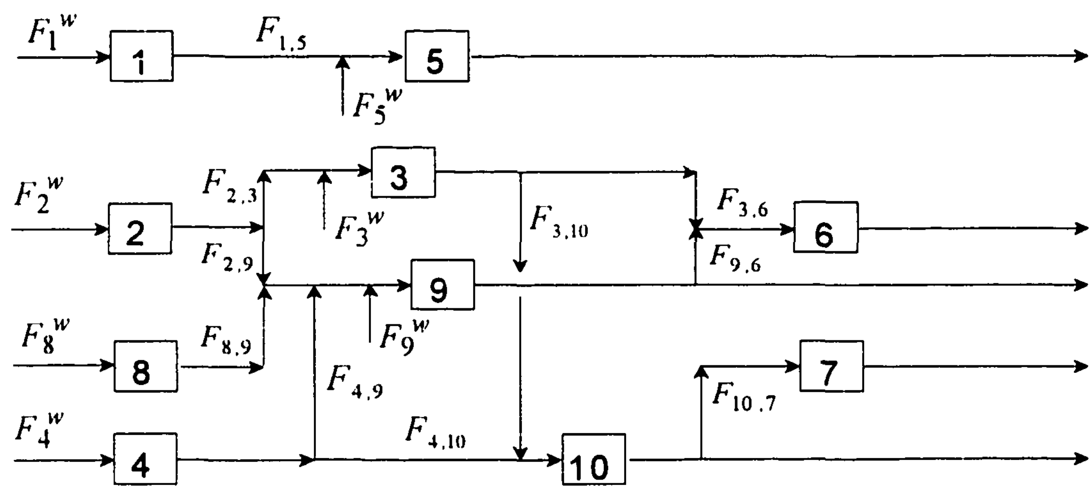


Figure 5-4
Network solution to Example 5-4.

The purpose of solving the same example using different objective functions is to show how many different alternative flowsheets can be obtained for the same optimal condition of minimum fresh water usage. When designing, the awareness of these alternatives is highly advantageous. Another important feature to observe from these solutions is that, without imposing flowrate constraints the last optimization removed all negligible streams from the flowsheet. The solution networks for Examples 5-2 and 5-3 have flowrates lower than 1.5 tons/h, which can be considered uneconomical. None of them appear in the last solution network. In all the following examples, GAMS has been used as the equation modeling system and GAMS/CIPLEX as the MILP solver.

Table 5-5: Solution of Example 5-4

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{2,3} = 6.349$	16.508	0.0
4	0.0	30.0	0.0
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{3,6} = 4.029$ $F_{9,6} = 5.166$	0.0	9.194
7	$F_{10,7} = 6.667$	0.0	6.667
8	0.0	10.0	0.0
9	$F_{2,9} = 25.651$ $F_{4,9} = 6.914$ $F_{8,9} = 10.0$	37.435	74.834
10	$F_{3,10} = 18.829$ $F_{4,10} = 23.086$	0.0	35.248
CONNECTIONS	**10**	**7**	**5**

5.3.2 Case 2: Minimum Fixed Costs

Reducing the number of interconnections is relevant for a cost-effective design. However, the networks obtained in previous examples do not guarantee minimum cost but only minimum number of connections. Since not all interconnections will require the same fixed capital investment, it seems most appropriate to minimize the fixed annualized cost.

5.3.2.1 Example 5-5

For this example, without loss of generality, a series of single cost values representing each interconnection is given as shown in Table 5-6. The columns for processes 1 and 8 has been eliminated because those are head processes, therefore they cannot reuse water. These values can be understood as the corresponding calculations of the annualized installed costs of piping, valves and pumps.

The new objective function can be written as:

$$\sum_{i,j} c_{i,j} Y_{i,j} \tag{5-27}$$

The rest of model (M_3) remains the same. The integer variables chosen are the interconnections among processes and those between processes and the wastewater treatment plant. The connections from the fresh water source cannot be different than those previously obtained hence; they have been excluded from the optimization.

The optimal cost is \$53,159. The resulting network is shown in Figure 5-5 and the flowrate values in Table 5-7.

Table 5-6: Cost data in $/year for Example 5-5

Process	2	3	4	5	6	7	9	10	WWT
1	2,419	2,981	3,169	3,544	3,544	3,544	2,981	2,794	5,419
2	----	2,794	2,981	3,544	3,544	3,544	3,169	2,981	5,419
3	----	----	----	2,981	3,169	3,544	3,544	3,544	4,669
4	----	2,419	----	2,794	2,981	3,544	3,544	3,544	4,669
5	----	----	----	----	----	----	----	----	3,919
6	----	----	----	----	----	----	----	----	3,919
7	----	----	----	2,981	2,794	----	----	----	3,919
8	----	3,544	----	3,169	2,981	2,419	2,794	2,981	3,919
9	----	----	----	3,544	3,544	2,981	----	----	4,669
10	----	----	----	3,544	3,544	3,169	----	----	4,669

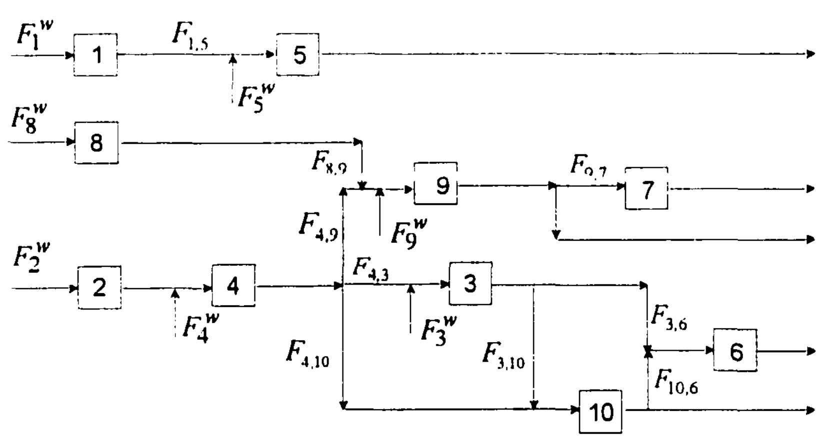


Figure 5-5
Solution network for minimum fixed cost example.

Table 5-7: Solution of Fixed Cost problem

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{4,3} = 5.714$	17.143	0.0
4	$F_{2,4} = 32.0$	26.80	0.0
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{3,6} = 4.028$ $F_{10,6} = 5.166$	0.0	9.194
7	$F_{9,7} = 6.667$	0.0	6.667
8	0.0	10.0	0.0
9	$F_{4,9} = 30.0$ $F_{8,9} = 10.0$	40.0	73.333
10	$F_{3,10} = 18.829$ $F_{4,10} = 23.086$	0.0	36.749
CONNECTIONS	**10**	**7**	**5**

5.3.3 Case 3: Forbidden / Compulsory Matches

It is quite often found that connections between certain processes are not allowed or must be imposed due to design or retrofit strategies. For example: heating and/or cooling limitations may render certain connections beneficial or undesirable; low flowrate interconnections, typically below 2.0 m^3/h, may be discarded due to economical or controllability reasons; finally, distance and space limitations may become decision variables as well.

When imposing such restrictions to any of the previous cases we can expect either feasible or infeasible solutions. The infeasibility may arise because no network can be found for the fresh water flowrate fixed at its minimum target.

Two example problems are presented below.

5.3.3.1 Example 5-6

This problem is a variance of Example 5-4 where a forbidden match between processes 2 and 3 ($Y_{2,3} = 0$), and a compulsory match between processes 4 and 3 ($Y_{4,3} = 1$) are imposed. Figure 5-6 and Table 5-8 show the new realizing network and the obtained flowrates, respectively.

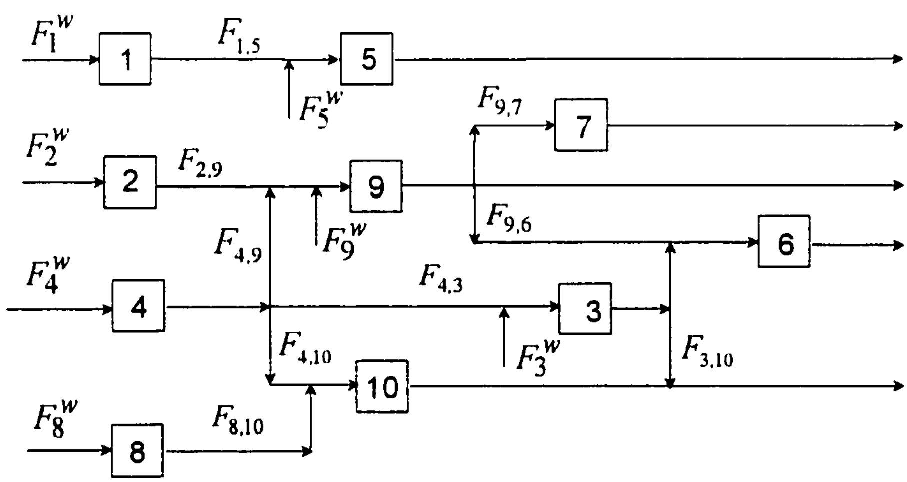


Figure 5-6
Solution network for Example 5-6.

Table 5-8: Solution of compulsory matches, Example 5-6

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{4,3} = 5.714$	17.143	0.0
4	0.0	30.0	0.0
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{3,6} = 4.028$ $F_{9,6} = 5.166$	0.0	9.194
7	$F_{9,7} = 6.667$	0.0	6.667
8	0.0	10.0	0.0
9	$F_{2,9} = 32.0$ $F_{4,9} = 11.20$	36.80	68.168
10	$F_{3,10} = 18.829$ $F_{4,10} = 23.086$ $F_{8,10} = 10.0$	0.0	41.914
CONNECTIONS	**10**	**7**	**5**

5.3.3.2 Example 5-7

Example 5-7 illustrates the increase in fixed costs when no process is allowed to send wastewater to more than two processes (including wastewater treatment units).

Reducing the number of stream splitting makes the system easier to control. This is accomplished by adding the constraint $\sum_j Y_{i,j} \leq 2\ \forall i \in N$. The new fixed cost is \$53,534 that is, only 0.7 % higher than the optimal. Figure 5-7 and Table 5-9 depict the corresponding network and flowrates, respectively.

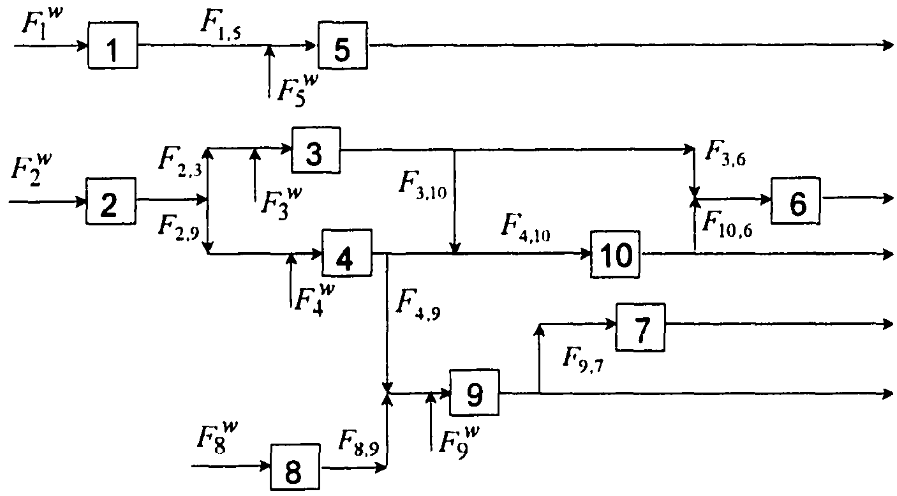


Figure 5-7
Solution network for Example 5-7.

Table 5-9: Solution of fixed cost with limited stream splitting

Process Number	$F_{i,j}$ (ton/h)	Minimum Fresh Water Flowrate with Reuse (ton/h)	Wastewater Flowrate (ton/h)
1	0.0	25.0	0.0
2	0.0	32.0	0.0
3	$F_{4,3} = 5.714$	17.143	0.0
4	$F_{2,4} = 32.0$	26.80	0.0
5	$F_{1,5} = 25.0$	15.0	40.0
6	$F_{3,6} = 4.028$ $F_{10,6} = 5.166$	0.0	9.194
7	$F_{9,7} = 6.667$	0.0	6.667
8	0.0	10.0	0.0
9	$F_{4,9} = 30.0$ $F_{8,9} = 10.0$	40.0	73.333
10	$F_{3,10} = 18.829$ $F_{4,10} = 23.086$	0.0	36.749
CONNECTIONS	**10**	7	5

5.4 Use of Degeneracy

Although the previous examples provide different alternatives, they are all build assuming that the outlet concentrations are at their maximum values. There are, however, solutions to the problem that satisfy the target minimum fresh water usage, but have outlet concentrations lower than their maximum. These cases are considered by the corollaries of the necessary conditions of optimum (Chapter 3). We will use the existence of these degenerate solutions to reduce the number of connections even further.

Consider the example problem proposed by Olesen and Polley (1997). The limiting data is shown in Table 3-3.

The authors solved this problem by inspection and proposed the network solution illustrated in Figure 5-8. The reported fresh water target is 157.14 ton/h.

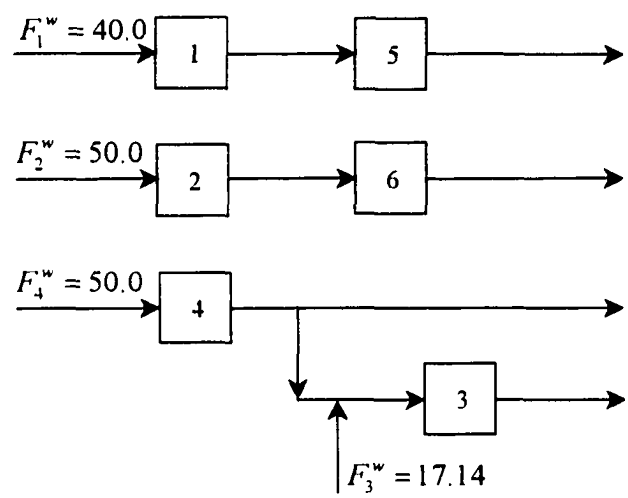


Figure 5-8
Design network proposed by Olesen and Polley.

From Figure 5-8 it can be observed that process 1 is consuming 15.0 ton/h more fresh water than the minimum required to pickup its entire load. As a consequence, its outlet concentration is 50 ppm instead of its possible maximum of 80 ppm. Therefore, Olesen and Polley solution can be understood as a degenerate solution. Its equivalent is the same network where process 1 reaches its maximum outlet concentration and $F_1^w = 25.0$, $F_5^w = 15.0$, with the rest of the values being the same. The wastewater produced by process 1 would be at 80 ppm.

Figure 5-9 shows a design network obtained when applying the LP targeting model. One can explore degenerate solutions where the fresh water intake of either process 3 or 4 is eliminated. Consider we want to eliminate the fresh water connection to process 3. In this case we will need wastewater available at 25 ppm which is the maximum inlet concentration allowed for process 3. To do that, the fresh water intake to process 1 should be increased to 80.0 ton/h. The minimum necessary reuse between units land 3 can be calculated to be 22.8571 ton/h. The remaining wastewater at process 1, 57.1429 ton/h, can then be sent to process 4 reducing its fresh water needs to 7.1428 ton/h. Thus, a new equivalent and feasible network can be obtained by increasing F_1^w, reducing F_4^w and eliminating F_3^w. The alternative flowrates are shown in Figure 5-9.

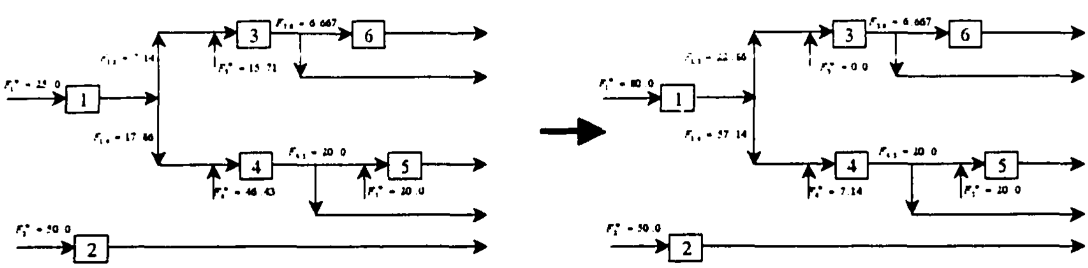


Figure 5-9
LP design network for the Olesen and Polley problem with degenerate alternatives.

In conclusion, one can always explore degenerate alternatives once the LP model network has been obtained and by applying the corresponding corollary of the necessary conditions.

5.5 Conclusions

A method to solve the water allocation problem in refineries and process plants using linear programming has been presented. It has been shown through multiple examples that the problem has several alternative optimal solutions, including degenerate cases where flows of water through the processes are larger than the minimum needed. Forbidden and compulsory water transfers from one process to another have also been solved. These findings have important consequences for the design and retrofit of water utilization systems, as it provides a tool to obtain several alternative solutions.

5.6 Notation

c fixed cost of interconnection, \$/year
C concentration of contaminant, ppm
F water flowrate, ton/h
L contaminant load, kg/h
$\boldsymbol{N}$ this set includes all water-using units
$\boldsymbol{H}$ this set includes all Head Processes

Subscripts:
in at inlet
out at outlet
j process j
Superscripts:
min minimum

max maximum
w *fresh water*

5.7 References

1. Alva-Argáez A., A.C. Kokossis and R. Smith. *Automated Design of Industrial Water Networks*. AIChE Annual Meeting, paper 13f, Miami, 1998.
2. Doyle, S. J. and R. Smith. *Targeting Water Reuse with Multiple Contaminants* Trans IchemE, 75, Part B, No. 3, pp. 181-189, 1997.
3. Olesen S.G. and G.T. Polley. *A Simple Methodology for the Design of Water Networks Handling Single Contaminants*. Trans IChemE, 75, part A, pp. 420-426, 1997.
4. Takama N., T. Kuriyama, K. Shiroko and T. Umeda, 1977. *Optimal Water Allocation in a Petroleum Refinery*. Comp. & Chem. Eng., 4, pp. 251-258, 1980.
5. Wang Y. P. and R. Smith. *Wastewater Minimization*. CES, 49, 7, pp. 981, 1994.

CHAPTER 6

Energy Efficient Water Utilization Systems in Refineries and Process Plants

6.1 Introduction

The influence of heat integration on the solution of the WAP problem has been ignored for a long time. Savelski and Bagajewicz (1997) first studied the problem pointing out the existence of a trade off. The design of an energy-efficient WAP was attempted by Savulescu and Smith (1998). They used a graphical procedure that does not seem suitable to be applied on all possible cases.

This chapter introduces a novel approach for the design of water utilization networks featuring minimum freshwater usage and minimum utility consumption. The procedure is based on a linear programming formulation, which relies on necessary conditions of optimality, and a heat transshipment model. An LP model is first used to obtain minimum water usage and minimum heating utility target values. Once the energy and water targets have been identified, an MILP model is constructed. This model, which accounts for non-isothermal mixing, provides the information needed to construct the water reuse structure as well as the corresponding heat exchanger network.

6.2 Problem Statement

Given is a set of water-using/water-disposing processes which required water of a certain quality and temperature. It is desired to determine a network of water streams interconnections among the processes, and design a network of heat exchangers between these streams, such that the freshwater usage and energy consumption are simultaneously minimized. The water minimization provides the processes with water of adequate quality, dictated by the given inlet and outlet concentrations limits, while the minimum energy consumption efficiently integrates the heat exchanger network.

6.3 Two Stage Approach

Savulescu and Smith (1998) presented a method based on the following steps:

6.3.1 Stage 1

1. Obtain a water allocation network maximizing the energy transfer by mixing. The authors propose to use a two-dimensional grid diagram and the concept of water mains. This diagram allows them to identify heating and cooling duties graphically.
2. Apply certain re-use rules. These rules suggest starting the reuse structure from the hottest source, connect processes near in temperature, and use non-isothermal mixing.

6.3.2 Stage 2

1. Construct the energy composite curves and identify the minimum utility.
2. Assume all the freshwater being sent to the processes as a single stream. Also, assume that the wastewater being sent to treatment is going to be merged appropriately.
3. Apply a set of splitting rules to obtain vertical matching of the composite curves portions.

The method is in reality a sequential procedure that makes use of certain heuristics in the first stage to obtain a network of process-to-process interconnections, such that the indirect heat exchange structure might feature minimum utility.

However, these rules cannot guarantee that the resulting structure is optimal. Moreover, the notion of connecting processes close in temperature may clash with the fact that monotonicity of outlet concentrations should hold (Chapter 3). In the illustration of the second stage, the authors assume that there are no process-to-process wastewater connections requiring heating or cooling in a heat exchanger. This allows them to introduce the so-called separate systems. There are, however, processes where indirect heating or cooling of process-to-process streams is needed. The method of separate systems proposed does not address this case. Finally, to build the heat exchanger network, it is assumed that the wastewater streams are merged and sent to treatment. If one wants to send these streams to water treatment individually, at the least the concept of separate systems has to be re-formulated.

Savulescu and Smith (1998) proposed and solved an example that will be used in this chapter to illustrate the features of our procedure. The data for this example is given in Table 6-1 and their proposed solution is illustrated in Figure 6-1.

Table 6-1: Example data from Savulescu and Smith (1998)

Process Number	Mass Load of Contaminant (g/s)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	2	0	100	40
2	5	50	100	100
3	30	50	800	75
4	4	400	800	50
Temperature of fresh water $T_w = 20^\circ C$				
Temperature of wastewater $T_{out} = 30^\circ C$				

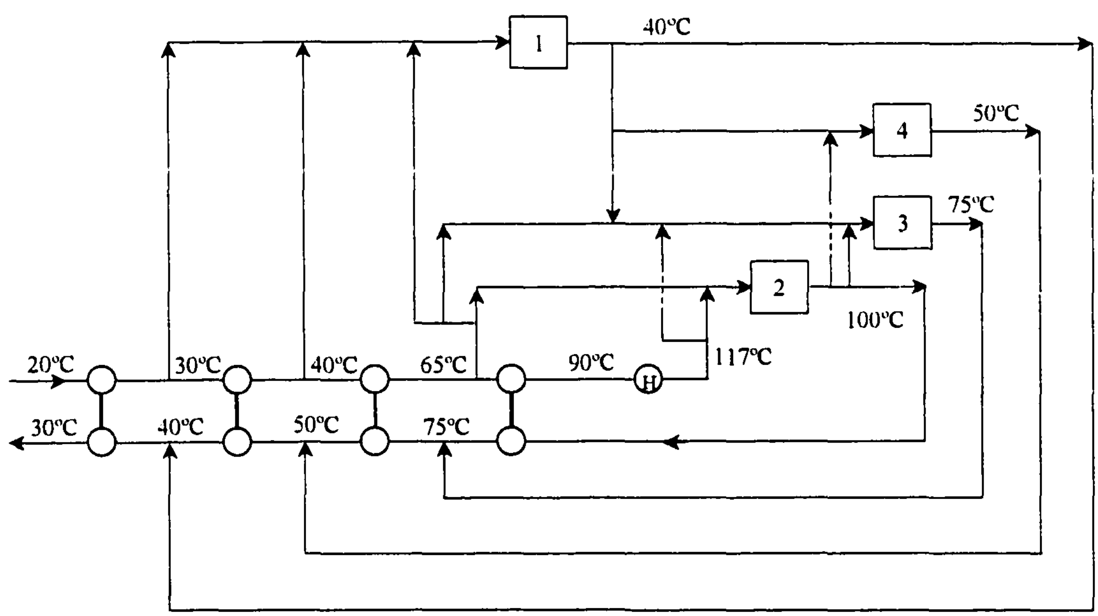


Figure 6-1
Solution network proposed by Savulescu and Smith (1998).

6.4 Minimum Fresh Water Targeting

The LP formulation for the Water Allocation Planning problem was presented in the previous chapter. First, an NLP representation, **M1**, was proposed. Then, after applying the necessary conditions of maximum outlet concentrations, problem **M1** was linearized to yield problem **M2**.

Figure 6-2 shows the water network obtained using **M2** for the problem proposed by Savulescu and Smith (1998).

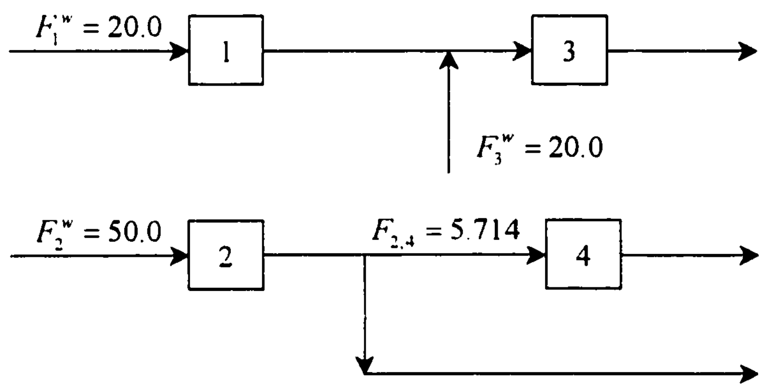


Figure 6-2
Water targeting of the problem proposed by Savulescu and Smith (1998).

6.5 Minimum Utility Targeting

In Chapter 5, it was showed that problem **M2** has several alternative solutions with the same water consumption. They exploited this property to find different networks featuring forbidden and compulsory matches, minimum number of interconnections, or minimum fixed cost. Furthermore, the degeneracy of this problem can be used to obtain the set of interconnections that feature minimum freshwater usage and minimum utility consumption simultaneously.

Once problem **M2** is solved, a target for minimum freshwater usage is obtained. In order to obtain the minimum heating/cooling utility, this freshwater usage is to remain fixed. Moreover, the water interconnections corresponding to this target can be ignored, as one is seeking a new set of interconnections, which features minimum-energy consumption while following the freshwater target found.

To build the model we consider the use of a Pinch Operator and a simplified version of the state-space representation of this problem, an approach proposed by Bagajewicz and Manousiouthakis (1992). This model was later used for heat exchanger networks and combined mass and heat exchange networks (Bagajewicz *et al.*, 1998). Figure 6-3 shows a state-space representation of the problem. A freshwater stream enters the distribution network where it is split and is sent to several junctions. These junctions also collect wastewater coming from processes (represented by the pollutant operator) and from heat exchangers (represented by a pinch operator). In turn, the pollutant operator has for this case the form of a superstructure operator (Bagajewicz *et al.*, 1998), that is, each of the junctions is connected to each of the process. This is schematically shown in Figure 6-4. Process streams transfer pollutants to the water.

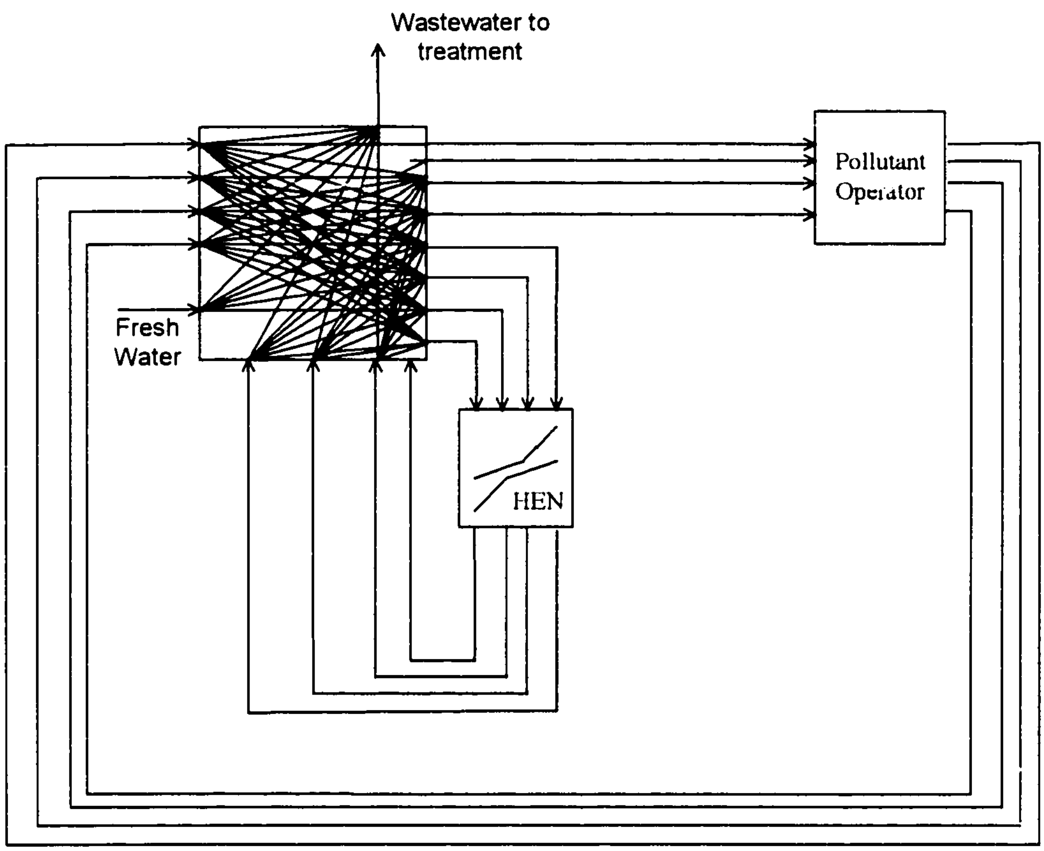


Figure 6-3
State Space Representation of the problem.

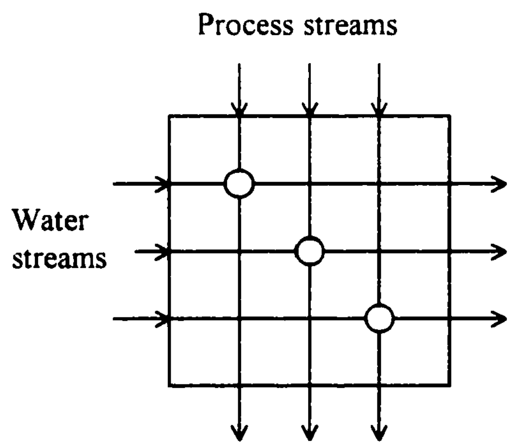


Figure 6-4
Pollutant Operator.

Several models can be used to represent the pinch operator. Bagajewicz and Manousiouthakis (1992) proposed an MILP model that makes use of integers to take into account the varying position of the inlet and outlet temperatures and flowrates. In our case, however, inlet and outlet temperatures can be considered fixed. This can be justified as follows. Assume that streams mix when they achieve their target temperature only. This means that the mixing junctions connected to the pinch operator receive a single stream coming from a process junction. This is illustrated in Figure 6-5 and the corresponding flowsheet is shown in Figure 6-6. Only one side of the heat exchangers is shown at each heating and cooling point.

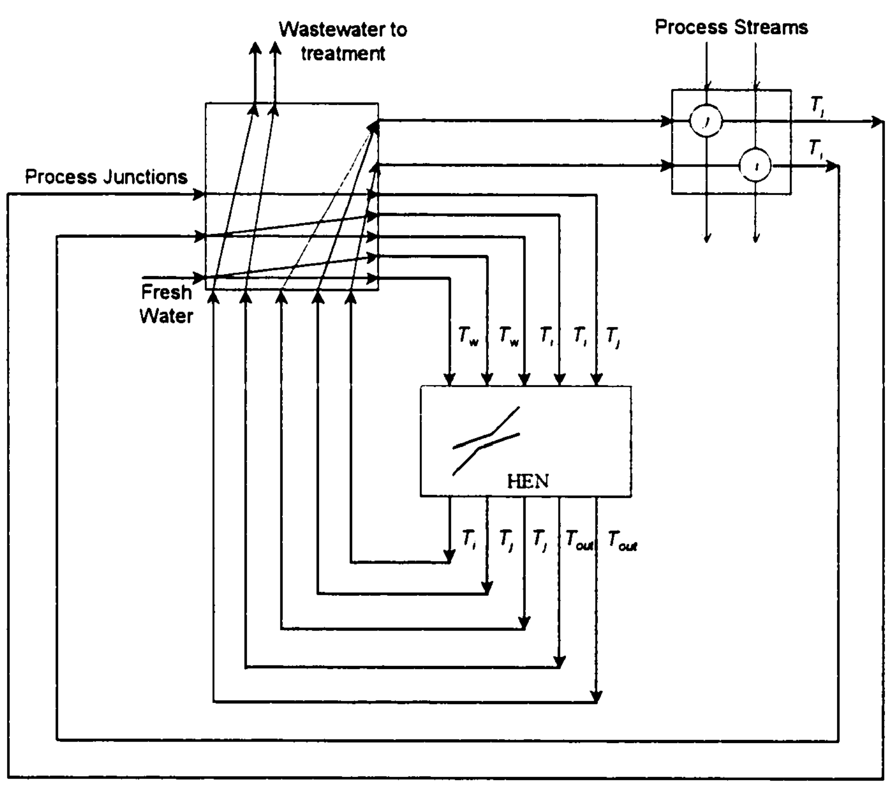


Figure 6-5
State Space Simplification for mixing streams.

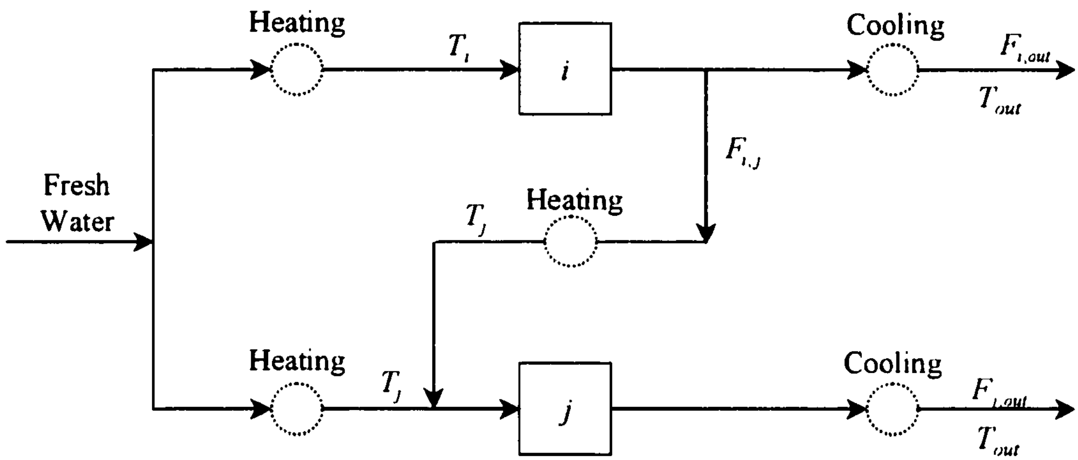


Figure 6-6
Traditional flowsheet representation of Figure 6-5.

The traditional version of the pinch operator considers indirect heat transfer only. Direct heat transfer, coming from mixing of streams can be represented by the same model. Consider a hot and a cold stream (H_1 and C_1, respectively). Figure 6-7(a) shows the transshipment model cascade diagram obtained by the classical approach of indirect heat transfer. In turn, Figure 6-7(b) considers that H_1 and C_1 have been mixed. The remaining stream C_1' is using the same amount of heating utility than in case a.

Consequently, the assumption that mixing is taking place does not alter the result of the targeting problem. All this is possible because the hot and cold streams that mix have the same target temperature.

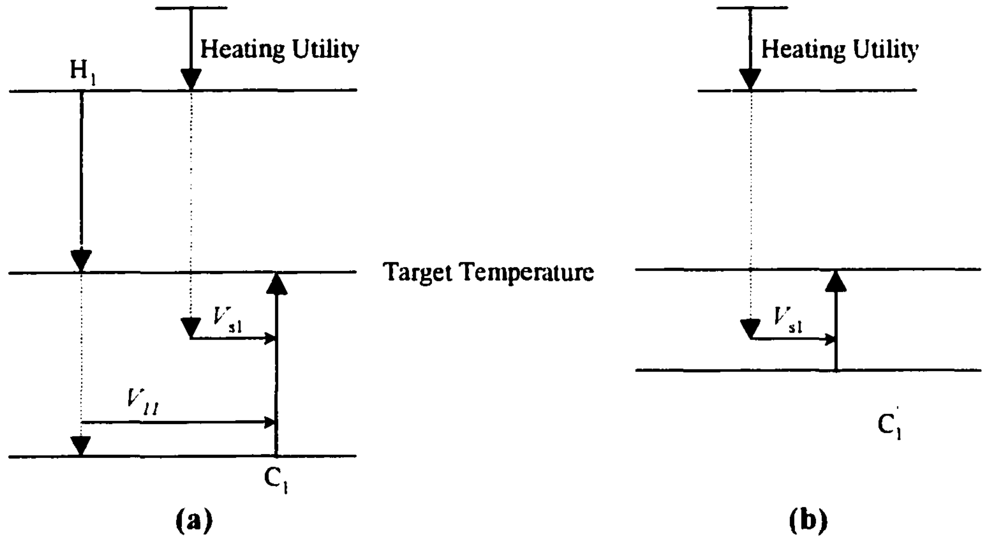


Figure 6-7
(a) Indirect heat transfer (no mixing). **(b)** Mixing of hot and cold streams.

In view of the previous analysis, the state space representation of the process can be simplified, eliminating splitting-to-mixing connections, maintaining the connections shown in Figure 6-6 only. The pinch operator has now fixed inlet and outlet temperatures and varying flowrates. Figure 6-8 shows the new situation.

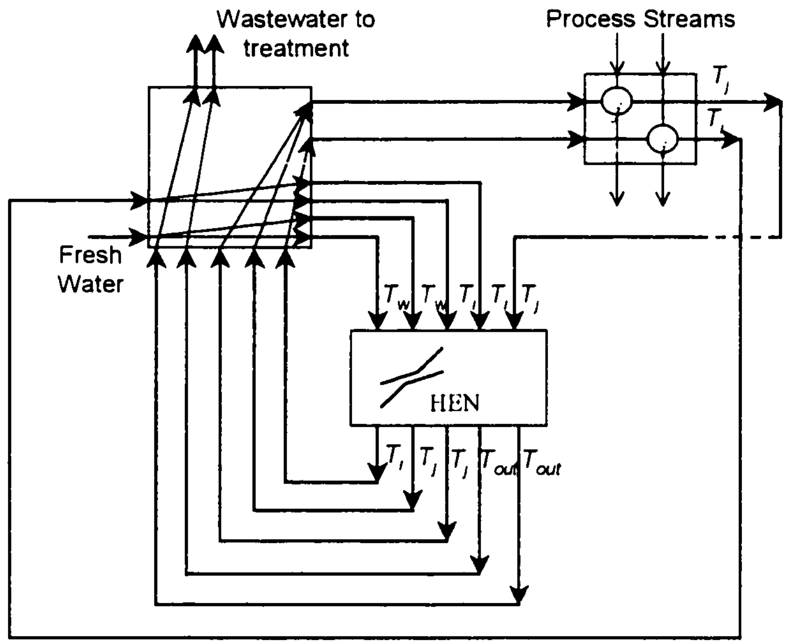


Figure 6-8
Eliminating splitting-to-mixing connections.

The complete model to obtain the heating utility target is the following:

$$\mathbf{M3}=Min\left(\sum_{\forall h \in HU} Q_h\right) \tag{6-1}$$

$s.t.$

$$\sum_j F_j^w = \alpha \tag{6-2}$$

$$F_j^w + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,out} = 0 \qquad \forall j \in \boldsymbol{N}, i \in \boldsymbol{P}_j, k \in \boldsymbol{R}_j \tag{6-3}$$

$$F_h^w - \frac{L_h}{C_{h,out}^{\max}} = 0 \qquad \forall h \in \boldsymbol{H} \tag{6-4}$$

$$\left.\begin{aligned} &\sum_i F_{i,j}\left(C_{i,out}^{\max} - C_{j,in}^{\max}\right) - F_j^w C_{j,in}^{\max} \le 0 \\ &\sum_i F_{i,j}\left(C_{i,out}^{\max} - C_{j,out}^{\max}\right) - F_j^w C_{j,out}^{\max} + L_j = 0 \end{aligned}\right\} \forall j \in \overline{\boldsymbol{H}}, i \in \boldsymbol{P}_j \tag{6-5}$$

$$\left.\begin{array}{l}\delta_{h,t}-\delta_{h,(t-1)}+\sum_{(w,j)\in DW_t}V_{h,wj,t}+\sum_{(r,s)\in D_t}V_{h,rs,t}+\sum_{(k,u)\in DE_t}V_{h,ku,t}=Q_h \quad t=t_h\\ \delta_{h,t}-\delta_{h,(t-1)}+\sum_{(w,j)\in DW_t}V_{h,wj,t}+\sum_{(r,s)\in D_t}V_{h,rs,t}+\sum_{(k,u)\in DE_t}V_{h,ku,t}=0 \quad t\geq t_h\end{array}\right\}\forall h\in \boldsymbol{HU} \tag{6-6}$$

$$\left.\begin{array}{l}\left.\begin{array}{l}\delta_{wj,t}-\delta_{wj,(t-1)}+\sum_{(r,s)\in D_t}V_{wj,rs,t}+\sum_{(k,u)\in DE_t}V_{wj,ku,t}\\ \quad+\sum_{\forall c\in CU_t}V_{wj,c,t}=F_j^w c_{p_w}(T_{t-1}-T_t)\end{array}\right\}\forall(w,j)\in \boldsymbol{SW}_t\\ \left.\begin{array}{l}\delta_{pq,t}-\delta_{pq,(t-1)}+\sum_{(w,j)\in DW_t}V_{pq,wj,t}+\sum_{(r,s)\in D_t}V_{pq,rs,t}\\ +\sum_{(k,u)\in DE_t}V_{pq,ku,t}+\sum_{\forall c\in CU_t}V_{pq,c,t}=F_{p,q}c_{p_p}(T_{t-1}-T_t)\end{array}\right\}\forall(p,q)\in \boldsymbol{S}_t\\ \left.\begin{array}{l}\delta_{ku,t}-\delta_{ku,(t-1)}+\sum_{(w,j)\in SW_t}V_{ku,wj,t}+\sum_{(r,s)\in D_t}V_{ku,rs,t}\\ \quad+\sum_{\forall c\in CU_t}V_{ku,c,t}=F_j^{out}c_{p_k}(T_{t-1}-T_t)\end{array}\right\}\forall(k,u)\in \boldsymbol{SE}_t\end{array}\right\}\forall t\in \boldsymbol{T} \tag{6-7}$$

$$\left.\begin{array}{l}\sum_{h\in HU_t}V_{h,wj,t}+\sum_{(p,q)\in S_t,q\neq j}V_{pq,wj,t}\\ +\sum_{(k,u)\in SE_t}V_{ku,wj,t}\leq F_j^w c_{p_w}(T_{t-1}-T_t)\end{array}\right\}\forall(w,j)\in \boldsymbol{DW}_t \qquad \forall t\in \boldsymbol{T} \tag{6-8}$$

$$\sum_{t\in T}\left(\begin{array}{c}\sum_{h\in HU_t}V_{h,wj,t}+\sum_{(p,q)\in S_t}V_{pq,wj,t}\\ +\sum_{(k,u)\in SE_t}V_{ku,wj,t}\end{array}\right)=F_j^w c_{p_w}(T_C^t-T_C^s) \qquad \forall(w,j)\in \boldsymbol{DW} \tag{6-9}$$

$$\left.\begin{array}{l}\sum_{h\in HU_t}V_{h,rs,k}+\sum_{(w,j)\in SW_t,j\neq s}V_{wj,rs,t}+\sum_{(p,q)\in S_t,q\neq s}V_{pq,rs,t}\\ \quad+\sum_{(k,u)\in SE_t}V_{ku,rs,t}\leq F_{r,s}c_{p_r}(T_{t-1}-T_t)\end{array}\right\}\forall(r,s)\in \boldsymbol{D}_t \quad \forall t\in \boldsymbol{T} \tag{6-10}$$

$$\sum_{t\in T}\left(\begin{array}{c}\sum_{h\in HU_t}V_{h,rs,k}+\sum_{(w,j)\in SW_t}V_{wj,rs,t}\\ +\sum_{(p,q)\in S_t}V_{pq,rs,t}+\sum_{(k,u)\in SE_t}V_{ku,rs,t}\end{array}\right)=F_{r,s}c_{p_r}(T_{t-1}-T_t) \quad \forall(r,s)\in \boldsymbol{D} \tag{6-11}$$

$$\left.\begin{array}{l}\sum_{h\in HU_t} V_{h,ku,t} + \sum_{(w,j)\in SW_t} V_{wj,ku,t} \\ + \sum_{(p,q)\in S_t} V^r_{pq,ku,t} = F_j^{out} c_{p_j} (T_{t-1} - T_t)\end{array}\right\} \quad \forall (k,u)\in \boldsymbol{DE}_t \quad \forall t\in \boldsymbol{T} \tag{6-12}$$

$$\sum_{(w,j)\in SW_t} V_{wj,c,t} + \sum_{(p,q)\in S_t} V_{pq,c,t} + \sum_{(k,u)\in SE_t} V_{ku,c,t} = Q_c \quad \forall c\in \boldsymbol{CU}_t \quad \forall t\in \boldsymbol{T} \tag{6-13}$$

$$F_j^w, F_{i,j}, F_j^{out}, \delta, V, Q \geq 0 \tag{6-14}$$

The model minimizes the heating utility and uses a fixed amount of freshwater (α), obtained by minimum water usage targeting. The proper degenerate set of water interconnections is found by the inclusion of the sets of constraints (6-3 through 6-5). Finally, constraints (6-6 through 6-14) consider the transshipment model representation of the Pinch operator.

6.5.1 Illustration

Note that, the example from Savulescu and Smith (1998) is such that the target temperatures can be achieved using mixing. Figure 6-9 shows the water network obtained solving the minimum utility targeting model **M3**. Note that the water network differs from the solution obtained using the water allocation problem **M2**. Another important observation is that the utility targeting model produced a non-monotonous network-interconnection between processes 3 and 4. Since the outlet concentrations of streams 3 and 4 are equal, the connection (although feasible) contributes nothing to the water requirement of process 4. It presence responds to an energy need only.

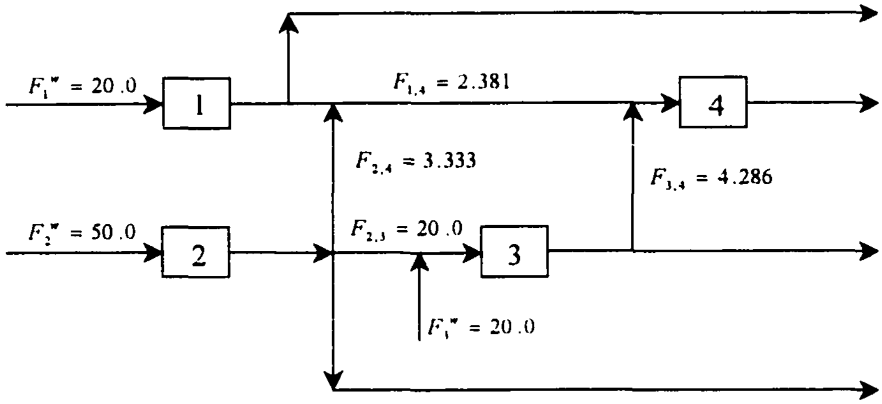


Figure 6-9
Water network for Savulescu and Smith example obtained using **M3**.

The heat-targeting model is useful in providing one of the feasible water networks that realizes the minimum heating utility. This minimum utility can also be predicted for certain cases in a more straightforward manner using the following equations:

$$HU = \alpha\, c_p\, Max\{T_{out} - T_{in}, \Delta T_{\min}\} \tag{6-15}$$

$$CU = \alpha\, c_p\, Max\{\Delta T_{\min} - (T_{out} - T_{in}), 0\} \tag{6-16}$$

For illustration, consider one process. The T-H diagram for this case is given is Figure 6-10. Notice that two cases are immediately apparent.

a) $T_{out} - T_{in} \geq \Delta T_{\min}$: In this case, the problem is unpiched and the heating utility is given by (6-15). Figure 6-10(a) illustrates this case.

b) $T_{out} - T_{in} < \Delta T_{\min}$: In this case, vertical alignment on the left is not possible (Figure 6-10 (b)). The heating and cooling utilities are given by (6-15) and (6-16) respectively.

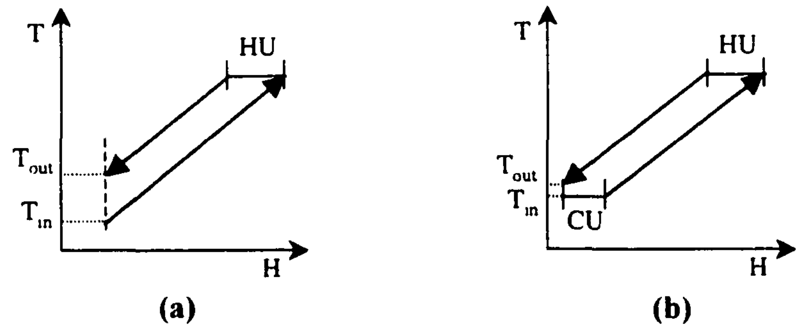


Figure 6-10
(a) Heating utility required only. **(b)** Both type of utility are required (6-15) and (6-16) apply.

For processes in which water undergoes continuous heating to a certain maximum temperature and this is followed by cooling, the previous result holds. Indeed, consider the case where no heat transfer occurs through mixing. That is, water is always being heated up, being pass through the processes a mere accident. This is shown in Figure 6-11.

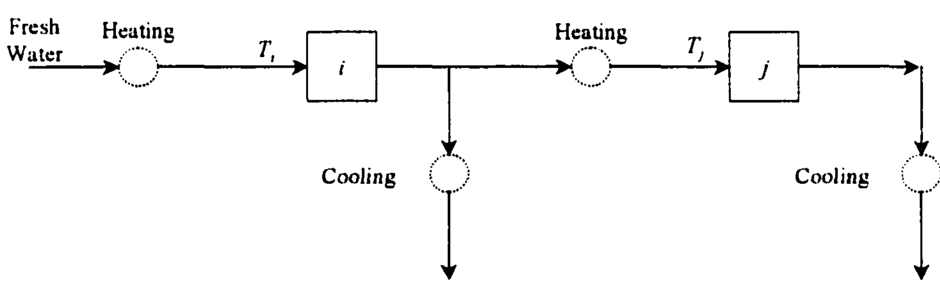


Figure 6-11
Water is always being heated up as it moves through the network.

One can immediately recognize that mixing is another way of heat transfer, and therefore, covered by the above scenario. Thus, the following consideration follows:

when all the wastewater has to reach the same outlet temperature, the heating and cooling utility is given by (6-15) and (6-16).

In the example solved above, $F^w = 90.0\ kg/s$, $c_p = 4.2\ kW/kg\ ^\circ C$ and $T_{out}^w - T_{in}^w = 10\ ^\circ C$, which gives 3,780 *kW*. Any unrestricted feasible alternative solution of the water allocation problem **M1** will in fact consume the same amount of utility regardless of the individual temperatures of the processes.

When water undergoes cycles of heating, followed by cooling at least one time, the above formulas may not hold. Consider the case of the problem given in Table 6-2. The solution is given in Figure 6-12. The *T-H* diagram is shown in Figure 6-13, revealing that this is a pinched problem. Water from process 1 has to be used to heat up water going to process 3, and there is a limitation imposed by minimum temperature approach, which raises the minimum utility.

Table 6-2: Water undergoes cycles of heating

Process Number	**Mass Load of Contaminant (g/s)**	C_{in}^{max} **(ppm)**	C_{out}^{max} **(ppm)**	**Temperature (°C)**
1	5.0	50	100	100
2	30.0	50	800	75
3	50.0	800	1,100	100
Temperature of fresh water $T_w = 20^\circ C$				
Temperature of wastewater $T_{out} = 30^\circ C$				

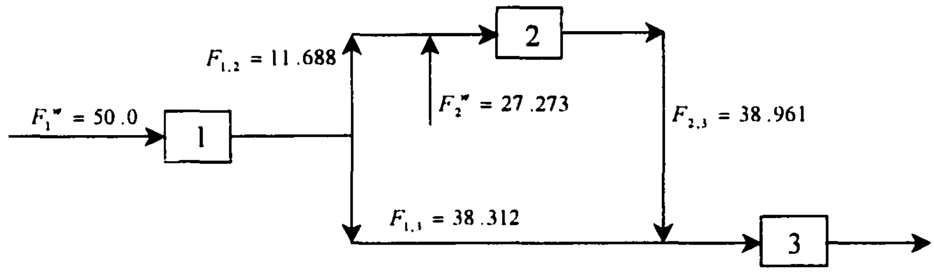


Figure 6-12
Water network solution to heating cycles example.

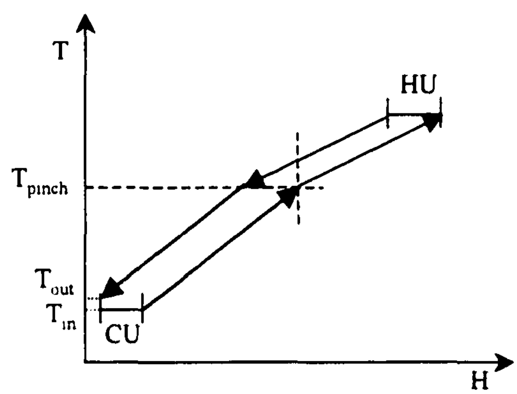


Figure 6-13
T-H representation of water streams of Figure 6-13.

Moreover, the use of equations (6-15) and (6-16) is not valid for the case in which one or more of the wastewater streams are sent to different treatment units and those units require different operating temperatures. This is illustrated using a modified version of the problem from Savulescu and Smith (1998). Consider the new temperature data given in Table 6-3.

Table 6-3: Modified example data for Savulescu and Smith (1998)

Process Number	Temperature (°C)	WWT Temperature (°C)
1	40	30
2	100	60
3	75	40
4	50	30
Temperature of fresh water $T_w = 20^{\circ}C$		

This problem has the same fresh water target than the original formulation. However, the minimum heating utility is now 8,520 kW. Figure 6-14 shows the resulting water network.

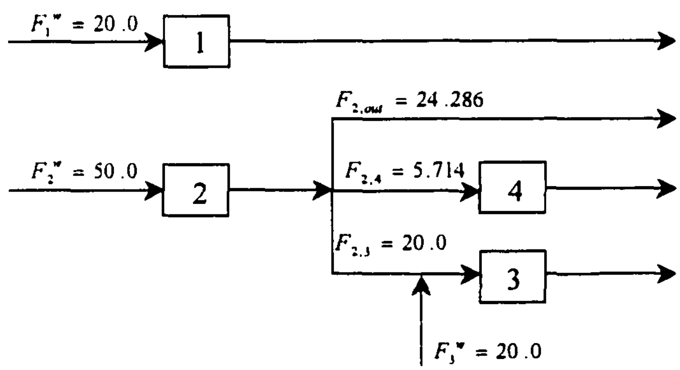


Figure 6-14
Different wastewater discharge temperatures.

A compulsory match between processes 1 and 3 is now imposed to reproduce the water network structure proposed by Savulescu and Smith (1998) (Figure 6-1). Figure 6-15 shows the resulting water network. The heating utility of the corresponding heat exchanger network is 11,040 kW.

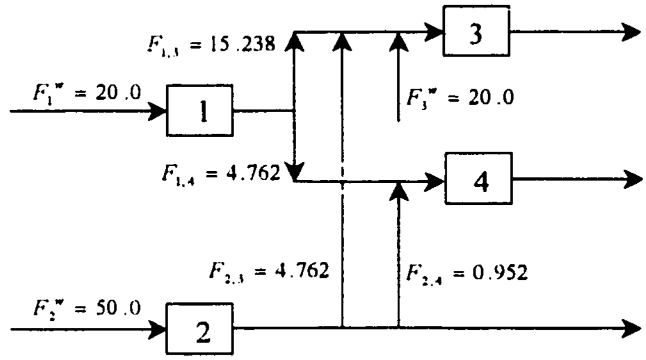


Figure 6-15
Savulescu and Smith network structure with different wastewater discharge temperatures.

This example clearly shows that a two-stage approach in which target temperatures are forced by mixing can actually lead to a much larger heating utility than needed. Therefore, the problem needs to be solved considering the water and heating utility targets, simultaneously.

6.6 Heat Exchanger Networks

Once the minimum utility target is obtained, a heat exchanger network can be constructed. If one uses the process-to-process flowrates and utility targets obtained form the previous steps, the problem reduces to a classical heat exchanger network design. However, one may decide to leave the constraints corresponding to the flowrate connections and build a generalized heat transshipment model. As this model is solved, new process-to-process connections and flowrates are chosen helping thus to achieve a lower capital investment target. The problem can be written in compact form as follows:

M4= $Min\,\{\text{Number of Matches}\}$

$s.t.$

Flowrate constraints

Heat Balance constraints

Constraints counting matches

In this formulation, the objective function is given by:

$$Min = \left(\begin{array}{l} \sum\limits_{\forall h\in HU,\forall(w,j)\in DW} Y_{h,wj} + \sum\limits_{\forall h\in HU,\forall(r,s)\in D} Y_{h,rs} + \sum\limits_{\forall h\in HU,\forall(k,u)\in DE} Y_{h,ku} \\ + \sum\limits_{\forall(w,j)\in SW,\forall(r,s)\in D;j\neq s} Y_{wj,rs} + \sum\limits_{\forall(w,j)\in SW;\forall(k,u)\in DE} Y_{wj,ku} + \sum\limits_{\forall(w,j)\in SW,\forall c\in CU} Y_{wj,c} \\ + \sum\limits_{\forall(p,q)\in S,\forall(w,j)\in D;q\neq j} Y_{pq,wj} + \sum\limits_{\forall(p,q)\in S,\forall(r,s)\in D;q\neq s} Y_{pq,rs} + \sum\limits_{\forall(p,q)\in S,\forall(k,u)\in DE} Y_{pq,ku} + \sum\limits_{\forall(p,q)\in S;\forall c\in CU} Y_{pq,c} \\ + \sum\limits_{\forall(k,u)\in SE,\forall(w,j)\in DW} Y_{ku,wj} + \sum\limits_{\forall(k,u)\in SE,\forall(r,s)\in D} Y_{ku,rs} + \sum\limits_{\forall(k,u)\in SE,\forall c\in CU} Y_{ku,c} \end{array} \right) \tag{6-17}$$

The flowrate constraints are given by (6-3) through (6-5), and the heat balance constraints are given by (6-6) through (6-14). The following target constraint is added.

$$\sum_{\forall h\in HU} Q_h = \beta \tag{6-18}$$

Finally, the following constraints used for counting heat matches are.

$$\left. \begin{array}{ll} \sum\limits_{t\in T} V_{h,wj,t} - U_{h,wj} Y_{h,wj} \leq 0 & \forall h\in \boldsymbol{HU};\forall(w,j)\in \boldsymbol{DW} \\ \sum\limits_{t\in T} V_{h,rs,t} - U_{h,rs} Y_{h,rs} \leq 0 & \forall h\in \boldsymbol{HU};\forall(r,s)\in \boldsymbol{D} \\ \sum\limits_{t\in T} V_{h,ku,t} - U_{h,ku} Y_{h,ku} \leq 0 & \forall h\in \boldsymbol{HU};\forall(k,u)\in \boldsymbol{DE} \end{array} \right\} \tag{6-19}$$

$$\left.\begin{array}{ll}\sum_{t\in T} V_{wj,rs,t} - U_{wj,rs} Y_{wj,rs} \leq 0 & \forall (w,j)\in \boldsymbol{SW}\,;\forall (r,s)\in \boldsymbol{D}\,; \boldsymbol{j\neq s} \\ \sum_{t\in T} V_{wj,ku,t} - U_{wj,ku} Y_{wj,ku} \leq 0 & \forall (w,j)\in \boldsymbol{SW}\,;\forall (k,u)\in \boldsymbol{DE} \\ \sum_{t\in T} V_{wj,c,t} - U_{wj,c} Y_{wj,c} \leq 0 & \forall (w,j)\in \boldsymbol{SW}\,;\forall c\in \boldsymbol{CU} \end{array}\right\} \quad (6\text{-}20)$$

$$\left.\begin{array}{ll}\sum_{t\in T} V_{pq,wj,t} - U_{pq,wj} Y_{pq,wj} \leq 0 & \forall (p,q)\in \boldsymbol{S}\,;\forall (w,j)\in \boldsymbol{DW}\,; \boldsymbol{q\neq j} \\ \sum_{t\in T} V_{pq,rs,t} - U_{pq,rs} Y_{pq,rs} \leq 0 & \forall (p,q)\in \boldsymbol{S}\,;\forall (r,s)\in \boldsymbol{D}\,; \boldsymbol{q\neq s} \\ \sum_{t\in T} V_{pq,ku,t} - U_{pq,ku} Y_{pq,ku} \leq 0 & \forall (p,q)\in \boldsymbol{S}\,;\forall (k,u)\in \boldsymbol{DE} \\ \sum_{t\in T} V_{pq,c,t} - U_{pq,c} Y_{pq,c} \leq 0 & \forall (p,q)\in \boldsymbol{S}\,;\forall c\in \boldsymbol{CU} \end{array}\right\} \quad (6\text{-}21)$$

$$\left.\begin{array}{ll}\sum_{t\in T} V_{ku,wj,t} - U_{ku,wj} Y_{ku,wj} \leq 0 & \forall (k,u)\in \boldsymbol{SE}\,;\forall (w,j)\in \boldsymbol{DW} \\ \sum_{t\in T} V_{ku,rs,t} - U_{ku,rs} Y_{ku,rs} \leq 0 & \forall (k,u)\in \boldsymbol{SE}\,;\forall (r,s)\in \boldsymbol{D} \\ \sum_{t\in T} V_{ku,c,t} - U_{ku,c} Y_{ku,c} \leq 0 & \forall (k,u)\in \boldsymbol{SE}\,;\forall c\in \boldsymbol{CU} \end{array}\right\} \quad (6\text{-}22)$$

$$F_j^w, F_{i,j}, F_j^{out}, \delta, V, Q \geq 0 \quad (6\text{-}23)$$

$$Y \in \{0,1\} \quad (6\text{-}24)$$

Thus, the heat transshipment part of this model is again an extension of the model presented by Papoulias and Grossmann (1983) that considers variable flowrates. A few modifications have been introduced. First, the heat exchange between streams that are fed to the same process $(F_{i,j}$ and $F_{m,j})$ is not counted as a match. Therefore, the integer variables associated with a match between streams that can be mixed do not exist.

The above model may count heat exchangers twice. Consider the case of two streams going to the same process. Assume the solution obtained by the model shows that each of these streams matches (exchanges indirect heat) with the same cold stream. This situation is presented in Figure 6-16, while Figure 6-17 shows two alternative possibilities. In Figure 6-17 (a), the hottest stream matches with the cold stream in the lowest interval. Therefore, one can assume that the two streams can merge before matching in a single heat exchanger. In Figure 6-17 (b), the hottest stream realizes heat transfer in the highest interval, and even if merging of streams occurs; two heat exchangers are needed.

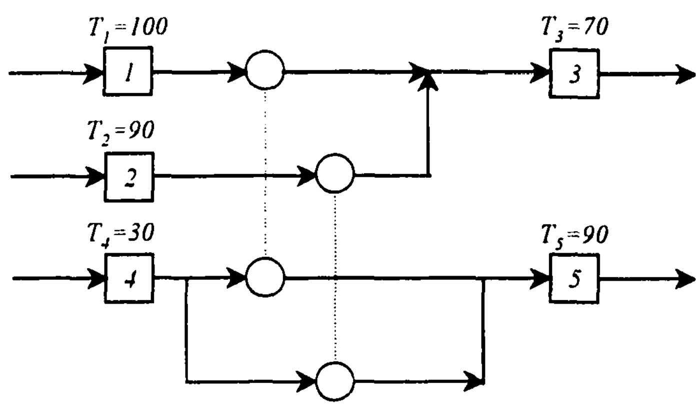


Figure 6-16
Two cold water streams going to the same process exchange heat with a unique hot stream.

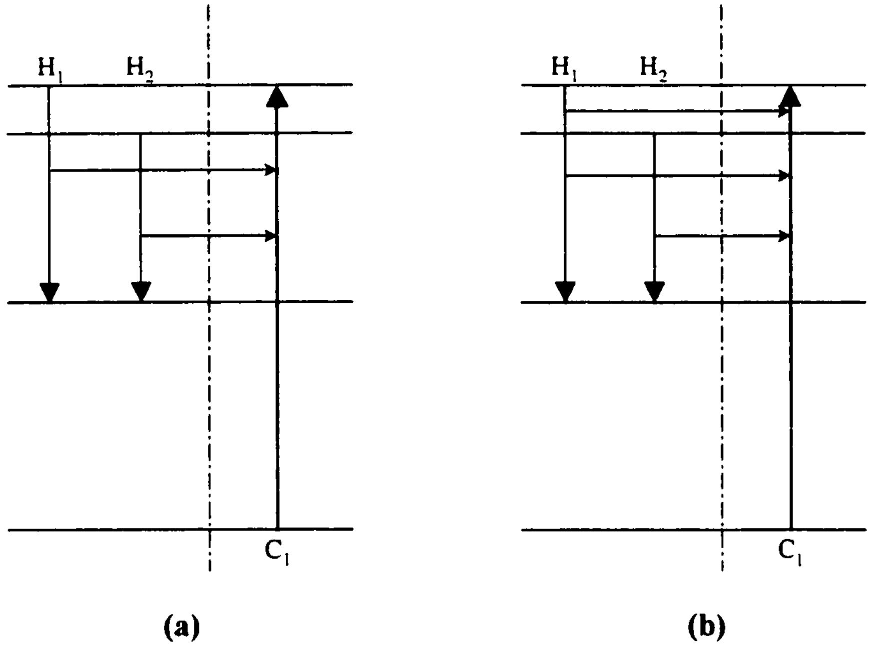


Figure 6-17
(a) Heat exchange between H_1 and C_1 occurs at a lower temperature interval only. (b) Heat exchange between H_1 and C_1 occurs at higher and lower temperature intervals.

Fortunately, this situation if it is accounted by a revised model will not lead to a different solution, except in the matches between these three streams. The rest of the network is not altered by this. Therefore, instead of developing a new model, these situations can be identified after the solution is obtained and the merging can be performed.

6.6.1 Illustration

Now, the heat transshipment model is applied to the problem proposed by Savulescu and Smith (1998). Figure 6-18 shows the resulting water network. The problem has no pinch and the objective function value is 7. Therefore, a heat exchanger network featuring only 7 heat exchangers is obtained. Figure 6-19 shows such network and Table 6-4 lists all 22 matches obtained by the model.

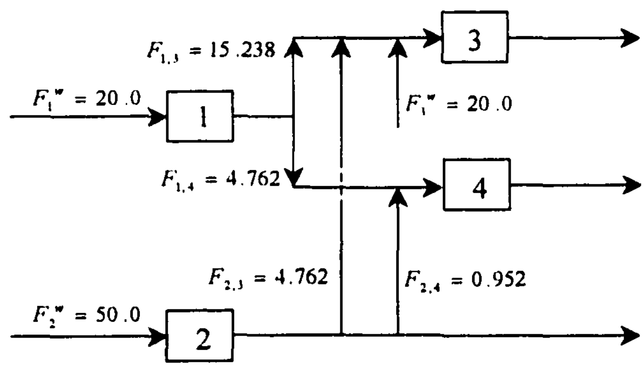


Figure 6-18
Water network obtained using M4 in the problem proposed by Savulescu and Smith.

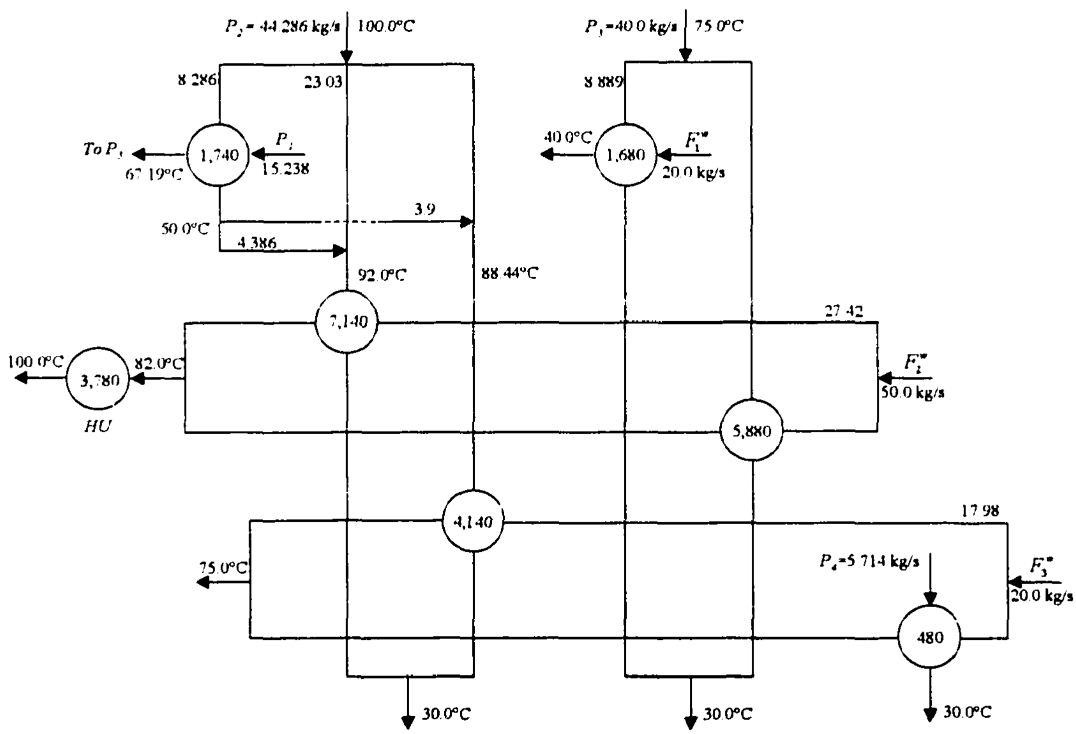


Figure 6-19
Heat Exchange Network obtained using **M4**.

Table 6-4: Matches obtained using **M4** in the Example problem

Hot Stream		**Cold Stream**		**Temperatures of Intervals (°C)**		**Heat Load (kW)**
From Process	To Process	From Process	To Process	In	Out	
2	wwt	Fw	2	30	40	1,260
2	wwt	Fw	3			600
3	wwt	Fw	1			840
3	wwt	Fw	2			840
4	wwt	Fw	3			240
2	wwt	Fw	2	40	50	1,260
2	wwt	Fw	3			600
3	wwt	Fw	1			840
3	wwt	Fw	2			840
4	wwt	Fw	3			240
2	wwt	Fw	2	50	60	420
2	wwt	Fw	3			840
2	wwt	1	3			600
3	wwt	Fw	2			1,680
2	wwt	Fw	2	60	75	630
2	wwt	Fw	3			1,260
2	wwt	1	3			900
3	wwt	Fw	2			2,520
2	wwt	Fw	2	75	85	2,100
2	wwt	Fw	3			840
2	wwt	1	3			240
2	wwt	Fw	2	85	100	1,470

6.7 Merging of Streams

The models previously presented do not consider the fact that the fresh water is coming from a unique source. Moreover, the freshwater to be sent to different processes can be progressively heated up in a set of exchangers at the exit of which splitting to feed the processes can take place. The network already presented in Figure 6-1 accounts for these observations. To achieve such a structure, the heat transshipment model was run allowing only for direct heat exchange (non-isothermal mixing) and indirect heat exchange between the fresh water inlet and wastewater streams. The water and heat exchanger networks are shown in Figures 6-20 and 6-21 respectively.

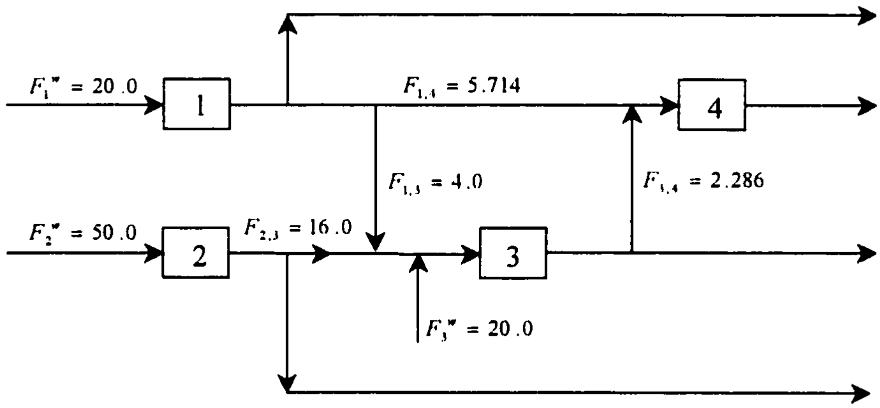


Figure 6-20
Water network obtained using M4 in Savulescu and Smith problem but allowing for direct heat exchange only.

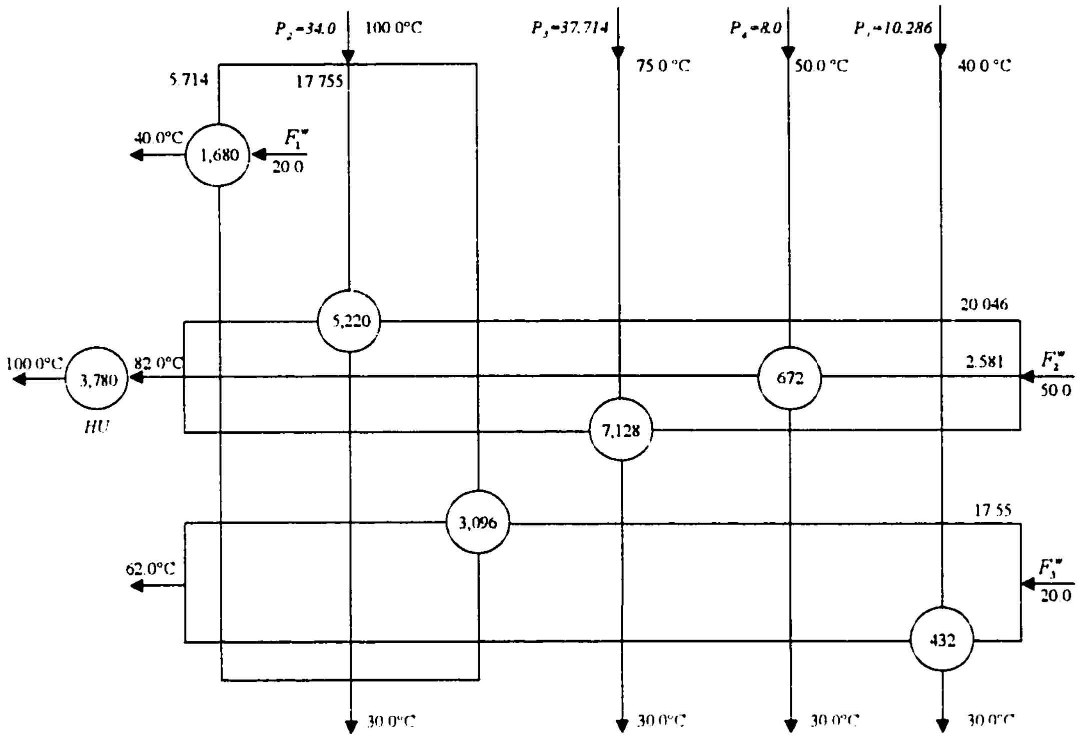


Figure 6-21
Heat Exchanger network of system of Figure 6-20

Consider the following merging procedure (Figure 6-22). The total heat load exchanged by the streams has been redistributed among the temperature intervals in which it is exchanged. Consequently, a structure with only four heat exchangers and a heater is obtained.

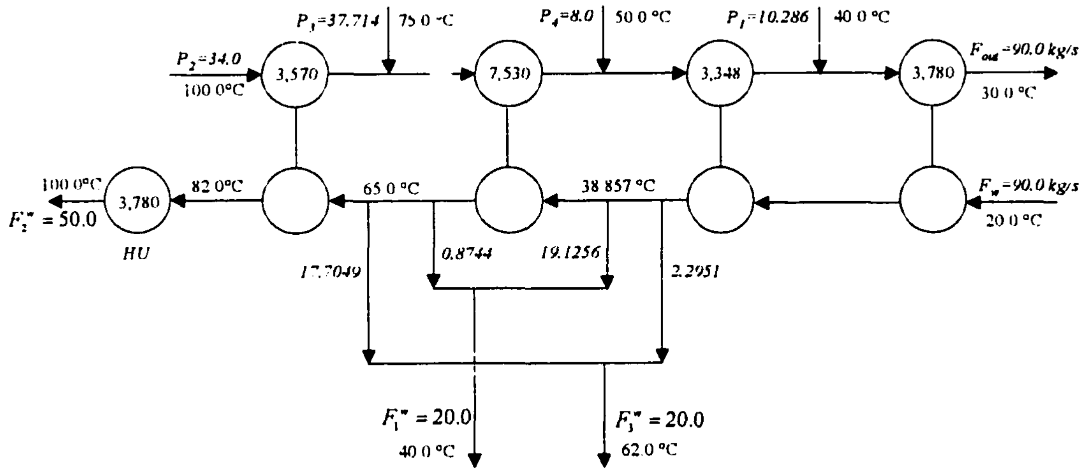


Figure 6-22
Merging.

Subsequent manipulations can be performed to reduce the number of exchangers even further (Figure 6-23).

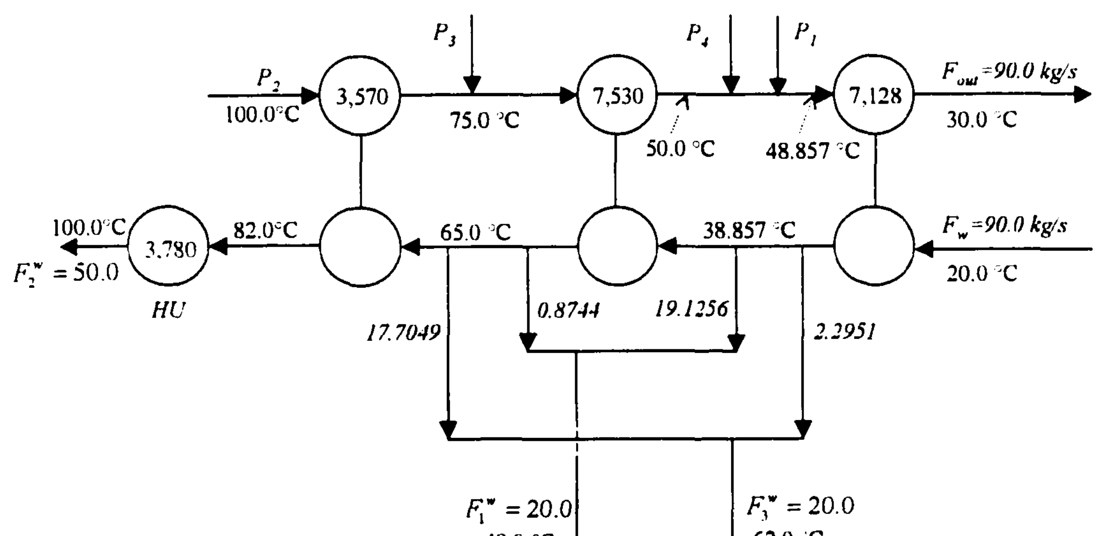


Figure 6-23
Four heat exchangers solution network.

Finally, an alternative solution with four heat exchangers is presented in Figure 6-24. This network is a simplified version of the previous one since it features a single split in the outlet stream of process 3 instead of drawing fresh water at different temperatures and mixing them to provide processes 1 and 3. Therefore, the solution proposed requires less number of connections and is easier to control.

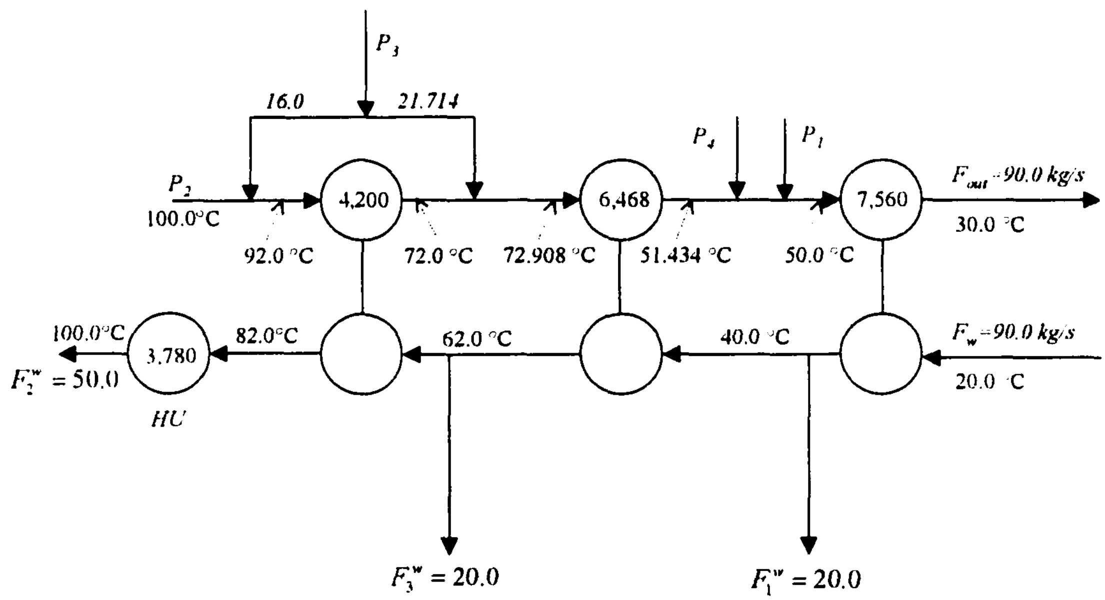


Figure 6-24
Alternative design for the four-heat exchangers network.

Remark: This merging procedure is not systematic and has been introduced to show that a structure of far less complexity than the one obtained by the two-step procedure suggested by Savulescu and Smith (1998) is possible.

6.8 Compulsory and Forbidden Connections and Matches

Forbidden connections and heat exchange matches can be obtained by simply setting the flowrate $F_{i,j}$ to zero or the heat transferred $V_{i,j,k}$=0. For compulsory matches one could resort to the introduction of constraints of the type $F_{i,j} \geq F_{i,j}^{min}$ and/or a similar one for heat transfer. However, this may lead to an infeasible problem if such connection prevents the structure to achieve the targeted freshwater usage. This is the case when a connection between two processes that do not satisfy monotonicity is imposed. In such cases, one needs to go back to the fresh water-targeting model and solve it again with the desired compulsory connection. However, instead of resorting to minimum values to force a match one may want to impose restrictions on low flows or heat loads in heat exchangers. This is accomplished by introducing the following constraints for flowrates.

$$\left.\begin{aligned} F_{i,j} &\leq F_{i,j}^{*} Z_{i,j} \\ F_{i,j} - U_{i,j} Z_{i,j} &\leq 0 \end{aligned}\right\} \qquad (6\text{-}25)$$

Similar constraints can be written for heat loads in terms of $Y_{i,j}$ and $V_{i,j,k}$.

6.9 Illustration of the Method for a Large System

Consider the system of eight processes. The limiting data and required water temperatures are shown in Table 6-5.

Table 6-5: Data for an eight-process Example problem

Process Number	Mass Load of Contaminant (g/s)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	2.0	25	80	40
2	2.88	25	90	100
3	4.0	25	200	80
4	3.0	50	100	60
5	30.0	50	800	50
6	5.0	400	800	90
7	2.0	400	600	70
8	1.0	0	100	50
Temperature of fresh water $T_w = 20^\circ C$				
Temperature of wastewater $T_{out} = 30^\circ C$				

Table 6-6 shows all the resulting flowrates and final concentrations of the processes. The heating utility and number of matches obtained are 5,289.6 kW and 12, respectively.

Table 6-6: Solution of Eight-process Example

Process Number	$F_{i,j}$ **(kg/s)**	C_{in} **(ppm)**	C_{out} **(ppm)**	**Minimum Fresh Water Flowrate with Reuse (kg/s)**
1	0.0	0	80	25.0
2	0.0	25	90	32.0
3	$F_{2,3} = 6.022$ $F_{4,3} = 0.294$	25	200	16.541
4	$F_{1,4} = 15.277$ $F_{2,4} = 19.754$	50	100	24.969
5	$F_{1,5} = 9.723$ $F_{2,5} = 6.224$ $F_{4,5} = 4.926$ $F_{8,5} = 1.694$	50	800	17.433
6	$F_{7,6} = 4.444$ $F_{8,6} = 5.873$	315.4	800	0.0
7	$F_{3,7} = 2.222$ $F_{4,7} = 2.222$	150	600	0.0
8	0.0	0	100	10.0
		Total minimum fresh water flowrate (kg/s)		**125.943**

6.10 Conclusions

A new method to obtain energy-efficient solutions to the water allocation problem in refineries and process plants has been presented. The method relies on two sequential LP problems to obtain the freshwater usage and energy consumption targets. An MILP transshipment model formulation allows the building of the corresponding heat exchanger network. Finally, a merging procedure has been proposed to obtain structures where freshwater is delivered to the corresponding processes, as a split from a main freshwater stream that is being heated up. A model to perform this step automatically using mathematical programming is the object of future work. The proposed methodology has been shown to take into account the interaction between water allocation and heat minimization simultaneously and with global optimality, proving that it can be superior to the two-step procedure proposed by Savulescu and Smith (1998), which cannot even guarantee local optimality. In addition, the procedure developed can incorporate forbidden and compulsory flow connections and heat transfer matches, an issue that is very important in the design of these systems as the processes can be geographically distant.

6.11 Notation

C	concentration of contaminant, ppm
c_p	calorific capacity at constant pressure
$\boldsymbol{CU}$	set of cooling utilities c
$\boldsymbol{CU}_t$	set of cooling utilities c existing in temperature interval $t \in \boldsymbol{T}$
$\boldsymbol{HU}$	set of heating utilities h
$\boldsymbol{D}$	set of cold streams that go from process p to process q
$\boldsymbol{D}_t$	set of cold streams that go from process p to process q existing in temperature interval $t \in \boldsymbol{T}$
$\boldsymbol{DE}$	set of cold streams that go from process k to wastewater collector u
$\boldsymbol{DE}_t$	set of cold streams that go from process k to wastewater collector u existing in temperature interval $t \in \boldsymbol{T}$
$\boldsymbol{DW}$	set of cold streams that go from fresh water source w to process j
$\boldsymbol{DW}_t$	set of cold streams that go from fresh water source w to process j existing in temperature interval $t \in \boldsymbol{T}$

f	component flowrate, g/s
F	water flowrate, kg/s
$\boldsymbol{H}$	set of Head Processes
L	mass load of contaminant, g/s
$\boldsymbol{N}$	this set includes all water-using units
Q_h	heating utility, kW
Q_c	cooling utility, kW
$\boldsymbol{P}_j$	set of precursors of j
$\boldsymbol{R}_j$	set of receivers of j
$\boldsymbol{SW}$	set of hot streams that go from fresh water source w to process j
$\boldsymbol{S}$	set of hot streams that go from process p to process q
$\boldsymbol{S}_t$	set of hot streams that goes from process p to process q existing in interval $\bar{t} \leq t; \bar{t}, t \in \boldsymbol{T}$
$\boldsymbol{SE}$	set of hot streams that go from process k to wastewater collector u
$\boldsymbol{SE}_t$	set of hot streams that goes from process k to wastewater collector u existing in interval $\bar{t} \leq t; \bar{t}, t \in \boldsymbol{T}$
$\boldsymbol{SW}_t$	set of hot streams that goes from fresh water source w to process j existing in interval $\bar{t} \leq t; \bar{t}, t \in \boldsymbol{T}$
$\boldsymbol{T}$	set of intervals t
t_h	interval where the heating utility h is used
T	water temperature, °C
V	heat transferred between streams, kW
δ	heat that cascades between intervals, kW

Other subscripts:

h	*heating utility*
in	at inlet
out	at outlet
i,j	connection going from process *i* to process *j*
j	process *j*

Other superscripts:

min	minimum
max	maximum
w	fresh water

6.12 References

1. Bagajewicz M. and V. Manousiouthakis. *Mass/Heat-Exchanger Network Representation of Distillation Networks*. AIChE Journal, 38, pp.1769-1800, 1992.
2. Bagajewicz M., R. Pham, and V. Manousiouthakis. *On the State Space Approach to Mass/Heat Exchanger Network Design*. CES, 53, 14, pp. 2595-2621,1998.
3. Papoulias S.A. and I.E. Grossmann. *A Structural Optimization approach in Process-synthesis-II: Heat recovery networks*. Comput. & Chem. Eng., 7, p. 707, 1983.
4. Savelski M.J. and M.J. Bagajewicz. *Design and Retrofit of Water Utilization Systems in Refineries and Process Plants*. Annual National AIChE Meeting, paper 188g. Los Angeles, 1997.
5. Savulescu L.E. and R. *Smith. Simultaneous Energy and Water Minimisation*. AIChE Annual Meeting, paper 41f, Miami, 1998.

CHAPTER 7

Summary

7.1 Introduction

Throughout this thesis, two different approaches are used to solve to single-component WAP problem. The first three chapters build on conceptual design and mathematically proven heuristics to introduce two procedures. Chapter 2 presents a systematic method, which depends on targeting the problem first. Chapter 4, conversely, introduces a robust method that provides the target and a realizing water network simultaneously. Furthermore, both methods can easily handle large-scale problems and allow for exploring different network alternatives.

The last three chapters approach the single-contaminant WAP problem by means of mathematical programming. In Chapter 5, the problem is first modeled as an NLP (M1) and then, based on necessary conditions of optimality, it is reduced to an LP problem (M2). It is also shown that the problem has several alternative solutions all with the same fresh water consumption. The latter is accomplished by using an MILP formulation where different objective functions (M3) are proposed and the minimum fresh water usage is added as a constraint. Finally, heat integration among water streams is included in the optimal water allocation problem. Fresh water targeting is once again done using M2. Model M3 is then used to target heating and cooling utility and finally a transshipment model, M4, provides with a water network featuring minimum number of matches for the optimal fresh water usage and minimum utility.

The multicomponent WAP problem has also been studied and solved by means of mathematical programming and optimality conditions. A brief description of the approach follows.

7.2 Multicontaminant Systems

Doyle and Smith (1997) proposed to solve the multicomponent version of (M1) as follows. They state that one can construct a linear problem by assuming that all contaminants are at their maximum outlet concentration, that is $C_{p,j,out} = C^{\max}_{p,j,out}$. This is obviously not true, so the solution would be infeasible. To make the problem feasible, they propose to relax the component balance as follows:

$$\sum_i F_{i,j}\left(C^{\max}_{p,i,out} - C^{\max}_{p,j,out}\right) - F_j^w C^{\max}_{p,j,out} \leq L_{p,j} \tag{7-1}$$

With the solution of such LP problem, they propose to solve the NLP multicomponent version of (M1). To aid in the search for such solutions, they propose to add several other constraints on maximum flows of wastewater that can go from one process to another. To illustrate their procedure, they present the data of Table 7-1. The solution obtained is the one given in Figure 7-1. They also show that forbidden matches can be handled by this procedure obtaining a solution where the connection from process 3 to process 2 (0.067 ton/h) is forbidden (Figure 7-2).

Table 7-1: Example from Doyle and Smith (1997)

Process Number	Contaminant	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	A	0	15
	B	0	400
	C	0	35
2	A	20	120
	B	300	12,500
	C	45	180
3	A	120	220
	B	20	45
	C	200	9,500

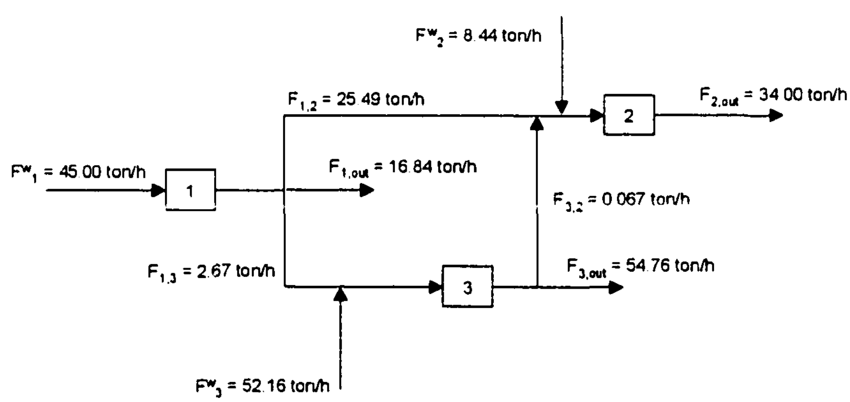


Figure 7-1
Optimal solution of the problem of Table 7-1 (F_{total}^{w} = 105.60 ton/h).

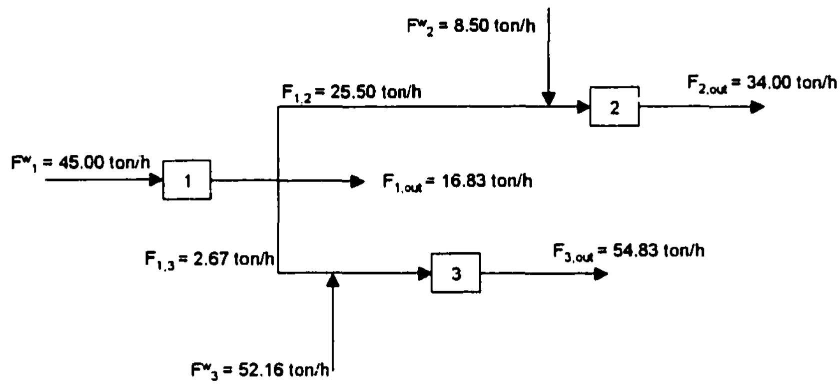


Figure 7-2
Sub-optimal solution of the problem of Table 7-1 (F^w_{total} = 105.66 ton/hr).

Alva-Argáez *et al.* (1998) presented a solution approach for multiple contaminant systems in combination with water treatment in which they include piping costs as well as treatment costs. However, one can use their model to solve the problem for the water allocation only. The objective function that they propose, reduced to the water allocation problem, is:

$$\alpha \sum_{i,j} C_{i,j} Y_{i,j} + \beta \sum_{i} F_i^w \tag{7-2}$$

where α and β are appropriate annualization factors and Y is the integer variable representing the connection between processes i and j. They use the same relaxation as in (7-1), but in this case, they solve the problem by adding a penalty function consisting of the summation of all the slack variables coming from (7-1). Thus, the linear problem can be solved to obtain a network of flows, which in turn can be used to obtain a new set of concentrations. These concentrations are substituted in (7-1) again, until convergence is achieved. This is the same procedure that Takama *et al.* (1980) used. The sequence of MILP obtained is a sequence of infeasible problems. At the end, the authors claim that a) the sequence converges, and in such case, b) the solution is near optimal. Global optimality is, of course, not guaranteed.

Recently, Benko *et al.* (1999) modeled the example problem proposed by Takama *et al.* (1980) as a non-convex MINLP problem. The authors updated the concentration limits in the desalter to make the problem more realistic. This approach cannot guarantee optimality and numerical limitations may limit its use to small-scale problems.

7.2.1 Necessary Conditions of Optimality for Multicontaminant Systems

Savelski *et al.* (1999) derived necessary conditions of optimality for multicontaminant systems. These necessary conditions are very similar to those presented for single component. The condition of maximum outlet concentration is replaced by a condition of at least one component reaching its maximum. The monotonicity condition is replaced by a monotonicity of key components. These key components are defined as those components that make reach their maximum when fresh water is used. These conditions are used later in an algorithmic design procedure. A brief description of the work performed in multicomponent systems is presented below.

7.2.2 Branch and Bound Algorithmic Procedure for Multicontaminant Systems

Consider the case where the pattern of flows is given, that is, all the potential precursors of each process are fixed. In such a case, Savelski *et al.* (1999) observed that a generalization of the maximum reuse rule derived for single components consists of an LP sub-problem. With this solution at hand, the only thing remaining is the construction of a tree of combinations. Such a tree is shown in Figure 7-3 and each branch of the tree can be interpreted by saying that every member of the combination is only a precursor of the processes that follow in the list.

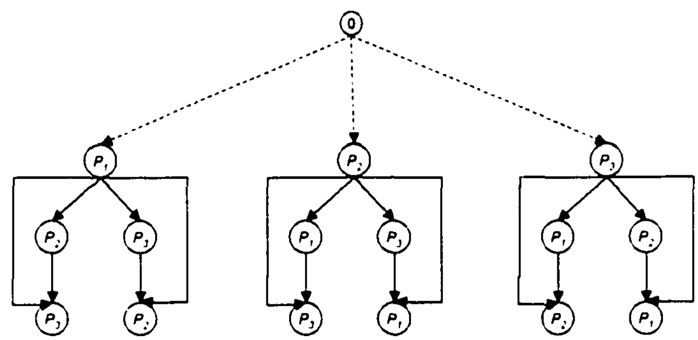


Figure 7-3
Tree of alternative sequences.

A first upper bound is obtained by developing one complete branch of the tree. This tree is then explored developing every branch and using stopping criteria. Monotonicity of key components, as well as definitions of fresh water user processes are used as branch cutting criteria. In addition, at each node of the tree, a partial count of freshwater intake is available, and when it is larger than the current upper bound, it is also used to cut the tree.

Therefore, the search allows exploring different design alternatives, capability that other methodologies fail to provide. Some of these alternative networks may consume more fresh water than the optimal case but they may still present an interesting option if the interconnections among processes are somehow limited. Forbidden and compulsory connections among processes are not unusual. This procedure guarantees global optimality for the case where all the wastewater users are terminal processes.

The method is very efficient. For example, the problem of Table 7-1 renders the solutions shown in Figures 7-1 and 7-2, and no others. For example, a four processes problem, presented also by Doyle and Smith (1997), has one head process and, monotonicity reduces the problem to only two sequences. A larger problem (ten processes) is shown in Appendix A.

The importance of this method stems from its ability of being able to provide several sub-optimal solutions that may be attractive to the practical engineer, but can also be useful for retrofit studies.

7.3 Challenges

In this last section, a few unresolved matters of the problem will be discussed.

7.3.1 Fixed Concentrations Vs. Fixed Mass Loads

Most of the previous work has approached the water reuse problem by assuming that 1) The water supplied to a process always removes fixed loads of contaminants, and 2) The solubility and corrosion limits can be used to establish maximum inlet and outlet concentration constraints imposed on pollutants. These assumptions came as a necessity to represent complex processes through simplifying approximations, making the problem easier to solve.

Consider briefly a desalter unit (Figure 7-4). In this process water is injected (F_w) with salt concentration C_w. The raw crude comes with a certain amount of water F_{wR_I} and some salt content. The desalted crude leaves the unit with a certain amount of residual water with salt.

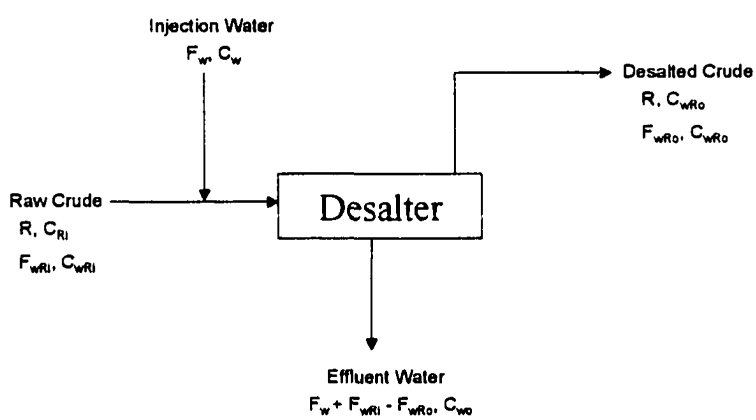


Figure 7-4
Balance on a Desalter.

Using material balances, assuming that the water in the crude and the effluent water stream have the same salt concentration and working with a constant salt removal (1-α) (independent of the flowrate and the concentration of the incoming water), one arrives at the following formula:

$$F_w^2 C_w + F_w Z C_w + F_w (S - RC_{Ro} - \alpha S) + Z(S - RC_{Ro}) - F_{wRi}\alpha S \geq 0 \qquad (7\text{-}3)$$

where $Z = F_{wRi} - F_{wRo}$ and $S = RC_{Ri} + F_{wRi}C_{wRi}$. This equation is quadratic in the water flowrate. If the contaminant is salt: $C_{Ri} = C_{Ro} = 0$ and the equation is slightly simplified. It becomes linear in F_w only when freshwater is used $(C_w = 0)$. For the case of H_2S instead of salt, one has $K = C_{Ro} / C_{wo}$ and another quadratic equation is obtained. Figure 7-5 shows the impact of these equations in the typical concentration vs. load diagram used by Wang and Smith (1994) and subsequent papers. In Figure 7-5 (a), the diagram proposed by Wang and Smith (1994) is shown. This contrast with Figure 7-5 (b), where the load and the exit concentration vary with the flowrate used.

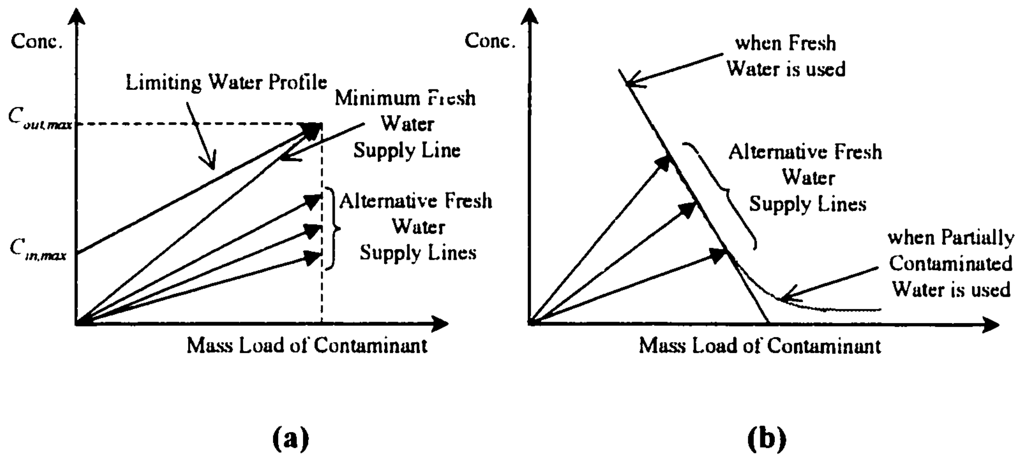


Figure 7-5
Concentration-Load Diagrams.

The problem is even richer in alternatives. In some other systems contaminate may reach solubility limits, in which case the outlet concentration is fixed and the load is, once again, variable with the flowrate. In addition, temperature and pressure set solubility limits and partition coefficients. Therefore, models should be at least temperature sensitive. Moreover, since contaminants have different solubility in water, a single water-using operation may need to respond to different models, one for each type of pollutant. This fact adds a new dimension of complexity to an already difficult multi-contaminant problem. Some of these issues are slowly surfacing in the literature. For example, Huang *et al.* (1999) already refer to the constant concentration in the outlet of some water using processes as well as treatment units.

7.3.2 Retrofit of Existing Plants

This problem needs to be focused differently than the design problem. As mentioned before, water reuse may be limited by geographical, process and/ or design constraints. Geographical constraints relate to actual distances or interconnection limitations among units and become of importance when retrofitting existing sites. In such cases, connections may need to be imposed (compulsory connections) or forbidden. The optimal reuse may demand connections that are technically impossible to fulfill. Consequently, full water reuse may be reduced, forcing an increase in fresh water usage. Design constraints deal with issues such as vessels, pipe lines, and pumps/compressors capacities as well as with corrosion limitations. For instance, replacing fresh water with reusable wastewater usually impiies an increase in flowrates and/or residence times. Such increase may not be feasible for existing equipment. Vessels and piping may to admit wastewater where corrosion limits exceed the original design allowances. The optimal water reuse scheme needs now to include other important variables such as re-piping and new pumping cost. Therefore, the objective may now depart from the minimization of fresh water consumption to include the aforementioned costs. Although retrofit options have been mentioned in several papers, (Alva-Argáez, 1998; Huang *et al.*, 1999), pumping costs have not been included and heat integration is absent. The burning challenge in these systems is the large number of integers that these MINLP models can have, which can induce a cumbersome integrality gap.

7.3.3 Uncertainty and Flexibility of Contaminant Loads

Wastewater flow rate as well as contaminant levels can vary. Especially in refineries, crudes carry more heavy hydrocarbons than others, and even the amount of aromatic and naphtenic components changes among crudes. Heavy crudes (low API gravity) have a larger proportion of heavier hydrocarbons and therefore the TBP curve is steep. This suggests that the design attempted should be resilient enough to be able to accommodate different pollutant levels.

Resiliency and flexibility have been addressed by several authors in the context of particular applications such as heat exchangers (Floudas and Grossmann, 1987; Colberg *et al.*, 1978). Some authors have addressed the overall plant resiliency problem (Morari, 1983). Recently, the problem has been initiated as part of what is called "Design with Uncertainties". Straub and Grossmann, (1993) and Pistikopoulos and Ierapetritou (1995) are some of the pioneering papers in the area. Many others follow.

7.3.4 Water Belt

This is a new concept that has been suggested as a model to incorporate realistically plant layout consideration to this problem. In this model, two sets of piping cruise an entire battery running along all water-using units. One pipe transports make-up fresh water while the second pipe(s) collects wastewater from the processes and delivers reusable wastewater at the same time. To avoid excessive wastewater degradation, the second pipe may actually be a bundle running together and selectively receiving and discharging wastewater as needed. Figure 7-6 illustrates the concept of the Water Belt in a simplified diagram. Two processes are shown receiving fresh water and wastewater from headers and discharging it in the wastewater header.

Such design presents a step ahead towards a zero discharge cycle achievement and breaks with the traditional process-to-process representation of this problem showing that significant savings in piping can be obtained.

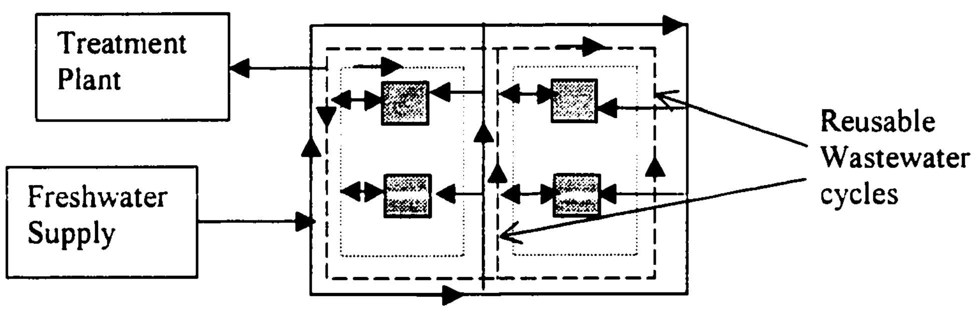


Figure 7-6
The Water Belt.

7.4 Notation

C concentration of contaminant, ppm

f	component flowrate, g/h
F	water flowrate, ton/h
L	mass load of contaminant, kg/h
$\boldsymbol{P}_j$	set of precursors of j
$\boldsymbol{R}_j$	set of receivers of j

Other subscripts:

in	at inlet
out	at outlet
i,j	connection going from process i to process j
p,i	pollutant p in stream i
j	process j

Other superscripts:

min	minimum
max	maximum
w	fresh water

7.5 References

1. Alva-Argáez A., A.C. Kokossis and R. Smith. *Automated Design of Industrial Water Networks.* AIChE Annual Meeting, paper 13f, Miami, 1998.
2. Benko N., E. Rev, Z. Szitkai and Z. Fonyo. *Optimal Water Use and Treatment Allocation.* Comp. & Chem. Eng., Vol. 23, Supp., pp. S589-S592, 1999.
3. Colberg R. D., M. Morari and D. W. Townsend, *A Resilience Target for Heat Exchanger Network Synthesis.* Comp. & Chem. Eng., 13, 7, 1978.
4. Doyle, S.J. and R. Smith. *Targeting Water Reuse with Multiple Contaminants.* Trans IChemE, 75, Part B, No. 3, pp. 181-189, 1997.
5. Floudas C.A. and I.E. Grossmann. *Synthesis of Flexible Heat Exchanger Networks with Uncertain Flowrates and Temperatures.* Comp. & Chem. Eng., 11,319, 1987.
6. Huang C-H, C-T. Chang, H-C. Ling and C-C. Chang. *A Mathematical Programming Model for Water Usage and Treatment Network Design.* Ind. Eng. Chem. Res., 38, pp. 2666, 1999.
7. Morari M. *Design of Resilient Processing Plants, III. A general Framework for the Assessment of Dynamic resilience.* CES, 38, 1983.
8. Pistikopoulos E. N. and M. G. Ierapetritou. *Novel Approach for Optimal Design under Uncertainty,* Comp. & Chem. Eng. 19,1089-1110, 1995.

9. Savelski M., M. Rivas and M. Bagajewicz. *A New Approach to the Design of Water Utilization Systems with Multiple Contaminants in Process Plant.* Annual AIChE Meeting, Dallas, 1999.
10. Straub D.A. and I.E. Grossmann. *Design Optimization of Stochastic Flexibility.* Comp. & Chem. Eng., 17,4,339-354, 1993.
11. Takama N., T. Kuriyama, K. Shiroko and T. Umeda. *Optimal Water Allocation in a Petroleum Refinery.* Comp. & Chem. Eng. 4, 251-258, 1980.
12. Wang Y.P. and R. Smith. *Wastewater Minimization.* CES, 49, 7, pp. 981, 1994.

APPENDIX A

Large-scale Multicomponent Example Problem

A.1 Problem Data

This appendix presents the results of the application of the algorithm explained in Chapter 7 to a ten-process system with three contaminants (Tables A-1 (a) and A-1 (b)). The minimum fresh water rate is 392.85 ton/hr. This solution is shown in Figure A-1.

Table A-1 (a): Limiting process data for processes 1 through 5

Process Number	Contaminants	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
1	A B C	3.40 414.80 4.59	20 300 45	120 12,500 180
2	A B C	5.60 1.40 520.80	120 20 200	220 1,000 9,500
3	A B C	0.16 0.48 0.16	0 0 0	20 60 20
4	A B C	0.80 60.80 0.48	50 400 60	150 8,000 120
5	A B C	0.75 20.00 1.75	0 0 0	15 400 35

Several sub-optimal solutions are also identified by the method. The two best sub-optimal solutions feature 393.20 and 393.31 ton/hr, Figures A-2 and A-3, respectively.

Table A-1 (b): Limiting process data for processes 6 through 10

Process Number	Contaminants	Mass Load of Contaminant (kg/h)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)
6	A B C	2.40 100.70 2.50	10 200 20	70 600 90
7	A B C	1.80 6.80 0.60	25 230 20	150 1,000 220
8	A B C	3.00 102.3 8.14	5 45 50	100 4,000 300
9	A B C	200.00 1.90 4.00	13 200 5	100 3,000 200
10	A B C	4.00 10.30 9.00	10 90 70	100 500 800

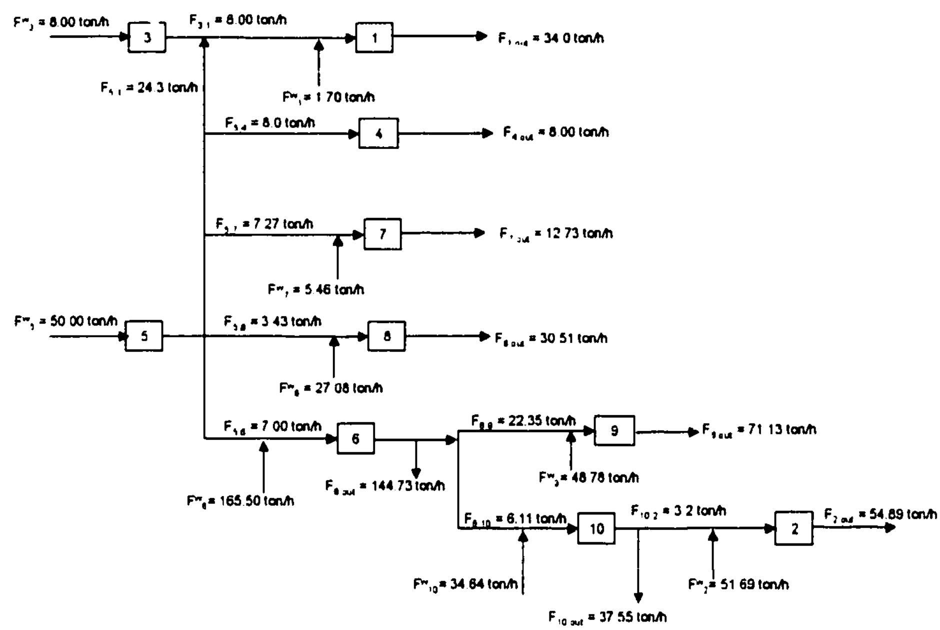


Figure A-1
Optimal Solution.

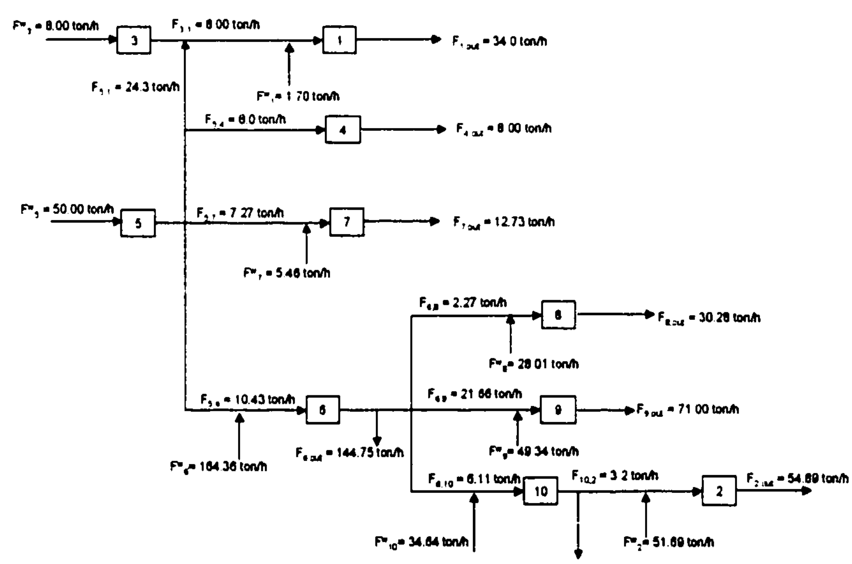


Figure A-2
Sub-optimal solution # 1.

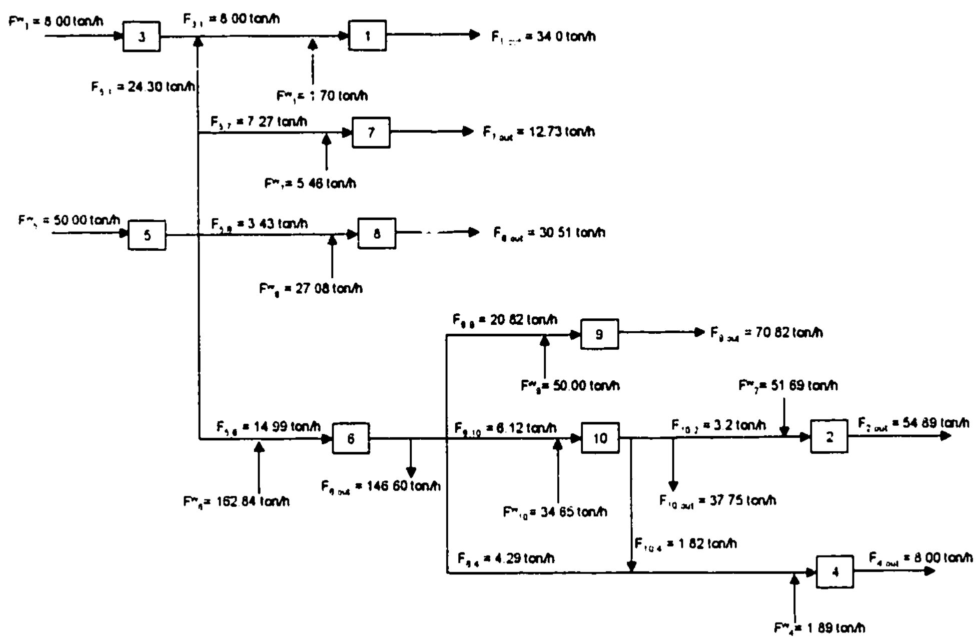


Figure A-3
Sub-optimal solution # 2.