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ADVANCED OPTIMIZATION TOOLS FOR THE DESIGN AND RETROFIT OF PROCESS PLANTS WATER NETWORKS

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SCHOOL OF CHEMICAL, BIOLOGICAL AND MATERIALS ENGINEERING

BY

Dr. Miguel J. Bagajewicz, Chair

Dr. Theodore B. Trafalis

Dr. Dimitrios V. Papavassiliou

Dr. Lance L. Lobban

Dr. Jeffrey H. Harwell

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ABSTRACT

Water is extensively used in industry and due to its increasing cost and the continuous quality deterioration of the available freshwater sources; its use is becoming also a cost concern in industries. An alternative to reduce costs associate to water consumption is the integration of the water system through reuses and recycles. This problem is often called Water Allocation Problem (WAP) and has been studied in the past three decades and several approaches to solve it have been presented. A comprehensive review of methods presented up to 2000 is given by Bagajewicz (2000); additional overviews can be found in a few books (Mann and Liu, 1999; Sikdar and El-Halwagi, 2001).

The methods to solve the WAP can be divided into two big classes: those based on mathematical programming, and those based on graphical, heuristic or algorithmic methods. The most promising class is the one based on mathematical programming, which is being increasingly used, especially because of the inability of graphical, heuristic or algorithmic procedures to effectively provide rigorous solutions to multiple contaminant problems. Additionally, more elaborate objective functions (cost, number of connections, etc.) are easier to handle using mathematical programming approaches.

Although this problem has been studied for three decades, some conceptual issues have been overlooked. The WAP first defined by Takama et al.(1980) considered two water subsystems commonly seen in the industry, the water-using subsystem and the wastewater treating subsystem, but left the water pre-treatment subsystem out of the systems integration. This work proves that the absence of this third subsystem has a strong effect on freshwater consumption targets and, in many cases, the use of the former

definition creates systems that are “impossible” to reach zero liquid discharge.

In the mathematical optimization group, approaches using LP, NLP, MILP, and MINLP have been presented. Aside from the linear models presented, which are only able to find the optimum solution for particular situations, the biggest challenge on the mathematical procedures is to overcome the difficulties generated by the non-linear and non-convex terms that arise from the contaminants balance (mixers and splitters). Such problems require good start points to find a feasible solution and most of the available solvers cannot guarantee global optimality if a solution is found. On the other hand, methodologies based on mathematical optimization are much easier to describe the problem in more detail and thus more complex problems can be approached.

Although the *integrated water system* problem has been solved by other authors for minimum freshwater consumption and cost (Takama et al., 1980; Alva-Argaez et al., 1998; Huang et al., 1999; Karuppiah and Grossmann, 2006; Bagajewicz and Faria, 2009; Faria and Bagajewicz, 2009), robust methods to find optimum and sub-optimum solutions, present the option of investigating alternative solutions and are able to analyze the problem from different perspectives are needed. To overcome this drawback, different global optimization methods to solve the WAP using the *complete water system* are presented. Additionally, a method to find several alternative solutions is described and a planning model is suggested.

1. INTRODUCTION

The first chapter aims to give a general overview of different approaches and methods used to address the water allocation problem (WAP). Additionally, the objectives of this work are presented.

Water is an indispensable component in processes plant especially because of its characteristic of being a good heat and/or mass transfer agent without being hazardous and being relatively cheap. However, nowadays its cost is increasing and its quality is becoming poorer, which makes the costs associated to its treatment also increase. Several industries, including refineries, hydrometallurgy, iron and steel, sugar factories, dairy facilities, breweries, the textile industry, pulp and paper, pharmaceuticals and electronics, among other, intensively use water in their processes and, in some of these cases, need high quality water to feed their processes.

In general, the conventional water cycle in processes plants includes a pre-conditioning step to make it suitable for being used in processes (which are often referred as water-using units), and after used, it is sent to an end-of-pipe treatment, which treats the water to appropriate environmental discharge limits. A scheme of this general water cycle is given in Figure 1.1.

The water pre-treatment subsystem normally treats water to different qualities and its size and complexity are much related to the quality of the water source available.

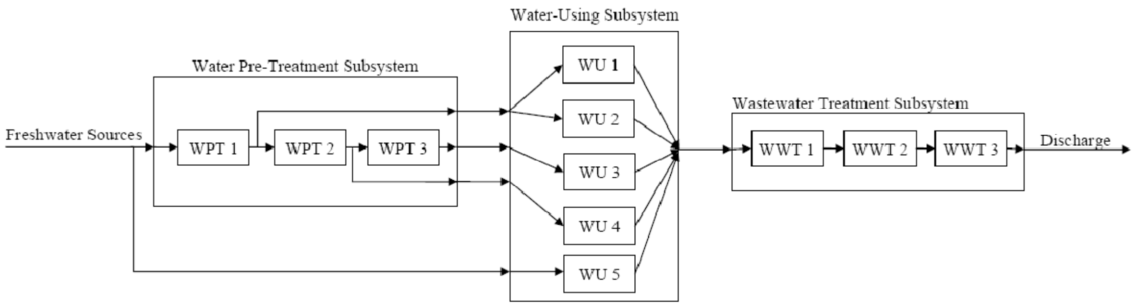

Figure 1.1 - Typical water cycle in process plants.

The water-using subsystem is composed by processes that need water, normally as a washing agent or steam. Some of the common contaminants in petroleum refineries for example are: hydrogen sulfide, suspended matter, ammonia, salts, organic matter, and hydrocarbons (Speight, 2005).

The wastewater treatment subsystem aims the conditioning of the stream to be discharged in the environment. In many instances, this subsystem is known as "end-of-pipe" treatment, which commonly consists in three types of operations: primary, secondary and tertiary.

Primary processes have the purpose of protecting the subsequent treatments from fouling by mechanically removing floatable and settleable solids. Secondary operations normally bring the wastewater to a desire quality level through biological oxidation processes. The tertiary process is responsible for polishing the wastewater. Common tertiary treatments are: membrane technologies, advanced oxidation methods, ozonation, distillation, electro-deionization, ion exchange, among others. More details regarding wastewater treatment subsystem and it primary, secondary and tertiary systems can be found in several books (Celenza, 1999; Tchobanoglous et al., 2003; Asano, 2007; among others).

Looking at these subsystems together, opportunities like minimizing freshwater consumption and/or costs can be achieved when they are optimized. The optimization of industrial water systems has been extensively studied and several approaches to solve it have been presented. A comprehensive review of methods presented up to 2000 can be found in Bagajewicz (2000). Additional overviews can be also found in a few books (Mann and Liu, 1999; Sikdar and El-Halwagi, 2001).

This class of optimization problems is often called Water Allocation Problem (WAP) and it can be generally defined as follows: *Given a set of process systems in need of water (water-using units), a set of freshwater sources and a set of potential regeneration processes, determine the optimum network that satisfies the system constraints.*

In fact, this problem statement has several variations depending especially on assumptions (conceptual and modeling) and the definition of "optimum network", that is the objective function. These variations do not only interfere on the kind of solution one is looking for, but they strongly influence the ability of finding its solution using different methods.

In these optimization problems, the water-using units are often described as quality controlled or quantity controlled (Polley and Polley, 2000). As quality controlled water-using units have been modeled as mass exchanger units with a fixed mass load and variable flowrates (Wang and Smith, 1994). When water-using units are defined as a combination of quality and quantity controlled units, they are modeled as mass exchanger units as well, but now with fixed flowrates (Takama et al., 1980; Wang and Smith, 1995). Another case of mass exchanger units is presented by Doyle and Smith (1997): they assume some water-using units are modeled by fixed outlet concentrations. This would be the case in which contaminants have limited solubility. Some works have assumed quantity controlled only in which outlet concentrations and flowrates are fixed (Polley and Polley, 2000). These models are often known as sources-sinks models. The two last classes of water-using unit models have the big advantages of allowing the use of a linear model if no other non-linearity exists. In reality, many water-using units have to be modeled using the first two alternatives and consequently non-linearities will appear.

Although the models used to describe water-using units have been extensively applied and are very acceptable, it is assumed that *process conditions are given beforehand*.

One of the weaknesses in currently methods for optimizing WAP in process plants is a lack of accurate modeling of water regeneration processes. In general, two kinds of model assumptions are made: regeneration processes have a fixed outlet concentrations (Koppol et al., 2003); and, regeneration processes have a fixed rate of removal (Takama et al, 1980; Guanaratnam, 2005; Karuppiah and Grossmann, 2006; Alva-Argáez, 2007). In reality, outlet concentration and/or rate of removal of regeneration process may vary with inlet concentrations and flowrates. This issue was approached by Lili et al. (2006), which show that when removal efficiency is variable, different solutions can be obtained.

In addition to how the processes are modeled, how these problems are solved is also an extremely important issue in WAP. Most of the methods presented can be divided into two big classes: those based on mathematical programming, and those based on graphical, heuristic or algorithmic methods. The most promising class is the one based on mathematical programming (Bagajewicz, 2000; Faria and Bagajewicz, 2009), originally proposed by Takama *et al.* (1980). The use of mathematical programming is being increasingly used, especially because of the inability of graphical, heuristic or algorithmic procedures to effectively provide rigorous solutions to multiple contaminant problems. Additionally, more elaborate objective functions (cost, number of connections, etc.) are easier to handle using mathematical programming approaches. In reality, sometimes, it is not that it is easier, but it is the only way to rigorously solve such problems.

The WAP was first defined by Takama et al.(1980) as the integration of two water subsystems commonly seen in the industry: the *water-using subsystem* and the *wastewater treating subsystem*. Before Takama and co-workers' paper, efforts were made to individually optimize the *wastewater subsystem* (see a review presented by Mishra et al, 1975). In this case, the sub-optimum conditions (amount of wastewater and concentrations of contaminants) of the *water-using subsystem* are used as input data in the optimization of the *wastewater treating subsystem*. Clearly, the integration of these two subsystems can generate important alternatives for the optimum design as shown by some authors (Kuo and Smith, 1998; Huang et al., 1999; Karuppiah and Grossmann, 2006; Alva-Argaz et al., 2007; Bagajewicz and Faria, 2009; Faria and Bagajewicz, 2009). After Takama et al. (1980), which solved the problem using mathematical optimization, different approaches have been presented. These approaches can generally be split in two big groups: one based on graphical methods; and another based on mathematical optimization.

The graphical methods, first presented by Wang and Smith (1994), are based on the well known pinch analysis for heat/mass integration problems and so called *water pinch*. Although many authors claim that these approaches can give "good insights" to the designers, they can be extremely time-consuming and very inefficient when multi-contaminants problems and/or complex networks are addressed. Moreover, minimum cost targets are virtually impossible to be solved with these methods and the supposed “good insights” are fairly obvious. Unexpected solutions, which are many times found using mathematical programming, are pretty much out of the scope of graphical methods and can represent interesting alternatives.

In the mathematical optimization group, approaches using LP, NLP, MILP, and MINLP have been presented (Takama et al., 1980; Huang et al. 1999; Gunaratnam et al., 2005; Karuppiah and Grossmann, 2006; Alva-Argaez et al., 2007). Aside from the linear models (Bagajewicz et al., 2000; Salveski and Bagajewicz, 2000), which are only able to find the optimum solution for particular situations, the biggest challenge on the mathematical procedures is to overcome the difficulties generated by the non-linear and non-convex terms that arise from the contaminants balance (mixers and splitters). Such problems require good start points to find a feasible solution and most of the available solvers cannot guarantee global optimality if a solution is found. On the other hand, methodologies based on mathematical optimization are much easier to describe the problem in more detail and thus more complex problems can be approached. More details about particularities of graphical methods and mathematical procedures and can be found in a review presented by Bagajewicz (2000).

Although the *integrated water system* problem has been solved by other authors for minimum freshwater consumption and cost (Takama et al., 1980; Alva-Argaez et al., 1998; Huang et al., 1999; Karuppiah and Grossmann, 2006; Bagajewicz and Faria, 2009; Faria and Bagajewicz, 2009), robust methods to find optimum and sub-optimum solutions, present the option of investigating alternative solutions and are able to analyze the problem from different perspectives are needed. To overcome this drawback, not only does a specific method have to be developed but also current concepts involving the WAP should be re-evaluated.

To achieve this end, this work approaches some of the different aspects of the WAP:

- The validity of simplifying assumptions in current models: the use of optimality conditions;
- Optimization of current models using different criteria (objective functions);
- Structures of current models (conceptual issues);
- A robust and reliable optimization method;
- The degeneracy of WAP;
- A planning model able to handle future expansions.

These issues are going to be presented and discussed throughout the chapters as summarized next.

Chapter 2 discusses a common assumption used in the design of water/wastewater systems for single components. This assumption is common used for single contaminant problems and fix the water-using units outlet concentrations of the pollutant to their maximum allowed value. This converts the problem from one with nonlinear constraints into one with linear constraints. For problems minimizing freshwater consumption in single contaminant systems, this assumption has been proven to lead to global optimal solutions (Savelski and Bagajewicz, 2000). However, it is shown in chapter 2 that the use of this assumption may not lead to global optimal solutions in certain cases, specifically when the number of connections is minimized and when the cost is minimized.

Chapter 3 evaluates the choice of different objective functions and presents a methodology to analyze the WAP using profit-based optimization criteria for both, grassroots design and/or retrofit of water systems. The maximization of Net Present Value (NPV) and/or Return of investment (ROI) is proposed and the examples show that the solutions where savings and/or profit are maximized can be different from those where freshwater is minimized. They also differ from each other when ROI or NPV are used. In addition, when the NPV objective is used, the optimum solutions also vary depending on the interest rate used to calculate the discount factor.

Chapter 4 re-evaluates the definition of the water/wastewater allocation problem as it was originally defined by Takama et al. (1980), how this concept was modified, and sometimes simplified through time, as well as additional issues that were still not properly addressed as the inclusion a the *water pre-treatment system* in the WAP optimization framework, which create a *complete water system*. Then the mathematical model of the *complete integrated water system,* which is based on the modifications discussed, is presented.

Chapter 5 presents optimization methods and discusses the issue of global optimality of WAP. The biggest challenges in solving these problems are rooted in the nonlinearities and non-convexities that arise from bilinear terms corresponding to component material balances and concave cost functions. Different approaches to address this issue are presented.

Chapter 6 discusses the degeneracy of WAP, the inability of graphical methods, how degeneracy may affect the robustness of optimization methods and how it can be reduced.

Chapter 7 presents a planning model for industrial water systems to address expected future changes in the system such as stricter environmental regulations, increasing costs of freshwater, variability on the quality of the available freshwater source, bottlenecks caused by expansion of the capacity plant, etc.

Finally, Chapter 8 concludes this work giving the main remarks obtained from the results and discussing important issues that should be approached in future works.

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2. DIFFERENT ASSUMPTION FOR SIMPLIFIED WAP MODELS

One common assumption used in the design of water/wastewater systems for single components is to fix the process outlet concentrations of the pollutant to their maximum allowed value. This converts the problem from one with nonlinear constraints into one with linear constraints. For problems minimizing freshwater consumption in single contaminant systems, this assumption has been proven to lead to global optimality (Savelski and Bagajewicz, 2000). In this chapter, the effect of using this assumption in cases where it may not lead to global optimal solutions is investigated, namely when the number of connections is minimized and when the cost is minimized.

2.1. Overview

The water/wastewater allocation problem has been widely formulated as a freshwater intake minimization problem. In addition, although there are several graphical/conceptual and also algorithmic methods that can be used, the problem has been efficiently addressed using mathematical programming, which is the focus of this work. Minimization of freshwater consumption can be achieved using reuse/recycle structures with the eventual addition of intermediate regeneration processes (Wang and Smith, 1994; Kuo and Smith, 1997; Feng et al., 2007; Ng et al., 2007a, b; Alva-Argaez et al., 2007).

The biggest challenge on the mathematical procedures is the presence of nonlinearities. Aside from stochastic approaches (Genetic algorithms; Xu et al.(2003), Prakotpol and Srinophakun (2004)), which do not guarantee global optimality, many mathematical programming approaches using linear programming (LP), non-linear programming (NLP), mixed integer linear programming (MILP), and mixed integer non-linear programming (MINLP) were developed for this problem (Takama et al., 1980; El-Halwagi and Manousiouthakis, 1990; Galan and Grossmann, 1998; Alva-Argaez et al., 1998; Bagajewicz et al. 2000; Bagajewicz and Savelski, 2001; Karuppiah and Grossman, 2006).

For single contaminant cases in which water-using units are handled as mass exchangers, many methodologies are based on the optimality conditions proved by Savelski and Bagajewicz (2000). One of these necessary optimality conditions states that the outlet concentrations in each process are at their maximum value. The other one is a condition of monotonicity in the outlet concentrations, which is useful when using algorithmic methods (Savelski and Bagajewicz, 2001). This last condition is not relevant for mathematical programming approaches, although it can be used as aid to exclude connections that do not comply with the monotonicity and thus accelerate computations. Both conditions are added in the appendix in more detail.

Using the maximum concentration condition allows transforming non-linear models into linear ones. However, it will be shown that the optimality conditions presented by Savelski and Bagajewicz (2000) are only valid when the objective function is freshwater consumption minimization and no structural constraints, like forbidden connections and/or combination of connections, exist. This was also pointed out by Doyle and Smith (1997), who focused on the multiple contaminant case.

Thus, this chapter analyzes the effects of using these particular conditions on problems involving costs and/or structural constraints. The original MINLP and the particular MILP models are presented and compared. The results prove that the necessary optimality conditions (every process at its maximum outlet pollutant concentration) cannot be used to optimize costs or freshwater when structural constraints exist. Additionally, we show that connections between units based on the monotonicity conditions should not be pre-excluded in these cases.

Similarly to the problem statement given in chapter 1, the problem to be analyzed in this chapter can be defined as: Given a set of water-using units, a freshwater source, a wastewater discharge sink and an available regeneration process (with a fixed outlet concentration), the optimum solution for different objectives are sought. Additionally, self recycle in water-using units is excluded, which is also an assumption used by several previous papers. The superstructure used to build these models is presented in Figure 2.2.

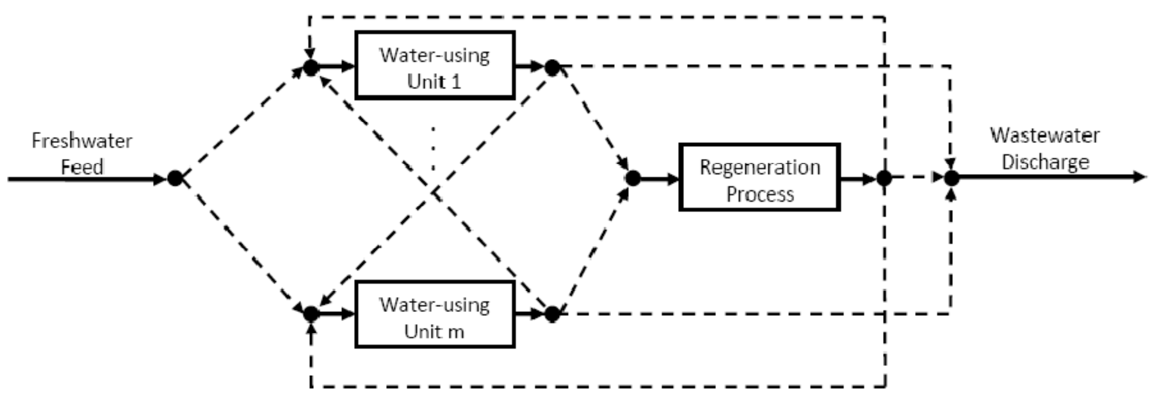

Figure 2.2 – Superstructure used in the models.

2.2. Non-Linear Model

The corresponding non-linear model to solve the water/wastewater allocation problem (WAP) previously defined is given by the following set of equations:

Balance of water on the units:

$$FW_{m*} + FNU_{m*} + \sum_{m \neq m*} FUU_{m,m*} = FUN_{m*} + FS_{m*} + \sum_{m \neq m*} FUU_{m*,m} \qquad \forall m* \tag{2-1}$$

where FW_{m*} is the freshwater consumption of unit $m*$, FNU_{m*} is the flowrate from the regeneration process to unit $m*$, $FUU_{m,m*}$ is the flowrate from unit m to unit $m*$, FUN_{m*} is the flowrate from unit $m*$ to the regeneration process, and FS_{m*} is the flowrate from unit $m*$ to the discharge.

Balance of water on the regeneration process (without loss of generality, we assume only one is needed):

$$\sum_{m} FUN_m = FNS + \sum_{m} FNU_m \tag{2-2}$$

where FNS is the water discharge to end-of pipe treatment from the regeneration process (we assume that the regeneration process has outlet concentration larger than the disposal limits). Thus, the mixture of all the streams sent to wastewater disposal has to be further treated by the end-of-pipe treatment.

Balance of the contaminant on the units:

$$FW_{m*}C^{ws} + FNU_{m*}C^{n} + \sum_{m \neq m*} FUU_{m,m*}C_{m}^{out} + \Delta m_{m*} =$$
$$\left(FUN_{m*} + FS_{m*} + \sum_{m \neq m*} FUU_{m*,m} \right) C_{m*}^{out} \quad \forall m* \tag{2-3}$$

where C^{ws} is the contaminant concentration of freshwater ws, C^{n} is the outlet contaminant concentration of the regeneration process (which is a pre-defined parameter), C_{m*}^{out} is the outlet concentration of unit $m*$ and Δm_{m*} is the contaminant mass load of unit $m*$.

Limit of inlet concentration on the units:

$$FW_{m*}C^{ws} + FNU_{m*}C^{n} + \sum_{m \neq m*} FUU_{m,m*}C_{m}^{out} \leq$$
$$\left(FW_{m*} + FNU_{m*} + \sum_{m \neq m*} FUU_{m,m*} \right) C_{m*}^{\max,in} \quad \forall m* \tag{2-4}$$

where $C_{m*}^{\max,in}$ is the inlet maximum contaminant concentration for unit $m*$.

Limit of outlet concentration on the units:

$$C_{m*}^{out} \leq C_{m*}^{\max,out} \quad \forall m* \tag{2-5}$$

Binary variables are added to identify the existence of connections and be used in cost objective functions:

$$FW_{m} \leq U \; YW_{m} \qquad \forall m \tag{2-6}$$

$$FUN_{m} \leq U \; YUN_{m} \qquad \forall m \tag{2-7}$$

$$FNU_{m} \leq U \; YNU_{m} \qquad \forall m \tag{2-8}$$

$$FUU_{m^*,m} \leq U\ YUU_{m^*,m} \qquad \forall m^*, m \tag{2-9}$$

$$FNS \leq U\ YNS \tag{2-10}$$

$$FS_m \leq U\ YS_m \qquad \forall m \tag{2-11}$$

In these equations, YW_m, $YUU_{m^*,m}$, YUN_m, YNU_m YNS and YS_m are binary variables used to determine the existence of flowrates going from the freshwater source to the units, from a unit to another unit, from a unit to the regeneration process, from the regeneration process to a unit, from the regeneration process and a unit to the discharge unit, respectively. U is the maximum value (upper bound) of flowrate allowed in the connections.

Objective Functions

Because it is known that the water allocation problem generally presents degenerate solutions (different sets of decision variables giving the same objective values) when freshwater is minimized (Bagajewicz and Savelski, 2000), it is possible to further use some economic objectives to sort the best solution among these degenerate ones. Some of the possible objective functions are presented below.

Minimum number of connections:

$$Min\left(\sum_m \left(YWU_m + YS_m + YUN_m + YNU_m + \sum_{m^* \neq m} YUU_{m,m^*}\right) + YNS\right) \tag{2-12}$$

Minimum capital cost:

$$Min\begin{pmatrix} RegCost_n + \sum_m \begin{pmatrix} YWU_m\, ICWU_m + YS_m\, ICS_m + \sum_{m^* \neq m}\left(YUU_{m,m^*}\, ICUU_{m,m^*}\right) \\ +YUN_m\, ICUN_m + YNU_m\, ICNU_m \end{pmatrix} \\ +YNS\ \ ICNS \end{pmatrix} \tag{2-13}$$

where $ICWU_m$, ICS_m , $ICUU_{m,m^*}$, $ICUN_m$, $ICNU_m$, $ICNS$ are the investment cost with connections. The cost of the regeneration unit $RegCost$ can be either a function of the treated flowrate (which can be linear or non-linear) or a constant value. The equations used to calculate the capital investment of the regeneration process is presented in each example.

In addition, the use of the maximum outlet concentrations assumption when total annualized cost is minimized is investigated:

Minimum annualized cost:

$$Min\left(\alpha \sum_m FWU_m + \beta \sum_m FUN_m + af \begin{pmatrix} RegCost_n \\ +\sum_m \begin{pmatrix} YWU_m\, ICWU_m + YS_m\, ICS_m + \\ \sum_{m^* \neq m}\left(YUU_{m,m^*}\, ICUU_{m,m^*}\right) \\ +YUN_m\, ICUN_m + YNU_m\, ICNU_m \end{pmatrix} \\ +YNS\ \ ICNS \end{pmatrix} \right) \tag{2-14}$$

where α is the freshwater cost, β is the operating cost of the regeneration process and af is the annual discount factor.

2.3. Linear Models

Savelski and Bagajewicz (2000) proved that when minimum freshwater is sought, then, there is an optimum solution in which the outlet concentration of each water-using units reaches its maximum value. As a result, equations (2-3) and (2-4) can be rewritten as follows (Bagajewicz and Savelski, 2001):

$$FW_{m^*} C^{ws} + FNU_{m^*} C^{n} + \sum_{m \neq m^*} FUU_{m,m^*} C_{m}^{out,\max} + \Delta m_{m^*} = \left(FUN_{m^*} + FS_{m^*} + \sum_{m \neq m^*} FUU_{m^*,m} \right) C_{m^*}^{out,\max} \quad \forall m^* \tag{2-15}$$

$$FW_{m^*} C^{ws} + FNU_{m^*} C^{n} + \sum_{m \neq m^*} FUU_{m,m^*} C_{m}^{out,\max} \leq \left(FW_{m^*} + FNU_{n,m^*} + \sum_{m \neq m^*} FUU_{m,m^*} \right) C_{m^*}^{\max,in} \quad \forall m^* \tag{2-16}$$

Next, the use of this assumption is investigated solving examples using different objective functions and/or structural constraints. The examples were implemented in GAMS (Brooke et al., 1998). The linear model is solved using GAMS/CPLEX and the non-linear model using GAMS/DICOPT.

2.4. Illustrations

Example 1

The first example involves a small-scale problem using the one posed by Wang and Smith (1994) with four water-using units. The configuration of the network without reuse (which we call conventional network) and its respective limiting data are presented in Figure 2.3.

Minimization of freshwater consumption using both models, linear and non-linear, renders the same minimum freshwater usage (90 t/h). However, there are degenerate solutions in which the maximum outlet concentration is reached and others in which the outlet concentration is lower than the maximum.

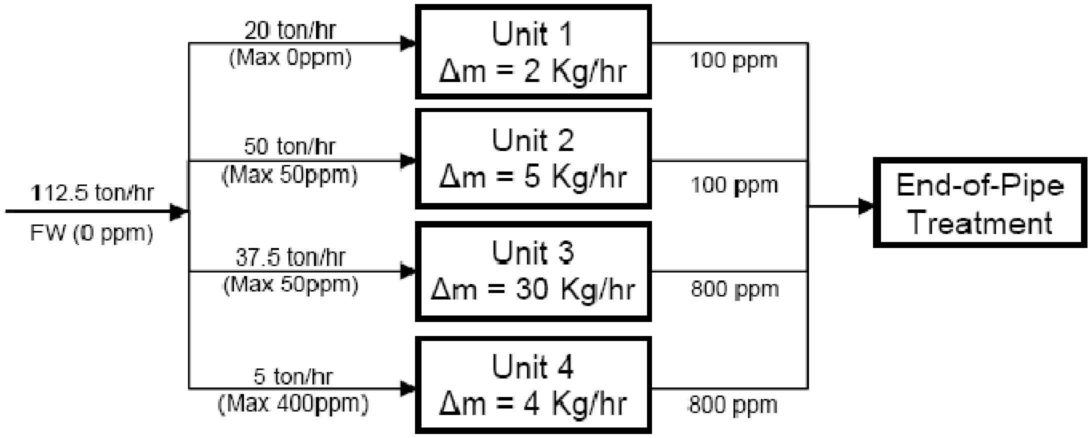

Figure 2.3 – Network configuration without reuse and its limiting data.

Minimizing the number of connections among degenerate solutions:

Both models were used to analyze the validity of the maximum outlet concentration condition when the minimum number of connections is used as the objective. In both cases, the freshwater consumption is set to be 90 t/h, which is the minimum that can be calculated using the water pinch and several other different methodologies.

The number of connections of the solution obtained by the linear model is 8 (Figure 2.4) while the non-linear model renders 6 connections (Figure 2.5). Note that the non-linear model also has a simpler structure.

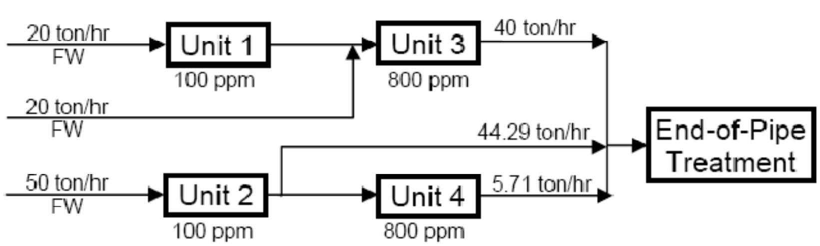

Figure 2.4 – Solution with minimum number of connections - linear model.

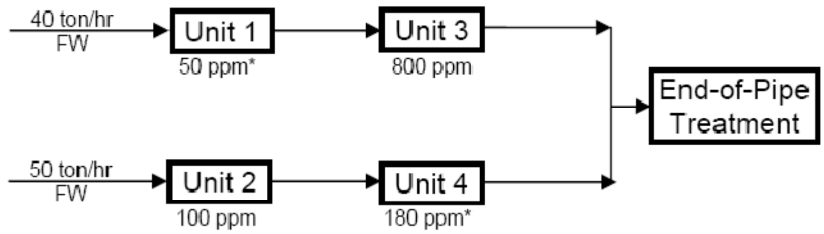

Figure 2.5 – Solution with minimum number of connections (non-linear model).
(*: Concentrations lower than the maximum)

Because the outlet concentration is fixed in the linear model, every unit that requires an inlet concentration lower than the minimum outlet concentration among the units has to be supplied by freshwater. In this example one can see that this happens for Units 2 and 3. Their maximum allowed inlet concentration is 50 ppm and the minimum outlet concentration among all the units is 100 ppm. Thus, there is no other option for these units than to be totally or partially supplied by freshwater. In other words, these two connections must exist when the maximum outlet concentration condition is used. Conversely, the nonlinear model can lower the outlet concentration of one (or more) unit(s) and remove the need for dilution. Indeed, Figure 2.5 shows that Unit 1 does not reach its maximum concentration and thus feeds Unit 3 without dilution. This issue can become significant when the physical distance between the freshwater source and the units is a concern (layout and/or cost issues).

Minimizing the cost of connections among degenerate solutions:

The cost of connections is now minimized maintaining the freshwater consumption at the minimum of 90 t/h. We set all costs to zero except the costs of connections between freshwater source and Units 2 and 3 ($10,000 each). As expected, the linear model reached a minimum cost of $20,000. This is the same solution found when the number of connection was minimized (Figure 2.4). The nonlinear model, in turn, shows a network with no costs, that is, both connections that had a cost were avoided. Figure 2.6 shows this solution. Note that Unit 1 reaches an outlet concentration (lower than its maximum and the one found in Figure 2.5) that allows the absence of connections between freshwater and Units 2 and 3.

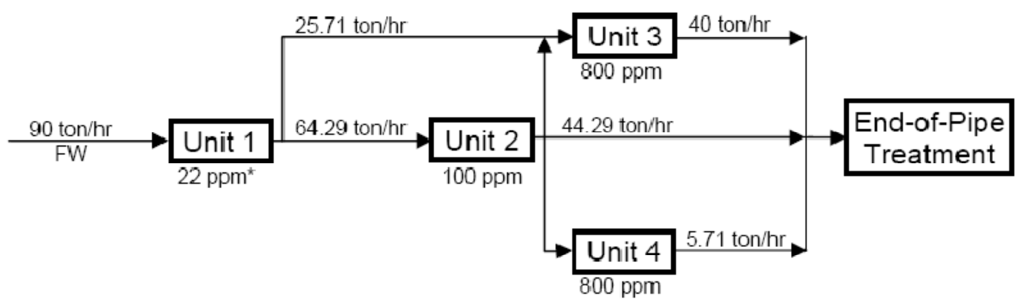

Figure 2.6 – Solution with minimum cost of connections - non-linear model.
(*: Concentrations lower than the maximum)

Feasible flowrate ranges feeding water-using units:

The flexibility given by the non-linear model is shown next. The nonlinear model has larger flexibility to vary flowrates in the water using units, which can have an impact on costs. To do that, the feasible regions are investigated.

In the case of Unit 1 (Figure 2.7), only one inlet concentration is possible (0 ppm). Then, a graph directly relating outlet concentration and flowrate is presented. The contaminant balance for the units (Equation 2-3) shows that the outlet concentration decreases when the flowrate through the unit increases. When the linear model is used, there is only one feasible flowrate for Unit 1 (20 t/h). Otherwise, the model with free outlet concentration can have a variety of flowrates, which will reduce the outlet concentration.

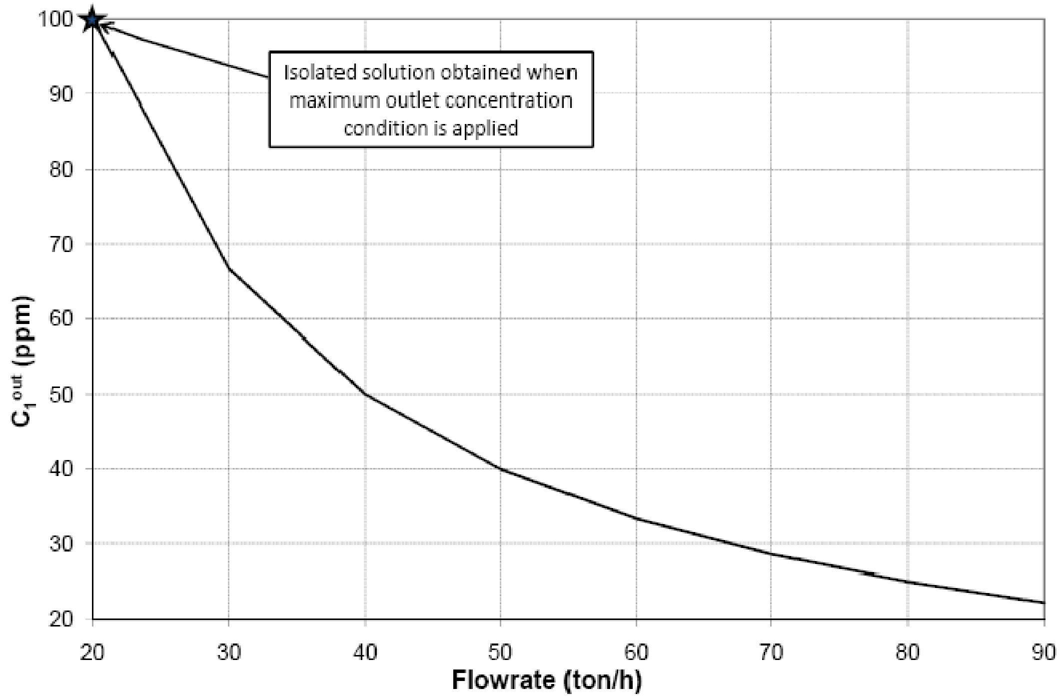

Figure 2.7 – Feasible flowrates through Unit 1

Figure 2.8 shows the outlet concentration as a function of the inlet concentration at different flowrates of Unit 2. The inlet concentration of Unit 2 was varied from zero to its maximum allowed inlet concentration. Note that the feasible solutions for the linear model are limited by a maximum flowrate (100 t/h). This does not happen when the outlet concentration is free (nonlinear model). Moreover, in the linear case each feasible flowrate has a unique inlet concentration, which does not happen in the nonlinear case. Indeed, the flexibility of the model when maximum outlet concentration condition is not applied can be observed by the larger feasible region (shadow region). Similar behavior is found for Units 3 and 4.

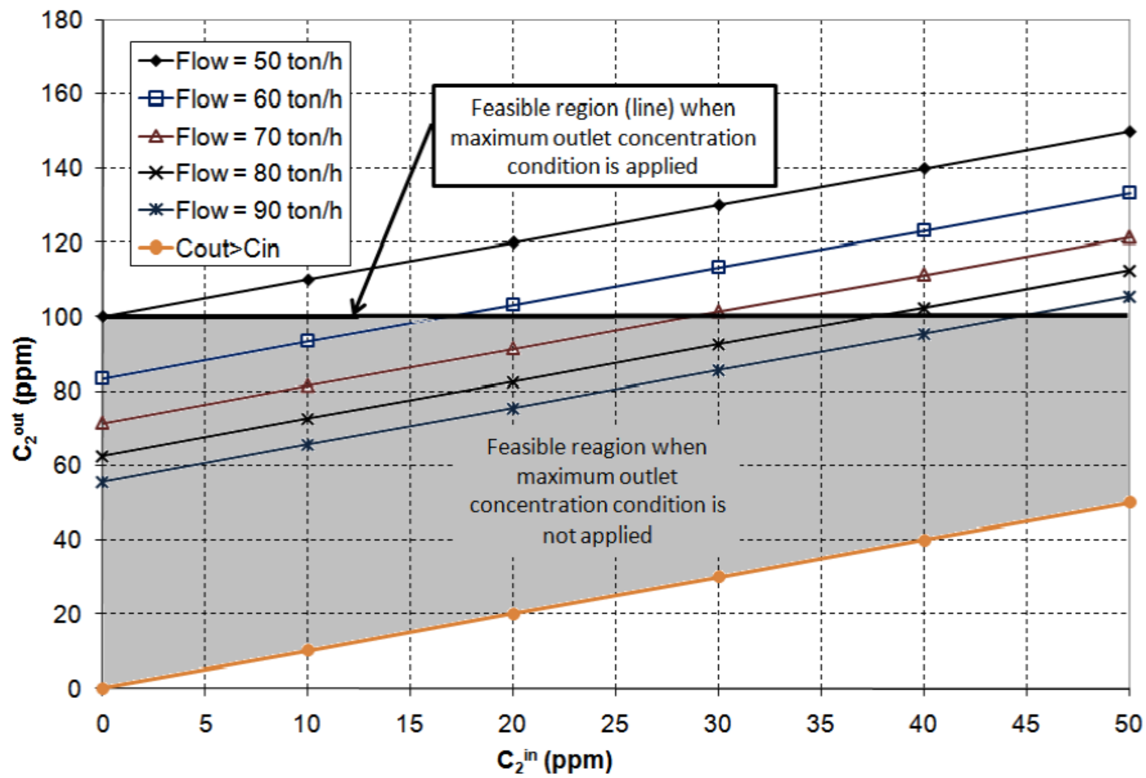

Figure 2.8 – Feasible flowrates through Unit 2.

Example 2

In example 2, the addition of a regeneration process in the problem studied in example 1 is allowed. The regeneration process added has a fixed outlet concentration of 10 ppm. When freshwater consumption is minimized, both models reach the same minimum flowrate (20 t/h) and obtain the same network structure. The solution is shown in Figure 2.9. The required connections between freshwater source and Units 2 and 3 are no longer needed. This is because now there is an option of using water coming from the regeneration process, which has outlet concentration (10 ppm) lower than the maximum allowed inlet concentration in Units 2 and 3 (50 ppm).

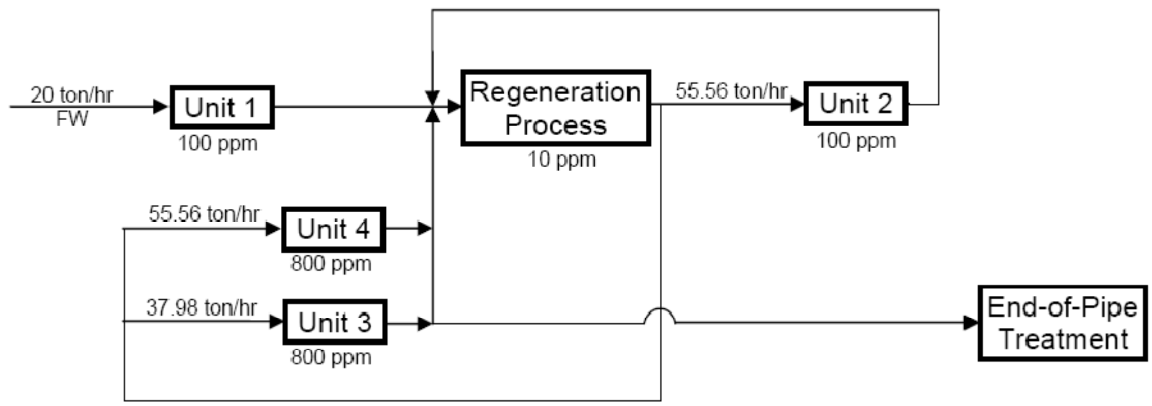

Figure 2.9 – Optimal solution for Example 2 - both models.

These observations characterize the existence of degenerate solutions, which can provide economical advantages for the design. Thus, the freshwater flowrate is fixed at 20 t/h and the following analyses are made:

a - Minimizing the number of connections among degenerate solutions:

The linear model shows a minimum of 8 connections (Figure 2.10) while the nonlinear model requires only 7 connections (Figure 2.11). Interestingly, both solutions present isolated zero discharge cycles, which is not always convenient due to control/flexibility reasons (the load in the units might vary and there is no freshwater to add to respond to the changes) and the need to prevent the accumulation of compounds that are not removed in the regeneration processes. In fact, this is not a situation that is often seen in industry, and, while feasible there are many impediments to implement them. It is not unthinkable that in the future, the pressure to reduce water consumption will increase and these impediments will be sorted out.

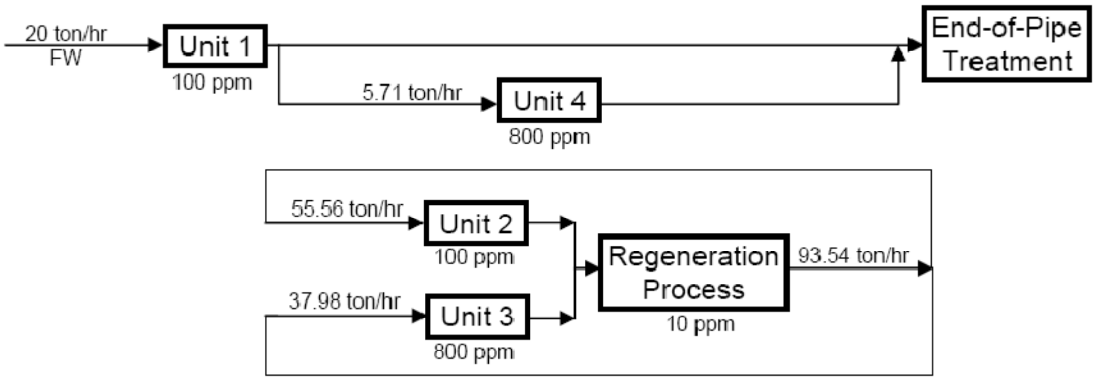

Figure 2.10 – Minimum number of connections for Example 2 - linear model.

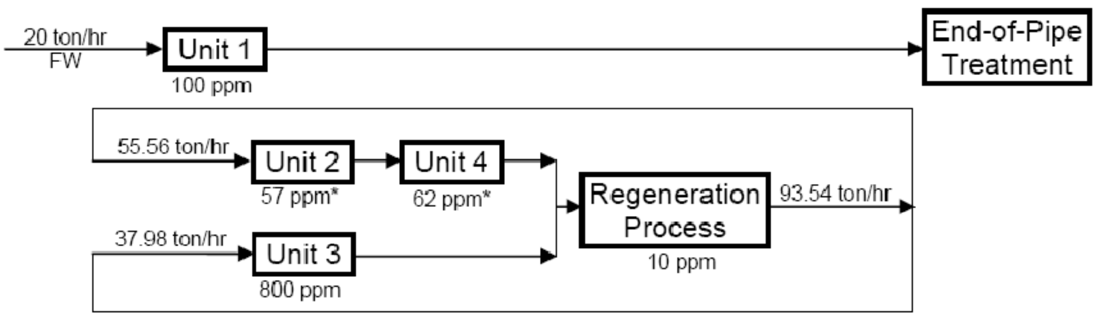

Figure 2.11 – Minimum number of connections for Example 2 - non-linear model.
(*: Concentrations lower than the maximum)

b - Elimination of Closed Cycles:

To avoid closed cycles, forbidden connections constraints are added to the models. The following constraint forbids a closed cycle between one unit and the regeneration process.

$$YUN_m + YNU_m \leq 1 \quad \forall m \tag{2-17}$$

Note that the idea here is not to forbid the recycles involving a unit and a regeneration process, but to avoid the isolated cycles. The suggested constraint cannot guarantee the non existence of these cycles since one involving two units and the regeneration process still can exist. However, it reduces the possibility of the existence of these cycles. If this constraint does not work for this example, a new one can be added. In the above solution, this constraint would forbid the loop between the regeneration process and Unit 3. Now, only isolated loops involving the regeneration and two units can exist. In such a case constraints similar to (2-17) can be written.

The minimum freshwater consumption is solved first. As a result, the linear model does not give the same minimum freshwater consumption than the nonlinear model. The first one gives 40 t/h of freshwater usage, while the nonlinear model renders 20 t/h of freshwater usage. These networks are shown in Figure 2.12 and Figure 2.13.

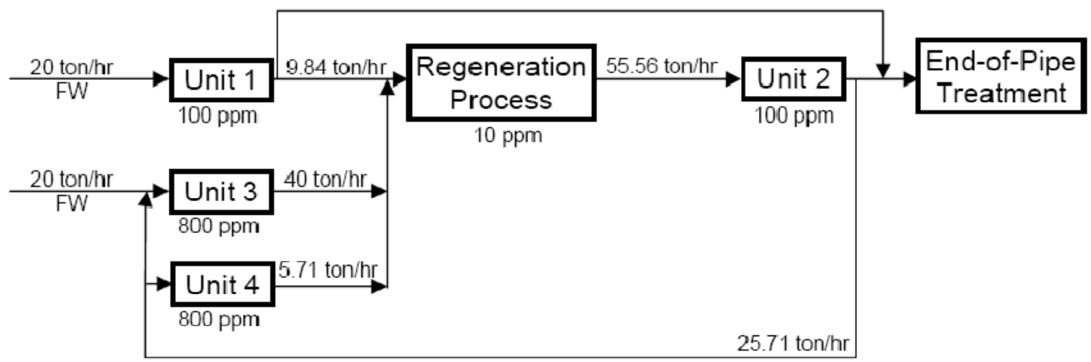

Figure 2.12 – Minimum freshwater usage for Example 2, forbidding cycles - linear model.

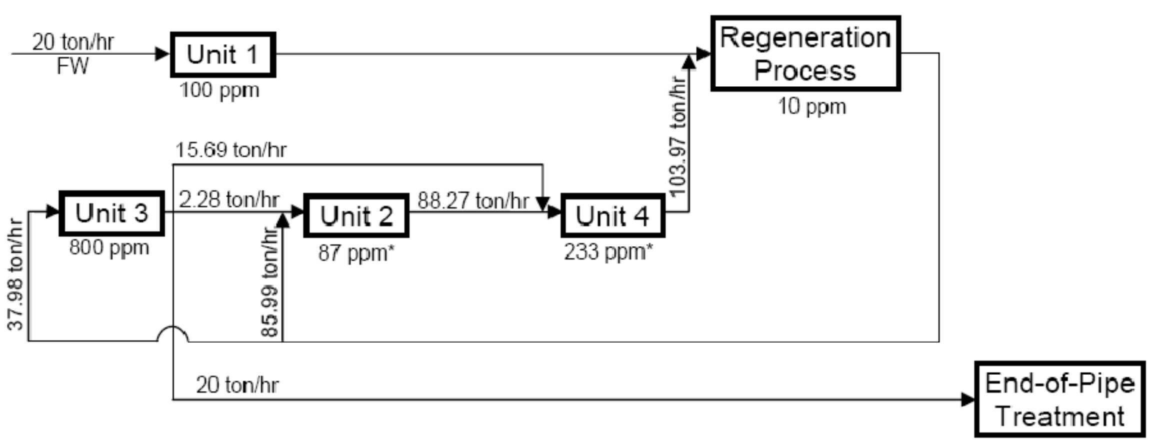

Figure 2.13 – Minimum freshwater use for Example 2, forbidding cycles - non-linear model.
(*: Concentrations lower than the maximum)

These results show that the maximum outlet concentration assumption does not only fail when other objective functions (cost or number of connections) are used, but also when minimum freshwater is targeted under structural constraints.

c - Minimizing the number of connections among degenerate solutions with forbidden cyclic connections:

The linear model solution finds the network presented in Figure 2.12, which was obtained by eliminating cycles. This network has 10 connections and does not have disconnected zero discharge cycles. Figure 2.14 shows the solution of minimizing the number of connections using the non-linear model with forbidden cycles between the regeneration process and units. The found solution has 8 connections and no isolated cycles.

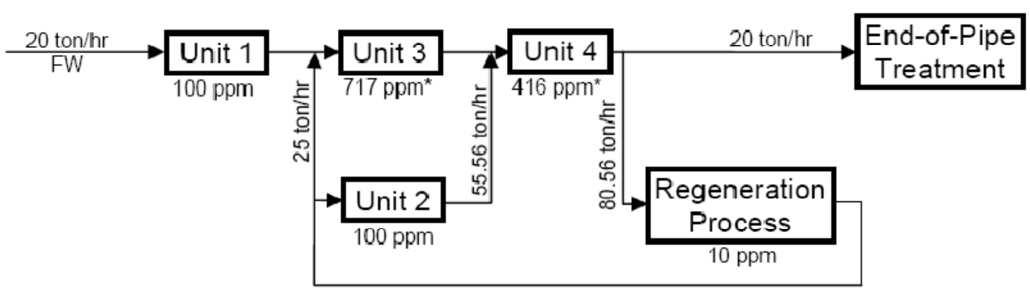

Figure 2.14 – Minimum number of connection (forbidding disconnected closed cycles) - non-linear model. (*: Concentrations lower than the maximum)

Note, that the nonlinear model renders a smaller number of connections (8 compared to 10 in the network found using the linear model) but a larger regeneration capacity (90.56 t/h compared to 55.56 t/h in the network found using the linear model).

d - Minimizing Capital cost among degenerate solutions with forbidden connections:

In this example the cost of the regeneration process is given by:

$$RegCost = 16,800\ RegCap^{0.7} \tag{2-18}$$

where $RegCap$ is the capacity of the regeneration process, which is in turn given by:

$$RegCap = \sum_{m} FUN_m \tag{2-19}$$

The capital costs of connections between the regeneration process and units, among units and between units and the end-of-pipe treatment are presented in Table 2-1. Both models (with forbidden connections) were applied over their range of reuse. Note that because the capital cost of the regeneration process is non-linear, both models need to be solved using a non-linear solver. The difference here is that in one case all outlet concentrations are fixed to be the maximum value. The solutions are presented in Figure 2.15.

Table 2-1 - Capital costs of the connections.

	Unit 1	Unit 2	Unit 3	Unit 4	Reg.	EoP treatment
FW	$30,000	$45,000	$25,000	$60,000		
Unit 1	-	$150,000	$110,000	$45,000	$145,000	$15,000
Unit 2	$50,000	-	$134,000	$40,000	$37,000	$30,000
Unit 3	$180,000	$35,000	-	$42,000	$91,000	$20,000
Unit 4	$163,000	$130,000	$90,000	-	$132,000	$34,000
Reg.	$33,000	$130,000	$50,000	$98,000	-	$45,000

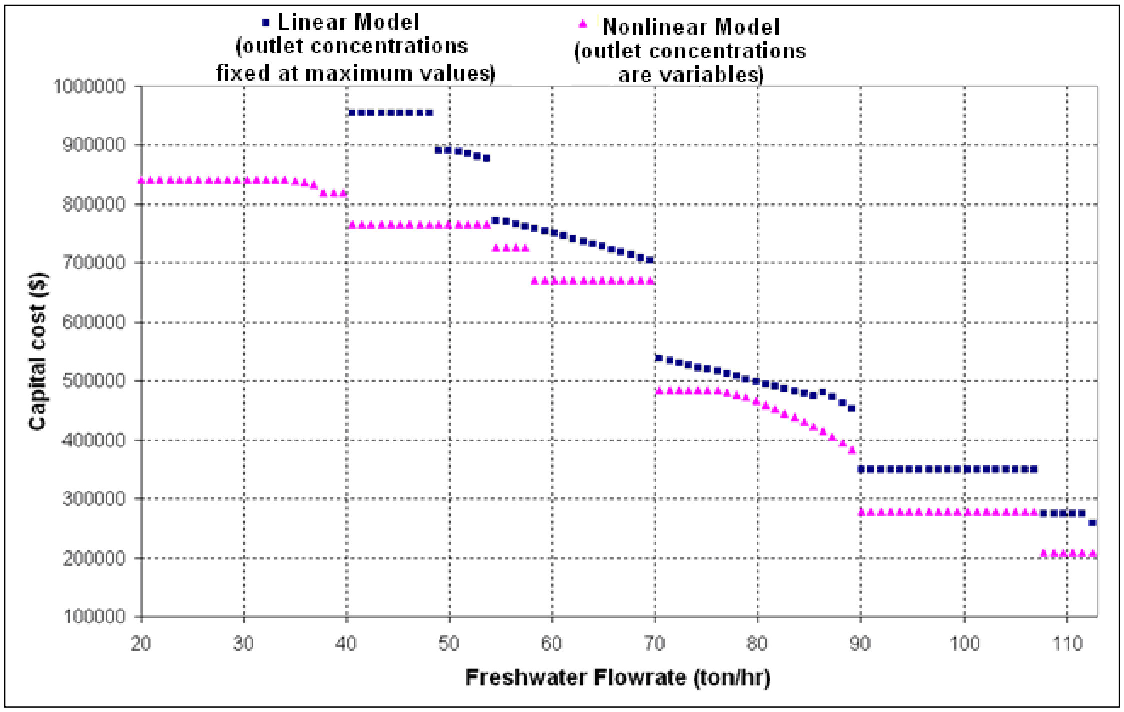

Figure 2.15 – Comparison of capital cost of networks of example 2 that operate at different freshwater consumption (forbidding disconnected closed cycles).

The solutions show that the use of maximum outlet concentration condition generates networks with higher capital costs for every freshwater flowrate inside its feasible range. Also, the linear model with forbidden connections cannot reach the same minimum freshwater consumption reached by the non-linear model.

An interesting observation here is that the nonlinear model is able to generate a network with a capital cost lower than the conventional one (network without reuse as in Figure 2.3), which is the minimum capital cost solution for the linear model. In both cases, the minimum capital cost corresponds to the network with the maximum flowrate (112.5 t/h). For this maximum flowrate, the capital cost of the network generated by the linear model is $259,000 and the one obtained by the non-linear model is $209,000. Additionally, it is worth noting the network generated by the non-linear model can operate with lower freshwater consumption. That is, the last 6 freshwater consumption points generated by the non-linear model (Figure 2.15) represent the same network, The optimum network at the last freshwater consumption point (112.5 t/h) for the linear model corresponds to the one presented in Figure 2.3 (no reuse). This network cannot operate at a freshwater consumption lower than 112.5 t/h. However, using a variable outlet concentration allows finding an optimum network at the same freshwater consumption that is not only cheaper, but also can operate at lower flowrates. This is only possible because the outlet concentrations are not set to their maximum value. This network is presented in Figure 2.16.

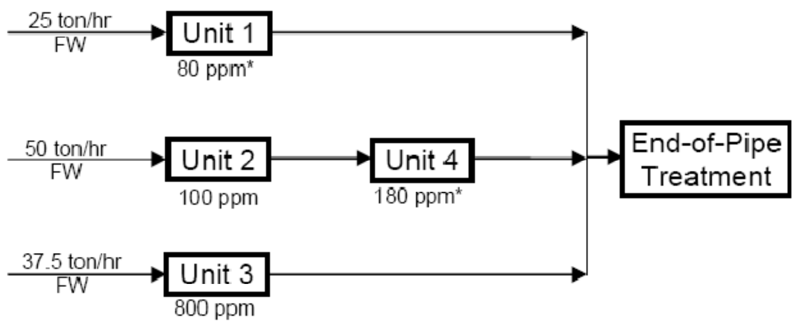

Figure 2.16 – Network with the lowest capital cost generated by the nonlinear model (*: Concentrations lower than the maximum)

Example 3

Example 3 presents the analysis of a larger scale network presented by Bagajewicz and Savelski (2001). This network has ten water-using units and the corresponding limiting data are presented in Table 2-2. Since this example was previously solved by Bagajewicz and Savelski (2001) applying the maximum outlet concentration conditions, both results are compared and discussed. It is worth noting that if the maximum outlet concentration condition is applied, one could already detect that processes 1 to 5 and 8 to 9 would need freshwater since their maximum inlet concentration is lower than the minimum outlet concentration of all processes. Using the non-linear model (outlet concentration as a variable), this conclusion cannot be made and, consequently, the feasible region is not reduced (as shown in previous example – Figure 2.7 and Figure 2.8).

The freshwater usage of the analyzed network was minimized and both models achieved 165.94 t/h as expected (Figure 2.17). This represents the same solution presented by Savelski and Bagajewicz (2000). The degenerate solutions are analyzed next.

Table 2-2 – Limiting data for example 3.

Process Number	Mass load of contaminant (kg/h)	C_{in} (ppm)	C_{out} (ppm)	Minimum freshwater flowrate (ton/h)
1	2.00	25	80	25.00
2	2.88	25	90	32.00
3	4.00	25	200	20.00
4	3.00	50	100	30.00
5	30.00	50	800	37.50
6	5.00	400	800	6.25
7	2.00	400	600	3.33
8	1.00	0	100	10.00
9	20.00	50	300	66.67
10	6.50	150	300	21.67

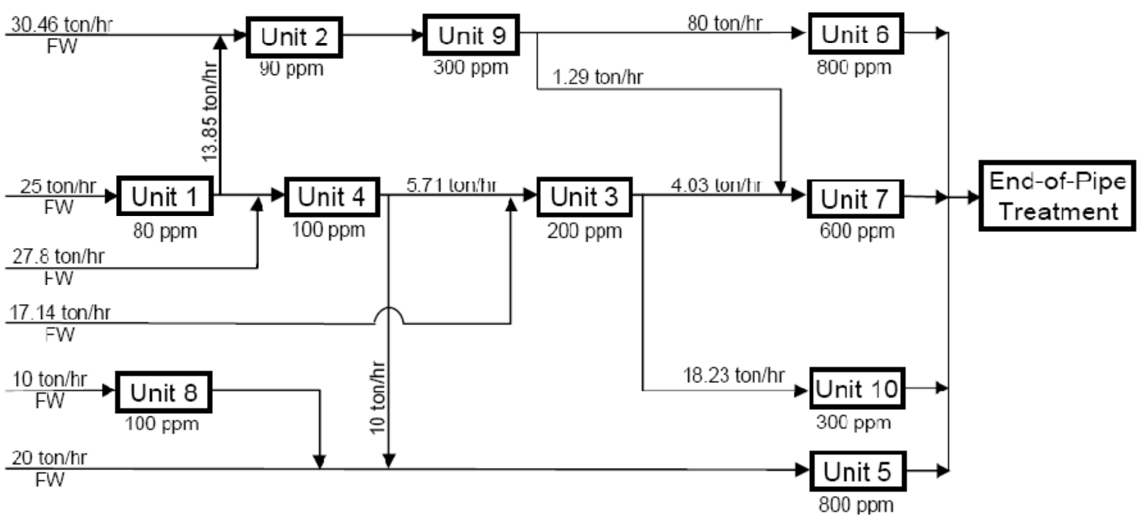

Figure 2.17 – Minimum freshwater consumption – Solution from both linear and nonlinear model.

Minimizing the number of connections among degenerate solutions:

The minimum number of connection of the network that features the minimum freshwater consumption is analyzed first. Thus, both models were run and the networks presented in Figure 2.18 and Figure 2.19 were found using the linear and non-linear model respectively. The minimum number of connections found by the linear model is 22. Conversely, the non-linear model is able to reduce this number to 21. Note that in the non-linear model (Figure 2.19) units 1, 2, 6, 7 and 10 do not reach their maximum outlet concentration.

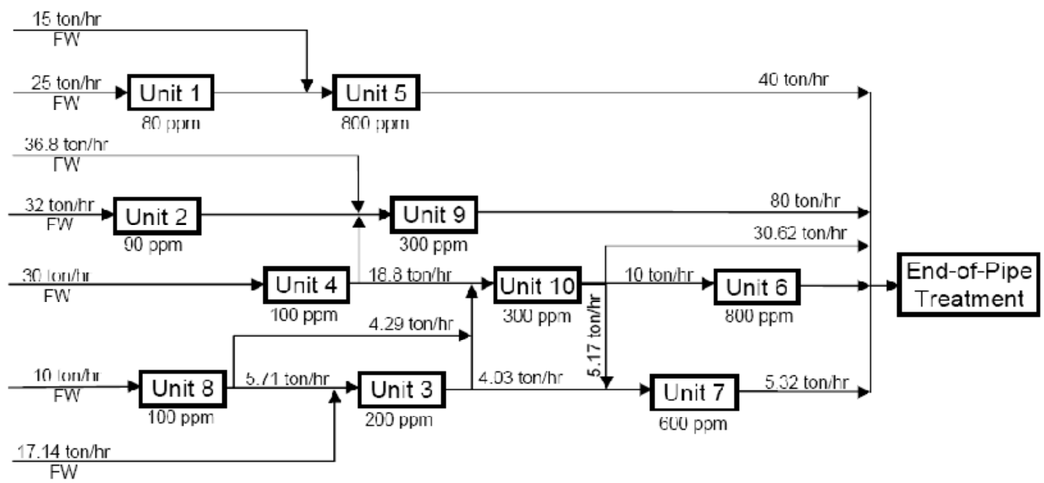

Figure 2.18 – Solution with minimum number of connections – linear model.

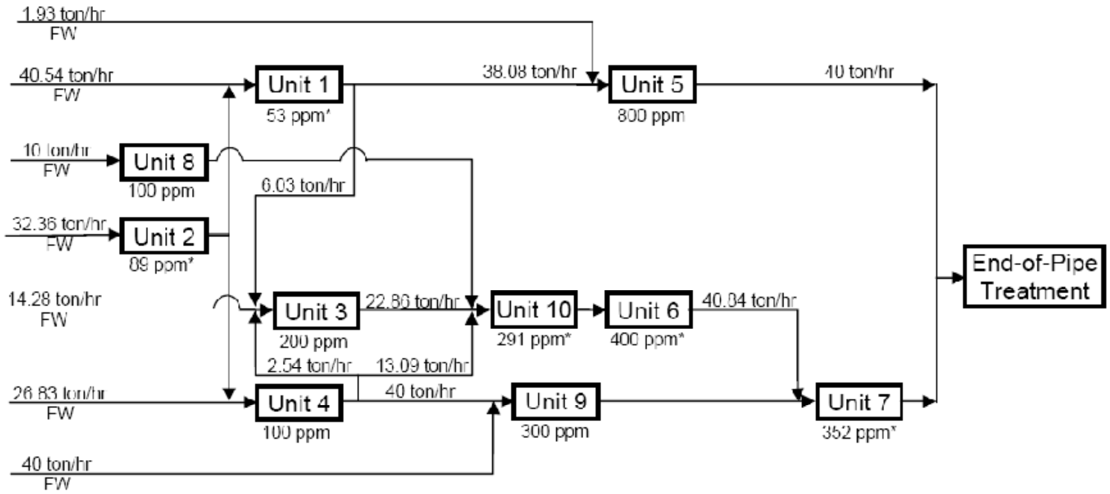

Figure 2.19 – Solution with minimum number of connections – non-linear model.
(*: Concentrations lower than the maximum)

Minimizing cost of connections among degenerate solutions:

The minimum cost of connections was also analyzed. The cost data proposed by Bagajewicz and Savelski (2001) are presented in Table 2-3. They pre-excluded some of the connections (the ones without costs associated) using the monotonicity condition proved by Savelski and Bagajewicz (2000). However, this condition may not be valid for the cases when one lets the outlet concentrations vary. In fact, the solution for the minimum number of connection previously shown (Figure 2.19) has connections that were excluded by the monotonicity conditions. To evaluate the validity of this condition on the minimization of costs and forbidden connections, the problem is solved first considering this pre-exclusion and then not considering it. The authors also excluded the costs between freshwater source and units claiming that connection from the freshwater source cannot be different from the ones gotten before (minimization of freshwater). However, as discussed in Example 1, these connections are always required only when the linear model is used. The non-linear model may not render some of these connections.

Table 2-3 – Cost of connections for example 3 ($ per year).

UNIT	1	2	3	4	5	6	7	8	9	10	WWT
1	-	2.42	2.98	3.17	3.54	3.54	3.54	-	2.98	2.79	5.42
2	-	-	2.79	2.98	3.54	3.54	3.54	-	3.17	2.98	5.42
3	-	-	-	-	2.98	3.17	3.54	-	3.54	3.54	4.67
4	-	-	2.42	-	2.79	2.98	3.54	-	3.54	3.54	4.67
5	-	-	-	-	-	-	-	-	-	-	3.92
6	-	-	-	-	-	-	-	-	-	-	3.92
7	-	-	-	-	2.98	2.79	-	-	-	-	3.92
8	-	-	3.54	-	3.17	2.98	2.42	-	2.79	2.98	3.92
9	-	-	-	-	3.54	3.54	2.98	-	-	-	4.67
10	-	-	-	-	3.54	3.54	3.17	-	-	-	4.67

The solutions obtained when the exclusion of some connections (by the monotonicity condition) is applied are presented first. The minimization of capital cost at the minimum flowrate (165.94 t/h) using the linear model gives a cost with connections of $53.16, where 22 connections are needed. This is the same solution found by Bagajewicz and Savelski (2001). The corresponding network is presented in Figure 2.20. For the nonlinear model, the minimum cost is $39.72, which is 25% lower. Note that the outlet concentrations of units 1, 2, 6, 7 and 10 did not reach their maximum outlet concentration. The network that represents the found solution, together with the outlet concentrations of the units, is presented in Figure 2.21. This solution has also 21 connections, which is the minimum obtained when the number of connections is minimized. Even when some of the connections are excluded by the monotonicity condition, the non-linear model is capable of reaching 21 connections.

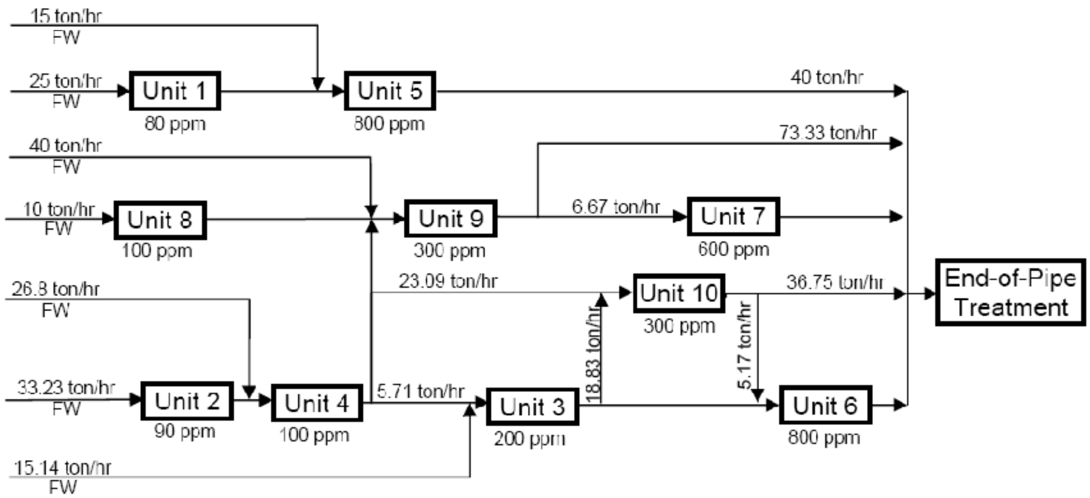

Figure 2.20 – Solution with minimum connections cost considering pre-defined connections –linear model.

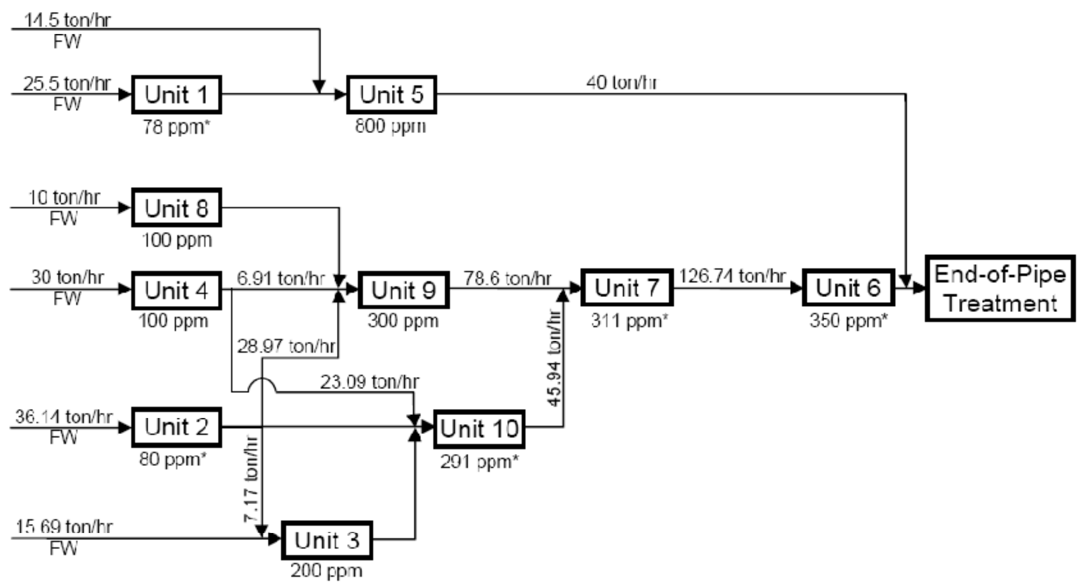

Figure 2.21 – Minimum connections cost considering pre-excluded connections – non-linear model. (*: Concentrations lower than the maximum)

Additionally, the minimum connection cost when all the possible combinations of connections are allowed is sought. To guarantee an analysis capable of only investigate the possibility of existence and not the decision due to cost, the cost of these previously excluded connections (the connections without the costs of Table 2-3) are set to zero. The solution obtained using the linear and non-linear model are presented in Figure 2.22 and

Figure 2.23 respectively. Interestingly, the linear model could now reach a lower cost of connections ($49.80) than when some connections were excluded by the monotonicity condition. This solution shows a connection from unit 8 to unit 4 that was excluded in the previous case and it substitutes the connection from unit 2 to unit 4 in the previous case. The non-linear model also reaches a lower cost ($38.40) and units 1, 6, 7 and 10 do not reach their maximum concentration.

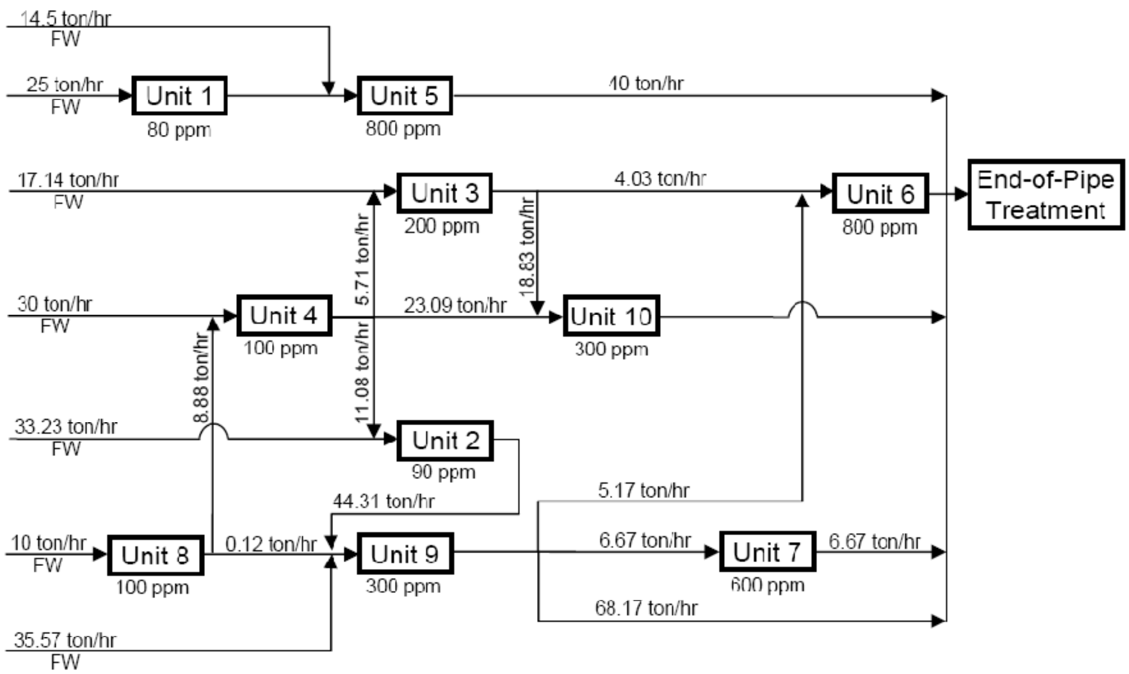

Figure 2.22 – Solution with minimum connections cost considering all possible connections –linear model.

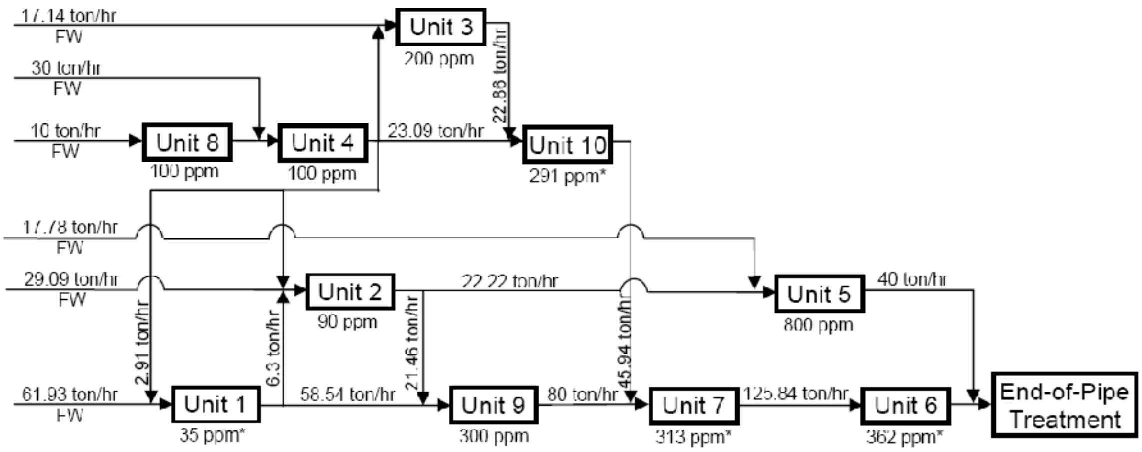

Figure 2.23 – Solution with minimum connections cost considering all possible connections –non-linear model) (*: Concentrations lower than the maximum)

Minimizing Total Annualized Cost:

Now, using the objective function presented in equation (2-14), the total annual cost is minimized. It is assumed the freshwater cost (α) is \$0.3/t and the annual discount factor (*af*) is 0.1 (over 10 years).

The linear model gives a minimum total annual cost of \$54.82 at 167.70 t/h. This solution (Figure 2.24) consumes slightly more freshwater than the minimum possible.

The minimum annual cost obtained using the non-linear model is \$53.60 for a network that consumes 166.74 ton of freshwater per hour. The found network is presented in Figure 2.25. Once again, units 1, 2, 6, 7 and 10 do not reach their maximum outlet concentration.

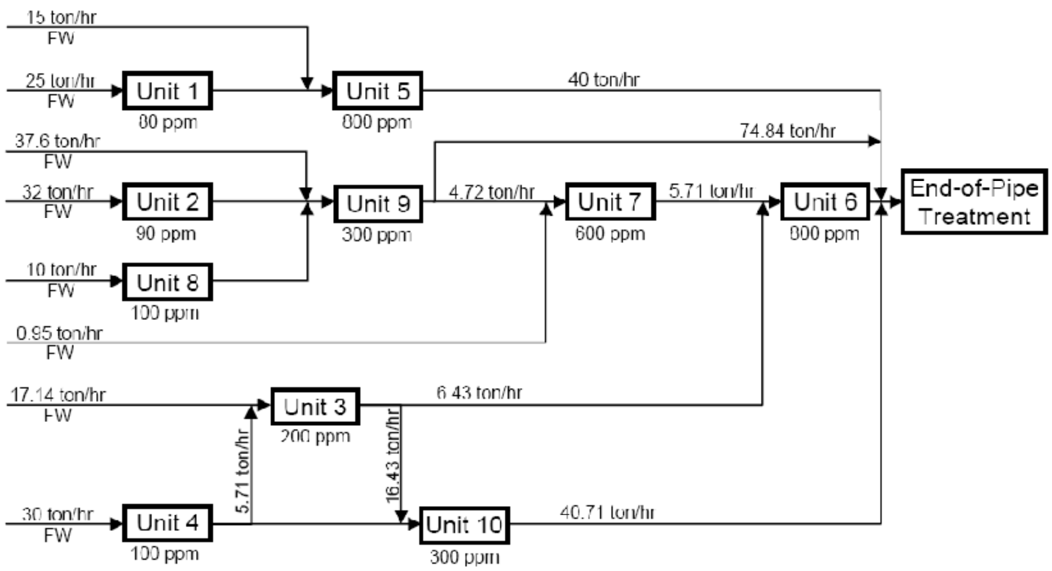

Figure 2.24 – Solution with minimum total cost considering all possible connections – linear model.

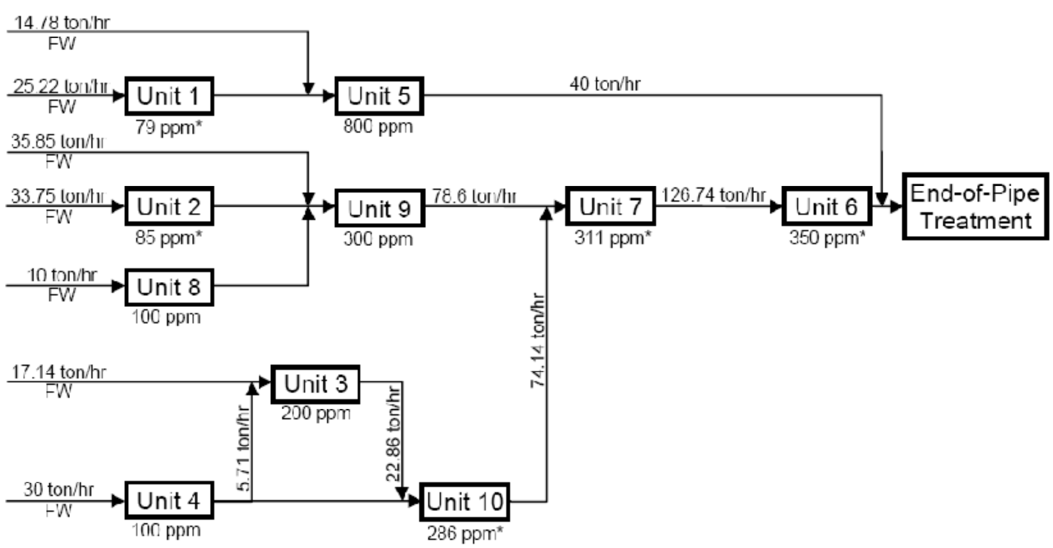

Figure 2.25 – Solution with minimum total cost considering all possible connections – non-linear model. (*: Concentrations lower than the maximum)

2.5. Conclusions

A comparative analysis of results obtained using the water allocation original MINLP model and a model that applies particular conditions to design single contaminants water networks was made. The comparison is based on the application of the optimality conditions (maximum outlet concentration and monotonicity conditions) to minimize objective functions other than minimum freshwater. The influence of structural constraints was also analyzed. Results show that in both cases these conditions should not be used.

2.6. References

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3. NETWORKS BASED ON A PROFIT-BASED OPTIMIZATION CRITERIA

In this chapter, profit-based optimization criteria are investigated and compared with the most used ones: freshwater consumption and total cost. A methodology for the grassroots design and/or retrofit of water systems using mathematical optimization to maximize Net Present Value (NPV) and/or Return of investment (ROI) is proposed. The examples show that the solutions where savings and/or profit are maximized can be different from those where freshwater is minimized. They also differ from each other when ROI or NPV are used. In addition, when the NPV objective is used, the optimum solutions also vary depending on the interest rate used to calculate the discount factor.

3.1. Overview

Consumption of water in the process industry, especially water re-use and regeneration, is a very well known and studied problem. Several review papers were recently written on the subject (Bagajewicz, 2000; Liu et al., 2004, Yoo et al, 2006), and a book (Mann and Liu; 1999). In order to design these systems, the tendency has been to minimize freshwater usage, sometimes as a true objective and sometimes as a substitute for a cost objective function using the assumption that freshwater costs is the dominant portion of the cost function.

Despite the aforementioned tendency to focus on freshwater consumption there are several articles that deal with minimizing cost objectives for grassroots design. Total annualized cost is used as the objective function by Chang and Li (2005), Guanaratnam et al. (2005), Karuppiah and Grossmann (2006), and Alva-Argáez et al. (2007).

Articles that discuss profitability objectives explicitly for grassroots design are: Zhelev (2005), Wan Alwi and Manan (2006, 2007) and Lim et al. (2006, 2007).

Zhelev (2005) uses a grid diagram analogous to Water Pinch, but targets optimum profitability. They applied the method for an energy recovery project and examples on water network systems are not explored. In the case study they analyze three options that generates the same energy saving and then they seek for the most profitable one.

Wan Alwi and Manan (2006) search for a cost-effective grassroots design of water networks involving a single contaminant. Their method is applied both for municipal and industrial sites and is not based on mathematical optimization. Instead, they suggest a hierarchical procedure in which a sequence of proprietary water management steps is established: after a payback limit is set, several water network options are investigated. In this sequential procedure, the maximum water recovery of each option is determined and the plot of investment vs. annual savings is generated. If the total payback period does not agree with the one previously set, some processes can be replaced in order to achieve the desired payback period. Wan Alwi et al. (2007) extend their previously presented hierarchical method to account for other steps of the hierarchy, which includes process changes.

Lim et al. (2006) consider an economic evaluation of a freshwater consumption-optimized water network. They analyze the profitability of the optimized network having the conventional water network as a baselined and applying incremental costs and benefits to rearrange the given network to a more operational friendly one. No regeneration processes are considered. Some insights of major contributors to the costs and benefits are presented. However, these findings cannot be necessarily generalized since they are based on a specific case example. In a second paper, Lim et at. (2007), the optimized water network is found directly by optimizing the net present value (NPV) using an NLP model (using MINOS). The formulation of the NPV equation is based on the principal contributors of the incremental costs and benefits found in their previous work. The addition of regeneration processes is not considered either and a maximum allowed flowrate is imposed for each water-using unit. Their results confirm that a network obtained minimizing costs or freshwater consumption is not necessarily the most profitable one.

In turn, retrofit projects for water systems are motivated by the need for capacity increase, product quality improvement, environmental regulations, among others. In particular, one of the important issues concerning retrofit projects of water/wastewater systems are new environmental targets. Sometimes, there are economic incentives that come from cost reductions. While performing a retrofit to meet environmental targets could be mandated, retrofits to reduce freshwater costs as well as water treatment costs are not. In the latter case, profit drives the decision making. Setting aside the need to approach the retrofit problem trying to meet environmental targets or maximize savings, the cost and finances management point of view (maximum profit) is still very important in any industrial competitive environment.

In retrofit projects there is the same need for profitable alternatives. A cost effective retrofit project looking at reducing the environmental impact should have a precise description of the plant, be realizable in practice and the pollution impact should be fully defined in practical terms (Nourai et al., 2001). Even if the physical features are very well defined, relatively precise cost estimation is still primordial to reach the best retrofit alternative. This important implication is discussed in detail by Taal et al. (2003), who conclude that the use of complex methods does not guarantee the success of a retrofit design if reliable cost estimation is not available.

Bagajewicz et al. (2000) proposed a retrofit method that minimizes total cost (including cost with freshwater, capital cost and pumping cost) using mathematical programming. Later, Tan and Manan (2004) adapted the mass exchangers networks retrofit methodology presented by Fraser and Hallale (2000). This is a systematic methodology in which the targets are obtained before the network is designed. However, the targeting step involves uses water pinch analysis to obtain a grassroots design. The retrofit is then proposed by comparing the existing network and the suggestions inferred by the targeting technique. The design rules applied follows the ones presented by Wang and Smith (1994) for a single contaminant. Later, Tan and Manan (2006) presented another systematic methodology for the retrofit of single contaminant water networks through the optimization of existing regeneration units. The methodology is based on pinch analysis and the addition of new regeneration processes is not allowed. As the majority of graphical methods, the procedure consists of two stages, with a targeting step followed by the network design step. The problem is solved maximizing savings in operating cost under certain limits on minimum payback period and/or maximum capital expenditure. Tan et al. (2007) extended their approach to consider the optimum capacity and/or outlet concentration of the regeneration process as targets. This is also done using a two step technique (targeting and design) based on pinch analysis. The procedure assumes both mass transfer and non mass transfer based water-using units, a single contaminant network and only one type of regeneration.

Finally, Hul et al. (2007) presented LP and MILP models to handle the retrofit of water networks where only source-sink type units are considered (fixed flowrates and outlet concentrations). Their approach evaluates different criteria in the optimization of water networks: Maximum water recovery with and without investment limits; wastewater reduction targets; processes constraint as forbidden connections; and, the combination of these criteria. The model cannot be applied for mass transfer type of water using units. To handle their combined objective they use fuzzy optimization.

Although successful methodologies have been presented by previous work, there is a lack of a methodology that can provide alternative designs so one can analyze them in a more comprehensive and profit related way and have a better understanding of the opportunities of each option as well as their costs and benefits.

This chapter is an extension of the methodology presented by Faria and Bagajewicz (2006), which presents a procedure for the grassroots design and retrofit of single and multi-components water networks using cost, consumption and profitability as objectives. In both cases, the addition of regeneration processes is allowed.

3.2. Problem Statement

To define the problem, definitions that are similar to those used in previous work and presented in chapters 2 are applied.

Grassroots: Given a set of process systems in need of water for washing *operations, a set of freshwater sources of different pollutants concentration and, a set of potential regeneration processes to be installed, it is desired to determine what freshwater use is needed in each process, what water reusing connections are needed and what capacity of regeneration processes (if any) is needed to maximize profit or minimize cost.*

It is assumed that any regeneration process has a fixed outlet concentration of at least one contaminant (sometimes a maximum capacity limitation for this process is added). This is particularly true for certain operations, like the removal of solids. Additionally, capital for investment may be limited.

<u>*Retrofit:*</u> *Given an existing water network (water-using units, freshwater sources, regeneration processes and end-of-pipe treatment), a set of new processes in need of water for washing operations to be added (if any), a set of required capacity expansions of existing processes, a set of regeneration processes that are available for installation (if needed) and, new freshwater sources available, it is desired to determine what re-piping and what capacity of a new treatment process (if any) is needed to maximize targets (profit or savings).*

Maximum inlet and outlet concentrations as well as fixed mass loads of the water-using units and freshwater concentrations are used. The economic parameters include the cost of freshwater, operational costs of the end-of-pipe treatment and the regeneration process, the capital cost of the new potential connections and the new potential regeneration processes.

3.3. Mathematical Model

The constraints of the mathematical model for both grassroots design and retrofit of water networks with multiple contaminants are the following WAP standard ones:

Balance of water in the units:

$$\sum_{w\in W} FW_{w,m*} + \sum_{r\in R} FNU_{r,m*} + \sum_{m\neq m*\in M} FUU_{m,m*} = \\ = \sum_{r\in R} FUN_{m*,r} + FS_{m*} + \sum_{m\neq m*;m\in M} FUU_{m*,m} \quad \forall m* \in M \tag{3-1}$$

Balance of water in treatment/regeneration processes:

$$\sum_{m\in M} FUN_{m,r*} + \sum_{r\neq r*;r\in R} FNN_{r,r*} = FNS_{r*} + \sum_{m\in M} FNU_{m,r*} + \sum_{r\neq r*;r\in R} FNN_{r*,r} \quad \forall r* \in R \tag{3-2}$$

Balance of contaminant in the units:

$$\sum_{w\in W} FW_{w,m*} * C_{w,j} + \sum_{r\in R} FNU_{r,m*} * CR^{out}_{r,j} + \sum_{m\neq m*;m\in R} FUU_{m,m*} * C^{out}_{m,j} + \Delta m_{m*,j} = \\ \left(\sum_{r\in R} FUN_{m*,r} + FS_{m*} + \sum_{m\neq m*;m\in M} FUU_{m*,m} \right) * C^{out}_{m*,j} \quad \forall m* \in M, \forall j \in J \tag{3-3}$$

Limit of inlet concentration of contaminants in the units:

$$\sum_{w\in W} FW_{w,m*} * C_{w,j} + \sum_{r\in R} FNU_{r,m*} * CR^{out}_{r,j} + \sum_{m\neq m*;m\in M} FUU_{m,m*} * C^{out}_{m,j} \leq \\ \left(\sum_{r\in R} FUN_{m*,r} + FS_{m*} + \sum_{m\neq m*;m\in M} FUU_{m*,m} \right) * C^{\max,in}_{m*,j} \quad \forall m* \in M, \forall j \in J \tag{3-4}$$

Limit of outlet concentration of contaminants in the units:

$$C^{out}_{m*,j} \leq C^{\max,out}_{m*,j} \quad \forall m* \in M, \forall j \in J \tag{3-5}$$

Balance of contaminants in treatment/regeneration processes: A material balance at the inlet of the regeneration process is needed to identify the outlet concentrations of the contaminants that are not being treated by the respective regeneration process. Additionally, an equation using a connective binary parameter $XNC_{r,j}$ equal to one if treatment/regeneration process r treats contaminant j; and, 0 otherwise, is necessary to establish what is the outlet concentration of that particular contaminant.

$$\sum_{m\in M} FUN_{m,r^*} * C_{m,j}^{out} + \sum_{r\neq r^*; r\in R} FNN_{r,r^*} * CR_{r^*,j}^{out} = CR_{r^*,j}^{in} * \left(\sum_{m\in M} FUN_{m,r^*} + \sum_{r\neq r^*; r\in R} FNN_{r,r^*} \right) \quad \forall r^* \in R, \forall j \in J \tag{3-6}$$

$$CR_{r,j}^{out} = CR_{m,j}^{in} * \left(1 - XNC_{r,j}\right) + CR_{m,j}^{fixed} * XNC_{r,j} \qquad \forall r \in R, \forall j \in J \tag{3-7}$$

Existence of new connections: Binary variables (*Y)* are used to determine if a new connection is established and the following classical "big M" constraints are used to count the capital cost of the new connections.

$$FW_{w,m} \le U_{WU}^{(w,m)} * YWU_{w,m} \quad \forall w \in W, \forall m \in M \tag{3-8}$$

$$FUN_{m,r} \le U_{UN}^{(m,r)} * YUN_{m,} \quad \forall m \in M, \ \forall r \in R \tag{3-9}$$

$$FNU_{r,m} \le U_{NU}^{(r,u)} * YNU_{r,m} \quad \forall m \in M, \ \forall r \in R \tag{3-10}$$

$$FUU_{m^*,m} \le U_{UU}^{(m^*,m)} * YUU_{m^*,m} \quad \forall m^* \in M, \forall m \in M \tag{3-11}$$

$$FNN_{r^*,r} \le U_{NN}^{(r^*,r)} * YNN_{r^*,r} \quad \forall r^* \in R, \forall r \in R \tag{3-12}$$

$$FS_m \le U_{MS}^{(m)} * YMS_m \quad \forall m \in M \tag{3-13}$$

$$FNS_r \le U_{NS}^{(r)} * YNS \quad \forall r \in R \tag{3-14}$$

When connections already exist the binary variables are set to one and the respective capital cost set to zero.

Treatment/Regeneration Capacity: The flowrate through the treatment/regeneration unit is limited by the unit capacity:

$$\sum_{m \in M} FUN_{m,r^*} + \sum_{r \neq r^*; r \in R} FNN_{r,r^*} \leq RegCap_{r^*} \quad \forall r^* \in R \tag{3-15}$$

As in the case of existing connections, the capacities of an existing treatment/regeneration processes are set and the capital cost parameters are zero. For the cases in which the new regeneration processes can be added, the regeneration capacity ($RegCap_r$) is in some instances treated as a variable (design mode) or as a parameter (evaluation mode), as described below.

Objective Functions:

The case of retrofit is considered because it is more general and then how the objectives can be derived to the grassroots case is shown. Let FW^{old} be the existing system freshwater consumption, which is a fixed value and assume that operating costs are direct function of flowrates (freshwater and regenerated flowrate); then, the following objective function maximizes net savings:

$$Max \left[\left(\begin{array}{l} \sum_{w \in W} \left(FW_w^{old} - \sum_{m \in M} FW_{w,m} \right) * \alpha_w \\ \quad + \sum_{r \in R_{ex}} OPN_r^{old} * \left(\sum_{m \in M_{ex}} FUN_{m,r}^{old} + \sum_{r^* \in R_{ex}} FNN_{r^*,r}^{old} \right) \\ \quad - \sum_{r \in R_{new}} OPN_r^{new} * \left(\sum_{m \in M_{new}} FUN_{m,r} + \sum_{r^* \in R_{new}} FNN_{r^*,r} \right) \end{array} \right) * OP - FCI * af \right] \tag{3-16}$$

In the case of grassroots design, we have $FW^{old}=0$, $FNN_{r^*,r}^{old} = 0$ *and* $FUN_{m,r}^{old} = 0$, which makes the problem one of minimizing costs.

The first part of the equation represents the savings obtained from freshwater and end-of-pipe treatment flowrate reduction. In this expression, FW_m and α are the flowrate and cost of freshwater, respectively. The model can be extended to make these costs function of inlet concentrations of pollutants. The next term is devoted to regeneration costs, where OPN_r^{new} *a*nd OPN_r^{old} are the operating cost of the regeneration processes (new and old), $FUN_{m,r}$ are the flowrates between the water-using units and the regeneration process r and $FNN_{r*,r}$ are the flowrates between two regeneration processes. Finally, OP represents the hours of operation per year. The last term is the annualized capital cost invested in the retrofit, where FCI is the fixed capital cost and af is any factor that annualizes the capital cost (usually $1/N$, where N is the number of years of depreciation). The fixed capital of investment is calculated using the sum of the piping costs and the new regeneration units costs as follows:

$$FCI = \sum_{m \in M} \left(\begin{array}{l} \sum_{w \in W} YWU_{w,m} * ICWU_{w,m} + \sum_{r \in R} \left(YUN_{m,r} * ICUN_{m,r} + YNU_m * ICNU_m \right) \\ + \sum_{m^* \neq m, m^* \in M} YUU_{m,m^*} * ICUU_{m,m^*} + YUS_m * ICUS_m \end{array} \right)$$
$$+ \sum_{r \in R} \left(\sum_{r^* \neq r; r^* \in R} YNN_{r,r^*} * ICNN_{r,r^*} + YNS_r * ICNS_r + ICN_r * \left(RegCap_r \right)^{0.7} + YNS_r * ICNS_r \right) \quad (3\text{-}17)$$

The first term represents the capital costs with connections between the regeneration process and water-using units, and the capital cost associated to connections between two water-using units and end-of-pipe treatment. The second term corresponds to the capital costs of the connections between two new regeneration processes, between the new regeneration processes and the end-of-pipe treatment and the capital cost of the new regeneration treatments. The cost of the regeneration units is assumed to be a function of the regeneration process capacity only.

Note that for the retrofit case and a single source of water, when there is no capital investment to depreciate (*af*=0), OPN_{FT}^{old} = OPN_{FT}^{new} (unchanged end of pipe treatment) and no regeneration is used, then equation (3-16) reduces to minimizing freshwater consumption. However, even if the end-of-pipe treatment cost does not change, when regeneration is present, even if $OPN_r^{new} = OPN_r^{old}$ the objective is not equivalent to minimizing freshwater consumption. Indeed, under these conditions, equation (3-16) becomes:

$$Min\left[\left(\sum_{w\in W}\sum_{m\in M} FW_{w,m} * \alpha_w + \sum_{r\in R_{new}} OPN_r^{old} * \left(\sum_{m\in M_{new}} FUN_{m,r} + \sum_{r^*\in R_{new}} FNN_{r^*,r}\right)\right)\right] \qquad (3\text{-}18)$$

which can be rewritten as follows when water from the final treatment is not recycled but entirely disposed of (the usual assumption in many methods):

$$Min\left[\left(\begin{array}{l}\displaystyle\sum_{w\in W}\sum_{m\in M} FW_{w,m} * (\alpha_w + OPN_{FT}^{old}) \\ \displaystyle\quad + \sum_{r\in R_{new};r\neq FT} OPN_r^{old} * \left(\sum_{m\in M_{new}} FUN_{m,r} + \sum_{r^*\in R_{new}} FNN_{r^*,r}\right)\end{array}\right)\right] \qquad (3\text{-}19)$$

This last expression cannot be argued to be equivalent to minimizing freshwater consumption. The reason stems from the costing, which in this expression is not tied to the amount of pollutant removal, but to flows. In other words, if the operating costs would be only the cost of chemicals needed to remove the pollutants, then this would be a fixed amount because the amount of pollutants to remove in the whole network is fixed. However, even if the same amount of chemicals is used, the treatment units may receive water at different concentrations, and therefore require to manipulate larger or smaller flows. The operating cost related to moving fluids, which is what is assumed here, can therefore vary. This invalidates arguments that freshwater consumption minimization is a valid economic goal when regeneration is used.

An alternative objective function for retrofit is the Net Present Value (*NPV*)

$$Max\left[\left(\begin{array}{l}\sum_{w\in W}\left(FW_w^{old}-\sum_{m\in M}FW_{w,m}\right)*\alpha_w\\ \quad+\sum_{r\in R_{ex}}OPN_r^{old}*\left(\sum_{m\in M_{ex}}FUN_{m,r}^{old}+\sum_{r^*\in R_{ex}}FNN_{r^*,r}^{old}\right)\\ \quad-\sum_{r\in R_{new}}OPN_r^{new}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\end{array}\right)*OP*df-FCI\right] \tag{3-20}$$

where the discount factor *df* is the sum over *N* years of the different discount factors, that is:

$$df=\sum_{n=1}^{N}\frac{1}{(1+i)^n} \tag{3-21}$$

Finally, the return of investment (ROI) for retrofit is given by:

$$Max\ \frac{\left(\begin{array}{l}\sum_{w\in W}\left(FW_w^{old}-\sum_{m\in M}FW_{w,m}\right)*\alpha_w\\ \quad+\sum_{r\in R_{ex}}OPN_r^{old}*\left(\sum_{m\in M_{ex}}FUN_{m,r}^{old}+\sum_{r^*\in R_{ex}}FNN_{r^*,r}^{old}\right)\\ \quad-\sum_{r\in R_{new}}OPN_r^{new}*\left(\sum_{m\in M_{new}}FUN_{m,r}+\sum_{r^*\in R_{new}}FNN_{r^*,r}\right)\end{array}\right)*OP}{FCI} \tag{3-22}$$

In the case of grassroots design $FW_w^{old}=0,\ FNN_{r^*,r}^{old}=0\ and\ FUN_{m,r}^{old}=0$, which in the case of equation (3-20), makes the problem one of minimizing the net present costs

(NPC). In the case of ROI, equation (3-22) turns into a minimization of operating costs per unit capital invested. One would not use ROI in a grassroots context because there is no profit to talk about, and therefore equation (3-22) leads to such an unusual concept. Thus, for grassroots design, ROI is redefined with respect to a reference network and it is here named *return on extra investment* (ROEI). More details about ROEI will be presented together with the examples.

3.4. Solution Methodology

The methodology consists of maximizing Net Savings first (Equation 3-16) subject to the set of constraints given by Equations 3-1 to 3-15 and then calculating *NPV* (Equation 3-20) and *ROI* (Equation 3-22). To do this, the range of feasible freshwater consumption is determined first. This range is defined as the interval from the minimum possible freshwater consumption of the network to its maximum freshwater consumption, which is considered to be the consumption under no reuse conditions (conventional network). The freshwater consumption under no reuse conditions, which is the maximum value of the range, considers that the water using units are operating under their minimum flowrate. The minimum consumption is obtained minimizing the freshwater consumption using the same model as above (equations (3-1) through (3-15) and the following objective:

$$Min \sum_{w \in W} \sum_{m \in M} FW_{w,m} \tag{3-23}$$

In turn, the maximum freshwater consumption is given by the consumption of a conventional network in which all the water-using units are fed by freshwater and operate at their minimum freshwater consumption (FW^{old} for the retrofit case, which is the flowrate of the existing network).

Subsequently, when savings (Equation 3-16) are maximized for fixed freshwater consumption inside the aforementioned range, the respective capital investments (Equation 3-17) are calculated and the corresponding *NPV* (Equation 3-20) and *ROI* (Equation 3-22) are obtained. When plotting these results (Savings, FCI, NPV or ROI vs. Freshwater flowrate), different points correspond to different networks and also different capacities of the new regeneration process (if any) are found. Once the networks are identified, they are ranked according to different criteria. Finally, incremental analysis is performed.

The following results are obtained using the MINLP formulation previously presented, which was solved using DICOPT (CONOPT/CPLEX) as the solver in the GAMS platform.

3.5. Illustrations

Example 1: Single Contaminant Case

The following one component example was adapted from Example 1 of Wang and Smith (1994). The limiting process data for this problem are shown in Table 3-1 and it has a freshwater consumption without reuse (conventional network configuration) of 112.5 t/h.

The cost of freshwater is $\alpha_i(\$/t)$=0.3 and the system operates *OP(h/year)*=8600. The freshwater concentration was assumed to be equal to zero. The end-of-pipe treatment has an operating cost $OPN_r(\$/t)=1.0067$ and an investment cost $ICN_r(\$/t^{0.7})=19{,}400$.

Table 3-1 – Limiting process water data.

Process Number	Mass load of contaminant	C_{in}(ppm)	C_{out}(ppm)
1	2 kg/h	0	100
2	5 kg/h	50	100
3	30 kg/h	50	800
4	4 kg/h	400	800

A potential new regeneration process is available for the grassroots design and the retrofit case. Its capital cost is $ICN(\$/t^{0.7}) = 16{,}800$ and the operating cost is assumed to be $OCN(\$/t) = 1.00$. Only one regeneration unit with outlet concentration of 10ppm is considered. Finally, in the profitability analysis a 10 years period (*af* = 0.1) is used.

Grassroots design case:

The costs of connections for the superstructure of this network are presented in Table 3-2. Other cost data were presented above.

The feasible range of freshwater usage of this system is determined to be between the minimum freshwater consumption (20 t/h) and the consumption required by a network with no reuse (112.5 t/h). Figure 3.1 gives the optimum annualized total cost profile obtained when it is minimized (Equation 3-16) through the range of freshwater usage. This MINLP problem has 59 constraints, 38 continuous variables and 29 binary variables.

Table 3-2 – Capital costs of the connections.

	Unit 1	Unit 2	Unit 3	Unit 4	Reg.	End of pipe treatment
FW	\$39,000	\$76,000	\$47,000	\$92,000	-	-
Unit 1	-	\$150,000	\$110,000	\$45,000	\$145,000	\$83,000
Unit 2	\$50,000	-	\$134,000	\$40,000	\$37,000	\$102,500
Unit 3	\$180,000	\$35,000	-	\$42,000	\$91,000	\$98,000
Unit 4	\$163,000	\$130,000	\$90,000	-	\$132,000	\$124,000
Reg.	\$33,000	\$130,000	\$50,000	\$98,000	-	\$45,000

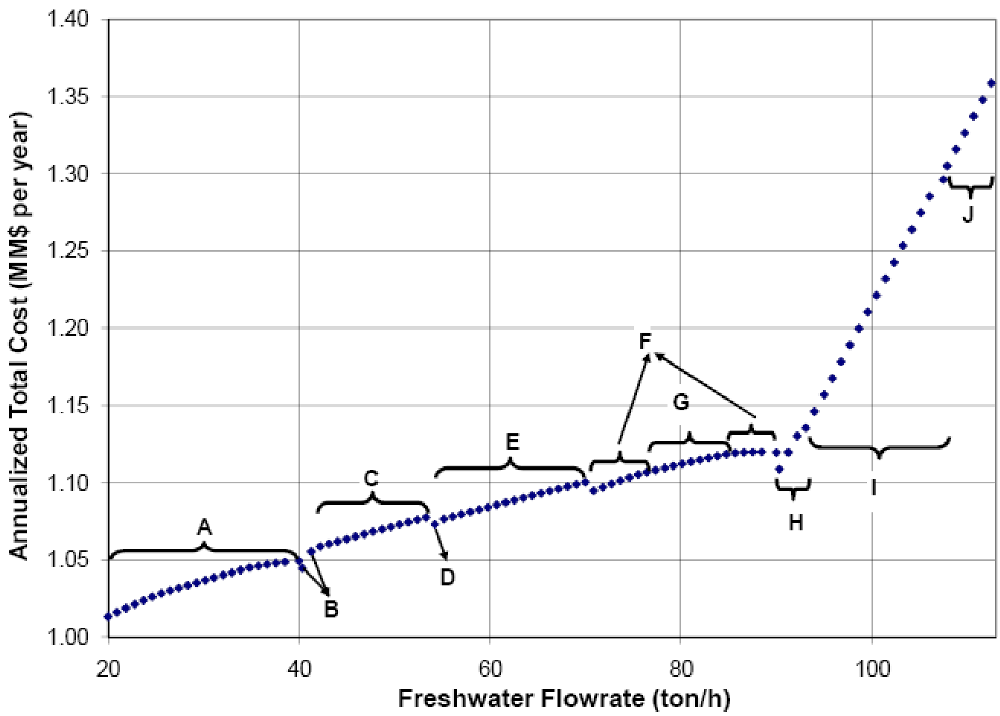


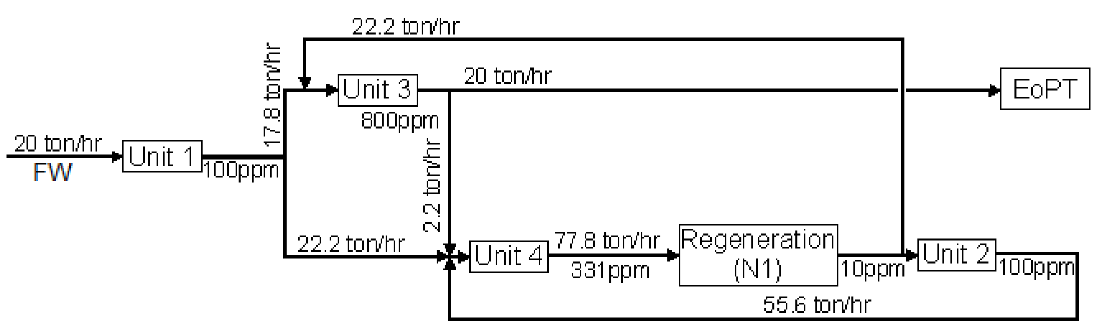
Figure 3.1 – Annualized total cost as a function of Freshwater flowrate for the grassroots design.

Ten different networks were found as optimum as a function of freshwater consumptions as shown by those profiles. The networks are summarized in Table 3-3, by indicating their connections and the minimum freshwater consumption they can reach. Network A represents the optimum solution when annualized total cost is minimized. For this case, it also represents a network that is able to reach the minimum consumption. Figure 3.2 shows networks A, B, H and I because they will become relevant in the discussion that follows. Network B exhibits one interesting feature: it is disconnected and exhibits a loop involving two units and a regeneration without discharge. Usually, because of possible build up of undesired contaminants, one would tend to disregard such a network. For the sake of completeness, it can be considered acceptable, assuming that all these other contaminants are somehow taken care of in the regeneration unit.

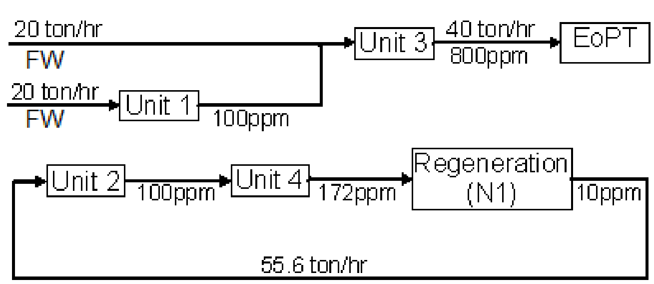
Table 3-3 – Networks for grassroots design (reuse of end-of-pipe wastewater not allowed)

Network	Connections	Min consumption
A	W-U1, U1-U3, U1-U4, U2-U4, U3-U4, N1-U2, N1-U3, U3-EoPT, U4-N1, EoPT-S	20 t/h
B	W-U1, W-U3, U1-U3, U2-U4, N1-U2, U3-EoPT, U4-N1, EoPT-S	40 t/h
C	W-U1, W-U2, W-U3, U1-U3, U2-U4, U3-U4, N1-U2, U4-N1, U4-EoPT, EoPT-S	40 t/h
D	W-U1, W-U2, W-U3, U1-U3, U2-U4, N1-U2, U3-N1, U4-EoPT, EoPT-S	54 t/h
E	W-U1, W-U2, W-U3, U1-U3, U2-U4, U3-U4, N1-U2, U3-N1, U4-EoPT, EoPT-S	54 t/h
F	W-U1, W-U2, U1-U3, U1-U4, U2-U4, N1-U3, U2-N1, U3-EoPT, U4-EoPT, EoPT-S	70 t/h
G	W-U1, W-U2, W-U3, U1-U3, U1-U4, U2-U4, N1-U3, U2-N1, U3-EoPT, U4-EoPT, EoPT-S	70 t/h
H	W-U1, W-U2, U1-U3, U2-U4, U3-EoPT, U4-EoPT, EoPT-S	90 t/h
I	W-U1, W-U2, U1-U3, U2-U4, U3-U4, U4-EoPT, EoPT-S	92.5 t/h
J	W-U1, W-U2,W-U3, U1-U4, U2-U4, U3-U4, U4-EoPT, EoPT-S	107.5 t/h

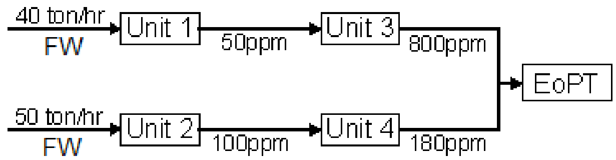
Abbreviations: W: freshwater, Ui: Unit *i*, N1: Treatment/Regeneration unit 1, EoPT: End of Pipe treatment, S: sink



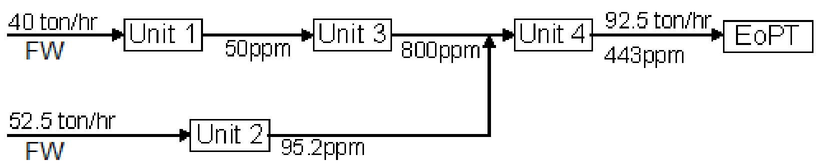
(a) Network A



(b) Network B



(c) Network H



(d) Network I

Figure 3.2 – Selected networks from Table 3.

If freshwater consumption is not a primordial issue (i.e. when freshwater is largely available and is cheap) and/or there are limitations in the investments, one may want to analyze this graph together with the FCI graph. Figure 3.3 shows the fixed capital cost profiles of the networks presented in Figure 3.1 along the range of freshwater usage. Although the costs of connections are constant for each network, the capital cost of the regeneration process and the end-of-pipe treatment vary. In fact as one increases the other decreases (Figure 3.4). From the FCI graph we can note that network C is the one in which the highest investment cost is required. If budget is an important issue for the project, network C may become an unattractive option. The effects of budgets limitations will be further discussed later.

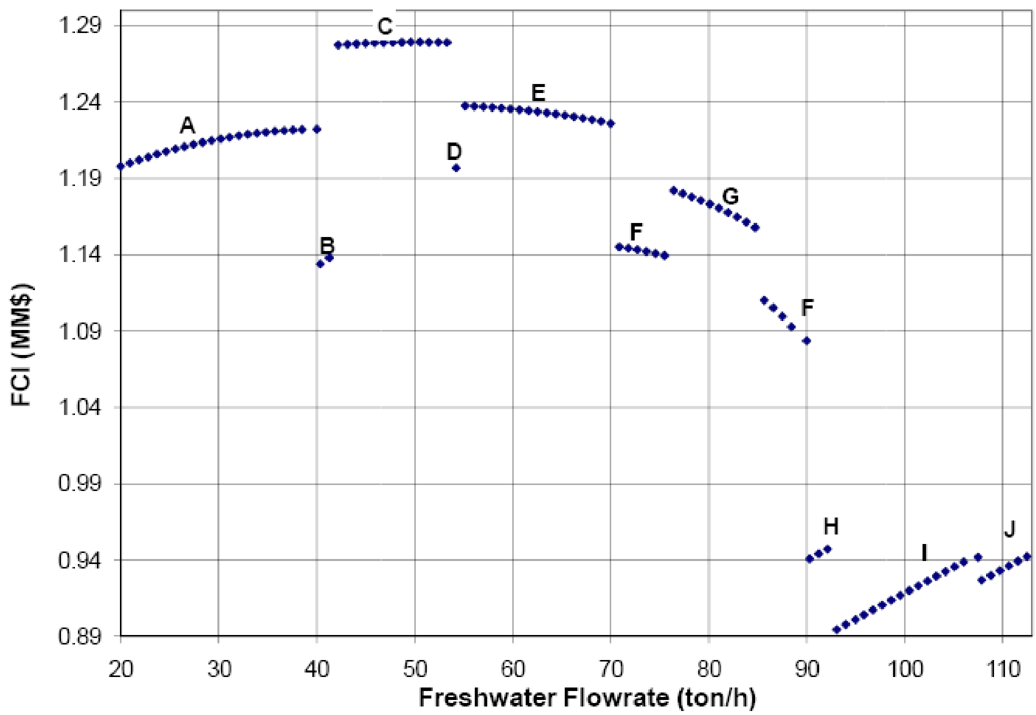


Figure 3.3 – FCI as a function of Freshwater flowrate grassroots design.

The same solutions are obtained when the NPC (Equation 20) is directly optimized (Figure 3.5). Variation on the rate of discount points at different optimal networks. The difference between the minimum and maximum NPC when a 5% rate of discount is used is around MM$2.6. When a 20% rate of discount is used, this difference reduces to approximately MM$1.3. Although larger discount rates are unlikely, their effects are investigated to analyze if the optimal solution might change (Figure 3.6) and it does in favor of solutions with lower FCI as one might expect.

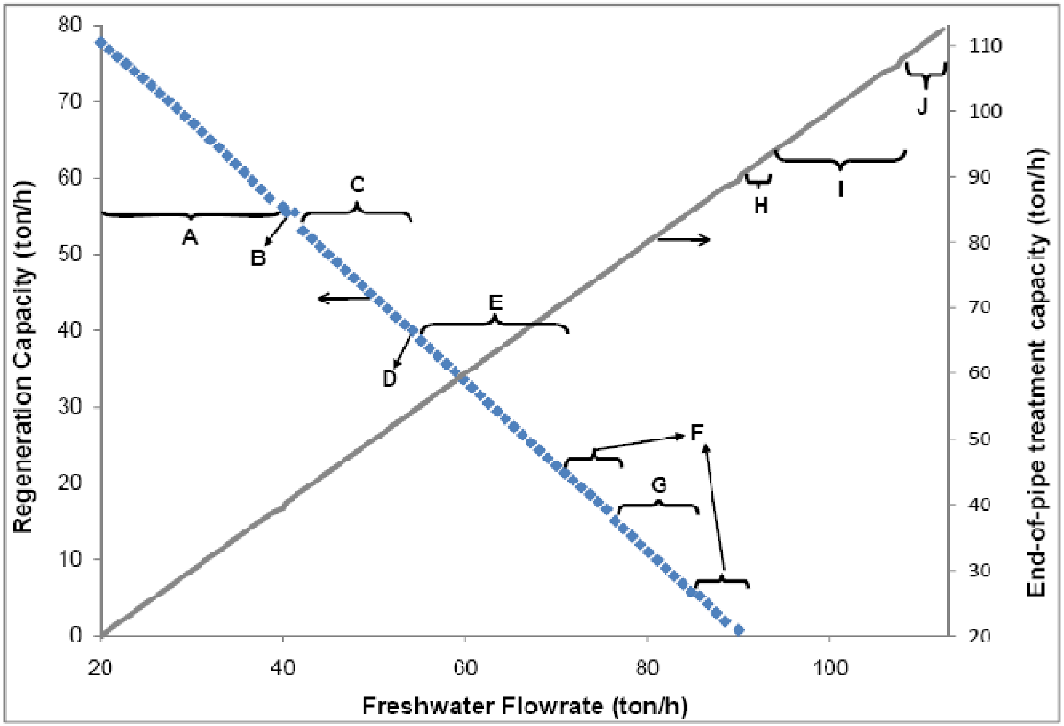


Figure 3.4 – Regeneration and end-of-pipe treatment capacities as a function of freshwater consumption.

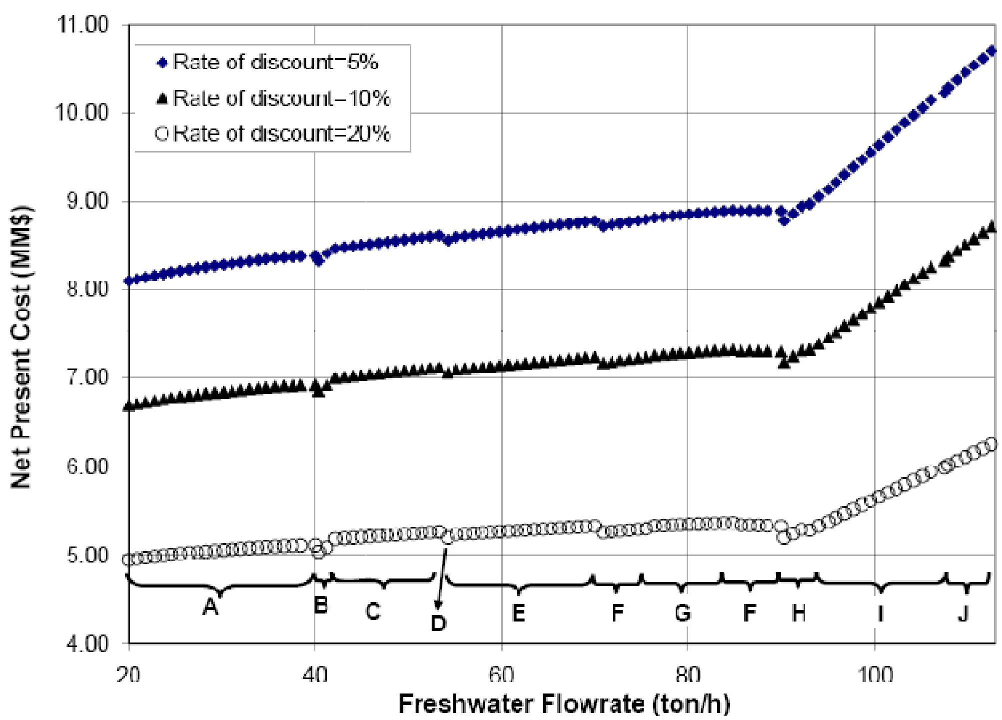


Figure 3.5 – NPC using different rates of interest as a function of Freshwater flowrate in the grassroots design.

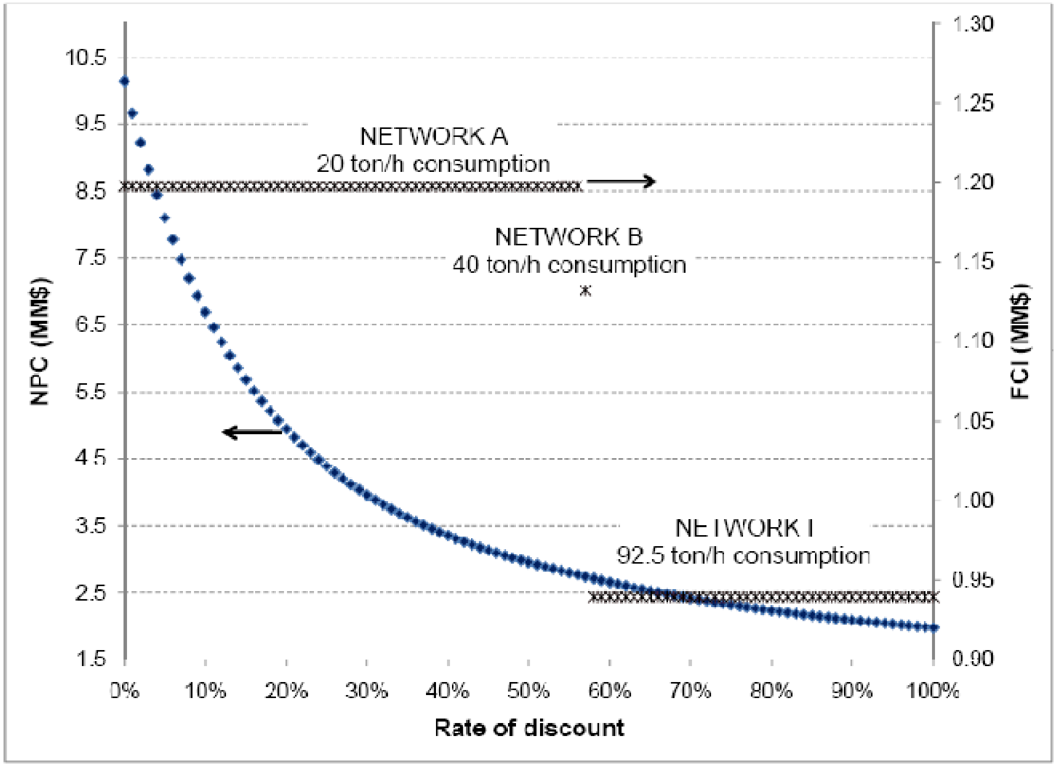
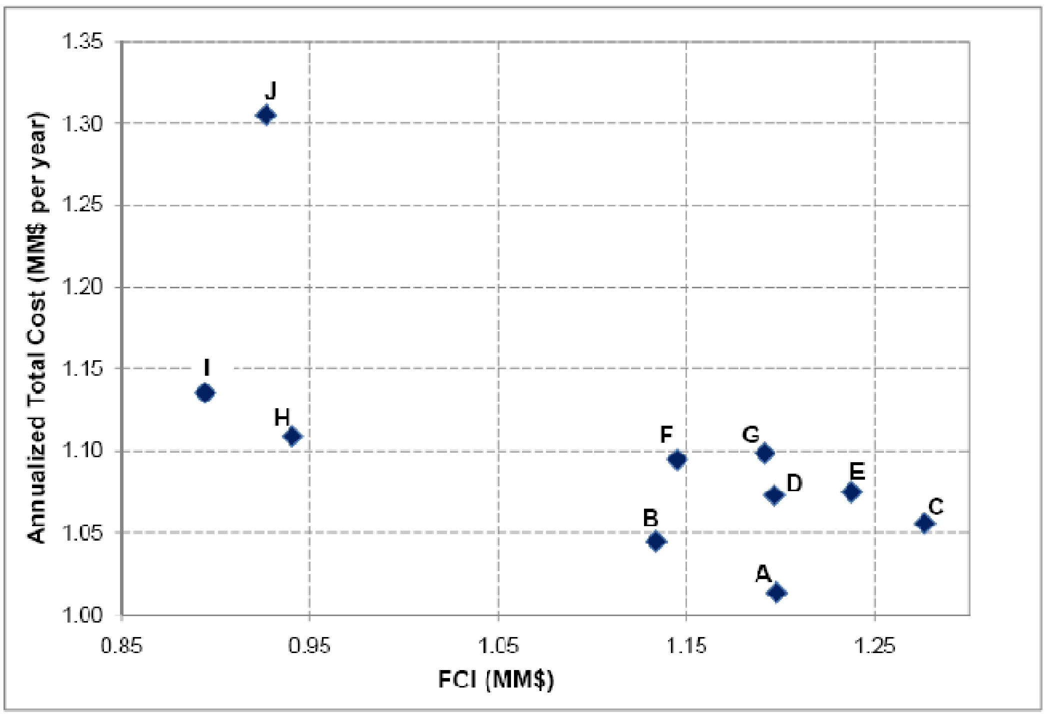


Figure 3.6 – NPC and FCI as a function of rate of discount.

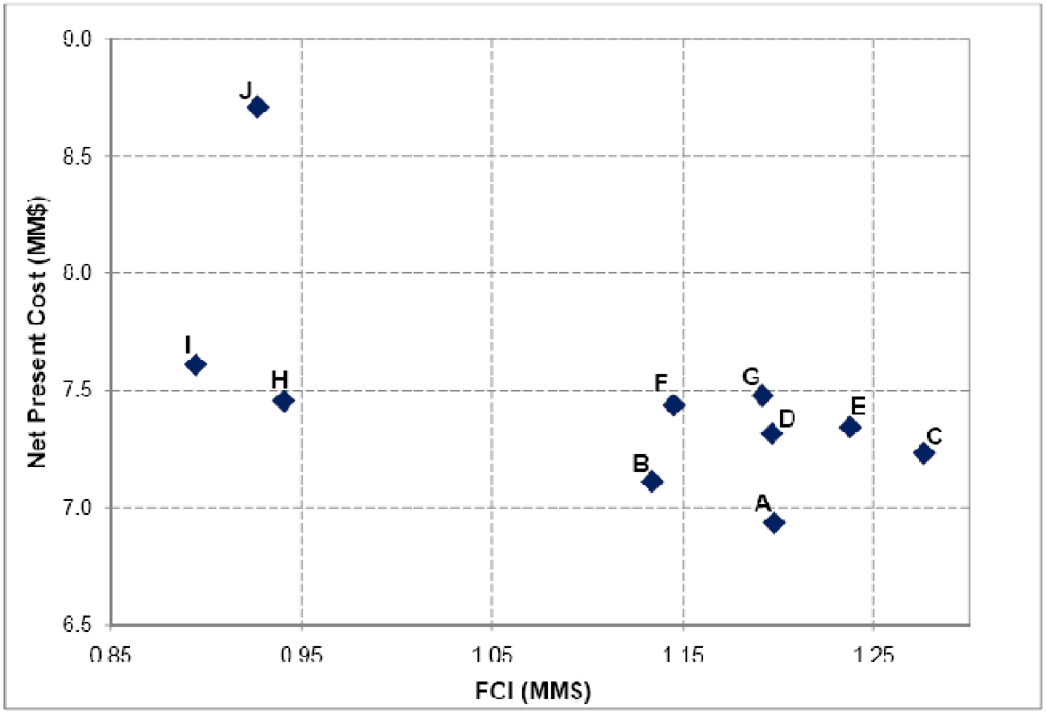
Next, the cost and profitability of the network options previously suggested in comparison to the initial investments is investigated. For that, a typical rate of discount of 9% is considered. In both cases (annualized total cost and NPC), network A shows the lowest objective value. However, if one considers also the initial investment (FCI), additional conclusions can be obtained. Figure 3.7 shows the Annualized total cost vs. FCI and NPC vs. FCI. The optimum capacities of the regeneration process and end-of-pipe treatment for each of the networks are presented in Table 3-4.

Table 3-4 – Regeneration and end-of-pipe treatment capacity of the networks analyzed in Figure 5.

	Regeneration Capacity	EOP Capacity
Network A	77.8 t/h	20 t/h
Network B	55.6 t/h	40 t/h
Network C	55.6 t/h	40 t/h
Network D	40 t/h	54 t/h
Network E	40 t/h	54 t/h
Network F	22.3 t/h	70 t/h
Network G	22.3 t/h	70 t/h
Network H	-	90 t/h
Network I	-	92.5 t/h
Network J	-	107.5 t/h



(a)



(b)

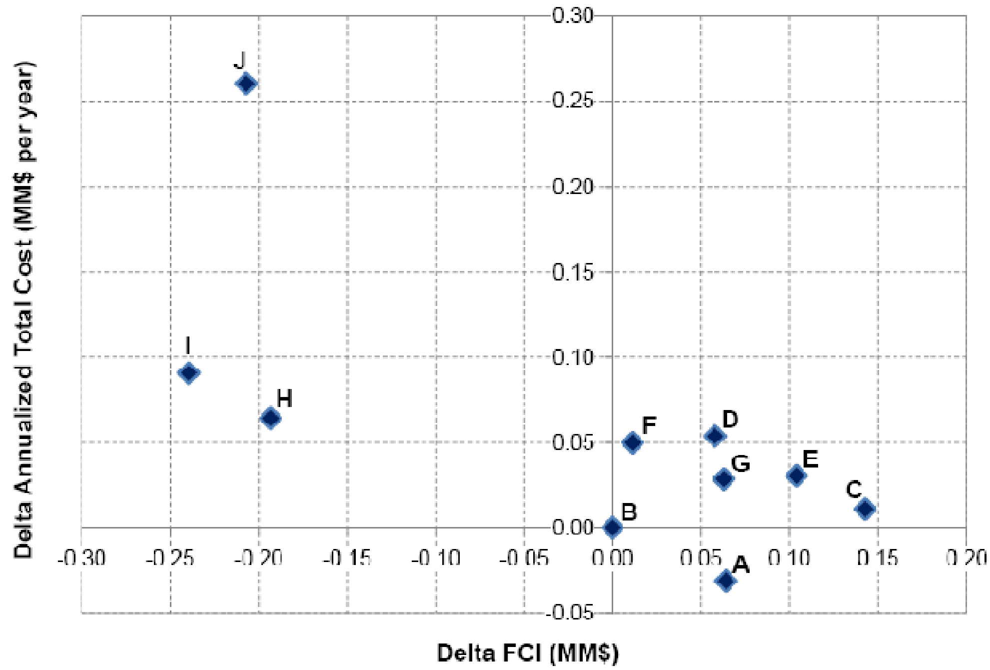
Figure 3.7 – a - Annualized total cost as function of FCI. b - NPC as a function of FCI.

Evaluation of Budget limitations:

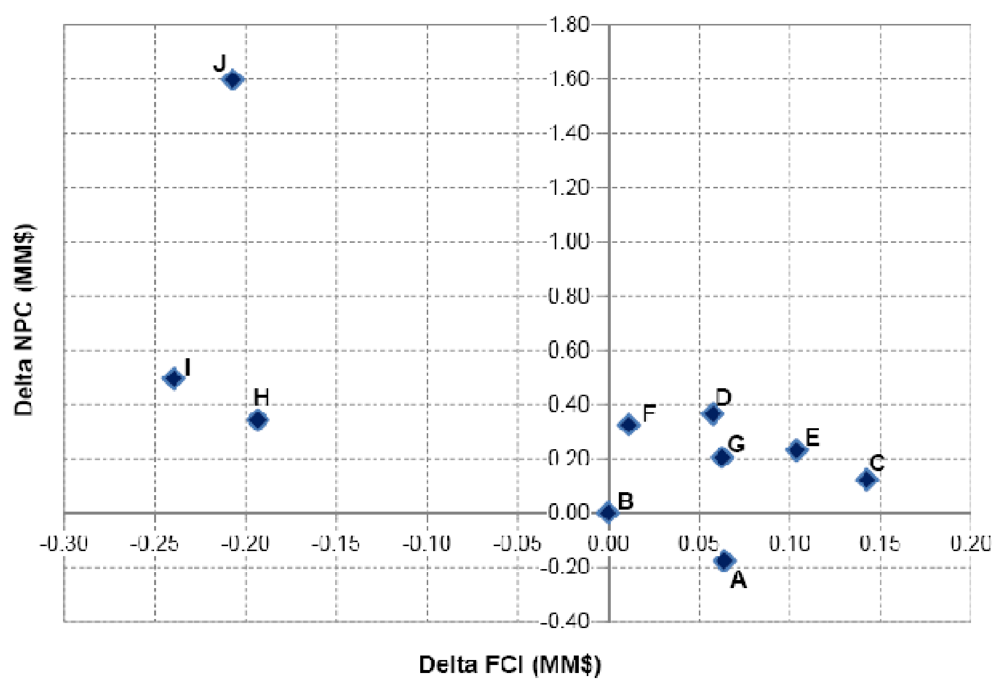
Considering the solutions previously obtained, note that if the budget is constrained to be lower than $1,190,000, the optimum solution (minimum NPC) is network B instead network A. Network B has a NPC of $7,112,219 (for a 9% discount rate). This network does not use the whole budget since it has an FCI around $1,134,000. Due to its isolated loop without discharge (or any other reason), one may not consider network B. In this case other options can be analyzed. To better organize this information, the marginal values of annualized total cost and NPC are calculated and presented in Figure 3.7. Network B is chosen as the reference network because it is the optimum solution for a $1,190,000 budget limit case. Thus, marginal values of the other suggested networks can be calculated by simply computing the change in costs (cost of a given network minus the optimum network). The first quadrant contains the solutions that do not give any advantages in terms of the analyzed objective, the second shows networks in which the budget constraint is violated, but they provide a better solution in terms of the objective function and, the third one is always empty since the graph is done using the optimum solution of a budget limited case. Finally, the last quadrant provides information of networks that require a lower investment, but result in a larger objective function. The second and fourth quadrants are the ones with interest in this analysis and will be discussed further.

First, we note that networks C, D, E, F and G do not give any advantage in terms of either annualized total cost or NPC. Then, one can look at the issue of how much one is losing for not having a higher budget (second quadrant). In this case the investment is $64,000 higher (which represents only $8,000 more than the budget), but it is able to decrease the annualized cost by $30,000 and NPC by $177,000 (network A).

Now if we look the graph considering the former discussion (how much more you are investing to gain a certain delta in NPC – fourth quadrant) and assuming that no more money can be put in this project (the maximum is $1,190,00), another interesting point can be made. In this case, network H would give an annualized total cost $64,000 higher and would increase the NPC by $343,000. On the other hand, network H has a lower investment ($193,000 lower than network B and $249,285 lower than the budget).



(a)



(b)

Figure 3.8 – a- Marginal annualized total cost. b – Marginal (grassroots case when reuse of end-of-pipe wastewater is not allowed).

A similar analysis can also be done considering a measurement of return on investment. Because this is a grassroots design, no direct profit can be calculated. However, it is known that one important objective function used by previous works (Hallale and Fraser, 19997, 2000a,b) is the minimization of capital cost (FCI). To evaluate this choice, one can now consider the optimum solution obtained when FCI is minimized (Equation 3-17) and use it as a reference solution. Thus, the Return on Extra Investment (ROEI) can be calculated as follows:

$$ROEI = \frac{OperatingCost^{ref} - OperatingCost}{FCI - FCI^{ref}} \tag{3-23}$$

This analysis is important when minimum freshwater is not an essential issue and capital cost is the main concern. In this case, one may think at first that the minimum capital of investment is the best choice. However, we show that some better opportunities can be missed.

For this example, network I presents the minimum FCI and accordingly is the reference network. Figure 3.9 shows the ROEI as function of the freshwater flowrate considering the optimum ranges found from the minimization of annualized total cost (Figure 3.1 to Figure 3.4).

The maximum ROEI as function of incremental FCI is shown in Figure 3.9. Because of its negative value (- 457%), network J was excluded from the figure. Now, from the ROEI point of view, the optimum network is network H, which gives a 67% return on extra investment. This network also corresponds to the one with the lowest extra investment. Note that network J represents a bad choice from the return on extra investment perspective since it has a higher FCI and a higher operating cost.

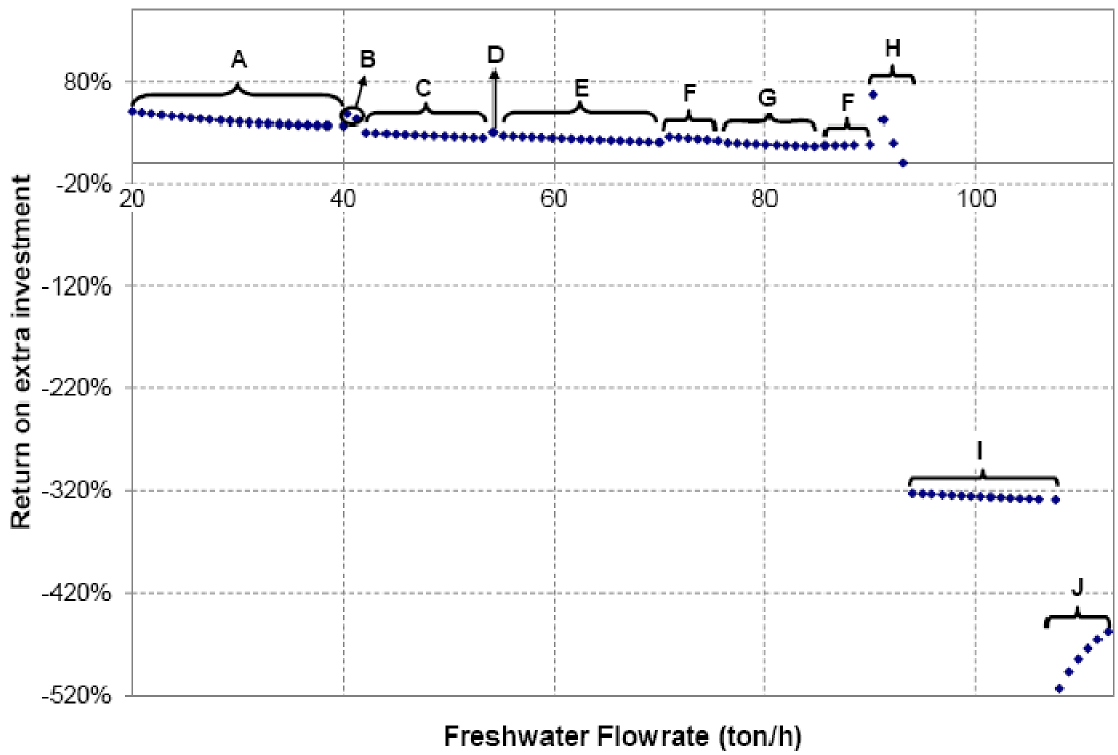


Figure 3.9 – Return on extra investment - grassroots case.

Table 3-5 summarizes the results (the FCI, Total cost, NPC and ROEI are calculated at the minimum freshwater consumption). One can see the importance of looking at this problem from a more comprehensive view of the opportunities, which allows the designer to make a decision based on the level of importance and priorities of the project, current financial situation of the company, available budget, etc.

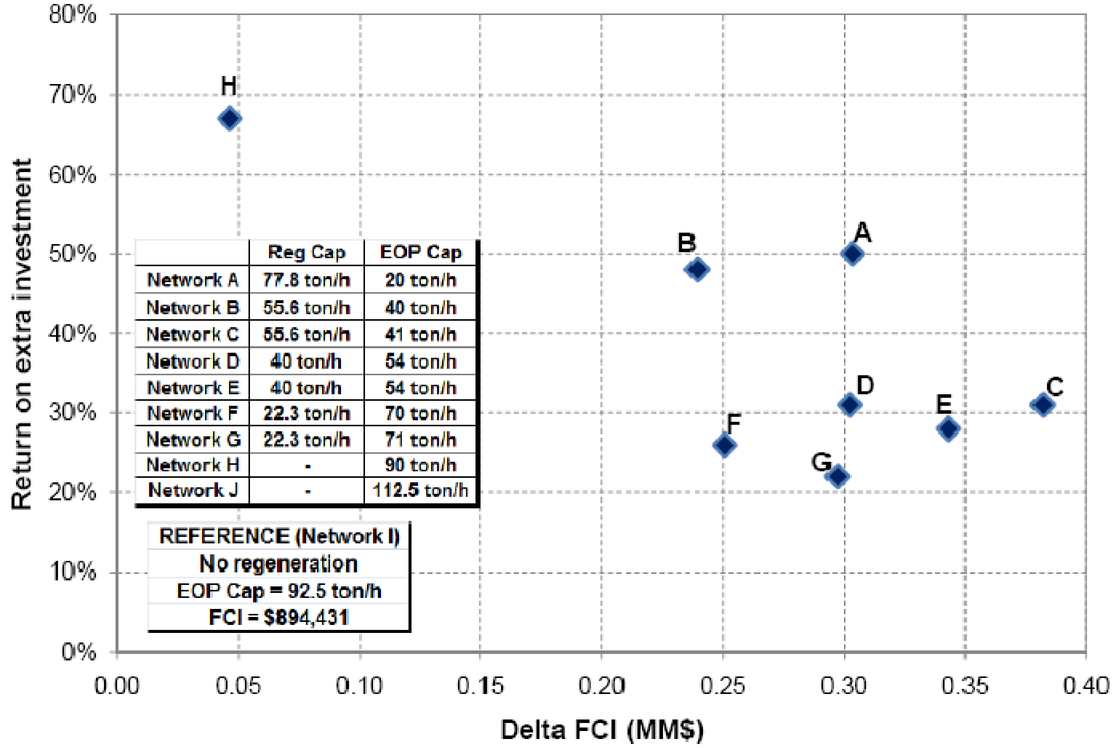


Figure 3.10 – Return on extra investment - grassroots case.

Table 3-5 – Summary of results - grassroots case.

Network	Minimum Freshwater Consumption	FCI	Total Cost	NPC	ROEI
A	20 t/h	$1,197,873	$1,013,429	$6,935,050	50%
B	40 t/h	$1,133,814	$1,044,597	$7,112,219	48%
C	40 t/h	$1,276,442	$1,055,516	$7,233,376	31%
D	54 t/h	$1,196,702	$1,073,030	$7,317,272	31%
E	54 t/h	$1,237729	$1,074,983	$7,344,497	28%
F	70 t/h	$1,145,154	$1,094,624	$7,437,454	26%
G	70 t/h	$1,191,666	$1,098,383	$7,478,235	22%
H	90 t/h	$940,715	$1,108,829	$7,455,456	67%
I	92.5 t/h	$894,431	$1,135,385	$7,609,375	Reference
J	107.5 t/h	$926,861	$1,304,944	$8,709,560	-513%

Retrofit case:

For the retrofit case, a conventional network (no water reuse) in which no regeneration process exists is assumed. That is, the current network has only the connection between the water source and water-using units and between water-using units and the end-of-pipe treatment. The investment costs of new connections and potential regeneration processes are needed. The costs previously presented are used in this case as well. However, the capital cost of existing connections (between freshwater and water using units and water using units and end of pipe treatment) and processes (in this case the end of pipe treatment) are set to zero.

The feasible range of freshwater usage found for the studied water network is between 20 t/h (the minimum flowrate using a regeneration process) and 112.5 t/h (flowrate of the current network). Figure 3.10 depicts the savings as a function of flowrate, where networks A through D make use of a regeneration unit and networks E, F and G do not use regeneration. Note that each point corresponds to a different regeneration unit capacity (when this applies).

The ranges of freshwater where each network is the economical optimal solution (maximum Net Savings – Equation 16), are shown in Table 3-6. Selected configurations (networks A, C, E and F) are presented in Figure 3.11. The thicker lines in the figures represent new connections and the values inside the boxes represent altered flowrates and concentration. The flowrates and concentrations shown in the figures correspond to the operating conditions to reach the maximum savings of each network.

The FCI as well as the ROI and NPV profiles corresponding to the savings presented in Figure 3.13 are shown in Figure 3.14 and Figure 3.15, respectively. Savings and FCI go down in a discontinuous manner. The ROI, however, increases. Therefore, one can conclude that maximizing savings does not necessarily generate the most profitable solution from the ROI point of view. *Indeed, the most profitable option from* *the ROI point of view happens at the limit of 95 t/h (Network F), where no regeneration process is needed. Conversely, Network A exhibits the highest savings.*

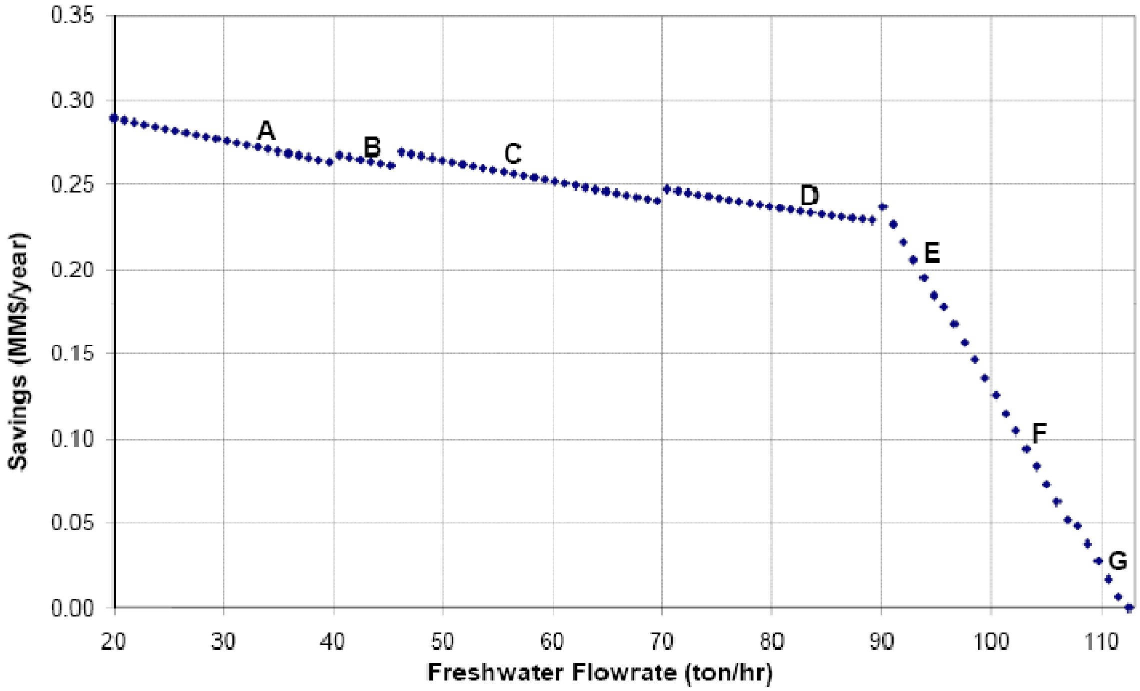
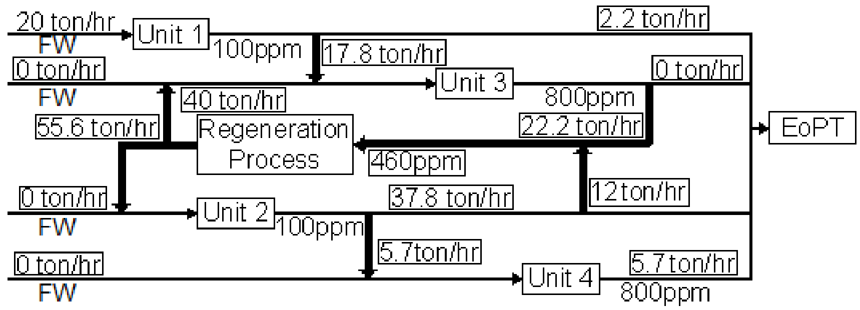


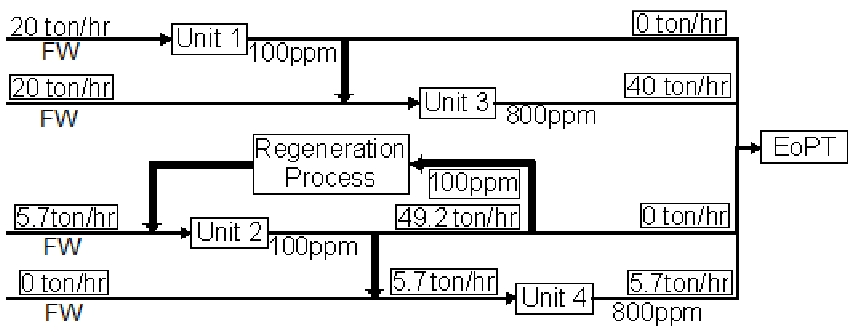
Figure 3.11 – Savings as a function of Freshwater flowrate for the retrofit design.

Table 3-6 – Network and corresponding range of freshwater flowrate (Figure 10).

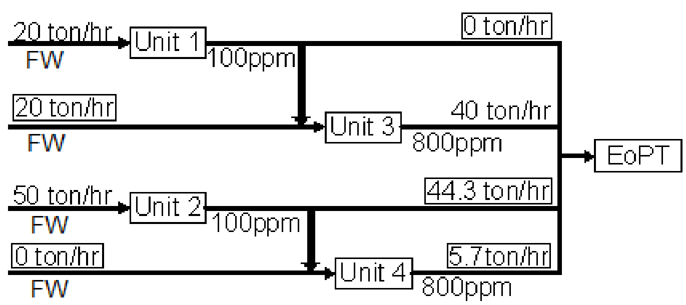
Network	Range of freshwater usage (discrete values)	New Connections	FCI of New Connections
A	20.00 to 39.621 t/h	U1-U3, U2-U4, N1-U2, N1-U3, U2-N1, U3-N1	$458,000.00
B	40.556 to 45.227 t/h	U1-U3, U2-U4, N1-U2, U2-N1, U3-N1	$408,000.00
C	46.162 to 69.520 t/h	U1-U3, U2-U4, N1-U2, U2-N1	$317,000.00
D	70.455 to 89.141 t/h	U1-U3, U2-U4, N1-U3, U2-N1	$237,000.00
E	90.076 to 94.747 t/h	U1-U3, U2-U4	$150,000.00
F	95.682 to 106.894 t/h	U1-U3	$110,000.00
G	107.828 to 111.566 t/h	U2-U4	$40,000.00



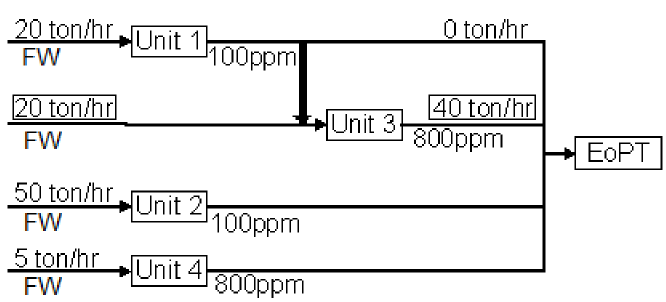
(a) Network A



(b) Network C



(c) Network E



(d) Network F

Figure 3.12 – Selected networks for the retrofit example.

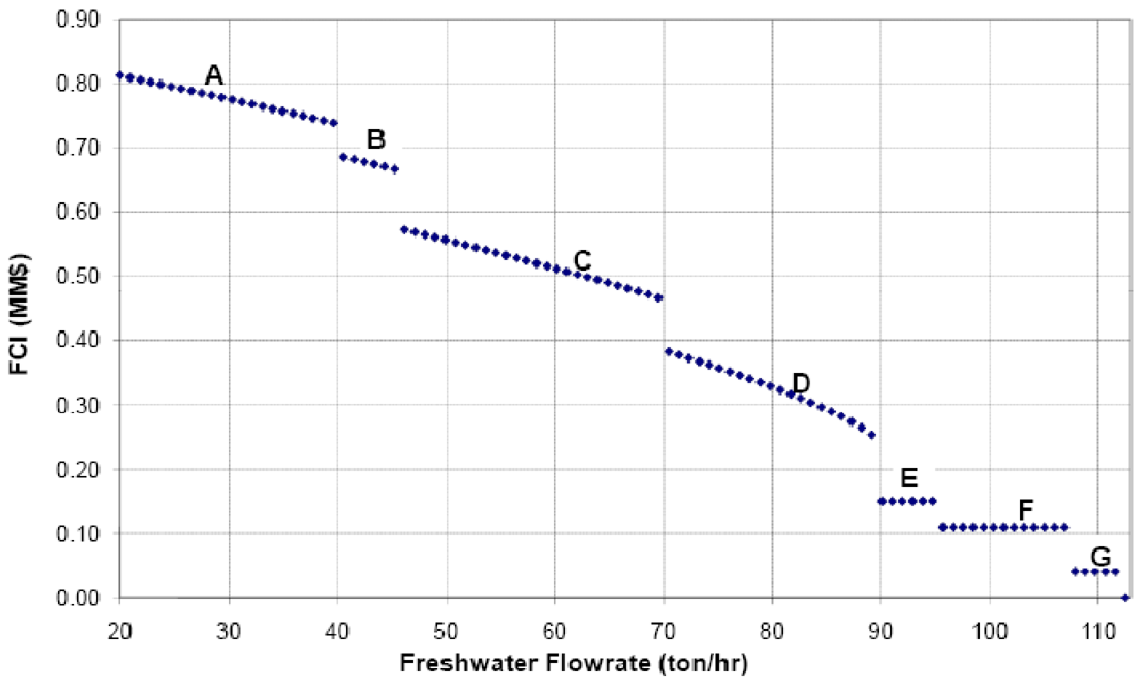


Figure 3.13 – FCI as a function of freshwater flowrate - retrofit.

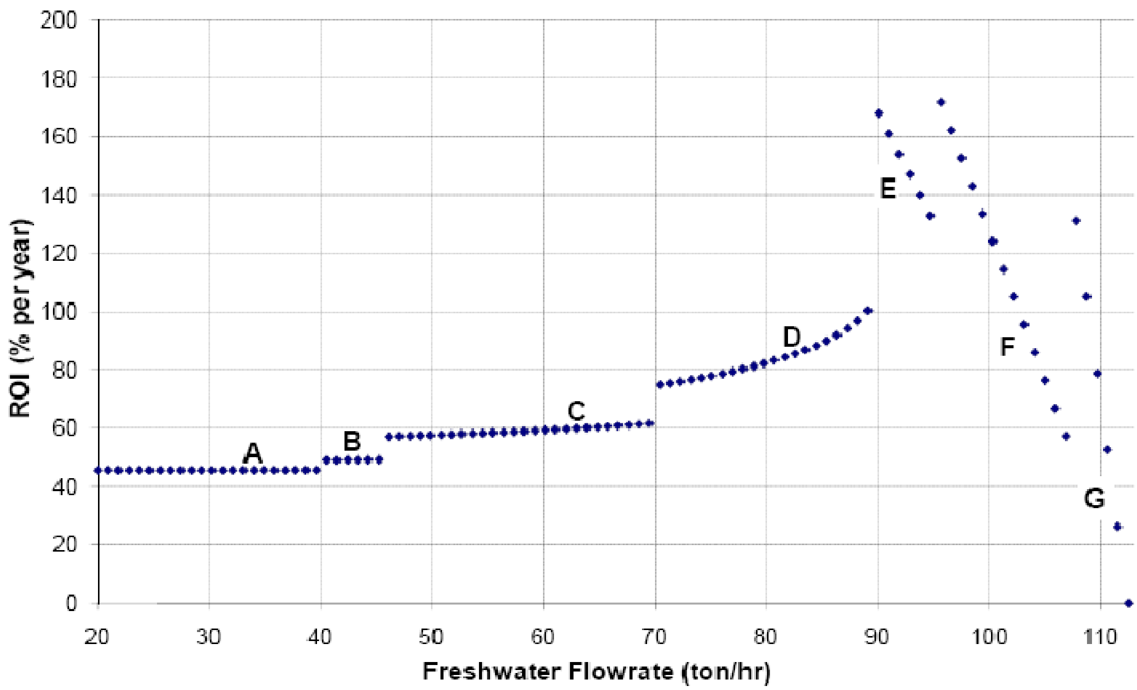


Figure 3.14 – ROI as a function of freshwater flowrate - retrofit.

Next, the net present value (NPV) is used as mean of looking at profitability. The same solutions are obtained optimizing either savings (Equation 3-16) or NPV (Equation

3-20). In this case, note that we are looking at true profitability of the retrofit, as opposed to using the net present cost as in the case of grassroots design. Figure 3.15 shows the NPV profiles of all the aforementioned solutions for different discount rates. The optimum solution varies according to the discount rate used. The 20% rate of discount gives network E as the one with the maximum NPV. On the other hand, the 10% rate of discount shows network A as having the maximum NPV. However, networks C and F also exhibit fairly good NPVs. For the 5% discount rate case, network A would be the best network from the NPV profitability based point of view. A better evaluation of what happens with the optimum solutions from the NPV point of view as function of rate of discount is shown in Figure 3.16. It is worth reminding the reader that each point has a different regeneration unit capacity (when this applies).

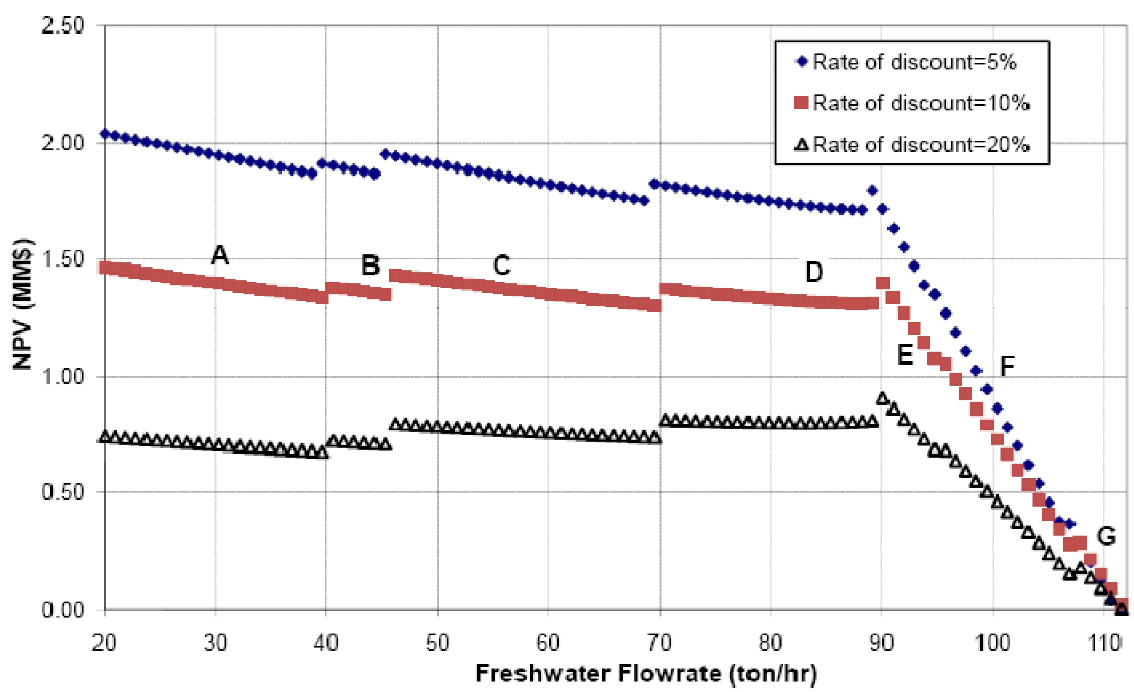


Figure 3.15 – NPV as a function of freshwater flowrate - retrofit design.

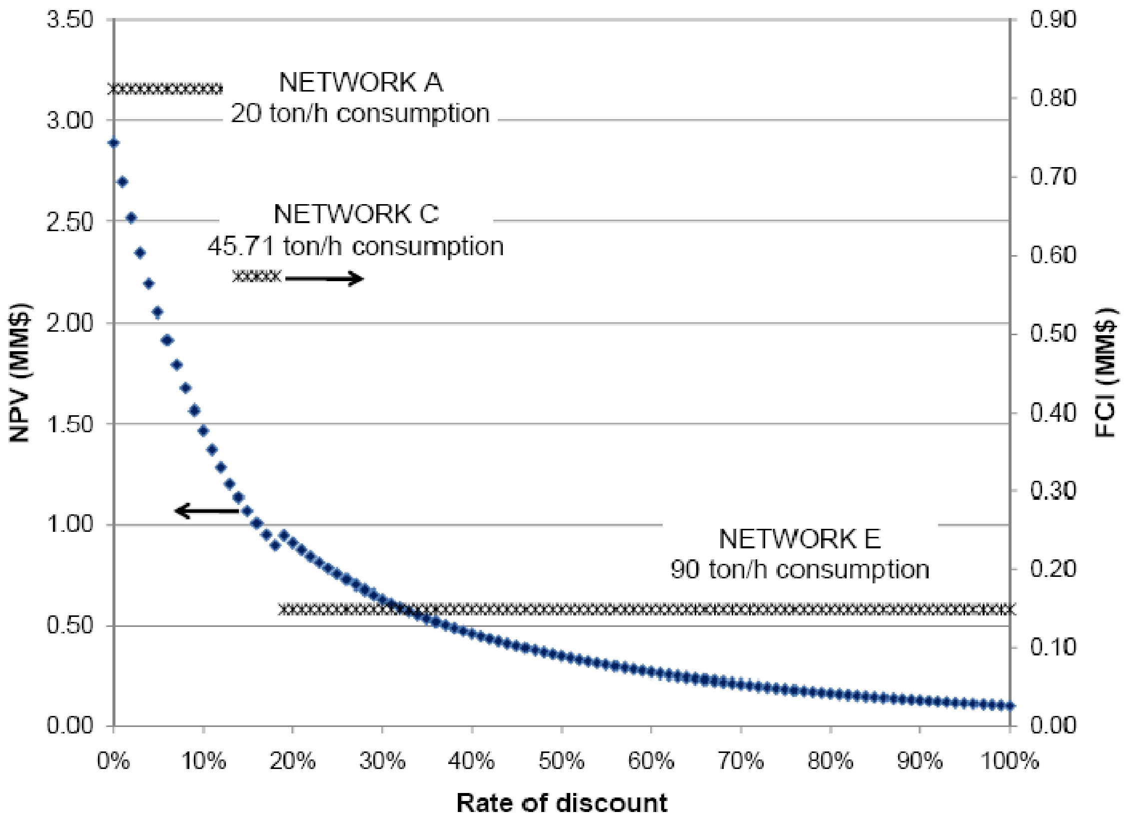


Figure 3.16 – NPC and FCI as a function of rate of discount - retrofit design.

Operability Range of the Networks:

The purpose of this section is to show the operability range (feasible variations of freshwater consumption) of each network and their relation with a chosen regeneration capacity. This can help in identifying adequate capacities of the regeneration process in each network and better understand the tradeoff between freshwater savings and cost with regeneration.

To make the operability range analysis, the feasibility range of each network is extended beyond the interval in which they are optimal by solving the same problem again for each of the networks. We fix the network connections (but not the size of the regeneration unit yet) and maximize savings (Equation 3-16) for each fixed freshwater flowrate. Unlike the previous problem, an NLP solver (GAMS/CONOPT) can be used here since the binary variables are now fixed. The results are shown in Figure 3.16.

Note the existence of overlapping solutions for all networks, which indicates that different networks can operate at certain same freshwater consumption. There is a linear relation between the regeneration capacity and the freshwater flowrate, which is also shown in the top scale of the figure. The interesting point to make here is that at certain freshwater flowrate, the network with maximum saving obeys this linear relationship and, all the other feasible networks with the same freshwater consumption have the same regeneration capacity. Another issue worth pointing out is that to construct the curves the minimum freshwater flowrate obtained for a fixed network may not coincide with the original minimum value of the freshwater usage range at maximum savings. When this happens, one may get isolated points like the one shown in Figure 3.16 for network C. This isolated point of network C represents a feasible operating condition of this network where it operates economically worse than at least another network. Since this point does not represent the maximum savings at this freshwater consumption, the regeneration flowrate scale is no longer valid for it. The corresponding ROI and NPV profiles for these extended ranges are shown in Figure 3.17 and Figure 3.18 respectively.

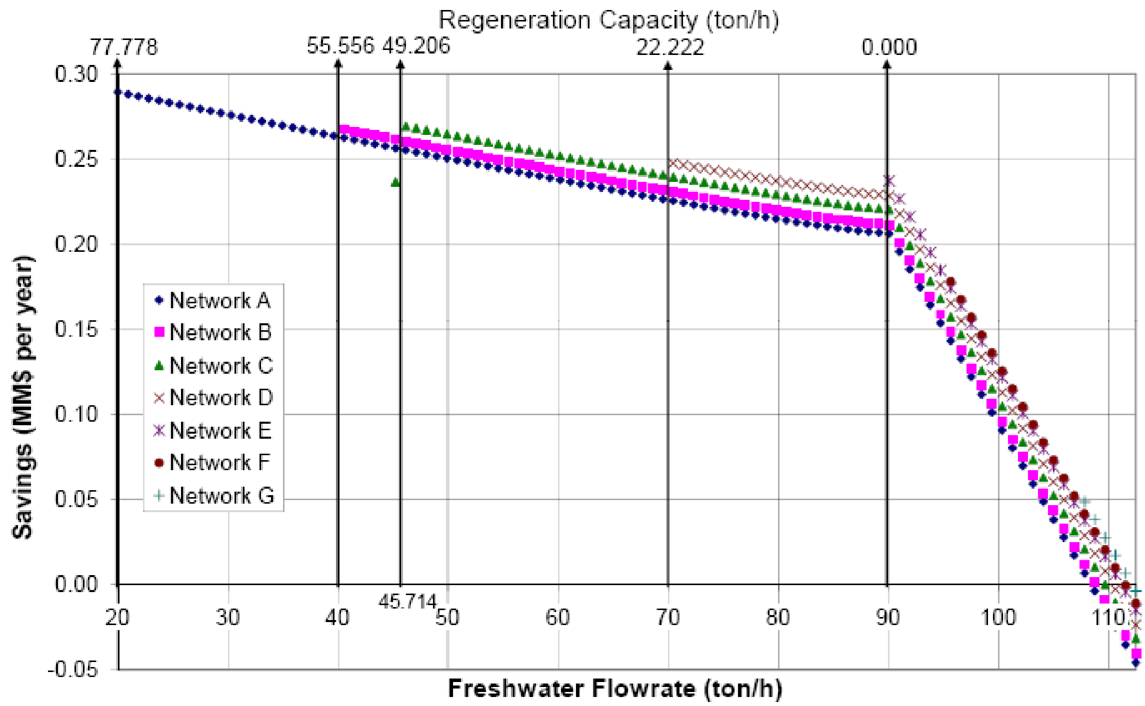


Figure 3.17 – Savings profile of the suggested networks.

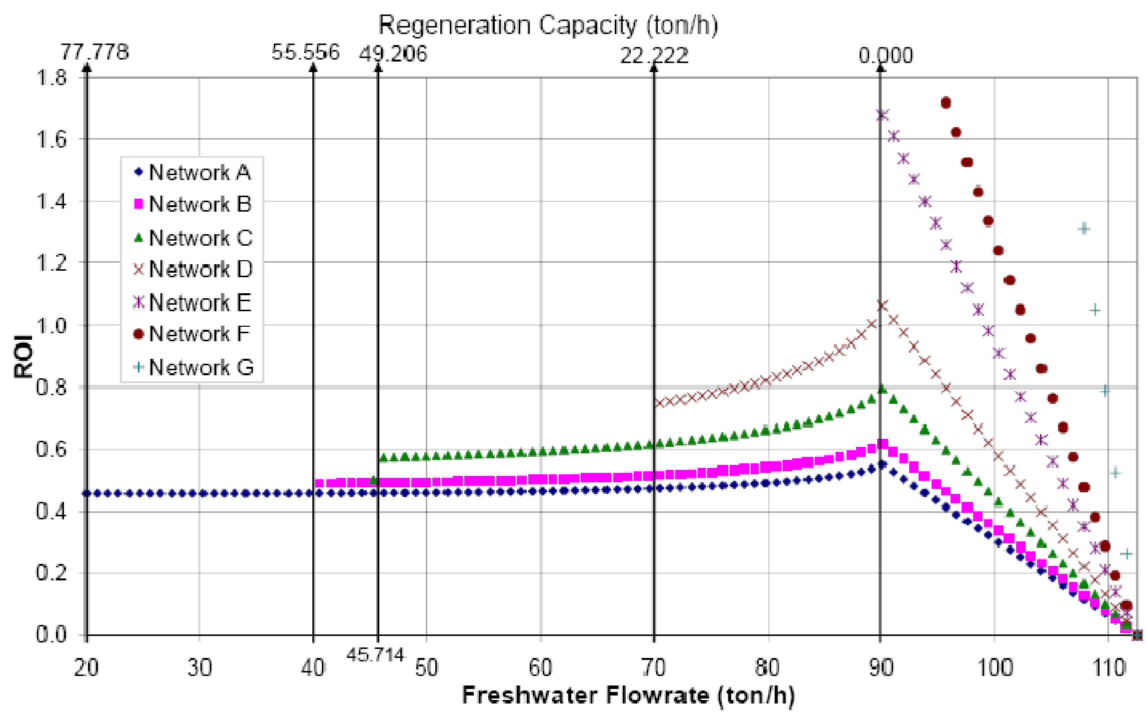


Figure 3.18 – ROI profile of the suggested networks - retrofit.

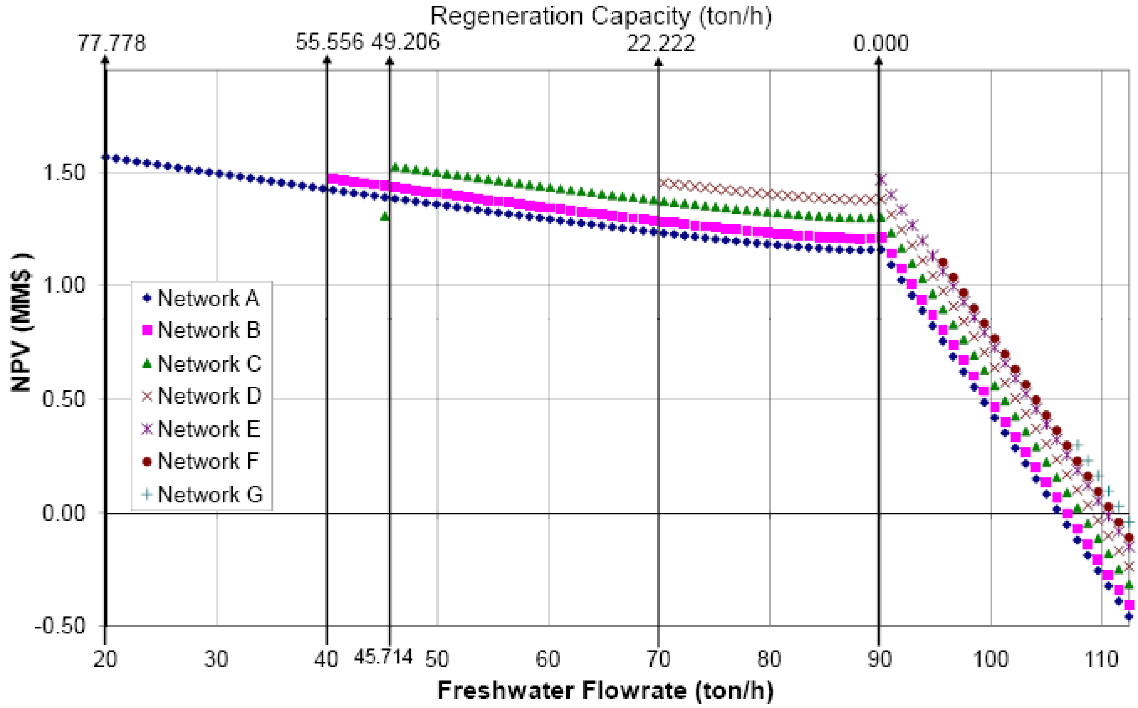


Figure 3.19 – NPV profile of the suggested networks for 9% rate of discount - retrofit design.

In the next step, the size of the regeneration ($RegCap_r$ is fixed in Equation 3-15) is fixed in addition to the connections. The sizes that correspond to the capacity obtained for the point with maximum savings of each network are chosen. Moreover, an additional lower size can be found using information of the other networks. For example, the lower size of network C is the capacity corresponding to the point where at least one other network can reach the same savings (in this case network D). The savings are now linear for the whole feasible freshwater consumption range, as shown in Figure 3.19. In this figure, the previous curves of the networks with regeneration are included for reference. The capacities of the regeneration units correspond to where the straight line touches its curved savings profile. Once the regeneration capacity is defined, the minimum freshwater consumption is determined by the freshwater flowrate scale (in the bottom).

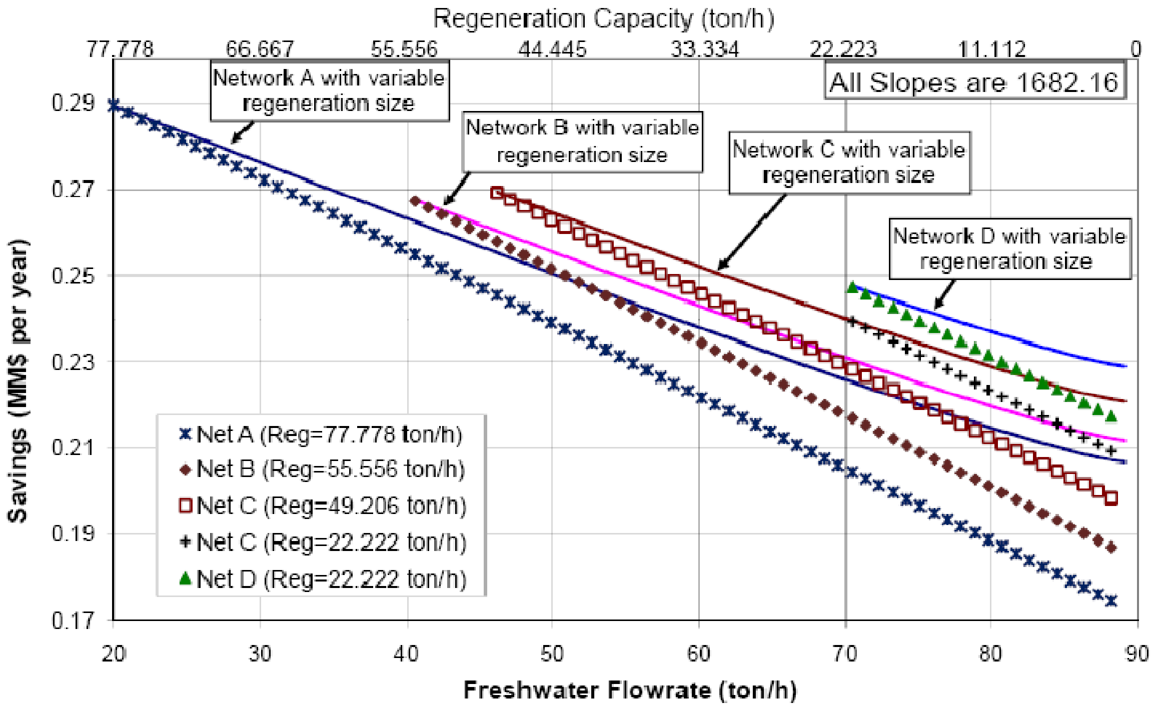


Figure 3.20 – Savings profile for fixed sizes of the regeneration process - retrofit design.

This evaluation is useful to define economical limit sizes of the regeneration process for the different networks. For each network, a regeneration process with capacity higher than the maximum values used to construct Figure 3.19 does not decrease the freshwater consumption without generating a saving that is lower than one of another network. Consequently, in the best case (when freshwater consumption does not decrease), the part of the savings equation related to operating cost does not change while FCI increases. Thus, a higher regeneration capacity generates economic loss.

In Figure 3.20 the lower limit of the regeneration capacities are analyzed. One can see that a regeneration process with capacity of 22.222 t/h will be economically superior when used in network D than when used in network C. This also happens with Network A and B with 22.222 t/h capacity. If we draw the profile, they will be below the one in network D. Similarly, a regeneration process with capacity of 49.206 t/h is economically superior when used in network C than when used by network B and one with 55.556 t/h capacity is economically superior in network B than in network A. Further, from the economical point of view, network A should not work with a regeneration process with capacity lower than 61.345 t/h and, as suggested before, it should not work with a regeneration process with capacity higher than 77.778 t/h. This lower capacity limit represents the regeneration capacity in network A that generates the same savings than the maximum savings generates by other network (in this case, network C) that can operate at the same freshwater consumption. This point is also the economically optimum upper limit of network C (49.206 t/h). Additionally, network B does not present any economical advantages. The only reason that it could be considered is due to freshwater consumption issues when compared to network C. Similarly, the limits for network C are between 49.206 t/h and 29.695 t/h (this lower limit generates the same savings as network D at its maximum savings). In turn, network D has the limit between 22.222 t/h and 12.104 t/h (this lower limit generates the same savings as the maximum savings in network E – the highest savings between the options without regeneration). Finally, the use of a regeneration process with capacity outside these intervals generates economical losses. This process of thought is illustrated in Figure 3.20.

The ROI and NPV profiles of the networks A to D with fixed size of regeneration process are presented in Figure 3.22 and Figure 3.23 respectively. The largest advisable sizes from the savings point of view are used in these profiles. The pattern of straight lines repeats, but they are not parallel anymore.

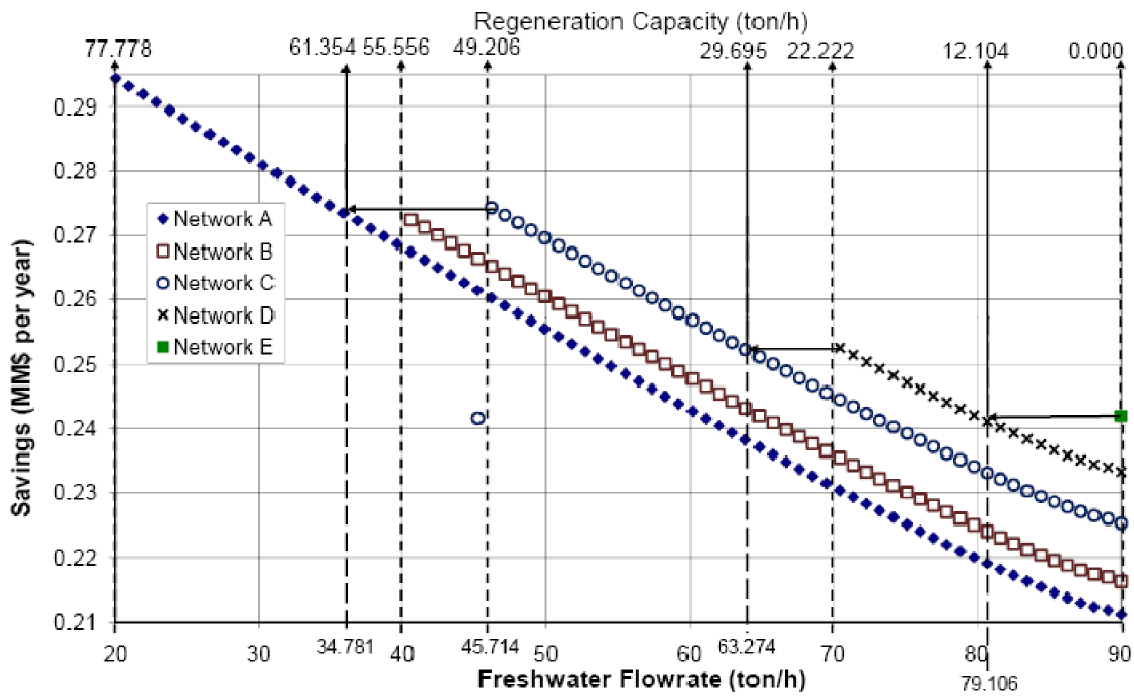


Figure 3.21 – Analysis of regeneration capacity - retrofit design.

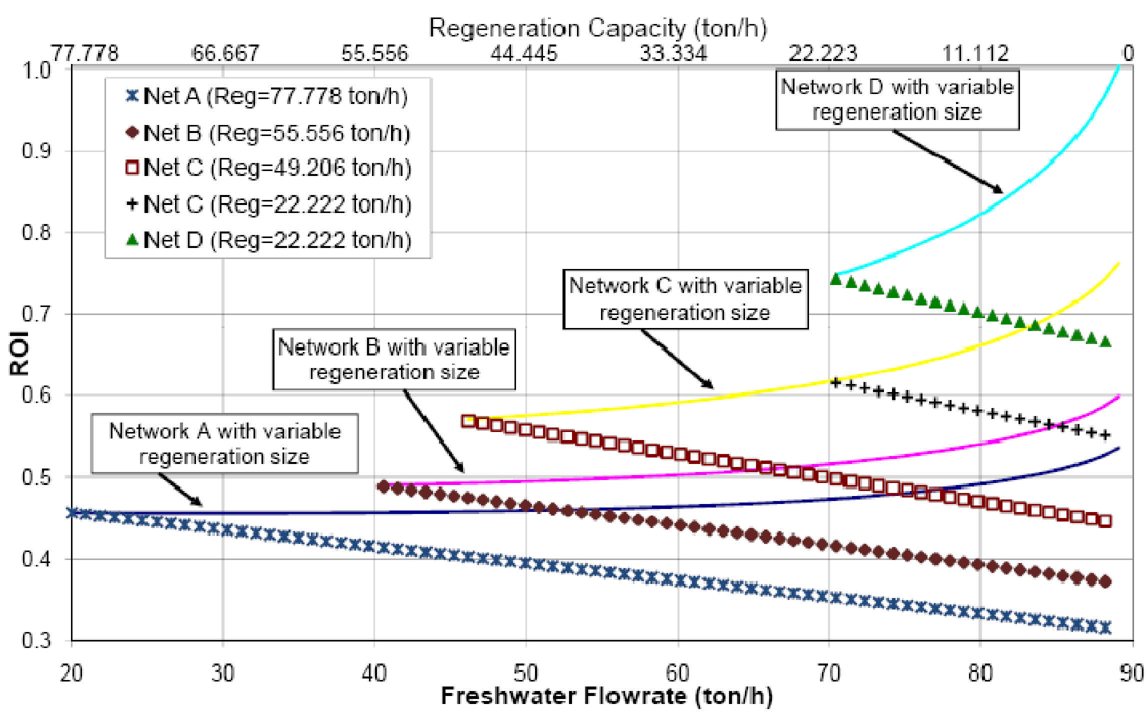


Figure 3.22 – ROI profile for the limit sizes of regeneration process - retrofit.

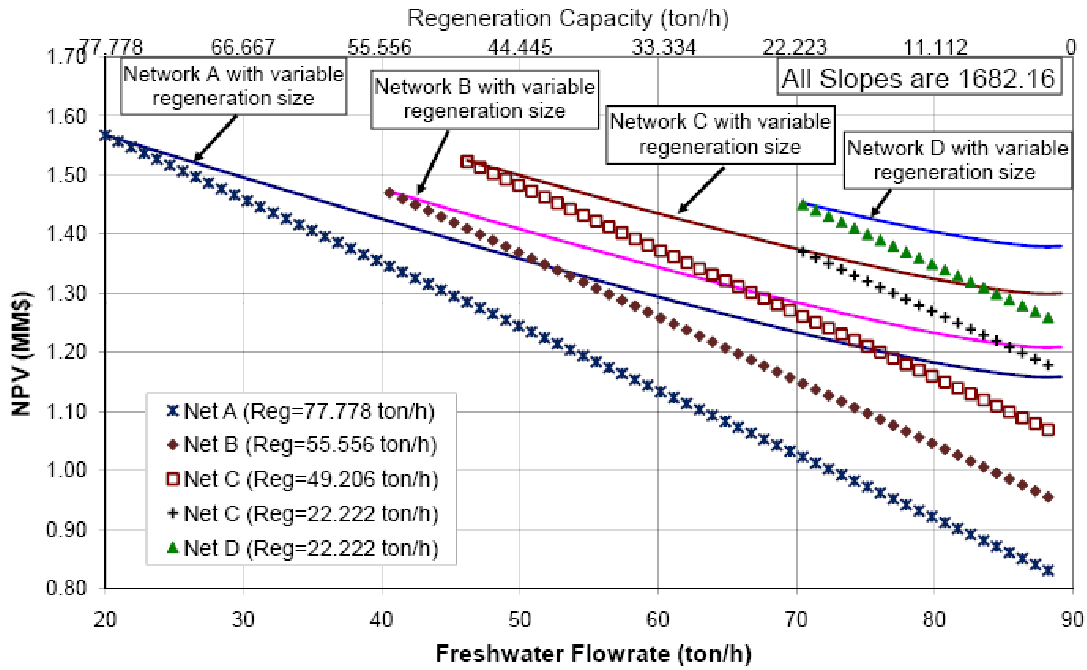


Figure 3.23 – NPV profile for the limit sizes of regeneration process - retrofit design.

Table 3-7 shows the summary of the results for the retrofit case of the single contaminant example. As before, all economics is computed for the minimum freshwater consumption.

Table 3-7 – Summary of results – retrofit design.

Network	Minimum Freshwater Consumption	FCI	Savings	NPV (i=10%)	ROI
A	20 t/h	$811,922	$289,398	$1,465,194	45.6%
B	40 t/h	$685,473	$267,467	$1,379,189	49.0%
C	45 t/h	$589,494	$236,631	$1,226,719	50.1%
D	70 t/h	$381,901	$247,533	$1,373,743	74.8%
E	90 t/h	$150,000	$236,995	$1,398,400	168.0%
F	95 t/h	$110,000	$177,996	$1,051,298	171.8%
G	107.5 t/h	$40,000	$48,499	$282,583	131.2%

Example 2: Multi Contaminant Case

To address the multi-contaminant case, the refinery example presented by Koppol et al. (2003) is investigated. It consists of six water using units and four key contaminants, which operates 8600 hours per year. Table 3-8 gives the limiting data of the six water-using units.

The cost of freshwater is \$0.32/t and its concentration is assumed to be zero. The operating cost of the end of pipe treatment is \$1.68/t and its capital cost factor is \$30,000/t$^{0.7}$. The financial analysis of the project is done for a period of 10 years (N=10 years and af = 0.1). This problem has 215 constraints, 139 continuous variables and 87 binary variables.

Table 3-8 – Limiting process water data for multi contaminant example.

Process	Contaminant	Mass Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1 - CausticTreating	Salts	0.18	300	500
	Organics	1.2	50	500
	H2S	0.75	5000	11000
	Ammonia	0.1	1500	3000
2 - Distillation	Salts	3.61	10	200
	Organics	100	1	4000
	H2S	0.25	0	500
	Ammonia	0.8	0	1000
3 – Amine Sweetening	Salts	0.6	10	1000
	Organics	30	1	3500
	H2S	1.5	0	2000
	Ammonia	1	0	3500
4 - Merox-I Sweetening	Salts	2	100	400
	Organics	60	200	6000
	H2S	0.8	50	2000
	Ammonia	1	1000	3500
5 - Hydrotreating	Salts	3.8	85	350
	Organics	45	200	1800
	H2S	1.1	300	6500
	Ammonia	2	200	1000
6 - Desalting	Salts	120	1000	9500
	Organics	480	1000	6500
	H2S	1.5	150	450
	Ammonia	0	200	400

Grassroots case:

For the grassroots case all design decisions need to be made. The capital costs of connections between processes are presented in Table 3-9.

Three intermediary regeneration processes are available (API separator followed by ACA, which reduces organics to 50 ppm; Reverse osmosis, which reduces salts to 20 ppm; and, Chevron wastewater treatment, which reduces H_2S to 5 ppm and ammonia to 30 ppm). The capital cost factor ICNr and the operation cost OPN_r are presented in Table 3-10.

Table 3-9 – Capital costs of the connections.

$(x10^3)	U1	U2	U3	U4	U5	U6	R1	R2	R3	EOP
W1	23	50	18	63	16	25	-	-	-	-
U1	-	50	110	45	70	42	23	15	11	53
U2	50	-	34	40	11	35	50	12	34	51
U3	110	34	-	42	60	18	18	35	47	62
U4	45	40	42	-	23	34	63	13	50	78
U5	70	11	60	23	-	28	16	21	19	58
U6	42	35	18	34	28	-	25	33	24	22
R1	23	50	18	63	16	25	-	50	31	44
R2	15	12	35	13	21	33	50	-	34	40
R3	11	34	47	50	19	24	31	34	-	52
EOP	53	51	62	78	58	22	44	40	52	-

The range of freshwater usage of this network is defined between its minimum consumption (33.6 t/h) and its freshwater consumption without reuse (144.8 t/h). Figure 3.24 shows the annualized total cost as function of freshwater consumption when the annualized total cost is minimized (Equation 3-16). The optimum solution from the annualized total cost point of view is network A, which can reach the minimum freshwater consumption.

Table 3-10 – Capital cost factor and operation cost for the regeneration processes.

Regeneration Process	ICN_r (\$/ton$^{0.7}$)	OPN_r (\$/ton)
1 - API separator followed by ACA	$25,000	0.12
2 - Reverse osmosis	$20,100	0.56
3 - Chevron wastewater treatment	$16,800	1.00

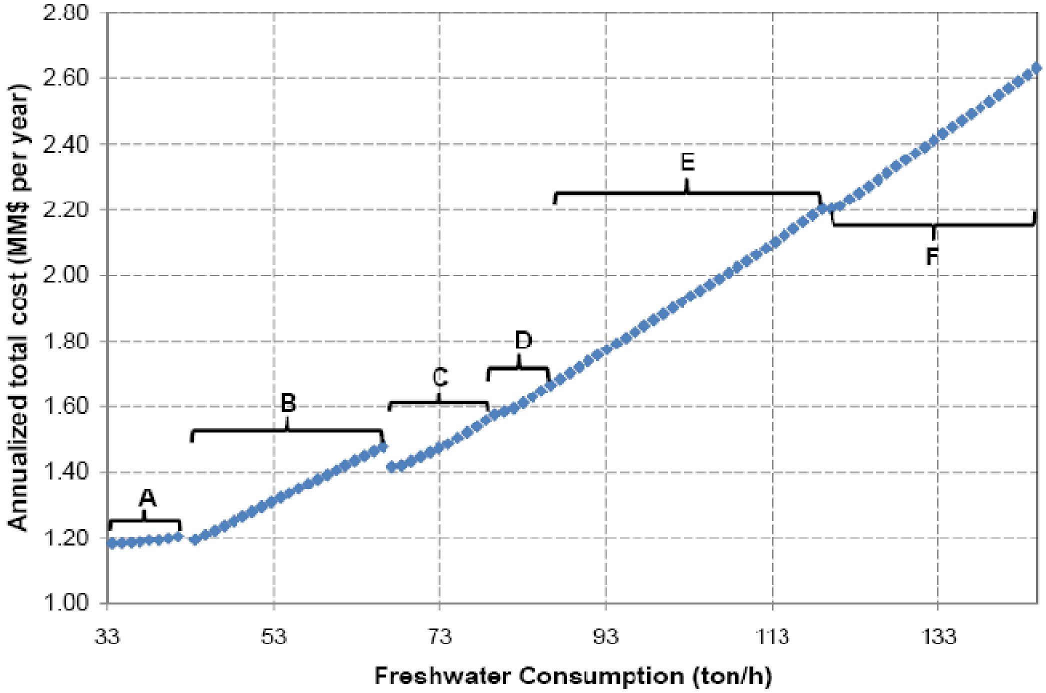


Figure 3.24 – Annualized total cost as a function of freshwater flowrate for the grassroots case of the multi contaminant example.

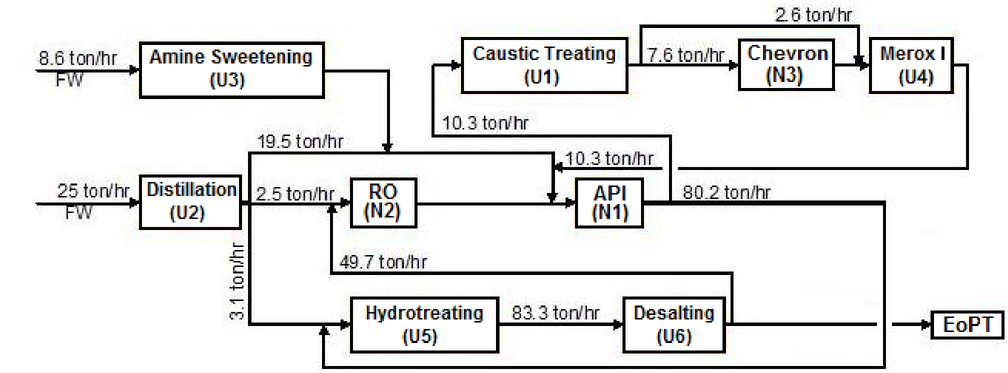
Table 3-11 shows the connections of all these networks and their corresponding minimum values of freshwater consumption (even when they are not optimal for those values). Relevant networks (A, B, C and F) are presented in Figure 3.24. Note that Table 3-11 indicates that network A has a connection between the freshwater source and water-using unit 4 (Merox I). In Figure 3.24a, however, this connection is not shown because this connection is not active at the specific condition of minimum freshwater consumption.

Table 3-11 – Network connections and minimum freshwater consumption of the networks – multi contaminant case.

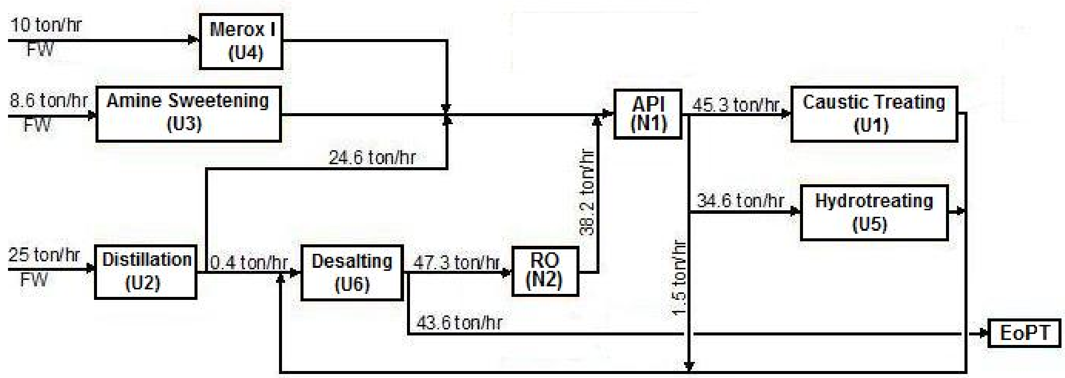
Network	Connections	Min Consumption
A	W-U2, W-U3, W-U4, U1-U4, U2-U5, U5-U6, N1-U1, N1-U5, N1-U6, N3-U4, U1-N3, U2-N1, U2-N2, U3-N1, U4-N1, U5-EoPT, U6-N2, U6-EoPT, N2-N1, EoPT-S	33.6 ton/h
B	W-U2, W-U3, W-U4, U1-U6, U2-U6, U5-U6, N1-U1, N1-U5, N1-U6, U2-N1, U2-N2, U3-N1, U4-N1, U6-N2, U6-EoPT, N2-N1, EoPT-S	43.6 ton/h
C	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U5, U1-U6, U5-U4, U5-U6, N1-U1, U2-N1, U3-N1, U4-N1, U5-N1, U6-N1, U6-EoPT, N1-EoPT, EoPT-S	68.1 ton/h
D	W-U2, W-U3, W-U4, W-U5, W-U6, U1-U6, U3-U6, U5-U6, N1-U1, N1-U5, U2-N1, U4-N1, U6-N1, U6-EoPT, EoPT-S	78.7 ton/h
E	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U6, U2-U5, U3-U6, U5-U6, N1-U6, U2-EoPT, U4-N1, U6-EoPT, EoPT-S	85.8 ton/h
F	W-U1, W-U2, W-U3, W-U4, W-U5, U1-U6, U3-U6, U5-U6, U2-EoPT, U4-EoPT, U6-EoPT, EoPT-S	120.6 ton/h

* N1 – API separator; N2 – RO; N3 – Chevron treatment; EoPT – End-of-pipe treatment.

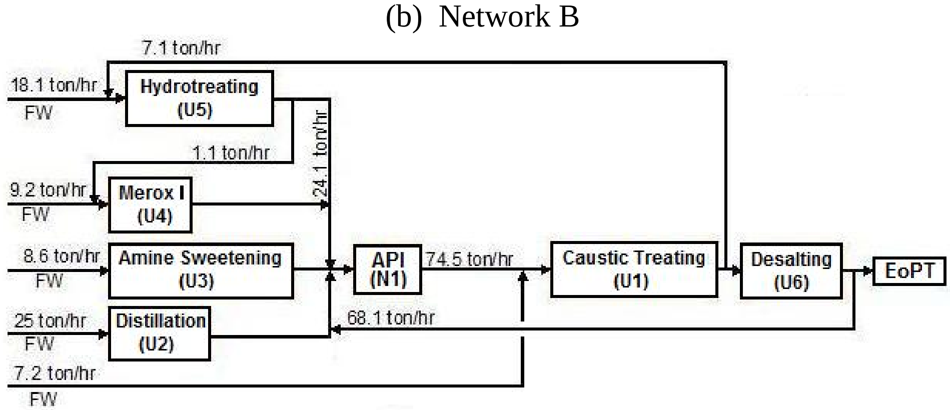
Figure 3.25 shows the regeneration capacities needed as function of the freshwater consumption of the networks previously found. The only regeneration process that is always used through the whole range of freshwater usage is the end-of-pipe treatment. API separator is used up to 120 t/h freshwater consumption (networks A to E), the reverse osmosis up to about 66 t/h (networks A and B) and the Chevron wastewater treatment is used only by network A (up to approximately 40 t/h). Note that only an extremely small capacity of Chevron treatment is needed, what is not acceptable in practice. As another option in which the total cost does not significantly increase, network B can be considered.



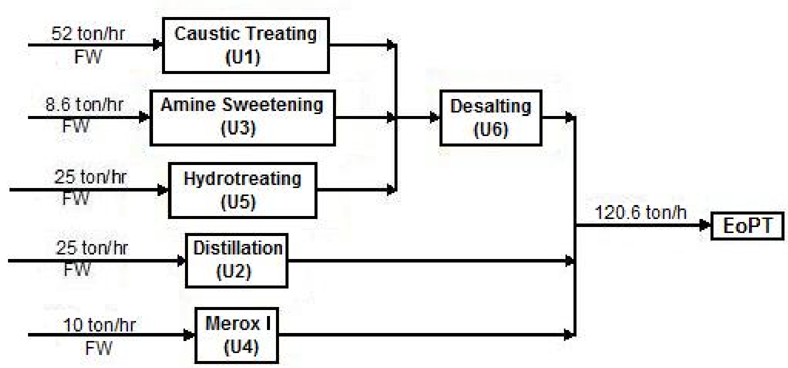
(a) Network A



(b) Network B



(c) Network C



(d) Network F

Figure 3.25 – Selected networks from Table 3-11.

The FCI of the networks presented in Figure 3.23 as function of the freshwater flowrate is presented in Figure 3.26. The discontinuities of the curves are caused by the different piping configurations, and the curvatures are due to the different regeneration capacities for each fixed freshwater consumption.

Figure 3.27 shows minimum NPC of those networks for different rates of discount as function of freshwater consumption. Note the optimum solution depends on the discount rate applied. At a 10% discount rate network A is the optimum solution. However, for rates of discount of 15% or 20%, the network B presents the lowest NPC.

Figure 3.28 shows the minimum NPC for a rate of discount of 10% of each network as function of FCI. The freshwater consumption where the minimum NPC happens is also presented in the graph.

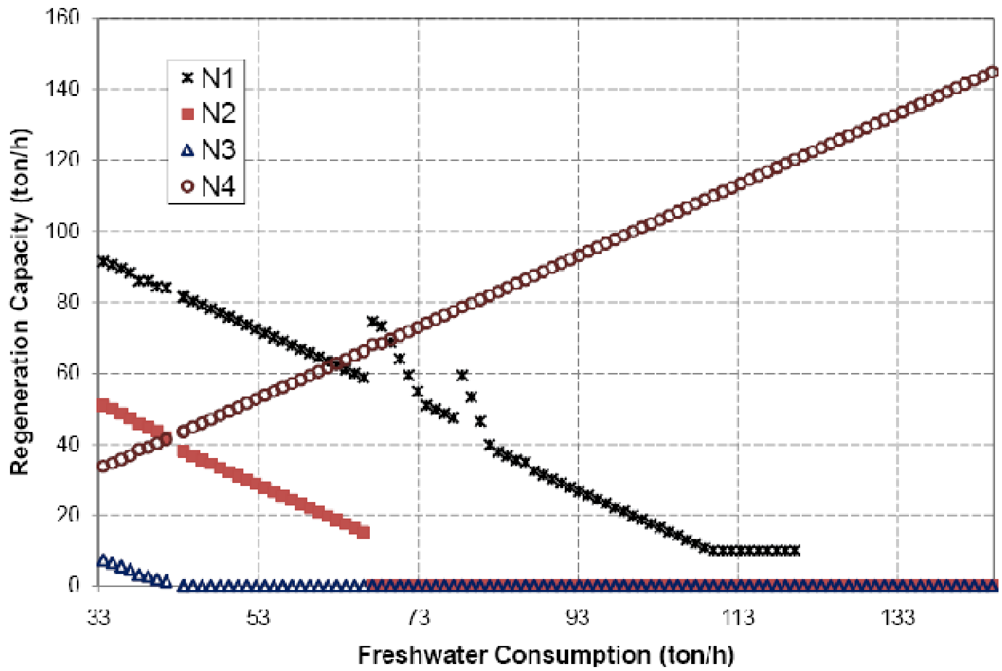


Figure 3.26 – Regeneration capacities as a function of freshwater flowrate for the grassroots case of the multi contaminant example.

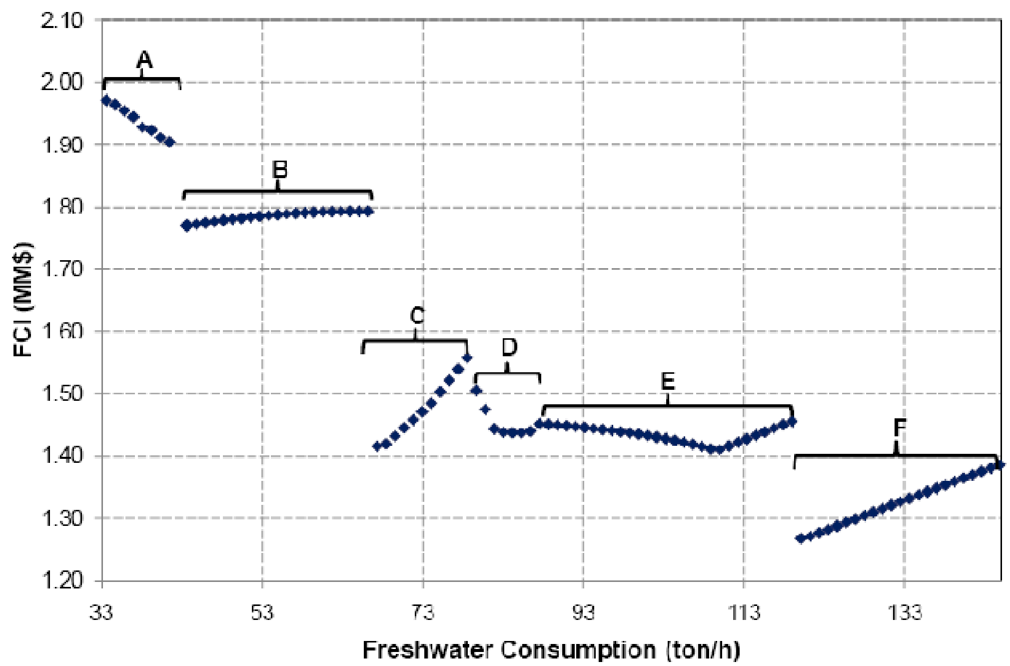


Figure 3.27 – FCI as a function of freshwater flowrate for the grassroots case of the multi contaminant example.

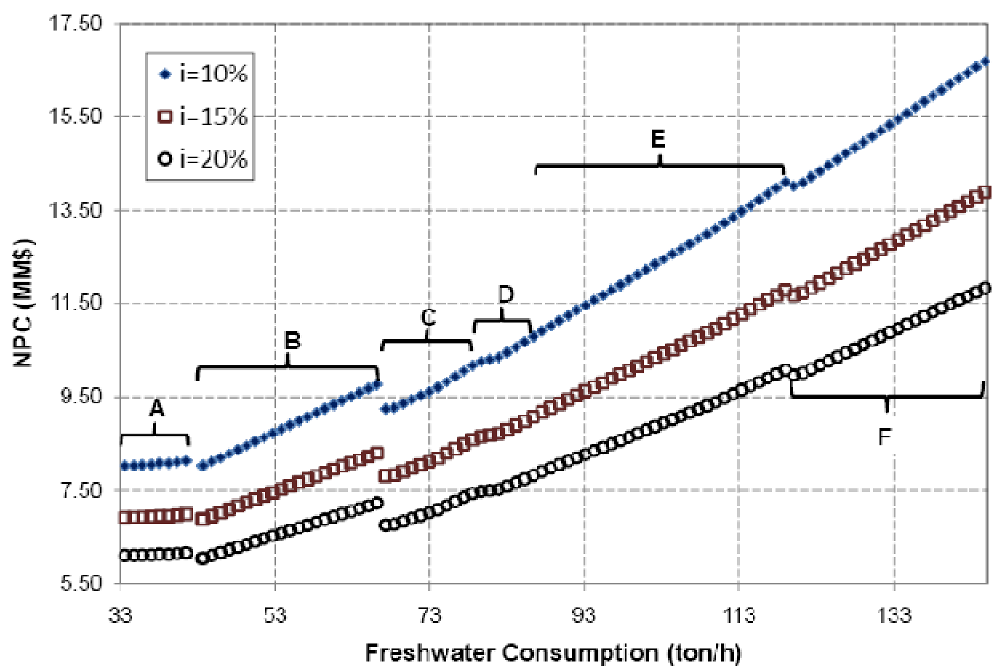


Figure 3.28 – NPC as a function of freshwater flowrate for the grassroots case of the multi contaminant example.

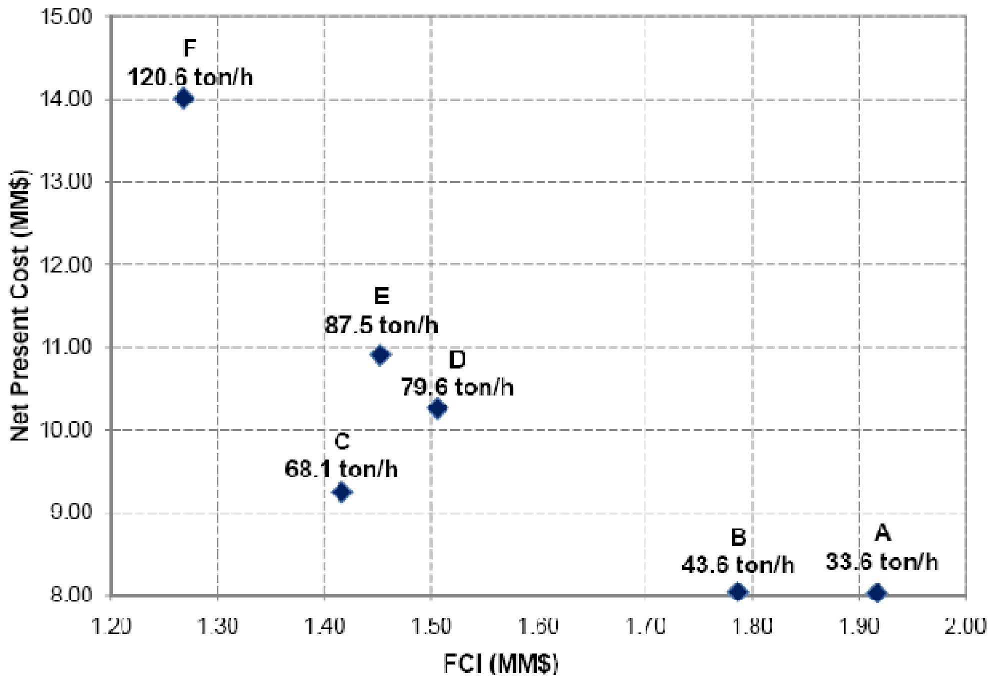


Figure 3.29 – NPC as a function of FCI for the grassroots case of the multi contaminant example (for rate of discount of 10%).

The return on extra investment is analyzed next. Network G features the minimum FCI operating at its minimum freshwater consumption (120.1 t/h). This network has a FCI of $1,267,987 and an annualized total cost of $2,200,590. Using this network as reference, the ROEI vs. freshwater consumption is calculated using Equation 3-23 and the solution is presented in Figure 3.29. Note that network G generates a negative ROEI. From the ROEI perspective, network C is the optimum solution when it is designed for a freshwater consumption of 68.1 t/h, which has an API regeneration process with capacity for 74.5 t/h.

A summary of the results for the multi contaminant example is presented in Table 3-12. Costs correspond to minimum freshwater consumption when the network is optimum. Network C has the highest ROEI (540%) when designed for a freshwater consumption of 67.3 t/h. The optimum solutions of each criterion are bolded.

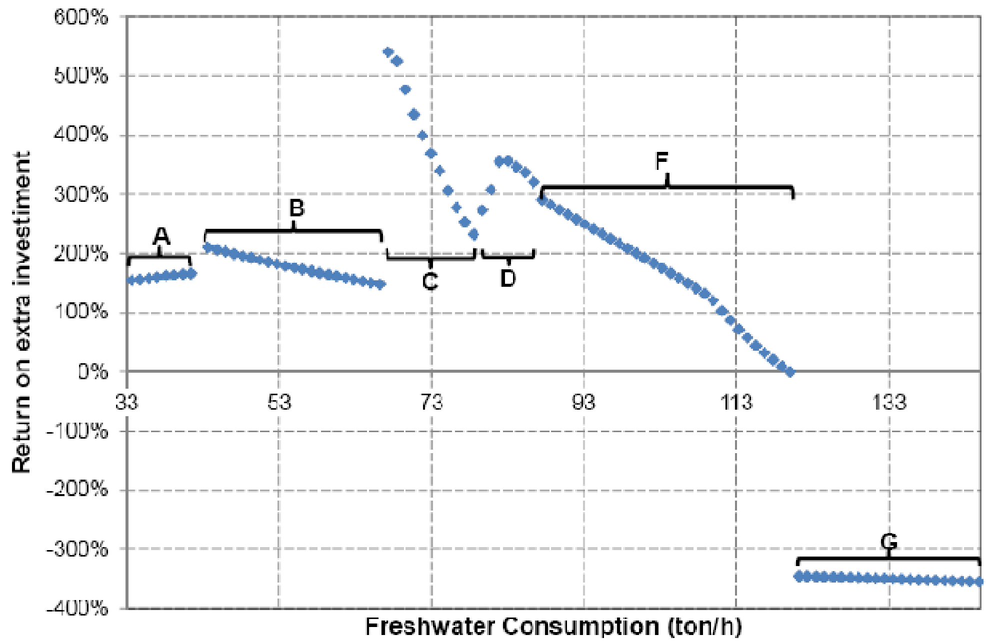


Figure 3.30 – Savings as a function of freshwater flowrate for the grassroots case of the multi contaminant example.

Table 3-12 – Summary of results for the multi contaminant case.

Network	Freshwater Consumption	FCI	Total Cost	NPC	ROEI
A	33.6 t/h	$1,917,204	$1,182,217	$8,024,198	155%
B	43.6t/h	$1,770,753	$1,194,671	$8,039,440	210%
C	68.1 t/h	$1,415,986	$1,415,986	$9,246,542	540%
D	79.6 t/h	$1,505,614	$1,575,265	$10,259,802	273%
E	87.5 t/h	$1,452,112	$1,683,807	$10,906,119	291%
F	120.6 t/h	$1,267,987	$2,200,590	$14,010,534	Reference

3.6. Conclusions

This chapter presented a methodology to perform the grassroots design and retrofit of water/wastewater systems based on mathematical optimization and profitability insights. The results point some important conclusions: Targeting maximum savings (or total annualized cost) does not necessarily generate the most profitable solution. In addition, different measurements for profitability can give different solutions. Moreover, when NPV is used as the measurement, the used discount rate can alter the optimum solution.

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4. WATER SYSTEMS CORRECT STRUCTURES

This chapter discusses the definition of the water/wastewater allocation problem as it was originally defined by Takama et al. (1980), how this concept was modified, and sometimes simplified through time, as well as additional issues that were still not properly addressed. Different architectures and assumptions used to model water system are discussed, a modification is suggested and the impact of proper modeling is investigated. A modified mathematical model is then presented.

4.1. Overview

Takama *et al.* (1980) discussed the architecture of the WAP and they made sure to include a wastewater treatment system and discharge concentration limits. Moreover, their model considers that a recycle of the water treated by these treatment units can be used to feed the water-using units. Later, Wang and Smith (1994), the work that gave rise to the "water pinch" method, ignored the discharge limits requirements. Thus, to comply with these requirements an implicit End-of-Pipe treatment (EoPT) had to be assumed. Because Wang and Smith (1994) only implicitly assumed it (it is not part of the model), they did not consider discussing the reuse and/or recycle of the stream treated by the EoPT. Several subsequent papers (Doyle and Smith, 1997; Polley and Polley, 2000; Bagajewicz et al., 2000; Hallale, 2002; Koppol et al., 2003; Prakotpol and Srinophakun, 2004; Teles *et al.*, 2008), including the review made by Bagajewicz (2000), have also omitted using discharge concentration limits, implicitly assuming that the End-of-pipe-

Treatment is able to bring the concentration of the contaminants down to these discharge limits. In addition, many of these papers used the regeneration processes as means of reducing freshwater consumption, but none explicitly assumed that an EoPT was present and its treated stream could be reused/recycled. This is the first issue investigated in this chapter.

Aside from these methodologies that model the units as mass exchangers, Gabriel and El-Halwagi (2005) used a source-sink model (El-Halwagi and Spriggs, 1998) in which “interceptors” were included to act as regeneration processes. They assumed that each interceptor could receive water from only one source, that is, that there is no mixing before interception. This assumption allowed discretizing the efficiency of each interceptor as function of the source only, something that rendered a linear model. In reality, the efficiency of each interceptor should be discretized as also function of possible range of concentration when sources are mixed, but this was not included in their model.

Much in the same way as it was suggested by Takama et al. (1980), it can be argued that if an end-of-pipe treatment has to be part of the water system, then its effluent should also be available as an option for reuse/recycle. *In fact, there is no water system without any kind of regeneration process (even those that were classified as “end-of-pipe”). Thus, all water allocation problems must at least include one treatment unit in which its treated stream can be reused/recycled.* When discussing regeneration, other articles (Takama *et al*., 1980; Wang and Smith, 1994; Kuo and Smith, 1998; Koppol *et al*., 2003; Gunaratnam *et al*., 2005; Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007; Ng *et al*., 2007a,b; Putra and Amminudin, 2008, among others) touch on this issue but do not explicitly come with this conclusion. Because of the lack of a discussion of the effect of implicitly assuming the EoPT and consequently ignoring a recycle from it, there is no established knowledge, rule, as of when this practice is appropriate, and when it is not. In this chapter, the intricacies and consequences of ignoring the existence of at least one end-of-pipe treatment (and consequently the reuse/recycle of the stream treated by it) and the different architectures the WAP problem models should be based on are discussed.

Then, a second issue is point out regarding appropriate modeling. Most of the papers, including Takama *et al.* (1980), have assumed that one source of freshwater was available, usually with zero contaminant concentration, and have not included the pre-treatments used to bring the freshwater to such quality. Occasionally, multiple sources of different contaminant concentration are mentioned, but rarely their use is discussed in detail, much less modeled.

Freshwater is usually sequentially processed in different pre-treatment units, some producing freshwater of stringent purities (like boiler water), and some producing water with less stringent qualities. However, to have a complete structure, the pre-treatment should be included when modeling the WAP. This system does not have to be necessarily a sequential set of treatment units where water of different quality is drawn from intermediate units, but it could be a distributed and/or decentralized system. Both the wastewater treatment system and the pre-treatment have to be modeled assuming a distributed configuration. Because the addition of these pre-treatment units has not been explicitly included in the WAP previously, the impact of considering it is discussed.

Finally, in addition to allowing water from the wastewater treatments (regeneration and/or EoPT) to be recycled to the water-using units, one could additionally include interaction with the pre-treatment units. Ultimately, it can be said that only when complete decentralization of the system is allowed, one is sure that the global optimum of the system is achieved, although such global optimum may feature centralized solutions. Moreover, when seeking zero liquid discharge cycles, this is the appropriate route to adopt. Indeed, it will be shown in the examples that some consumption targets presented in the literature are not true anymore if pre-treatment units are included. Even if only one pre-treatment is considered, and its output is a stream free of contaminants, water from any water-using unit could be recycled back to the pre-treatment to reduce the amount of freshwater needed. What determines how much smaller freshwater usage can be achieved are the constraints at the inlet of this pre-treatment unit (maximum allowed inlet concentrations and/or pre-treatment capacity). If these constraints allow this pre-treatment process receive some amount of water from any other process, this will reduce the minimum consumption.

4.2. Water Systems Architectures

A *Complete Water System* (CWS) in process plants is typically composed of three subsystems (water pre-treatment, water-using and wastewater treatment). A conventional, sequentially ordered, non-integrated CWS is shown in Figure 4.. Note that freshwater is treated in different units in a sequential manner, lowering the concentration of key contaminants after each treatment. All units receive freshwater of a quality that corresponds to its maximum inlet concentration and therefore, the corresponding water is taken after each treatment. For example, WU3 may be a steam consumer and WPT3 could be a boiler preceded by a boiler-feed treatment unit. In turn, WU4 could be a scrubbing unit that does not require boiler quality water and WU1, WU2 could be units that have less stringent quality requirements, like for example, desalters. In some cases, freshwater, purchased or taken from natural sources can be directly used. This is illustrated by unit WU5.

Another feature of the current architecture is that all wastewaters are mixed and sent to EoPT, which is usually sequential, as indicated. Water is cleaned to below discharge limits and usually not recycled.

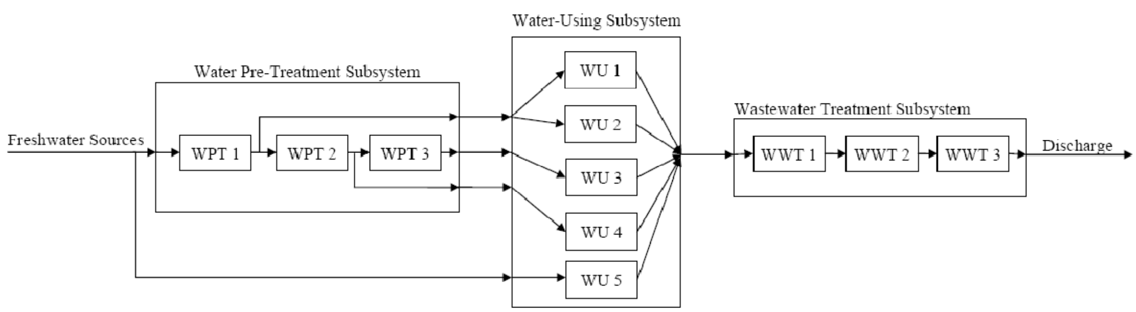

Figure 4.1 - Typical complete water system in process plants.

The WAP can be modeled in various forms depending on:

- The boundaries of the problem (i.e., which subsystems are considered and where are their boundaries),
- The architecture of the subsystems (i.e., how their units are arranged: in series, parallel, distributed, etc).
- Whether the recycle and reuse within subsystems is or isn’t allowed.
- Whether the recycle between subsystems is or isn’t allowed
- The level of detail of the model (fixed loads vs. variable loads, fixed vs.

variable flowrates through the units, etc.) and,

- The nature of the objective function.

The simplest form of the problem is simply a freshwater fed and the water-using subsystem followed by an assumed end-of-pipe treatment to adjust the wastewater to the discharge limits. This simplified version of water system is presented in Figure 4.2. The problem solved using this definition of the WAP is the one limited by the dashed line. Inside this line all the possible reuses among the water-using units are allowed. Here, the wastewater subsystem is treated as a single EoPT, which is not part of the optimization problem but has to exist to bring the contaminants concentration down to the discharge limits. This is the first problem addressed by the popular technology called "water pinch" (Wang and Smith, 1994), which is very useful when a single component is assumed, and several other methods (Doyle and Smith, 1997; Polley and Polley, 2000; Bagajewicz *et al*, 2000; Savelski and Bagajewicz, 2003; Teles *et al*, 2008;, among others), some also used for the multicontaminant case. The objective is usually not cost, but freshwater consumption.

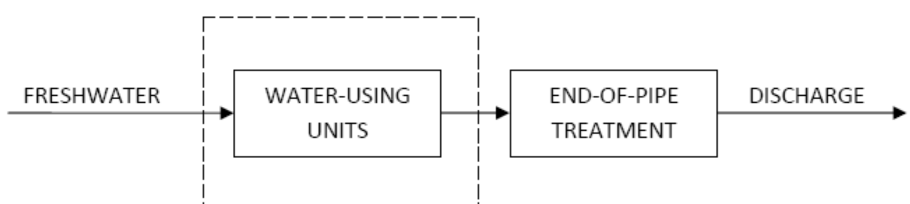

Figure 4.2 - Water-using units with an implicit end-of-pipe treatment.

Wang and Smith (1994) also discussed the possibility of having regeneration processes, but they did not include a discharge limit. Thus they implicitly assumed that an end-of-pipe treatment would help reaching these limits. We illustrate this system in Figure 4.3. In this case the interaction of the water-using units and some regeneration processes are allowed through three different options, reuse, regeneration-reuse and regeneration recycle. As in Wang and Smith (1994), several subsequent papers (Doyle and Smith, 1997; Polley and Polley, 2000; Bagajewicz et al., 2000; Koppol et al., 2003; Prakotpol and Srinophakun, 2004; Teles et al., 2008; among others) have also used this implicit end-of-pipe treatment assumption.

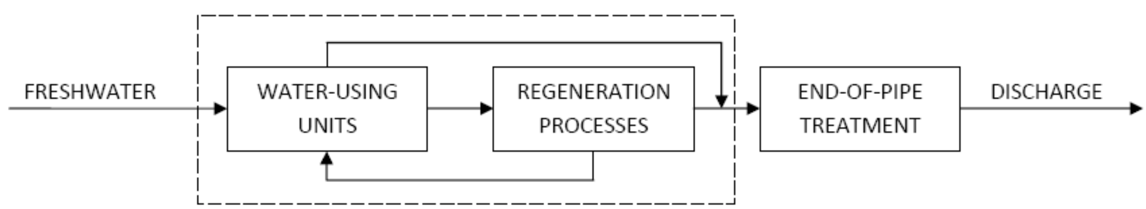

Figure 4.3 - Water-using units and regeneration processes with an implicit end-of-pipe treatment.

Thus, in its simplest form, the problem does not explicitly consider re-using the water that is ready for discharge. It is worth pointing out, however, that the seminal paper of the water management problem (Takama et al., 1980) had already included such a recycle when they introduced the existence of a wastewater treatment subsystem and added discharge limits to the whole system. They state that the system showed in Figure 4.4 is a typical system used in refineries and is formed by two subsystems, water-using subsystem and wastewater treating subsystem, which are often individually optimized regardless of the interaction introduced by the recycle. In reality, their definition of the wastewater subsystem together with the addition of discharge limits integrates all the possibilities of regeneration without clearly defining or singling out specifically an end-of-pipe treatment. In other words, this definition considers that the regeneration processes and the end-of-pipe treatment are part of a unique subsystem called wastewater treatment. Additionally, note that their system does not consider the existence of a water pre-treatment subsystem.

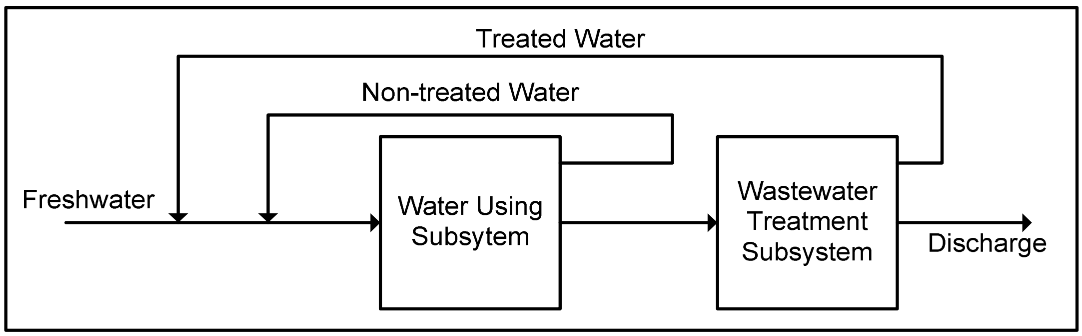

Figure 4.4 - Independently distributed freshwater and wastewater networks (Following Takama et al., 1980).

Thus, when considering only these two subsystems, Takama *et al.* (1980) suggest their integration in a *total system* (or *integrated system*). Their model handled the water-using units and wastewater treatment processes assuming a decentralized model, one that has no subsystem boundaries. Although their model allows connections from any process (water-using or treatment units) to any other process, the solution they presented did not show any recycle from a regeneration unit to a water using process. The solution to their example has a water reuse subsystem followed by a wastewater treatment subsystem that is distributed.

Later, Kuo and Smith (1998) reminded of the importance of the interaction between water-using units, regeneration processes and effluent treatment system. They presented an improvement of Wang and Smith's (1994) method, which had only considered the interaction between water-using units and regeneration processes. On the other hand, some authors (Gunaratnam *et al*., 2005; Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007; Ng *et al*., 2007a,b; Putra and Amminudin, 2008) have used the structure proposed by Takama *et al*. (1980) to solve the multiple component WAP, that is, they solved the problem that is often called *total water system*.

The use of the stream treated by the end-of-pipe treatment (or the addition of discharge limits) starts to play an important role not only from the freshwater consumption point of view, but also from the cost of the whole system point of view. Increasing freshwater costs, declining of water quality in the available freshwater sources and costs ratio between end-of-pipe treatment and intermediate regeneration processes can influence the trade-offs of recycling the stream treated by the end-of-pipe treatment. End-of-pipe treatment recycling can also show enormous advantages when retrofit projects are analyzed. For this case an end-of-pipe treatment already exists and therefore eventually no or very small capital cost is required.

As we stated above, Takama *et al.* (1980) consider the *total water system*, which the water-using units and wastewater treatment processes individually interact. However the way the subsystems interact is also important and different subsystems structures may be preferred for technical and/or layout issues. The discussion of some of these possibilities is presented next using the water system structure presented by Takama et al. (1980): Water-using subsystem and wastewater subsystem (Figure 4.4).

First, let us consider a water-using subsystem and a centralized/sequential wastewater treatment subsystem with a recycle of water that complies with discharge limits (Figure 4.5). In fact, this is the problem that should be solved when only water-using units are optimized. Note that the wastewater treatment subsystem is here understood as a single system (that could be what was previously called end-of-pipe treatment), but now the recycle of the discharge stream is allowed.

Figure 4.6 shows a centralized/distributed wastewater treatment subsystem. In both centralized cases, the centralization is more than geographical: it includes collecting all wastewaters and mixing them in one single stream before treatment.

As an alternative, one can envision a centralized and distributed wastewater treatment subsystem in the sense that no mixing of all wastewaters takes place and multiple streams feed it. This is shown in Figure 4.7.

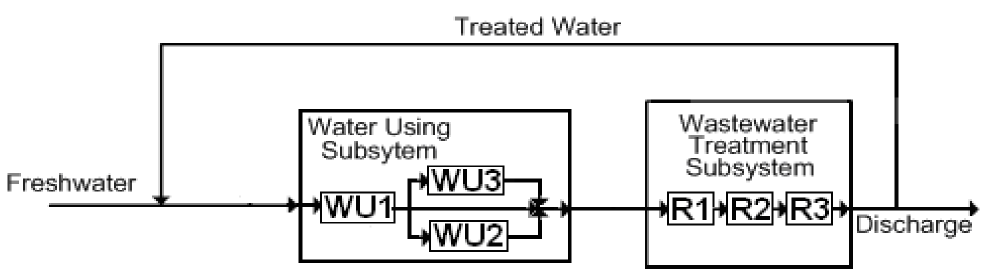

Figure 4.5 - Water Reuse and Sequential Centralized Treatment System.
(WU: water using unit; R: regeneration unit)

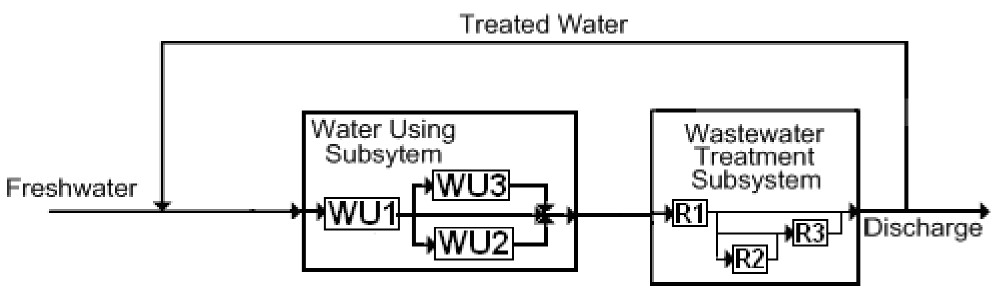

Figure 4.6 - Water Reuse and End-of-pipe Distributed Centralized Treatment System.
(WU: water using unit; R: regeneration unit)

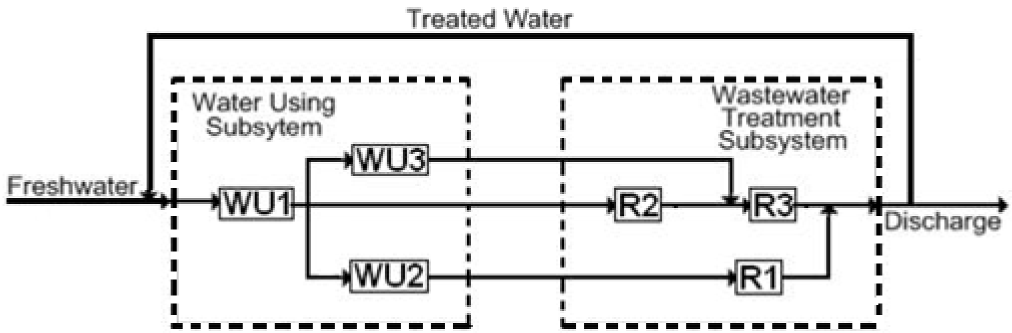

Figure 4.7 - Water Reuse and Distributed Centralized Treatment System.
(WU: water using unit; R: regeneration unit)

Finally, Figure 4.8 shows a completely decentralized wastewater treatment subsystem, which is often called as *integrated system* (or *total water system*). Note that allowing flows from any treatment unit in Figure 4.7 to be recycled is equivalent to the system of Figure 4.8. In the limit, Figure 4.8 can be a zero-liquid discharge cycle. These are extensions of the classification proposed by Bagajewicz (2000).

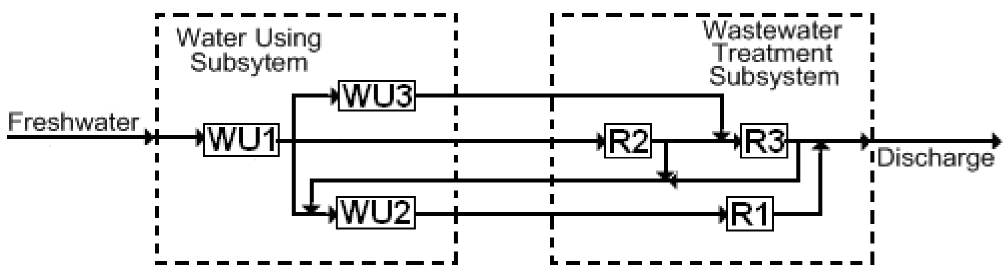

Figure 4.8 - Water Reuse and Decentralized Water/Wastewater System (integrated system).
(WU: water using unit; R: regeneration unit)

However, to achieve zero-liquid discharge cycle in the type of system presented in Figure 4.8, which is the most general case presented so far in the literature (including the model presented by Takama et al., 1980), one needs to achieve certain conditions:

- Every contaminant in all water-using units must have the maximum inlet concentration higher than the freshwater source with the lowest concentrations, and/or;

- Regeneration processes should be able to bring the concentration of the contaminants down to at least the lowest maximum inlet concentration among the water-using units.

These are conditions that are not often seen in the WAP. Current models often assume only the highest quality of freshwater available. Even when other qualities are assumed, the pre-treatment processes producing the available freshwater are not considered. This is a very important opportunity when zero-liquid discharge is targeted. Note that pre-treatment processes exist in the water pre-treatment subsystem shown in Figure 4. and they are responsible for producing freshwater at different qualities. When considering the *complete water system*, the water pre-treatment subsystem can receive water/wastewater from the water-using subsystem and/or from the wastewater treatment subsystem. Indeed, Figure 4.9a shows the architecture as it is understood nowadays, and Figure 4.9b shows the proposed architecture. This new architecture allows the used water to pass through the pre-treatment again and so comply with the quality required by some (or all) of the water-using units. *This is how the zero-liquid discharge cycle can be more easily identified*.

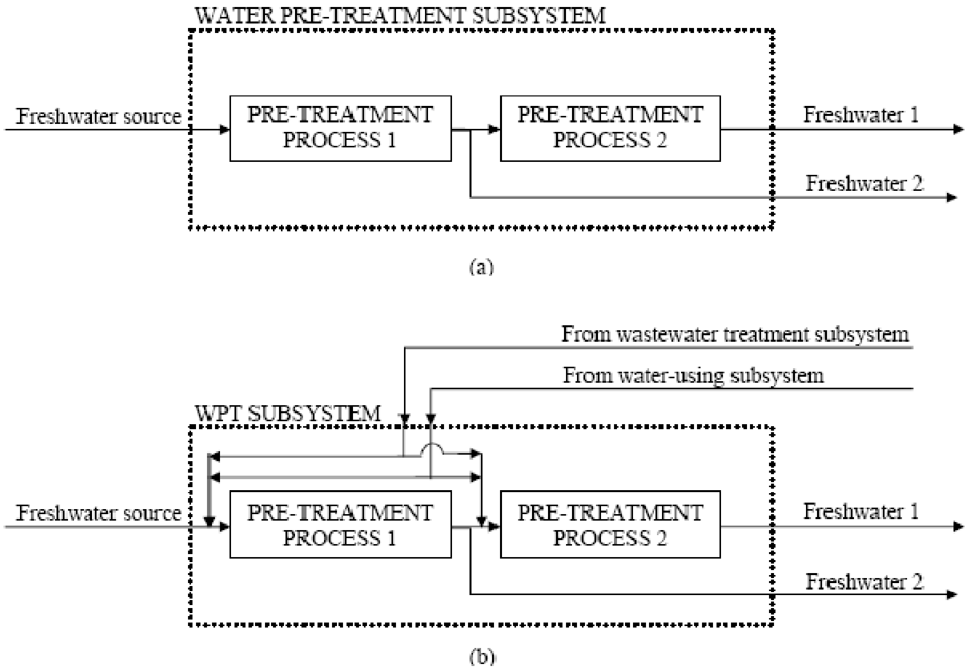

Figure 4.9 - a - Water pre-treatment subsystem sequential scheme; b – Recycles to the water pre-treatment subsystem.

Figure 4.10 shows the different definitions of the water allocation problem in relation to the boundary assumed for the analysis of the whole system, the architecture of each subsystem and the interaction among the subsystems. In other words, each of the subsystems can exhibit different options of reuse/recycle among their own units (or processes), i.e. they can be distributed systems within their own boundaries.

Figure 4.10a represents the optimization of the water-using subsystem only. This corresponds to the architecture presented in Figure 4.2. Thus, one could state this problem as follows:

Given a set of water-using units, a set of freshwater sources with corresponding contaminant concentrations (some usually zero), one wants to obtain a water-using network that optimizes a given objective (freshwater consumption, cost, etc.)

Figure 4.10b represents the optimization of the water using and treatment subsystems simultaneously. This is similar to the architectures presented in Figure 4.3 and Figure 4.4. In the first case (Figure 4.3), discharge limits are not imposed and the problem could be stated as follows:

Given a set of water-using units, a set of freshwater sources with corresponding contaminant concentrations (some usually zero) and potential intermediate regeneration processes, one wants to obtain a water-using/wastewater treatment system network that optimizes a given objective (freshwater consumption, cost, etc.)

For the case presented in Figure 4.4 we would have the following definition:

Given a set of water-using units, a set of freshwater sources with corresponding contaminant concentrations (some usually zero), potential intermediate regeneration processes and/or a wastewater end-of-pipe treatment unit, one wants to obtain a water-using/wastewater treatment system network that complies with the discharge limits and optimizes a given objective (freshwater consumption, cost, etc.)

Note that in this later case, discharge limits are imposed and the regeneration processes are not used only for reuse/recycle purpose but also to condition the wastewater stream to be discharged. In the literature, the dotted box around the water using and water treatment subsystem presented in Figure 4.10b is known and *total water system*. As stated above, this was solved by Gunaratnam *et al*., 2005; Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007; Putra and Amminudin, 2008, using different methodologies and assumptions.

Although all these definitions of the problem state that a set of freshwater sources is available, the issue of having more than one freshwater quality sources with different processes associated to them has not been studied yet. In fact, we can define these different freshwater qualities as part of another subsystem: the water pre-treatment subsystem. The addition of this subsystem has not been investigated and can generate further trade-offs in the water allocation problem and consequently new opportunities. Figure 4.10c exemplifies the suggested new water allocation problem structure that we believe should be solved to completely include all the possibilities of water integration. Thus, this problem can be stated as follows:

Given a set of water pre-treatment processes with corresponding their corresponding specifications, a set of water-using units, potential intermediate regeneration processes and/or a set of wastewater treatment units, one wants to obtain a water system network that complies with the discharge limits and optimizes a given objective (freshwater consumption, cost, etc.)

As in the wastewater treatment subsystem, both capital and operating cost are associated to the existence and capacity of water pre-treatments that determine the availability of each quality of freshwater. One of the reasons for omitting this subsystem is the fact that such analysis only becomes relevant when cost is considered as an objective. Otherwise, when freshwater consumption is the target, the source with highest quality (that is, lowest contaminant concentration) is the preferred one and this issue becomes irrelevant. It is also important to note here that the different freshwater sources are not only competing with each other, but they are competing with water reuse and/or recycles from regeneration processes.

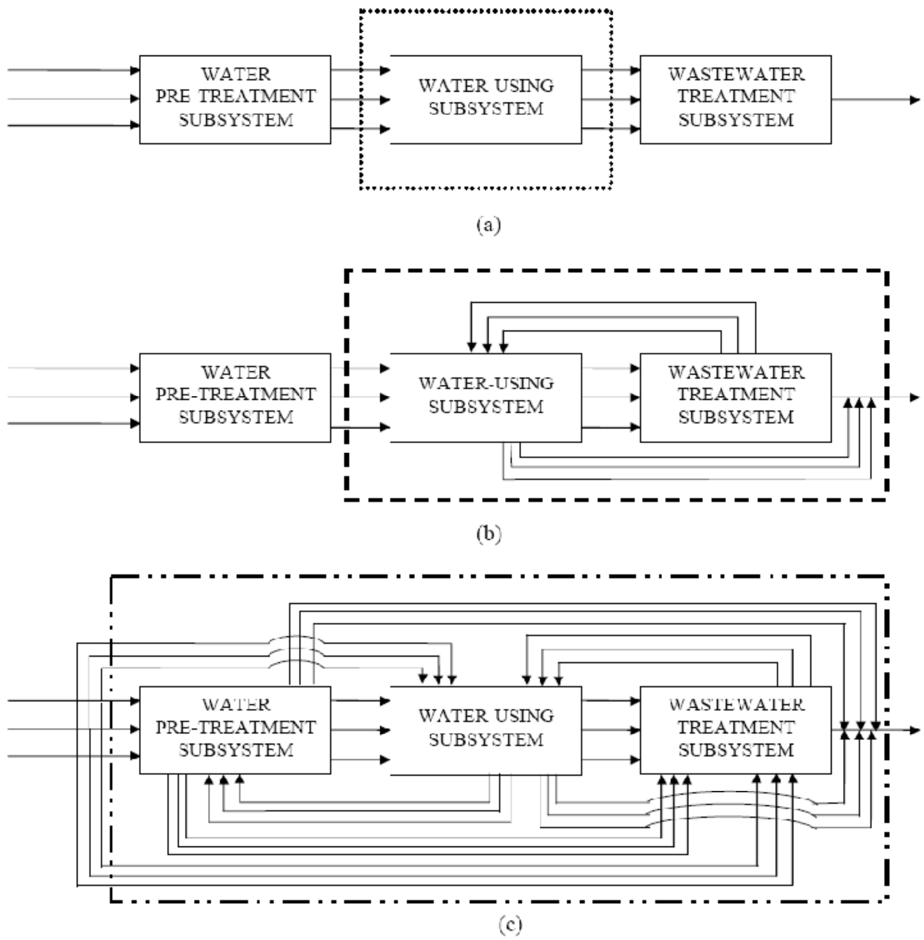

Figure 4.10 - Evolution of water allocation problem regarding the boundary of the water system (a – Optimization of the water-using subsystem; b – Optimization of the water-using/wastewater treatment subsystems; c – Optimization of the complete water system).

In conclusion, it can be said that the complete integration of water system is obtained breaking the boundaries of the subsystems and making use of all available regeneration processes, including the ones available in the water pre-treatment system. This follows the same idea of the *total water system* (or *integrated system*) previously discussed, but now we include the water pre-treatment subsystem to generate a *complete integrated water system*.

4.3. Mathematical Model of the *Complete Integrated Water System*

Based on the *complete integrated water system* structure previously discussed, a modified mathematical model is proposed to describe the WAP. Aside from the inclusion of the water pre-treatment sub-system, this model is well known and uses simple model to describe the water-using units and the regeneration processes. Later, the issue of proper modeling these units/processes is discussed.

A general non-liner model to solve the water allocation problem is given by the following set of equations:

Water balance at the water-using units

$$\sum_{w} FWU_{w,u} + \sum_{u^*} FUU_{u^*,u} + \sum_{r} FRU_{r,u} = \sum_{s} FUS_{u,s} + \sum_{u^*} FUU_{u,u^*} + \sum_{r} FUR_{u,r} \qquad \forall u \tag{4-1}$$

where $FWU_{w,u}$ is the flowrate from freshwater source *w* to the unit *u*, $FUU_{u^*,u}$ is the flowrates between units *u** and *u*, $FRU_{r,u}$ is the flowrate from regeneration process *r* to unit *u*, $FUS_{u,s}$ is the flowrate from unit *u* to sink *s* and $FUR_{u^*,r}$ is the flowrate from unit *u* to regeneration process *r*.

Water balance at the regeneration processes

$$\sum_{w} FWR_{w,r} + \sum_{u} FUR_{u,r} + \sum_{r^*} FRR_{r^*,r} = \sum_{u} FRU_{r,u} + \sum_{r^*} FRR_{r,r^*} + \sum_{s} FRS_{r,s} \qquad \forall r \tag{4-2}$$

where $FWR_{w,r}$ is the flowrate from freshwater source *w* to the regeneration process *r*, $FRR_{r^*,r}$ is the flowrate from regeneration process *r** to regeneration process *r* and $FRS_{r,s}$ is the flowrate from regeneration process *r* to sink *s*. In fact, we assume here that the set of regeneration processes existing in the system is formed by the set of water pre-treatments and the set of wastewater treatments. If one wants to differentiate between these two categories of regeneration processes, two subsets for the regeneration processes set can be easily created and different constraints applied to each subset.

Contaminant balance at the water-using units

$$\left.\begin{aligned}&\sum_{w}\left(CW_{w,c}\ FW_{w,u}\right)+\sum_{u^*}\left(FUU_{u^*,u,c}C^{out}_{u^*,c}\right)+\sum_{r}\left(FRU_{r,u,c}CR^{out}_{r,c}\right)+\Delta M_{u,c}\\&\qquad=\sum_{u^*}\left(FUU_{u,u^*,c}C^{out}_{u,c}\right)+\sum_{s}\left(FUS_{u,s,c}C^{out}_{u,c}\right)+\sum_{r}\left(FUR_{u,r,c}C^{out}_{u,c}\right)\qquad\forall u,c\end{aligned}\right\} \tag{4-3}$$

where $CW_{w,c}$ is concentration of contaminant c in the freshwater source w, $\Delta M_{u,c}$ is the mass load of contaminant c extracted in unit u, $C^{out}_{u,c}$ is the outlet concentration of contaminant c in unit u, and $CR^{out}_{r,c}$ is the outlet concentration of the not treated contaminant c in regeneration r .

Maximum inlet concentration at the water-using units

$$\left.\begin{aligned}&\sum_{w}\left(CW_{w,c}\ FW_{w,u}\right)+\sum_{u^*}\left(FUU_{u^*,u,c}C^{out}_{u^*,c}\right)+\sum_{r}\left(FRU_{r,u,c}CR^{out}_{r,c}\right)\\&\qquad\le C^{in,max}_{u,c}\left(\sum_{w}FUW_{w,u}+\sum_{u^*}FUU_{u^*,u}+\sum_{r}FRU_{r,u}\right)\qquad\forall u,c\end{aligned}\right\} \tag{4-4}$$

where $C^{in,max}_{u,c}$ is the maximum allowed concentration of contaminant c at the inlet of unit u.

Maximum outlet concentration at the water-using units

$$C^{out}_{u^*,c}\le C^{out,max}_{u,c}\quad\forall u,c \tag{4-5}$$

where $C_{u,c}^{out,max}$ is the maximum allowed concentration of contaminant *c* at the outlet of unit *u*.

Flowrate through the regeneration processes

$$FR_r = \sum_w FWR_{w,r} + \sum_u FUR_{u,r} + \sum_{r^*} FRR_{r^*,r} \quad \forall r \tag{4-6}$$

where FR_r is the flowrate through the regeneration process *r*.

Contaminant balance at the regeneration processes

$$FR_{r,c} CR_{r,c}^{in} = \sum_w \left(FWR_{w,r} CW_{w,c} \right) + \sum_u \left(FUR_{u,r} C_{u,c}^{out} \right) + \sum_{r^*} \left(FRR_{r^*,r} CR_{r^*,c}^{out} \right) \quad \forall r, c \tag{4-7}$$

$$CR_{r,c}^{out} = CR_{r,c}^{in} (1 - XCR_{r,c}) + CRF_{r,c}^{out}\ XCR_{r,c} \quad \forall r, c \tag{4-8}$$

where $CR_{r,c}^{in}$ is the concentration of contaminant *c* at the inlet of regeneration process *r*, $CRF_{r,c}^{out}$ is the outlet concentration of contaminant *c* in regeneration process *r* and $XCR_{r,c}$ is a binary parameter that indicates if contaminant *c* is treated by regeneration process *r*. We assume that $CRF_{r,c}^{out}$, the concentration of the treated contaminant is known and constant.

Maximum inlet concentration of the regeneration processes

$$CR_{r,c}^{in} \leq CR_{r,c}^{in,max} \quad \forall r, c \tag{4-9}$$

where $CR_{r,c}^{in,\max}$ is the maximum concentration of contaminant *c* allowed at the inlet of regeneration process *r*.

Maximum allowed discharge concentration

$$\sum_u \left(FUS_{u,s,c} C_{u,c}^{out} \right) + \sum_r \left(FRS_{r,s,c} CR_{r,c}^{out} \right) \le C_{s,c}^{discharge,max} \left(\sum_u FUS_{u,s} + \sum_r FRS_{r,s} \right) \quad \forall s,c \quad (4\text{-}10)$$

where $C_{s,c}^{discharge,max}$ is the maximum allowed concentration at sink *s*.

Minimum flowrates

It is well known that many solutions of the water problem may include small flowrates that are impractical. To avoid these we use the following constraints:

$$FWU_{w,u} \ge FWU_{w,u}^{Min} \, YWU_{w,u} \quad \forall w,u \qquad (4\text{-}11)$$

$$FWR_{w,r} \ge FWR_{w,r}^{Min} \, YWR_{w,r} \quad \forall w,r \qquad (4\text{-}12)$$

$$FUU_{u,u*} \ge FUU_{u,u*}^{Min} \, YUU_{u,u*} \quad \forall u,u* \qquad (4\text{-}13)$$

$$FUS_{u,s} \ge FUS_{u,s}^{Min} \, YUS_{u,s} \quad \forall u,s \qquad (4\text{-}14)$$

$$FUR_{u,r} \ge FUR_{u,r}^{Min} \, YUR_{u,r} \quad \forall u,r \qquad (4\text{-}15)$$

$$FRU_{r,u} \ge FRU_{r,u}^{Min} \, YRU_{r,u} \quad \forall r,u \qquad (4\text{-}16)$$

$$FRR_{r,r*} \ge FRR_{r,r*}^{Min} \, YRR_{r,r*} \quad \forall r,r* \qquad (4\text{-}17)$$

$$FRS_{r,s} \ge FRS_{r,s}^{Min} \, YRS_{r,s} \quad \forall r,s \qquad (4\text{-}18)$$

which uses a set of binary variables ($YWU_{w,u}$, $YWR_{w,r}$ $YUU_{u,u*}$, $YUS_{u,s}$, $YUR_{u,r}$, $YRU_{r,u}$, $YRR_{r,r*}$ and $YRS_{r,s}$) that are equal to one when the corresponding flowrate is different from zero and zero otherwise.

Maximum flowrates

To ensure that the connections do not surpass maximum values, we use the following constraints:

$$FWU_{w,u} \le FWU_{w,u}^{Max}\, YWU_{w,u} \quad \forall w,u \tag{4-19}$$

$$FWR_{w,r} \le FWR_{w,r}^{Max}\, YWR_{w,r} \quad \forall w,r \tag{4-20}$$

$$FUU_{u,u*} \le FUU_{u,u*}^{Max}\, YUU_{u,u*} \quad \forall u,u* \tag{4-21}$$

$$FUS_{u,s} \le FUS_{u,s}^{Max}\, YUS_{u,s} \quad \forall u,s \tag{4-22}$$

$$FUR_{u,r} \le FUR_{u,r}^{Max}\, YUR_{u,r} \quad \forall u,r \tag{4-23}$$

$$FRU_{r,u} \le FRU_{r,u}^{Max}\, YRU_{r,u} \quad \forall r,u \tag{4-24}$$

$$FRR_{r,r*} \le FRR_{r,r*}^{Max}\, YRR_{r,r*} \quad \forall r,r* \tag{4-25}$$

$$FRS_{r,s} \le FRS_{r,s}^{Max}\, YRS_{r,s} \quad \forall r,s \tag{4-26}$$

Objective functions

Minimum freshwater consumption:

$$Min \sum_{w} \left(\sum_{u} FWU_{w,u} + \sum_{r} FWR_{w,r} \right) \tag{4-27}$$

Minimum total annual cost:

$$Max \left[OP \left(\sum_{w} \alpha_{w} \left(\sum_{u} FWU_{w,m} + \sum_{r} FWR_{w,r} \right) + \sum_{r} OPN_{r}\, FR_{r} \right) - af\ FCI \right] \tag{4-28}$$

where OPN_r are the operational cost of the regeneration processes, OP is the hours of operation per year. The last term is the annualized capital cost, where *FCI* is the fixed capital cost and *af* is any factor that annualizes the capital cost (usually 1/*N*, where *N* is the number of years of depreciation). The fixed capital of investment is calculated using the sum of the piping costs and the new regeneration units costs as follows:

$$\left.\begin{array}{l} FCI=\sum_u\left(\begin{array}{l}\sum_w YWU_{w,u}\,CCWU_{w,u}+\sum_r YUR_{u,r}\,CCUR_{u,r}\\ +\sum_{u^*\neq u} YUU_{u,u^*}\,CCUU_{u,u^*}+\sum_s YUS_{u,s}\,CCUS_{u,s}\end{array}\right)\\ +\sum_r\left(\begin{array}{l}\sum_w YWR_{w,r}\,CCWR_{w,r}+\sum_{r^*\neq r} YRR_{r,r^*}\,CCRR_{r,r^*}+\\ \sum_u YRU_u\,CCRU_u+\sum_s YRS_{r,s}\,CCRS_{r,s}+CCR_r\left(FR_r\right)^{0.7}\end{array}\right)\end{array}\right\} \tag{4-29}$$

which uses a set of capital cost parameters to assign cost to the connections ($CCWU_{w,u}$, $CCWR_{w,r}$ $CCUU_{u,u^*}$, $CCUS_{u,s}$, $CCUR_{u,r}$, $CCRU_{r,u}$, $CCRR_{r,r^*}$ and $CCRS_{r,s}$) and to the regeneration processes (CCR_r).

All the above equations need to be tailored to the specifics of each system. If one considers the conventional problem stated by Takama et al. (1980), that is, the one in which the water pre-treatment subsystem is not considered, $FWR_{w,r}$ does not exist and thus should be set to zero. In this case all the regeneration processes are part of the wastewater treatment subsystem. In the same way, when only the water-using units are considered, all the parameters that relate regeneration processes should be set as zero.

Another point that should be made here is related to the interactions among the subsystems and their boundaries. Again, we take the case in which we have the only water-using subsystem and the wastewater treatment subsystem (Figure 4.5 to Figure

4.8).

- In the case of the system of Figure 4.5, that is, for a centralized treatment system with fixed structure, but now with the recycle allowed, we set $FUS_{u,s}$ to zero and we consider only one treatment with all fixed outlet concentrations, which can be the called end-of-pipe treatment. Thus, considering the end-of-pipe treats all the involved contaminants, equations (4-7) and (4-8) are not necessary and $CR_{r,c}^{out}$ can be substitute by $CRF_{r,c}^{out}$, which is a parameter.

- In the case of the system of Figure 4.6, the treatment is centralized but it can be individually optimized. In fact, for this system the water using subsystem could be first optimized and then the treatment subsystem is optimized using the output of the water subsystem as input of the treatment subsystem. However a better procedure would be to individually optimize both systems while a connection between then still exist. To achieve that, we introduce a fictitious unit u_f can be introduced. This unit is actually a mixer and have all $\Delta M_{u_f,c} = 0$ =0. The connection between the two systems is done allowing only the fictitious unit to send water/wastewater to the regenerations: $FUS_{u,s} = 0 \quad \forall u,s$, $FUR_{u,r} = 0 \quad \forall u \neq u_f, r$. In addition, the distributed treatment system has also to be individually optimized and may render concentrations that are smaller than the discharge limits. Thus we introduce a fictitious regeneration unit r_T with all $XCR_{r_T,c}$ =0 (no treatment) and we then make $FRS_{r,s}^{Max} = 0 \quad \forall r \neq r_T, s$ as well as $FRU_{r,u}^{Max} = 0 \quad \forall r \neq r_T, u$.

- In the case of Figure 4.7, we keep the concepts presented for Figure 4.3, but the fictitious unit is no longer needed. On the other hand, the fictitious regeneration is still needed. In the case of Figure 4.8, we keep all our equations.

4.4. Illustrations

A single contaminant case that was originally solved as a water-using unit subsystem problem (no regeneration processes – pre-treatment and/or wastewater treatment - and consequently no discharge limits) is presented first. This example shows that freshwater consumption can be reduced if the recycle of the end-of-pipe treatment is allowed.

Example 2 is an extension of the previous one, but allowing the addition of a regeneration process from the wastewater treatment subsystem. In this example it is possible to verify that even if the recycle of the end-of-pipe treatment does not show any advantage from the freshwater consumption point of view, it can sometimes bring reductions in costs.

In a third example, the single contaminant case is modified to include the water pre-treatment subsystem. Thus, the impact of considering this subsystem is analyzed.

Example 4 shows a small multi-contaminant water-using subsystem example in which there is a reduction in freshwater consumption when the reuse/recycle of the EoPT is considered.

Then a lager multiple contaminant problem is analyzed (examples 5 to 7). This problem was originally solved without discharge limits. Different networks that have different arrangements of the pre-treatment subsystem, water-using subsystem and wastewater treatment subsystem are presented. It is also shown that the recycle of the stream treated by the end-of-pipe treatment can reduce costs and the addition of the pre-treatment subsystem can generate more realistic possibilities of zero discharge cycles.

The examples were solved using GAMS/DICOPT. Because some of the examples could not be solved directly in DICOPT, starting points were generated using a linear relaxation of the non-linear model. The relaxed model was built using the convex and concave envelopes of the bilinear terms (McCormick, 1976) and linear underestimators for the concave terms, and was solved using GAMS/CPLEX.

Example 1

Example 1 is a single contaminant network adapted from Wang and Smith (1994), which they solved using pinch analysis. The limiting process data for this problem are shown in Table 4-1 and it has a freshwater consumption without reuse (conventional network configuration) of 112.5 t/h.

Table 4-1 - Limiting data for example 1.

Process Number	Mass load of contaminant	C_{in} (ppm)	C_{out} (ppm)
1	2 kg/hr	0	100
2	5 kg/hr	50	100
3	30 kg/hr	50	800
4	4 kg/hr	400	800

When the end-of-pipe recycling is not allowed, the freshwater consumption can reach a minimum of 90 t/h. With the recycle (assuming an end-of-pipe exit concentration of 5 ppm), the minimum consumption is 20 t/h. This minimum consumption could also be calculated using the “water-pinch” graphical method as shown by Wang and Smith (1994). Although the water pinch is also able to perform the design of this single component network complying with minimum consumption, costs cannot be used to drive the design. One could consider several network possibilities (degenerate solutions, that is, different network structures that are able to achieve minimum consumption) and then compare their costs, but in this case there is no guarantee that all possibilities are analyzed. Moreover, if one wants the optimum network from the cost point of view the resulting network does not have to operate at minimum freshwater consumption. Therefore, the number of options to be analyzed is much larger and the likelihood to miss the optimal network is smaller, not to mention the amount of work involved.

For an analysis of this problem using economic objectives freshwater cost is assumed to be $\alpha_i(\$/ton)$=0.3 and the system operates 8600 hours/year. There is one freshwater source, which is free of contaminants, and the end-of-pipe treatment has an outlet concentration of 5 ppm, which is the maximum concentration allowed for disposal. The operating cost of the end of pipe treatment is $OPN_r(\$/ton) = 1.0067$ and the investment cost is $CCR_r\left(\frac{\$}{ton^{0.7}}\right) =$ 19,400. The capital costs with connections are presented in Table 4-2.

Both the grassroots design and the retrofit of this network are analyzed in this first example.

Table 4-2 - Capital costs of the connections.

	Unit 1	Unit 2	Unit 3	Unit 4	End of pipe treatment
FW	$39,000	$76,000	$47,000	$92,000	-
Unit 1	-	$150,000	$110,000	$45,000	$83,000
Unit 2	$50,000	-	$134,000	$40,000	$102,500
Unit 3	$180,000	$35,000	-	$42,000	$98,000
Unit 4	$163,000	$130,000	$90,000	-	$124,000
EoPT	$83,000	$102,500	$98,000	$124,000	-

For the retrofit case, it is assumed that a conventional network (no water reuse) is the starting point, that is, the current network has only the connection between the water source and units and between units and the end-of-pipe treatment without any reuse among units or recycle of the water treated by the end-of-pipe treatment. The costs previously presented are used in the retrofit case as well. However, the capital cost of existing connections (between freshwater and water using units and water using units and end-of-pipe treatment) and processes (in this case the end-of-pipe treatment) are set to zero. Finally, when retrofitting, one has to assume that any increase in water throughput in the EoPT is possible (there is extra capacity installed), or has to put a limit to the maximum capacity, especially when recycles that were not present in the first place are now allowed. In this problem, the capacity of the EoPT is considered to be the volume of wastewater treated by the conventional network (112.5 t/h). First, the networks are obtained for minimum cost (TAC) using equations (4-28) and (4-29), but featuring the minimum freshwater consumption without recycle. Notice that in this situation the operating costs are fixed because the freshwater consumption and the EoPT flowrates have been fixed (there is no recycle). The networks obtained for the grassroots design and retrofit case are presented in Figure 4.11 and Figure 4.12 respectively.

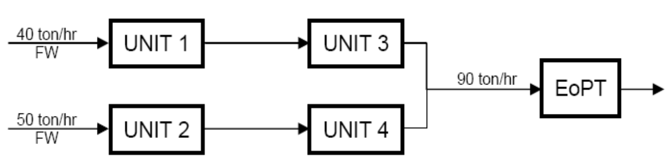

Figure 4.11 - Grassroots network design for Example 1 – no EoPT recycle- Minimum TAC at minimum consumption.

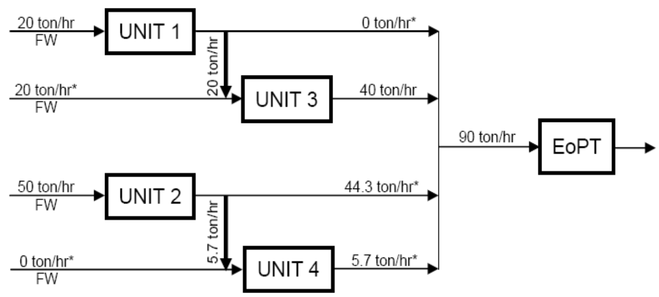

Figure 4.12 - Retrofit network design for Example 1 – no EoPT recycle- Minimum TAC at minimum consumption.

Allowing the option of recycling the stream treated by the end-of-pipe treatment reduces the minimum freshwater consumption to 20 t/h. This represents a reduction of approximately 78% in freshwater consumption, which is very significant. Figure 4.13 and Figure 4.14 show the minimum TAC networks at their minimum consumption (20 t/h) for grassroots design and retrofit case respectively.

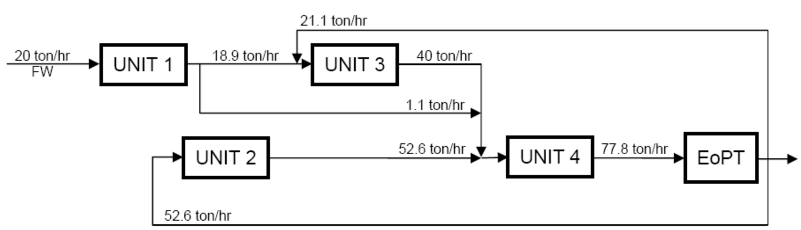

Figure 4.13 - Grassroots network design for Example 1 –EoPT recycle allowed- Minimum TAC at minimum consumption.

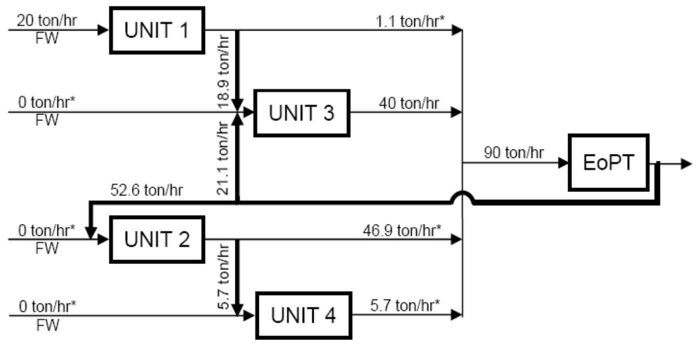

Figure 4.14 - Retrofit network design for Example 1 –EoPT recycle allowed- Minimum TAC at minimum consumption.

Example 2

Example 2 is a special case of Example 1 in which the addition of a regeneration process is allowed. It has a capital cost of $CCR_r\left(\frac{\$}{ton^{0.7}}\right) = 16{,}800$ and the operational cost is assumed to be $OCN(\$/ton) = 1.00$. This regeneration process has a fixed outlet concentration of 10ppm.

The capital costs of connections involving the regeneration process are presented in Figure 4.3 and the minimum TAC is calculated the same way as in example 1.

Table 4-3 - Capital costs of the connections.

	Unit 1	Unit 2	Unit 3	Unit 4	Reg.	End of pipe treatment
FW	$39,000	$76,000	$47,000	$92,000	-	-
Unit 1	-	$150,000	$110,000	$45,000	$145,000	$83,000
Unit 2	$50,000	-	$134,000	$40,000	$37,000	$102,500
Unit 3	$180,000	$35,000	-	$42,000	$91,000	$98,000
Unit 4	$163,000	$130,000	$90,000	-	$132,000	$124,000
Reg.	$33,000	$130,000	$50,000	$98,000	-	$45,000
EoPT	$83,000	$102,500	$98,000	$124,000	$45,000	-

The grassroots design case is investigated first. Now, both cases of allowing and not allowing the recycle of the end-of-pipe treatment stream, can reach the minimum freshwater consumption of 20 t/h. Unlike Example 1, this example does not show any advantage of allowing end-of-pipe recycling when looked from the minimum freshwater consumption perspective. However, advantages may be seen when the total annualized cost (TAC) is minimized. The minimum TAC obtained for the case in which the end-of-pipe recycling is not allowed (Figure 4.15) is $1,013,429 per year. When the end-of-pipe recycle is allowed, the minimum TAC decreases to $969,237 per year, which is 4.4% less than the former case. This is the network presented in Figure 4.13, obtained when consumption was minimized.

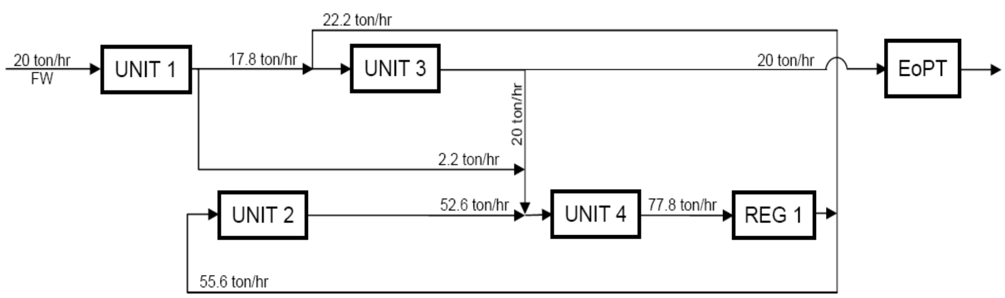

Figure 4.15 - Grassroots network design for Example 2 – no EoPT recycle- Minimum TAC at minimum consumption.

Note that when the recycle of the stream treated by the end-of-pipe treatment is allowed, the minimum freshwater consumption can be achieved without using the availible regeneration process.

Next, the retrofit design for the given network is analyzed. As before, a conventional network (no water reuse) is assumed. In this case, the current network does not have the regeneration process and so the only existing connections are the ones between the water source and water-using units and between water-using units and the end-of-pipe treatment. As expected, both cases (with and without end-of-pipe recycle) can reach the minimum freshwater consumption of 20 t/h. As presented by Faria and Bagajewicz (2009), for the retrofit case we maximize savings instead minimize total annualized cost. The maximum savings at the minimum consumption of the network presented in Figure 4.16 (no EOP treatment allowed) is $289,399 per year. If recycle of end-of-pipe is allowed (Figure 4.17), the saving goes up to $366,550 per year, which is approximately 27% higher.

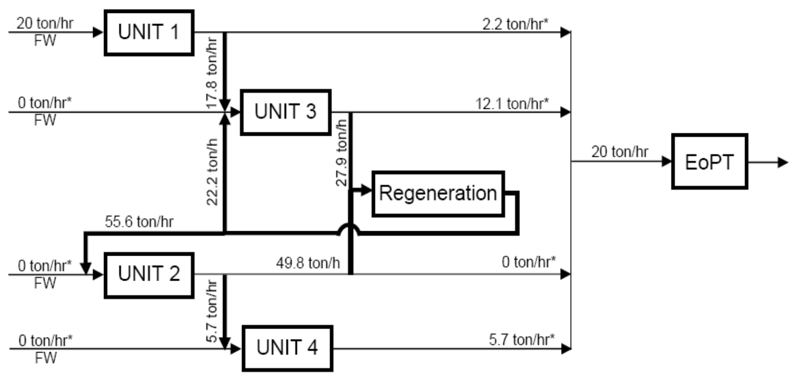

Figure 4.16 - Retrofit network design for Example 2 – no EoPT recycle- Minimum TAC at minimum consumption.

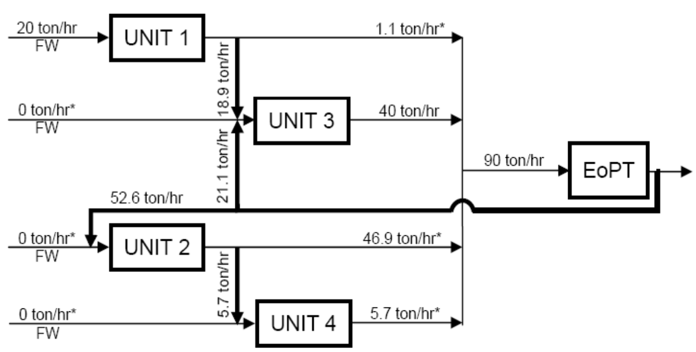

Figure 4.17 - Retrofit network design for Example 2 –EoPT recycle allowed- Minimum TAC at minimum consumption.

Example 3

This example discusses the suggested *complete water system* using a single contaminant problem. The simplest form of the *complete water system,* which assumes that the water pre-treatment subsystem cannot receive water from the other two subsystems, is analyzed first. In this case, the pre-treatment subsystem is added without allowing it to receive streams from the other two subsystems. However, the water-using subsystem and wastewater treatment subsystem are handled as in the *total water system* previously discussed. The limiting data is presented in Table 4-4 - Limiting data for example 3. Note that unit two has a maximum outlet concentration of 20 ppm and the end-of-pipe treatment has an outlet concentration of 25 ppm, which coincides with the discharge limit. The same capital and operating cost of the end-of-pipe treatment as well as connection costs of Example 1 are applied.

Table 4-4 - Limiting data for example 3.

Process Number	Mass load of contaminant	C_{in} (ppm)	C_{out} (ppm)
1	2 kg/hr	0	100
2	5 kg/hr	20	100
3	30 kg/hr	50	800
4	4 kg/hr	400	800

One external freshwater source is used, but two water treatment units are considered thus providing two different qualities of freshwater. In other words, the pre-treatment subsystem is a sequential system that does not necessarily need to treat all freshwater to the highest quality. This is the scheme presented in Figure 4.9a.

Note that there is also the possibility of recycling water from the water-using subsystem and/or wastewater treatment subsystem to the water pre-treatment subsystem

(Figure 4.9b). However, this is analyzed later in this example.

In this first case it is assumed that pre-treatment 1 can bring the freshwater down to 10 ppm and pre-treatment 2 can further treat it down to 0ppm. Pre-treatment 1 has an operating cost of \$0.30/ton and a capital cost of \$8,500/ton$^{0.7}$. The maximum inlet concentration of this pre-treatment is 500 ppm. The operating cost of pre-treatment 2 is \$0.50/ton and the capital cost is \$10,500/ton$^{0.7}$. Pre-treatment 2 has a maximum inlet concentration of 20 ppm. With the exception of capital cost, this problem could be solved using the conventional *Total Water System* model: equations (4-1) through (4-27) and TAC given by the sum of operating costs (4-28) and the annualized FCI, in turn given by equation (4-29). Then, one would have to consider two sources of water with different qualities and different costs. Thus, the two pre-treatment units would be eliminated from the problem description and the only regeneration processes existing in this problem would be the ones that are part of the wastewater treatment subsystem.

Figure 4.18 shows the solution found when the *complete water system* is solved assuming a sequential water pre-treatment and the total annual cost is minimized. Recycles from the water-using units to the water pre-treatment units are not allowed here. Figure 4.18 shows that both types of freshwater are used and that freshwater treated by only pre-treatment 1 is mixed with the recycle of the end-of-pie treatment before it feeds unit 2. This network has a TAC of \$1,275,915.

The same problem can be solved using the common assumption of one freshwater source free of contaminants. This is accomplished by disallowing any split after WPT 1 and forcing the use of water from WPT 2.

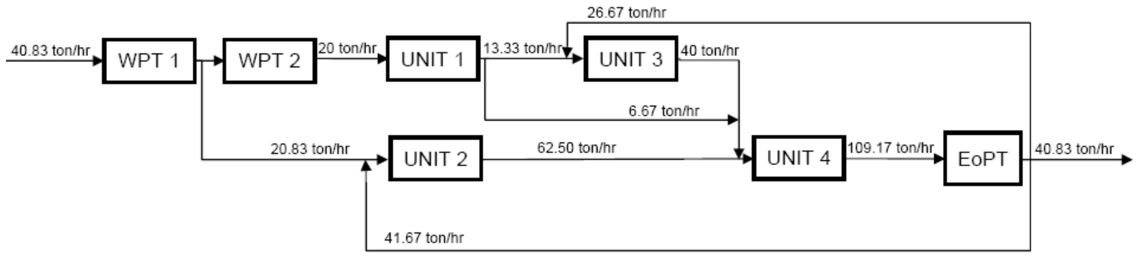

Figure 4.18 - Grassroots network design for Example 3 –EoPT recycle allowed-Wastewater recycle to pre-treatment units not allowed- Two freshwater sources-Minimum TAC.

The minimum TAC found was $1,309,950 and the network found is shown in Figure 4.19. It is the same as in the case of Figure 4.18 (except of course for the pre-treatment, which has been forced to be sequential). The two networks, however, differ substantially in the freshwater consumption. If one looks at this problem from the freshwater consumption point of view, the solution presented in Figure 4.19 is better than the one in Figure 4.18. However, in Figure 4.19 the overall cost of the water pre-treatment system is higher the one in Figure 4.18. This new trade-off created by the addition of the water pre-treatment subsystem is one of the reasons why the *complete water system* becomes very important when costs are analyzed.

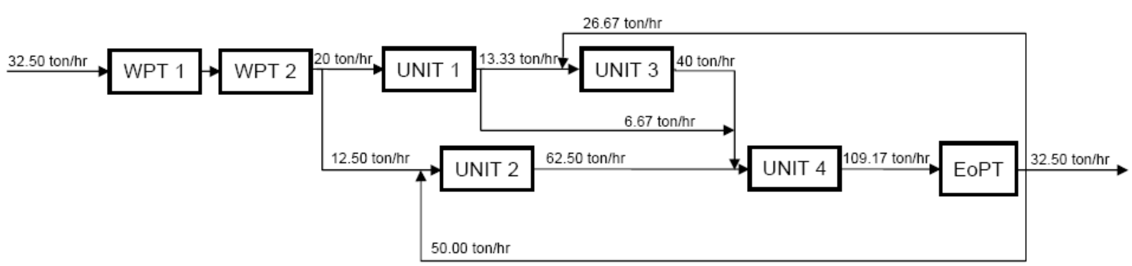

Figure 4.19 - Grassroots network design for Example 3 – EoPT recycle allowed-Wastewater recycle to pre-treatment units not allowed - One freshwater source used-Minimum TAC.

Here one can conclude that ignoring the modeling and constraints emerging from pre-treatment and seeking minimum freshwater consumption, or even minimum TAC, leads to the wrong solution.

We also investigated forbidding the recycle of the end-of-pipe treatment in the previous cases. Figure 4.20 shows the solution, which features a total annual cost of $1,314,652. For the integrated system scheme case, the optimum network found has a TAC of $1,536,684 and consumes 90t/h of freshwater. This network has the same structure presented in example 1 (Figure 4.11).

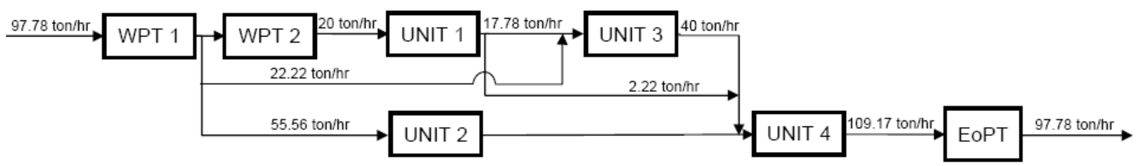

Figure 4.20 - Grassroots network design for Example 3 – no EoPT recycle - Wastewater recycle to pre-treatment units not allowed - Two freshwater sources - Minimum TAC.

Now the *Complete Integrated Water System*, which allows all interactions within subsystems and between subsystems, is considered. In other words, this case considers each pre-treatment, water-using unit and wastewater treatment as a single process inside one only boundary that is the *Complete Water System*. The solution of this case is presented in Figure 4.21. This network has a zero liquid discharge cycle and a total annualized cost of $410,277. Note that allowing the integration of the water pre-treatment subsystem eliminates the existence of the end-of-pipe treatment.

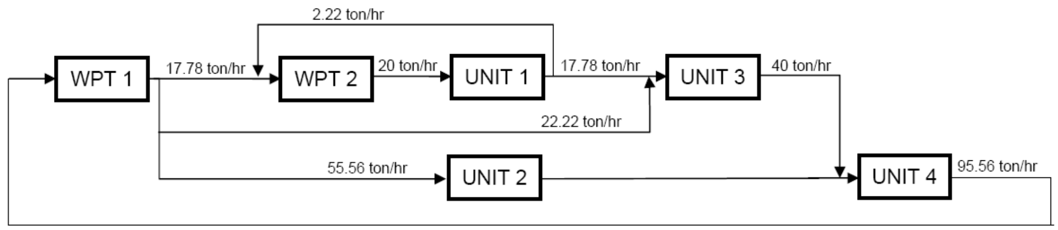

Figure 4.21 - Zero Liquid discharge solution for Example 3 obtained using a Complete Integrated Water System Model.

Example 4

Example 4 presents a simple multi-contaminant example from Wang and Smith (1994). This example has two water-using units and two contaminants and minimum freshwater consumption is the target. The example is meant to show that the same effects as in single contaminant cases are observed.

Table 4-5 presents the limiting data of this problem. The minimum freshwater consumption of this network without reuse is 63.33 t/h.

Table 4-5 – Limiting data of example 4.

Process	Contaminant	Mass Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	4	0	100
	B	2	25	75
2	A	5.6	80	240
	B	2.1	30	90

Because no regeneration process exists in this example, only two cases are analyzed: first, the case in which there is no recycle of the end-of-pipe treatment; and second the case where the stream treated by the end-of-pipe treatment can be reused by the water using units.

For the end-of-pipe treatment is assumed outlet concentration of 10 ppm for both contaminants. These concentrations are in agreement with the maximum allowed to disposal.

Consider the first case where no recycle of end-of-pipe treatment is allowed. The minimum freshwater consumption is 54 t/h, which is approximately 15% less than the freshwater usage without integration (straight use of freshwater in all units). The 54 t/h freshwater consumption network is presented in Figure 4.22.

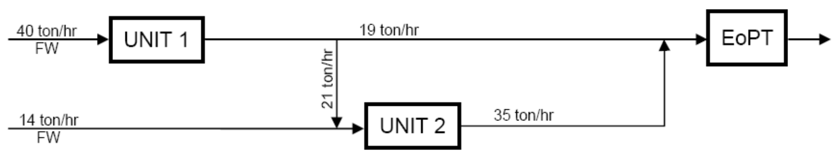

Figure 4.22 - Grassroots network design for Example 4 – no EoPT recycle.

The minimum freshwater consumption can be further reduced when the recycle of the stream treated by the end-of-pipe treatment is allowed. Indeed, the answer is that 40 t/h freshwater are only needed. This is 26% lower than the previous case (and 36.8% lower than the consumption without reuse). The network corresponding to 40 t/h freshwater consumption is presented in Figure 4.23.

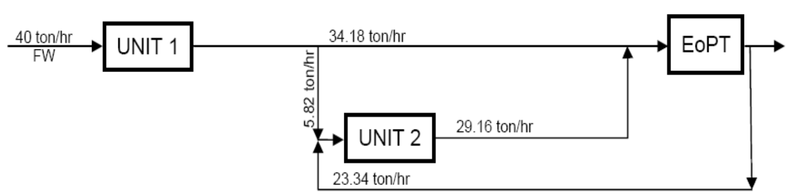

Figure 4.23 - Grassroots network design for Example 4 – EoPT recycle allowed.

Note that this example is focused on the minimum freshwater consumption. It shows clearly the advantage of allowing the recycle of the stream treated by the end-of-pipe treatment: a reduction of 26%%. However, one could argue that the capacity of the end-of-pipe treatment is larger when the freshwater consumption is reduced by means of adding the recycle and therefore it has a higher capital cost and may have also a higher operating cost.

The increase in capital cost due to the increase of end-of-pipe treatment capacity can be an important factor for networks. The influence of this increase can only in reality be observed when all the portions of capital cost (other regeneration processes, piping, etc) are also simultaneously considered. In this example, the influence seems to be significant (the end of pipe treatment now treats 9.34 t/h more than in the case of reuse without recycle). In addition, both options have the same number of connections. On the other hand, if this is a retrofit project and the end-of-pipe treatment already exists, the capital cost would only be related to new connections (assuming the original network had no reuse and therefore the available end-of-pipe treatment would be 63.33 t/h). In this case, the option allowing end-of-pipe treatment recycling needs only one extra pipe, which may not be a significant extra capital. The importance of having a capital cost should be investigated together with the benefits obtained with each option, which economically can be related to the operating cost. Here, the operating cost favors the non-recycling option once the ratio between cost of freshwater and end-of-pipe treatment cost decreases. In fact, when economics is the driven factor, all these issues should be considered together in a more general measurement such as total annualized cost, net present value (NPV) and/or return on investment (ROI). Some of these objectives will be addressed in the next few examples.

Example 5

Example 5 is applied to a refinery case presented by Koppol et al. (2003). This example has four key contaminants (salts, H2S, Organics and ammonia) and six water-using units. The limiting data of the water-using units are shown in Table 4-6. This network without reuse (conventional network) consumes 144.8 t/h of freshwater. The discharge limits are: 15 ppm for salts, 5 ppm for H_2S, 45 ppm for organics and 20 ppm for ammonia. The existing end-of-pipe treatment is able to reduce the contaminant to these discharge limits and no concentration limit is imposed at the treatment inlet.

Table 4-6 – Water-using units data of example 5.

Process	Contaminant	Mass Load (kg/hr)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1 - Caustic Treating	Salts	0.18	300	500
	Organics	1.2	50	500
	H2S	0.75	5000	11000
	Ammonia	0.1	1500	3000
2 - Distillation	Salts	3.61	10	200
	Organics	100	1	4000
	H2S	0.25	0	500
	Ammonia	0.8	0	1000
3 – Amine Sweetening	Salts	0.6	10	1000
	Organics	30	1	3500
	H2S	1.5	0	2000
	Ammonia	1	0	3500
4 - Merox-I Sweetening	Salts	2	100	400
	Organics	60	200	6000
	H2S	0.8	50	2000
	Ammonia	1	1000	3500
5 - Hydrotreating	Salts	3.8	85	350
	Organics	45	200	1800
	H2S	1.1	300	6500
	Ammonia	2	200	1000
6 - Desalting	Salts	120	1000	9500
	Organics	480	1000	6500
	H2S	1.5	150	450
	Ammonia	0	200	400

Some of the different cases previously described are discussed in this example: First, only the water-using subsystem is considered. Then, interactions with the wastewater subsystem are included. Finally, the pre-treatment subsystem is considered and the *Complete Water System* is investigated. Consideration of recycling (or not) the stream treated by an End-of-pipe treatment are also made for all the aforementioned cases.

Case 1: Water-using Subsystem only: In this case only the water-using units and the conventional end-of-pipe treatment are assumed. The original problem solved by Koppol et al. (2003) had an implicit end-of-pipe treatment, that is, it did not include it in the problem and so the recycle of the stream treated by the EoPT was not considered. Here both cases are investigated.

The minimum freshwater consumption achieved when end-of-pipe recycling is not allowed is 119.332 t/h. The minimum total annual cost (TAC) is found to be $2,291,652, which is also a network that consumes 119.332 t/h of freshwater. The solution is presented in Figure 4.24.

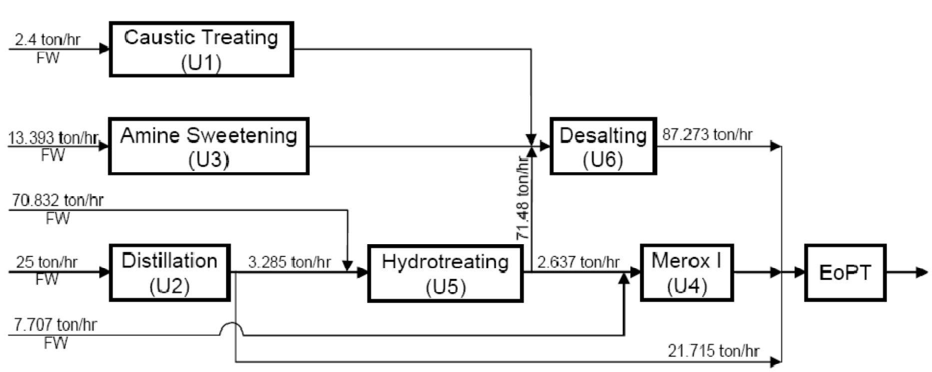

Figure 4.24 - Grassroots network design for Example 5 - No regeneration processes included- no EoPT recycle – Minimum TAC.

When end-of-pipe recycling is allowed, the minimum consumption is 33.571 t/h, which is approximately 72% lower than the earlier solution. The minimum TAC ($2,062,797) for this case is also found featuring the minimum freshwater consumption (33.571 ton/h). Figure 4.25 shows the network correspondent to this solution.

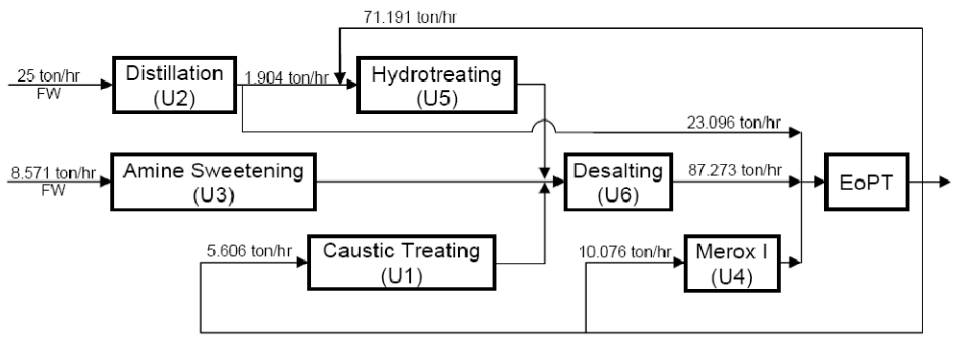

Figure 4.25 - Grassroots network design for Example 5 - No regeneration processes included - EoPT recycle allowed – Minimum TAC.

Case 2: Interaction between Water-using and Wastewater Treatment Subsystems allowed: The previous example is now solved for the case in which the wastewater treatment subsystem is also included. There are other three regeneration processes available in this wastewater treatment subsystem: Reverse osmosis, which reduces salts to 20 ppm; API separator followed by ACA, which reduces organics to 50 ppm; and, Chevron wastewater treatment, which reduces H_2S to 5 ppm and ammonia to 30 ppm.

Solutions for a centralized sequential wastewater treatment system (as in Figure 5) are presented first. For both solutions (allowing and not allowing the end-of-pipe recycling) the minimum freshwater consumption is 33.571 t/h. Freshwater cost is $0.32/t and the plant operates 8600 hours/year. The end-of-pipe treatment has a capital cost of $30,000/t$^{0.7}$ and an operating cost of $1.80/t. The costs of the potential additional regeneration processes are presented in Table 4-7.

Table 4-7 – Costs of the wastewater treatments for example 5.

Wastewater treatments	Capital Cost ($/ton$^{0.7}$)	Operating Cost ($/ton)
API separator followed by ACA	$25,000	0.12
Reverse osmosis	$20,100	0.56
Chevron wastewater treatment	$16,800	1.00

The costs of connections are presented in Table 4-8. Only the costs from the units to the centralized system are considered. The costs of connections between regeneration processes are ignored.

Table 4-8 – Capital costs of the connections for example 5

$(x10^3)	U1	U2	U3	U4	U5	U6	Centralized System	EOP
W1	23	50	18	63	16	25	10	10
U1	-	50	110	45	70	42	5.3	5.3
U2	50	-	34	40	11	35	5.1	5.1
U3	110	34	-	42	60	18	6.2	6.2
U4	45	40	42	-	23	34	7.8	7.8
U5	70	11	60	23	-	28	5.8	5.8
U6	42	35	18	34	28	-	2.2	2.2
Centralized System	5.3	5.1	6.2	7.8	5.8	2.2	-	-
EOP	5.3	5.1	6.2	7.8	5.8	2.2	-	-

Next the case in which the wastewater treatment subsystem is sequential and centralized is analyzed. The minimum total annual cost of the networks that are able to operate at minimum freshwater consumption is obtained both when end-of-pipe recycling is allowed and when it is not. Figure 4.26 shows the centralized sequential regeneration system network in which end-of-pipe recycling is not allowed. This network has a total annual cost of $2,065,383. When end-of-pipe recycling is allowed (Figure 4.27), the total annual cost goes down to $1,292,425, which represents only 37% of the previous value. Note that, allowing the end-of-pipe recylcing, only API separator is needed as additional regeneration process.

The minimum TAC is also obtained without forcing the minimum consumption. The same solution is found for the case in which the end-of-pipe recycling is allowed (Figure 4.27). However, for the case in which the recycle of the end-of-pipe treatment is not allowed, the minimum TAC happens at a freshwater consumption larger than the minimum (38.983 t/h). This network is presented in Figure 4.28. It has a total annual cost of $1,351,259 and uses two of the three available additional regeneration processes.

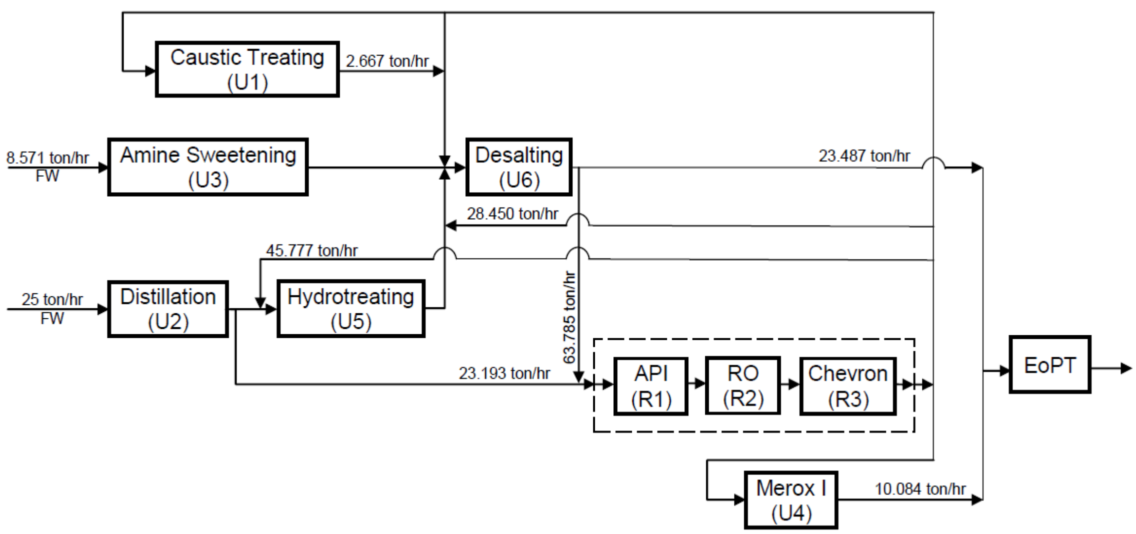

Figure 4.26 - Grassroots network design for Example 5 –Centralized sequential regeneration processes –no EoPT recycle– Minimum TAC at minimum consumption.

Now, the centralized distributed system is analyzed (as in Figure 4.6). The solution for minimum TAC without recycle of the end-of-pipe treatment is presented in Figure 4.29. Note that again the minimum TAC for this case does not happen at the minimum freshwater consumption of the system. This network also operates at 38.983 t/h and has a TAC of $1,330,142. Like the previous case, the suggested network has two regeneration processes. The major difference is due to the distributed system that allows different flowrates to be treated by the different regeneration processes.

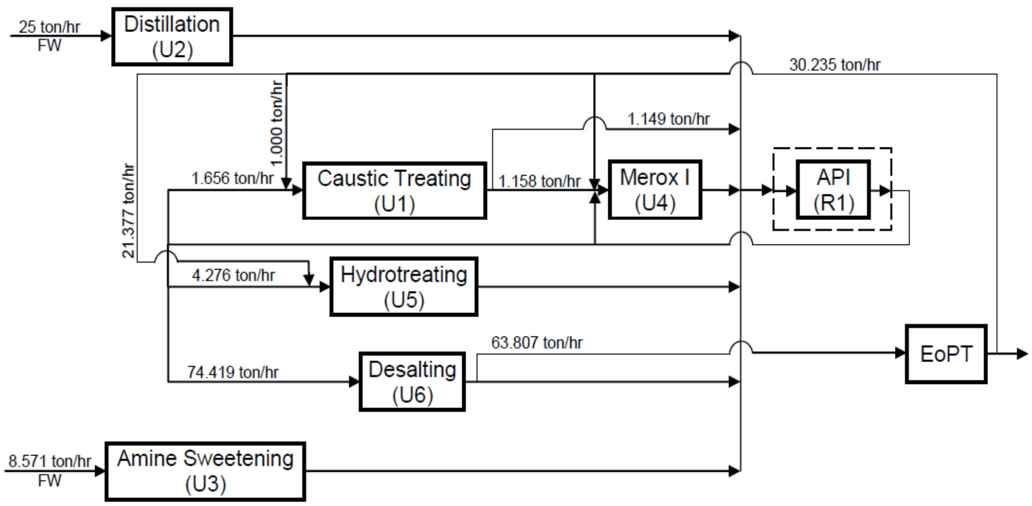

Figure 4.27 - Grassroots network design for Example 5 – Centralized sequential regeneration processes – EoPT recycle allowed – Minimum TAC at minimum consumption.

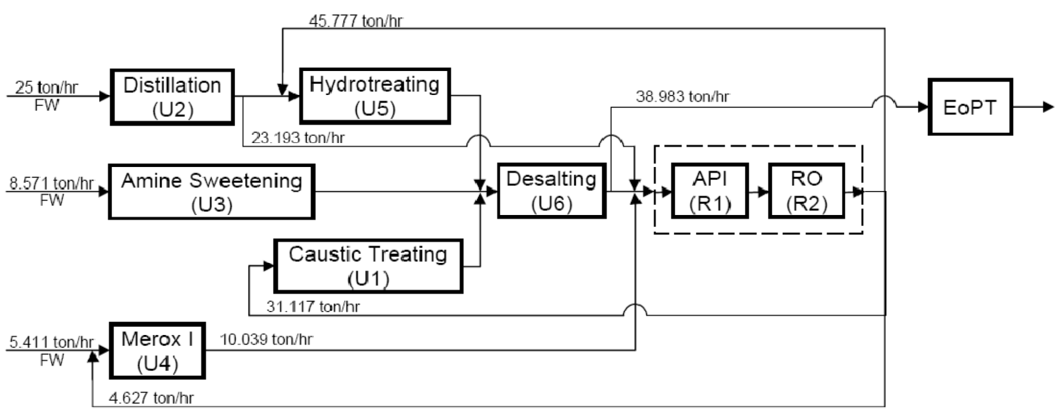

Figure 4.28 - Grassroots network design for Example 5 – Centralized sequential regeneration processes – no EoPT recycle – Minimum TAC.

When end-of-pipe recycling is allowed, the minimum TAC is found to feature the minimum consumption. This network is the same found when centralized sequential system was analyzed (Figure 4.27).

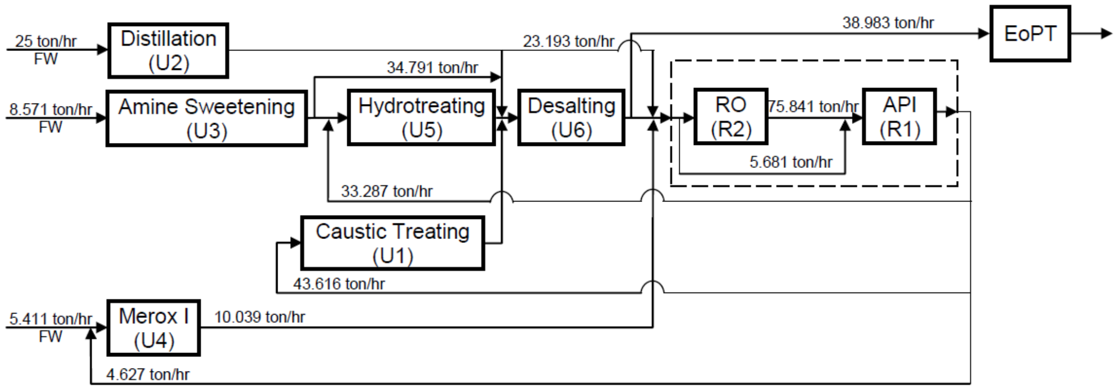

Figure 4.29 - Grassroots network design for Example 5 –Centralized distributed regeneration processes –no EoPT recycle– Minimum TAC.

Analyzing the network presented in Figure 4.29, the minimum TAC is also minimized maintaining the freshwater consumption at the minimum possible. This solution is presented in Figure 4.30 and has a total annual cost of $1,476,784. All the three additional regeneration processes are needed in this case.

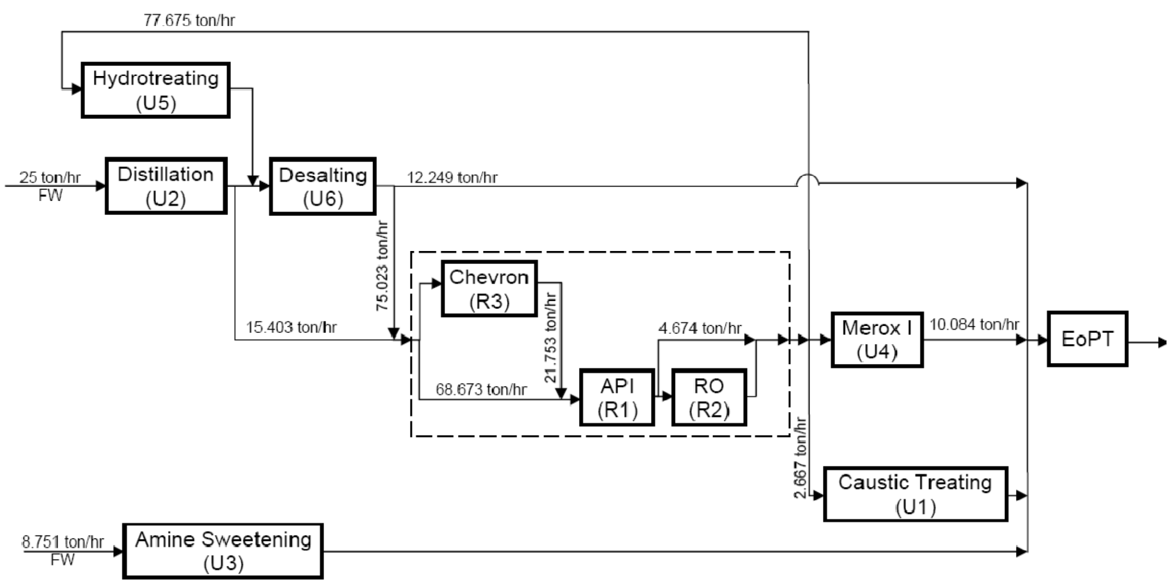

Figure 4.30 - Grassroots network design for Example 5 – Centralized distributed regeneration processes – no EoPT recycle – Minimum TAC at minimum freshwater consumption.

Now the integrated system is considered (as in Figure 4.8). Both cases, allowing and not allowing the recycle of the stream treated by the end-of-pipe treatment, can reach a minimum freshwater consumption of 33.58 t/h.

Networks corresponding to the case in which end-of-pipe recycling is not allowed are presented in Figure 4.31 and Figure 4.32 respectively. The first one has the minimum total annual cost ($1,093,011), which has a freshwater consumption (38.876 t/h) higher than the minimum possible. The second (Figure 4.32) gives the minimum TAC of $1,123,957. This solution is found for a network that operates at the minimum freshwater consumption that can be obtained for this system. Once again, the former case requires only two of the three regeneration process while the later needs all of the three regeneration processes to allow the minimum freshwater consumption.

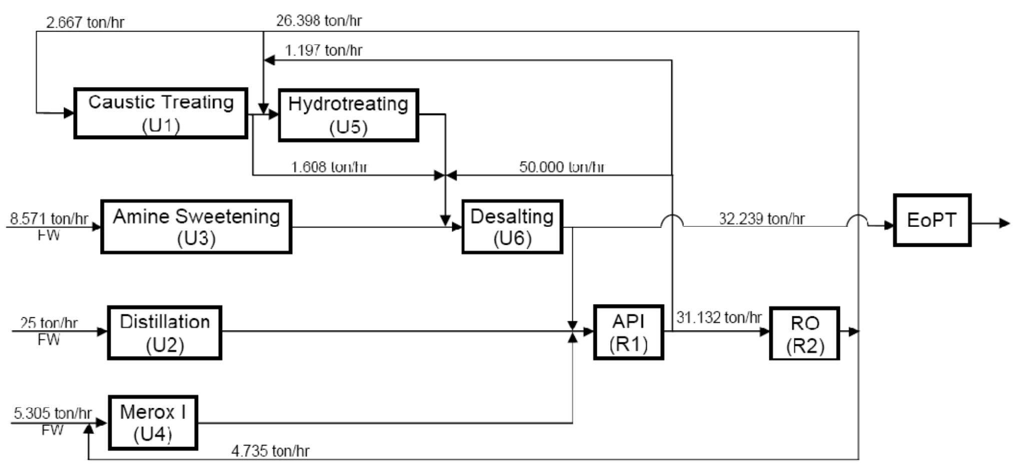

Figure 4.31 - Grassroots network design for Example 5 – Integrated Case –no EoPT recycle– Minimum TAC.

When end-of-pipe recycling is allowed in the *Total Water System* scheme, the minimum total annualized cost becomes $1,065,451. This solution is referred to a network that operates at the minimum freshwater consumption of the system. This network has two regeneration system that treat different flowrates.

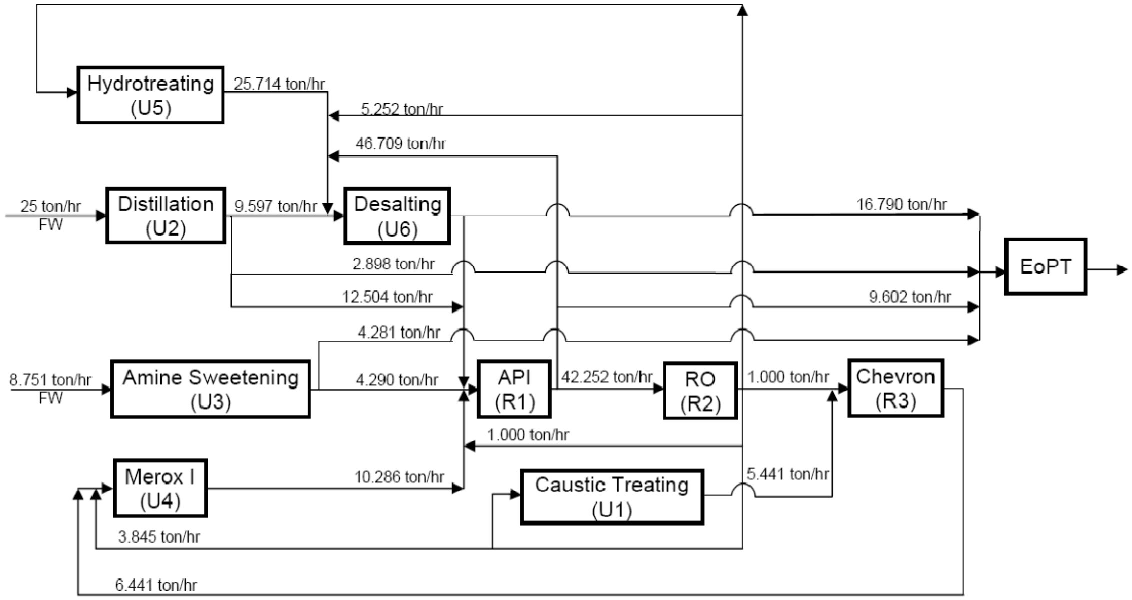

Figure 4.32 - Grassroots network design for Example 5 – Integrated Case – no EoPT recycle – Minimum TAC at minimum consumption.

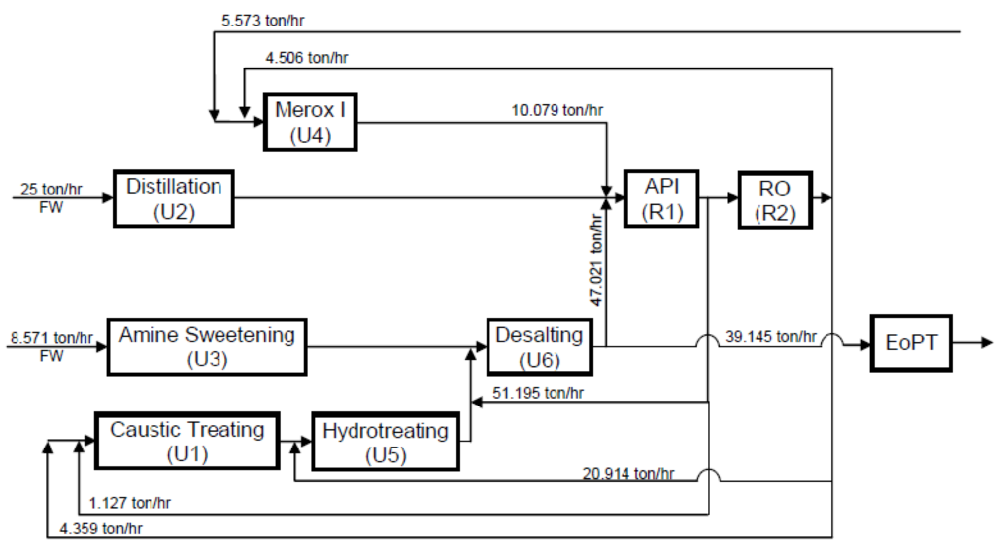

Figure 4.33 - Grassroots network design for Example 5 – Integrated Case –EoPT recycle allowed– Minimum TAC.

Table 4-9 presents a summary of all the costs and freshwater consumptions for this problem when only the water-using units subsystem is considered and when it is considered together with the wastewater subsystem. These results will be later analyzed considering the water pre-treatment subsystem.

Table 4-9 - Costs and Freshwater consumption comparison of the different options in which only water-using subsystem is considered; or, water-using and wastewater subsystems are simultaneously considered.

System	Recycle of EoPT	TAC ($/year)	Freshwater consumption
Water-using Subsystem only	No	$2,291,652	119.332 t/h
Centralized sequential WWT subsystem at minimum consumption (*WUU-WWT)*	No	$2,065,383	33.571 t/h
Water-using Subsystem only	Yes	$2,062,797	33.571 t/h
Centralized distributed WWT subsystem at minimum consumption (*WUU-WWT)*	No	$1,476,784	33.571 t/h
Centralized sequential WWT subsystem (*WUU-WWT)*	No	$1,351,259	38.983 t/h
Centralized distributed WWT subsystem (*WUU-WWT)*	No	$1,330,142	38.983 t/h
Centralized sequential WWT subsystem* (*WUU-WWT)*	Yes	$1,292,425	33.571 t/h
Centralized distributed WWT subsystem* (*WUU-WWT)*	Yes	$1,292,425	33.571 t/h
Integrated Water System at minimum consumption (*WUU-WWT)*	No	$1,123,957	33.571 t/h
Integrated Water System (*WUU-WWT)*	No	$1,093,011	38.876 t/h
Integrated Water System* (*WUU-WWT)*	Yes	$1,065,451	33.571 t/h

WUU-WWT : Case 2 - Interaction between Water-using and Wastewater Treatment Subsystems

* Same solution was fond either forcing or not the minimum freshwater consumption

Case 3: Complete Water System: Along with the water-using units data of Table 4-6 and the wastewater treatment data of Table 4-7, case 3 uses the water pre-treatment subsystem data of Table 4-10, which considers two regeneration processes.

There is one freshwater source that contains 150 ppm of salts, 200 ppm of organics, 3 ppm of H_2S and 2 ppm of ammonia. The connection costs applied here are the same ones presented in Table 4-8. Connections between freshwater source and pre-treatments and between pre-treatments are not considered. The cost for the connection between pre-treatments and any other processes (water-using units and wastewater treatments) are assumed to be the same as the ones from freshwater source and these other processes as presented in Table 4-8.

Table 4-10 – Data for the water pre-treatment subsystem.

		$CR^{in, max}$ (ppm)	CR^{out} (ppm)	Capital Cost ($/t$^{0.7}$)	Operating Cost ($/t)
Pre-Treatment 1	Salts	2000	10	$10,000	0.10
	Organics	2000	10		
	H2S	500	N/A		
	Ammonia	1000	N/A		
Pre-Treatment 2	Salts	10	0	$25,300	1.15
	Organics	10	0		
	H2S	5	0		
	Ammonia	5	0		

If this problem is solved considering an implicit freshwater source with 0 ppm for all the contaminants, (that is, a total water system - no recycles to water pre-treatment is allowed) the best found solution has a TAC of $1,467,640. This network is the same presented in Figure 4.33, but now it includes the water pre-treatment subsystem and the costs associated to it.

If we still consider only one quality of water (free of contaminants), but we have an explicit water pre-treatment subsystem (that is, the whole water pre-treatment subsystem is part of the model and thus recycling to the WPT is allowed), we are able to achieve a TAC of $1,422,786. This solution is presented in Figure 4.34. Note that not only the TAC is lower, but the freshwater consumption is also reduced to 31.256 t/h.

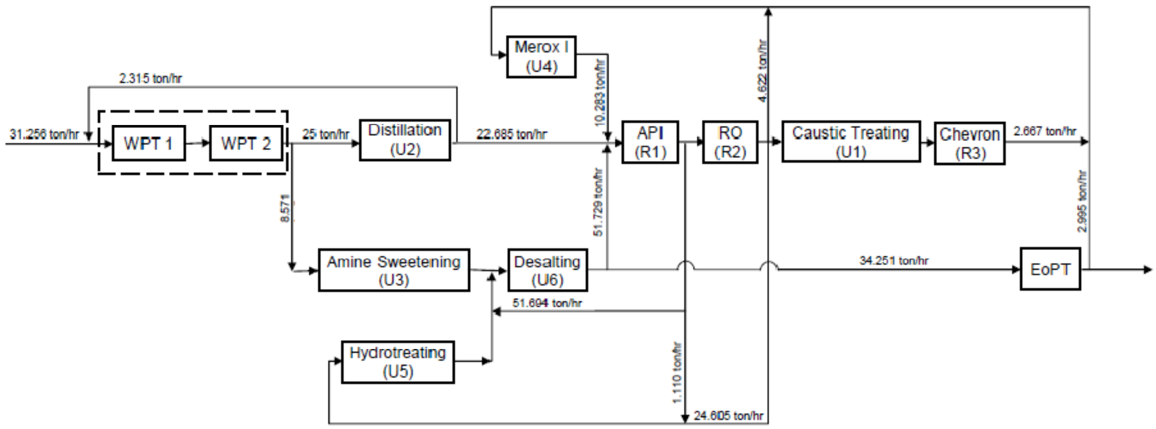

Figure 4.34 - Grassroots network design for Example 5 – Integrated Case with an explicit water pre-treatment–Minimum TAC.

Additionally, one also can assume the different water pre-treatments as individual regeneration process to which recycling can take place. When this case was analyzed, the optimum found solution was the same as the one found in the previous case where the recycles are to each pre-treatment individually was not considered. In fact, the previous solution is a special case and the found solutions indicate that, for this set of cost data, there is no advantage on considering individual water pre-treatments instead of considering the water pre-treatment subsystem as a “black box”. Example 3 had shown a different situation in which assuming individual water pre-treatment rendered advantages to the *complete water system*. We will later show that a few changes in cost data may show advantages on considering individual water pre-treatment.

Moreover, the system presented in Example 5 is able to achieve zero discharge when consumption is minimized. However, zero discharge cycles are not always wanted from the cost point of view. Figure 4.35 shows he best solution found for a zero discharge option of this system when TAC is minimized. This network has a TAC of $2,526,620. In this network ,water from WPT 2, which is free of contaminants, is used to dilute the water from the EoPT with the purpose of bringing the concentration of this mixing down to the maximum allowed inlet concentration in WPT1.

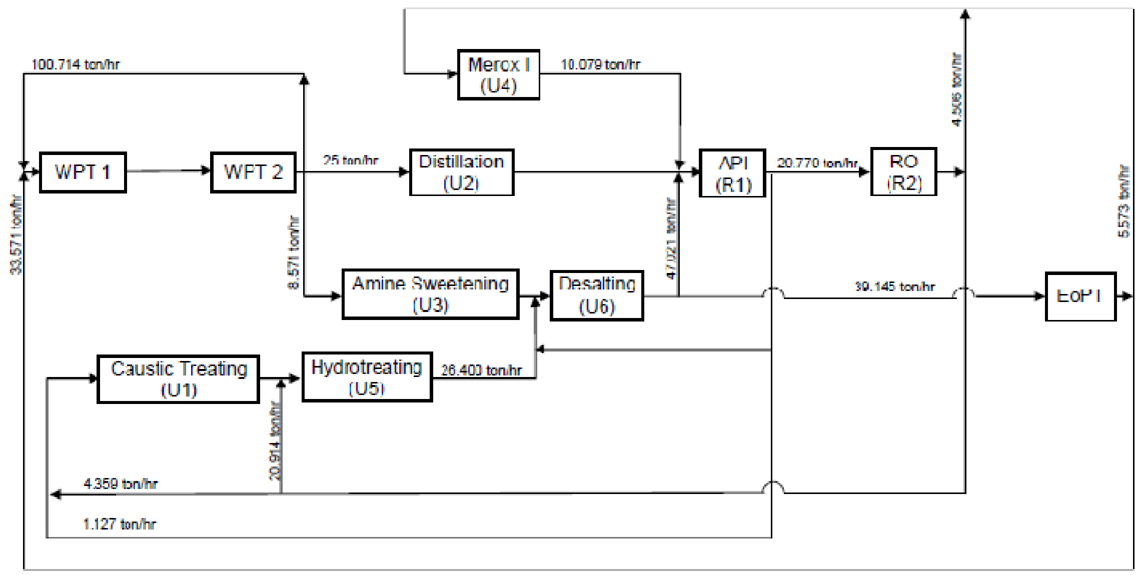

Figure 4.35 - Grassroots network design for Example 5 – Integrated Case with pre-treatment-–Minimum TAC at zero liquid discharge

Note that because self recycle is not allowed, the dilution happens before WPT 1. In reality, this dilution is necessary to bring the ammonia concentration of the other stream (EoPT) from 30 ppm down to 5 ppm, which is the maximum concentration allowed in WPT 2. To eliminate this issue, we also investigate the case in which self recycle of regeneration processes as well as pre-treatment processes are allowed. The network correspondent to the best found solution is presented in Figure 4.36, which has self recycle in both WPT 1 and WPT 2.

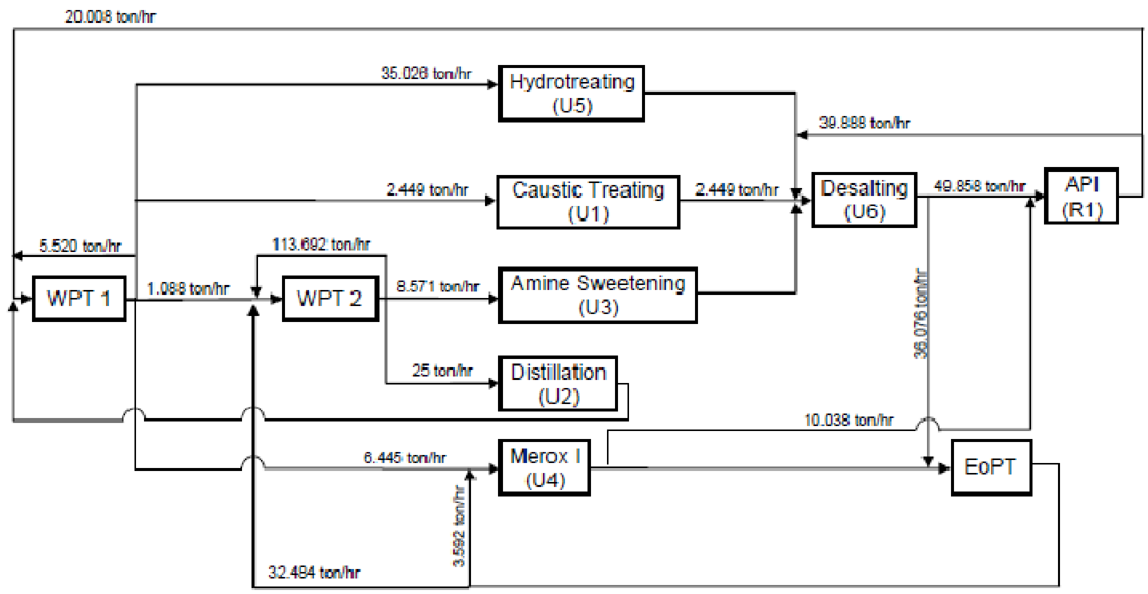

Figure 4.36 - Grassroots network design for Example 5 – Integrated Case with pre-treatment – Minimum TAC at zero liquid discharge – Self recycle on regeneration and pre-treatment allowed.

Table 4-11 presents a summary of all the costs and freshwater consumptions for this problem considering the water pre-treatment costs (even if they were not included in the model). Thus, for the networks presented in Table 4-9, the extra cost with water pre-treatment to have freshwater free of contaminants was added.

As previously mentioned, depending on the costs, a split up of the water pre-treatment subsystem in individual water pre-treatments, allowing recycles to each of them individually and allowing self recycles can be advantageous. Here the only altered data was the freshwater cost. Instead of considering a cost of \$0.32/t, it is assumed that water is free. In this case, the best found solution indicates the use of the intermediate water quality from WPT 1. This network is presented in Figure 4.37. Note that now WPT 1 send water to water-using unit 4.

Table 4-11 – Costs and Freshwater consumption comparison of the different options - considering the complete water system.

System	Recycle of EoPT	TAC** ($/year)	Freshwater consumption
Water-using Subsystem only	No	$3,674,818	119.332 t/h
Complete Water System (Zero Liquid Discharge)	Yes	$2,526,620	0 t/h
Centralized sequential WWT subsystem at minimum consumption (*WUU-WWT)*	No	$2,467,571	33.571 t/h
Water-using Subsystem only	Yes	$2,464,985	33.571 t/h
Centralized distributed WWT subsystem at minimum consumption (*WUU-WWT)*	No	$1,878,971	33.571 t/h
Centralized sequential WWT subsystem (*WUU-WWT)*	No	$1,816,182	38.983 t/h
Centralized distributed WWT subsystem (*WUU-WWT)*	No	$1,795,064	38.983 t/h
Centralized sequential WWT subsystem* (*WUU-WWT)*	Yes	$1,694,613	33.571 t/h
Centralized distributed WWT subsystem* (*WUU-WWT)*	Yes	$1,694,613	33.571 t/h
Integrated Water System (*WUU-WWT)*	No	$1,556,695	38.876 t/h
Integrated Water System at minimum consumption (*WUU-WWT)*	No	$1,526,146	33.571 t/h
Integrated Water System* (*WUU-WWT)*	Yes	$1,467,640	33.571 t/h
Complete Water System	Yes	$1,422,786	31.256 t/h
Complete Water System (one water quality)	Yes	$1,422,786	31.256 t/h

WUU-WWT : Case 2 - Interaction between Water-using and Wastewater Treatment Subsystems

* Same solution was fond either forcing or not the minimum freshwater consumption

**Considering the costs for the Complete Water System

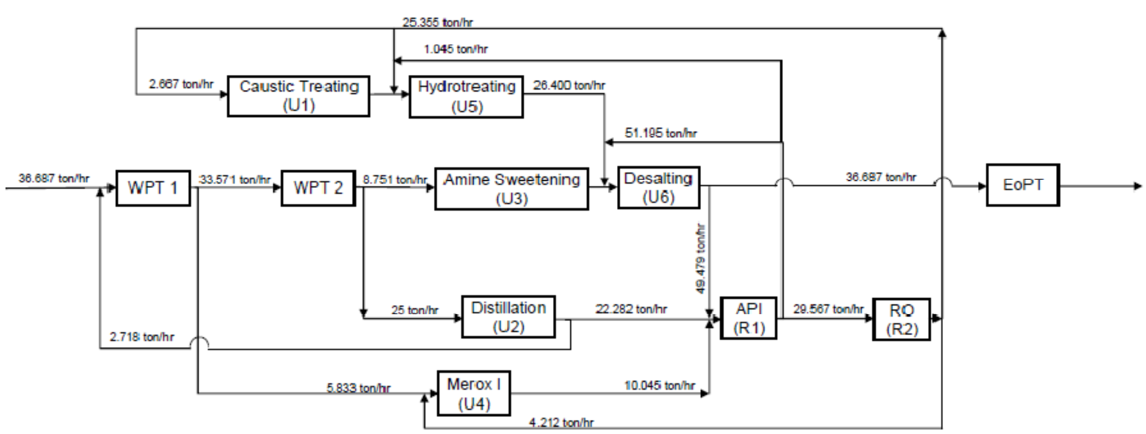

Figure 4.37 - Grassroots network design for Example 5 – Integrated Case that uses more than one pre-treatment water quality.

4.5. Final Remarks

This chapter discussed some of the different structures used to model the water allocation problem. These structures vary according to the different assumption used in each of the subsystems as well as with the interaction among the subsystems. It was shown through examples that different structural choices can make significant changes. Additionally, the inclusion of one more subsystem, the water pre-treatment subsystem, to form a *Complete Water System,* was suggested and the examples showed the importance of considering it.

In essence, it was concluded that when the proper architecture is used, i.e. all subsystem and all recycles among these subsystems are allowed, then the boundaries among these subsystems can be erased, reducing the problem to one big superstructure where all connections are allowed. This is, in many instances, an essential route to achieve zero liquid discharge cycles.

4.6. References

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5. GLOBAL OPTIMIZATION METHODS

One of the biggest challenges in solving the water allocation problems are rooted in the nonlinearities and non-convexities that arise from bilinear terms corresponding to component material balances and concave cost functions. To address these issues, an approach that discretizes the feasible region resulting in a lower bound MILP model is presented in this chapter. To reduce the gap between the lower bound and an upper bound (which can be found using the original NLP or MINLP model), different procedures are discussed.

5.1. Overview

The use of mathematical programming in the water allocation problems was first presented by Takama et al. (1980). This problem is usually modeled using non-linear programming (NLP) and it involves non-convexities in the contaminants mass balances.

Although mathematical programming has been used for a long time to solve these problems, several methods do not guarantee global optimality and many times cannot find a feasible solution. This is one of the drawbacks in the WAP that has not received much attention. Except for a few papers (Karuppiah and Grossmann, 2006a,b; Meyer and Floudas, 2006; Bergamini et al., 2008) that solve this problem to global optimality, all the other work done on multi-component WAP can only guarantee local solutions (Galan and Grossmann, 1998; Koppol et al., 2003; Gunaratnam et al., 2005; Alva-Argaez et al., 2007; Teles et al., 2008 to name a few). In fact, the biggest challenges of solving these problems to global optimality are the non-convex bilinear terms arisen from the contaminant balances (mixer and splitters) and other nonlinear terms stemming from concave cost functions.

In this chapter different optimization strategies are presented and global optimization is discussed. Global optimization methods are important not only to guarantee global optimality, but also because they are able to generate lower bounds that allow us to know how far we can be from the global optimum solution and, in many instances, generate good starting points for non-linear solvers. Although in some cases there is no strict need of finding the global optimum solution, it is very important to have at least an idea of how much better the solution could be. Another important advantage of global optimization methods is that initial starting points are often not required and a good solution is many times found in the first iterations of the method (Galan and Grossmann, 1998).

To address bilinear terms in generalized pooling problems, which are similar in nature to water management problems and also include wastewater treatment network problems, Meyer and Floudas (2006) proposed a piece-wise linear formulation based on reformulation-linearization technique (RLT). They first use partitioning of the continuous space (applied to the flowrates) to generate a MINLP and then they apply the RLT to linearize the model. Some constraints generated by the RLT that are redundant in the original problem and non-redundant in the MILP are also added to the relaxed model, which is a lower bound. The method is used just to verify the gap relative to the best known optimum solution and no procedure is presented to reduce the gap between lower and upper bounds. Different numbers of partitions of the continuous variables are considered to obtain the best lower bound. The method is able to generate very tight lower bounds at a cost of significant computational efforts due to the increase in numbers of binary variables and additional constraints.

Karuppiah and Grossmann (2006a), in turn, presented a methodology to globally optimize an integrated water system. The problem is formulated as a non-convex NLP problem and solved using a deterministic spatial branch and contract algorithm. To obtain a lower bound for the original NLP model, the bilinear terms are relaxed using the convex and concave envelopes (McCormick, 1976) and the concave terms of the objective function are replaced by underestimators generated by the secant of the concave term. To improve the tightness of the lower bound, piece-wise underestimators generated from partitioning of the flow variables are used to construct tighter envelopes and concave underestimators. As in Meyer and Floudas (2006), the number of partitions can make the lower bound tighter, but extra computational effort is needed. In an additional step, Karuppiah and Grossmann (2006) perform a bound contraction, which is a relaxed version of the bound contraction method presented by Zamora and Grossmann (1999).

In a second paper, Karuppiah and Grossmann (2006b) extended the previous method to solve the multi-scenario case of the integrated water systems. In both cases, the relaxed model, which renders a lower bound, is used in a LB/UB framework. In the first case (Karuppiah and Grossmann, 2006a) a spatial branch and bound procedure is used. For the multi-scenario case (Karuppiah and Grossmann, 2006b), a spatial branch and cut algorithm is applied. The cuts are generated using a decomposition based on Lagrangean relaxation.

An example of *total water system* previously presented in the literature is globally optimized by Bergamini et al. (2008). They present an improvement of their previous outer approximation method (OA) for global optimization (Bergamini et al., 2005). The major modifications are related to a new formulation of the underestimators (which replace the concave and bilinear terms) using delta-method of piecewise functions (see Padberd, 2000); and, the replacement of the most expensive step (global solution of the bounding problem) by a strategy based on the mathematical structure of the problem, which searches for better feasible solutions of fixed network structures. The improved outer approximation method relies in three sub-problems that need to be solved to feasibility instead to optimality. In turn, the model always look for solutions that are strictly lower (using a tolerance) than the current optimum solution.

Aside from the global optimization methods directly applied to water problems, other approaches to globally solve generic bilinear problems have been presented, many of which became popular in the chemical engineering community (Quesada and Grossmann, 1995; Adhyla, Tawarmalani and Sahinidis 1999; Zamora and Grossmann, 1999; Bergamini et al., 2005; Meyer and Floudas, 2006), some having reached commercial status, like BARON (Sahinidis, 1996), COCOS, GlobSol, ICOS, LGO, LINGO, OQNLP, Premium Solver, or others that are well-known like the αBB (Androulakis, et al., 1995).

5.2. GO Method Using Interval Elimination on Discretized Variables

Here a discretization methodology to obtain lower bounds and a new bound contraction procedure is suggested. The lower bound model uses some modified versions of well-known over and underestimators (some of which used in the literature review above), to obtain MILP models. Our procedure differs from previous approaches based on LB/UB schemes because the branch and bound strategy is not the most important step and a different interval elimination strategy is attempted to contract the bounds of the variables. A B&B is only used as a last resort in difficult cases where bounds cannot be further contracted. In essence, the suggested bound contraction procedure eliminates intervals from a range for each discretized variable.

5.2.1. Solution Strategy

After discretizing one of the variables in the bilinear terms, the method consists of a bound contraction using a procedure of eliminating intervals. Once the bound contraction is exhausted, the method relies on increasing the number of intervals, or on a branch and bound strategy in which the interval elimination takes place at each node. The discretization methodology (outlined below), generates linear models that guarantee to be lower bounds of the problem. Upper bounds are needed for the bound contraction procedure. These upper bounds can be usually obtained using the original MINLP model often initialized by the results of the lower bound model, although upper bounds can sometimes also be obtained using linear models.

Before the strategy is outlined, some important variables are defined:

Discretizing Variables: These are the variables that are discretized into intervals and used to construct linear relaxations of bilinear terms. The resulting models are MILP.

Bound Contracted Variables: These are the variables that are discretized into intervals, only for the purpose of performing their bound contraction. The lower bound model will simply identify the interval in which the variable to be bound contracted lies and use this information in the elimination procedure. Clearly, these variables need not be the same as the discretizing variables.

Branch and Bound Variables: These are the variables for which a branch and bound procedure is tried. It need not be the same set as the other two variables.

For example, in water management problems the bilinear terms are composed of the product of flowrates and concentrations. Thus, one can have a problem in which the discretizing variables are all or part of the concentrations, the bound contracted variables, be the flowrates and the B&B variables the flowrates as well. As discussed below, the B&B is more efficient when the variables used are different from the discretizing variables when using McCormick's envelopes, which has information of the non-discretized variable. Alternatively, one can use concentrations for both the discretizing and BC variables, with flowrates for B&B, or the discretizing variables could be both flowrates and concentrations (in which case the LB model is more efficient), the BC variables as well as the B&B variables the flowrates or the concentrations or both, and so on.

Although the bound contract variable and branch and bound variable do not need to be the same as the discretized one it is normal to have them being bound contracted or branched, as opposed to picking other variables. In some cases, picking the variable to bound contract different form the one to discretize renders tighter lower bounds as bound contraction takes place. However, it is important to point out that the feasible region of the lower bound model can only become entirely close to the feasible region of the upper bound when the discretized variables have discrete values within an ε tolerance and this can only be done through bound contraction and/or branching.

Then, the global optimization strategy is now summarized as follows:

- Construct a lower bound model discretizing bilinear and quadratic terms, relaxing the bilinear terms as well as adding piece-wise linear underestimators of concave terms of the objective function. If the concave terms are not part of the objective function, then overestimators can be used, but this is not included in our current paper.
- The lower bound model is run identifying certain intervals as containing the solution for specific variables that are to be bound contracted. These variables need not be the same variables as the ones using to construct the lower bound.
- Based on this information the value of the upper bound found by running the original MINLP using the information obtained by solving the lower bound model to obtain a good starting point. Other ad-hoc upper bounds can be constructed.
- A strategy based on the successive running of lower bounds where certain intervals are temporarily forbidden is used to eliminate regions of the feasible space. This is the bound contraction part.
- The process is repeated with new bounds until convergence or until the bounds cannot be contracted anymore.
- If the bound contraction is exhausted, there are two possibilities to guarantee global optimality:
    - Increase the discretization of the variables to a level in which the

discrete sizes are small enough to generate a lower bound within a given acceptable tolerance to the upper bound; or,

- Recursively split the problem in two or more sub-problems using a strategy such as the ones based on branch and bound procedure.

The first option of increasing discretization will not lead to further improvement in bound contraction if degenerate solutions (or very close to the global solutions) exist for different values of the discrete variables.

5.2.2. Discretization Methodology

We show here two different discretization strategies. The proposed approach consists of discretizing one of the variables of the bilinear terms, but one could also discretize both.

<u>*Bilinear Terms:*</u>

There are different ways to linearize the bilinear terms using discrete points of one (or both) given variable(s). Two alternatives are presented:

- *Direct Discretization* (our nomenclature). Some details of this technique were presented earlier (Faria and Bagajewicz, 2008).
- *Convex Envelopes* (McCormick, 1976) as used by Karuppiah and Grossmann (2006a).

To deal with the product of continuous variables and binary variables, three variants of each procedure are considered.

Consider z to be the product of two continuous variables x and y:

$$z = x\,y \tag{5-1}$$

where both x and y subject to certain bounds:

$$x^L \le x \le x^U \tag{5-2}$$

$$y^L \le y \le y^U \tag{5-3}$$

Assume now that variable y is discretized using *D-1* intervals. The starting point of each interval is given by.

$$\hat{y}_d = y^L + (d-1)\,\frac{\left(y^U - y^L\right)}{D-1} \quad \forall d = 1..D \qquad y^L \le y \le y^U \tag{5-4}$$

In the case of the *direct discretization,* we simply substitute the variable y by its discrete values and allow the bilinear term (z) to be inside of one of the intervals, that is, between two successive discrete values. Binary variables (v_d) are used to assure that only one interval is picked.

$$\sum_{d=1}^{D-1} \hat{y}_d\, v_d \le y \le \sum_{d=1}^{D-1} \hat{y}_{d+1}\, v_d \tag{5-5}$$

$$\sum_{d=1}^{D-1} v_d = 1 \tag{5-6}$$

$$z \le x \sum_{d=1}^{D-1} \hat{y}_{d+1}\; v_d \tag{5-7}$$

$$z \ge x \sum_{d=1}^{D-1} \hat{y}_d\; v_d \tag{5-8}$$

Equation (5-5) states that y falls within the interval corresponding to the binary variable v_d, of which only one is equal to one (Equation (5-6) enforces this). This is done for the discretization variables, but if x (or a subset of it) is the BC variable, then a similar discretization as the one in (5-5) and (5-6) is included.

In turn, equations (5-6) and (5-7) bound the value of *z* to correspond to a value of *y* in the given interval.

In the case of using *McCormick's envelopes* for each interval, the equations are:

$$z \geq x^L y + \sum_{d=1}^{D-1} \left(x \hat{y}_d v_d - x^L \hat{y}_d v_d \right) \tag{5-9}$$

$$z \geq x^U y + \sum_{d=1}^{D-1} \left(x \hat{y}_{d+1} v_d - x^U \hat{y}_{d+1} v_d \right) \tag{5-10}$$

$$z \leq x^L y + \sum_{d=1}^{D-1} \left(x \hat{y}_{d+1} v_d - x^L \hat{y}_{d+1} v_d \right) \tag{5-11}$$

$$z \leq x^U y + \sum_{d=1}^{D-1} \left(x \hat{y}_d v_d - x^U \hat{y}_d v_d \right) \tag{5-12}$$

which are used in conjunction with equations (5-5) and (5-6).

When *x* (or a subset of it) is the BC variable, then we only add equations (5-5) and (5-6) for these variables, but do not incorporate the bounds of each interval in the above equations (5-9) through (5-12).

Note that even if the bilinearity generated by the multiplication of *y* and *x* was eliminated, we still have variable *x* being multiplied by the binary variable v_d in both cases. Once again there are different ways to linearize the product of a continuous and binary variable. These methods, in various forms, are very well known and we present next our implementation.

Direct Discretization Variants:

When using the *direct discretization*, the linearization of the product of *x* and the binary variable v_d can be done using three different procedures.

Direct Discretization Procedure 1, (DDP1); Let w_d be a positive variable ($w_d \geq 0$), such that $w_d = x\, v_d$. Then (7) and (8) are substituted by:

$$z \leq \sum_{d=1}^{D-1} \hat{y}_{d+1}\ w_d \tag{5-13}$$

$$z \geq \sum_{d=1}^{D-1} \hat{y}_d\ w_d \tag{5-14}$$

and w_d is now obtained from the following linear equations:

$$w_d - x^U v_d \leq 0 \tag{5-15}$$

$$(x - w_d) - x^U (1 - v_d) \leq 0 \tag{5-16}$$

$$x - w_d \geq 0 \tag{5-17}$$

Indeed, if v_d =0, equation (5-15) together with the fact that $w_d \geq 0$ renders, $w_d = 0$. Conversely, if v_d =1, equations (5-16) and (5-17) render $w_d = x$, which is what is desired. There is, however, an alternative more compact way of writing the linearization: Indeed, the following equations accomplish the same linearization.

Direct Discretization Procedure 2 (DDP2): In this case, the product of the binary variable and the continuous variable is linearized as follows:

$$w_d \leq x^U v_d \qquad \forall d = 1..D-1 \tag{5-18}$$

$$w_d \geq x^L v_d \qquad \forall d = 1..D-1 \tag{5-19}$$

$$x = \sum_{d=1}^{D-1} w_d \tag{5-20}$$

Equations (5-18) and (5-19) guarantee that only one value of w_d (when v_d =1) can be greater than zero and in between bounds (all other w_d, for when v_d =0, are zero). Thus, equation (5-20) sets w_d to the value of *x*.

Direct Discretization Procedure 3 (DDP3): This procedure uses the following equations to linearize equations (5-7) and (5-8):

$$z \le x\,\hat{y}_{d+1} + x^U\left(y^U - \hat{y}_{d+1}\right)\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-21}$$

$$z \ge x\,\hat{y}_d - x^U\,\hat{y}_d\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-22}$$

$$z \le x^U y \tag{5-23}$$

Equations (5-21) and (5-22) force z to be inside a chosen interval d^* (the one for which v_{d^*} =1). Indeed, when v_{d^*} =1, (5-21) and (5-22) reduces to the following inequalities: $x\,\hat{y}_{d^*} \le z \le x\,\hat{y}_{d^*+1}$. In turn, equations (5-5) and (5-23) reduce to $z \le x^U y^* \le x^U\,\hat{y}_{d^*+1}$ (we use y^* to denote the optimal value of y). In the other intervals where v_d =0, equations (5-22) and (5-23) reduce to $\left(x - x^U\right)\hat{y}_d \le z \le x^U y^* \le x^U\,\hat{y}_{d^*+1}$, which puts *z* between a lower negative bound and the right upper bound. Finally, equation (5-21) reduces to $z \le x\,\hat{y}_{d+1} + x^U(y^U - \hat{y}_{d+1})$, which is a valid inequality. We now need to show that equation (5-22) is also satisfied. For this, we recall that $x\,\hat{y}_{d^*} \le z \le x\,\hat{y}_{d^*+1}$. Then, for *d* $\ge d^*$ we have $\hat{y}_{d^*+1} \le \hat{y}_{d+1}$ and then, $z \le x\,\hat{y}_{d+1} + x^U(y^U - \hat{y}_{d+1}) \le x\hat{y}^*_{d+1} + x^U(y^U - \hat{y}_{d+1})$, which is a valid upper bound for that *d*. Conversely, when *d*<*d**, we have $\hat{y}_{d^*+1} > \hat{y}_{d+1}$ and then, $z \le x\,\hat{y}_{d+1} + x^U(y^U - \hat{y}_{d+1}) \le x\hat{y}_{d+1} + x^U(y^U - \hat{y}^*_{d+1})$. Adding and subtracting $x\hat{y}^*_{d+1}$ to the last term and rearranging, we get $z \le x\hat{y}^*_{d+1} + x^U(y^U - \hat{y}^*_{d+1}) - x(\hat{y}^*_{d+1} - \hat{y}_{d+1})$. Finally, noticing that $\hat{y}_{d+1} \le y^U$, one can write $z \le x\hat{y}^*_{d+1} + (x^U + x)(y^U - \hat{y}^*_{d+1})$

With all these substitution any MINLP model containing bilinearity is transformed into an MILP, which is a lower bound of the original problem; this is because of the relaxation introduced.

McCormick Envelopes Variants:

In this case, equations (5-9) through (5-12) are substituted by the following equations:

$$z \geq x^L y + \sum_{d=1}^{D-1} \left(\hat{y}_d w_d - x^L \hat{y}_d v_d \right) \tag{5-24}$$

$$z \geq x^U y + \sum_{d=1}^{D-1} \left(\hat{y}_{d+1} w_d - x^U \hat{y}_{d+1} v_d \right) \tag{5-25}$$

$$z \leq x^L y + \sum_{d=1}^{D-1} \left(\hat{y}_{d+1} w_d - x^L \hat{y}_{d+1} v_d \right) \tag{5-26}$$

$$z \leq x^U y + \sum_{d=1}^{D-1} \left(\hat{y}_d w_d - x^U \hat{y}_d v_d \right) \tag{5-27}$$

and several variants of how to linearize $w_d = x v_d$ follow:

McCormick's Envelopes Procedure 1 (MCP1): It is when equations (5-15) to (5-17) are used.

McCormick's Envelopes Procedure 2 (MCP2): In this case equations (5-18) to (5-20) are used instead of equations (5-15) to (5-17).

McCormick's Envelopes Procedure 3 (MCP3): In this case, equations (5-5) and

(5-6) are still used, but equations (5-9) to (5-12) are substituted by:

$$z \geq x^L\, y + x\;\; \hat{y}_d - x^L\, \hat{y}_d v_d - \left(x^L y^U + x^U \hat{y}_d\right)\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-28}$$

$$z \geq x^U\, y + x\;\; \hat{y}_{d+1} - x^U\, \hat{y}_{d+1} v_d - x^U\left(y^U + \hat{y}_{d+1}\right)\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-29}$$

$$z \leq x^L\, y + x\;\; \hat{y}_{d+1} - x^L\, \hat{y}_{d+1} v_d + \left(x^U y^U - x^L\left(y^L + \hat{y}_{d+1}\right)\right)\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-30}$$

$$z \leq x^U\, y + x\;\; \hat{y}_d - x^U\, \hat{y}_d v_d + \left(x^U\left(y^U - y^L\right) - x^L\, \hat{y}_d\right)\left(1 - v_d\right) \qquad \forall d = 1..D-1 \tag{5-31}$$

$$z \leq x^U y \tag{5-32}$$

The case $x^L = 0$ is a very common situation in flowsheet superstructure optimization where connections between units exist formally but a flowrate of zero through some of these connections is almost always part of the optimal solution. If x represents the flowrates and y the composition of the stream, (5-28) would reduce to $z \geq x\;\; \hat{y}_d - x^U \hat{y}_d\left(1 - v_d\right)$ and (5-30) would reduce to $z \leq x\;\; \hat{y}_{d+1} + x^U y^U\left(1 - v_d\right)$. It is obvious that (5-28) is equal to (5-22), but when $v_d = 0$, (5-22) would be tighter than (5-30), which can help computationally when the MILP code tries to solve a relaxed problem.

As in the case of the direct discretization, when these equations are substituted in the original MINLP, they transform it into an MILP, which is a lower bound of the original problem.

In addition, it is worth point out that the decision of which variables should be discretized in a bilinear term is also not straightforward. In many cases, the number of binary variables is much higher for one variable, but the solution could be found faster. This is the case of problems with component balances: flowrates participate in all the balances, whereas each balance contains its own composition. Conversely, discretizing flowrates may render a smaller number of integers but may affect speed of convergence. This is discussed in more detail below when the method is illustrated.

<u>*Concave Terms:*</u>

Univariate functions used to estimate capital cost are often concave and expressed as functions of equipment sizes as follows:

$$z = \Omega\ y^{\alpha} \tag{5-33}$$

where α is often a value between 0 and 1, and y is the equipment capacity.

Let us first consider that variable y is discretized in several intervals as shown in equation (5-4). Then the linearizization of this concave function in each interval can be done following Karuppiah and Grossmann (2006):

$$y^{\alpha} = \overline{y} \geq \sum_{d=1}^{D-1} v_d \left(\left(\hat{y}_d\right)^{\alpha} + \left(\frac{\left(\hat{y}_{d+1}\right)^{\alpha} - \left(\hat{y}_d\right)^{\alpha}}{\hat{y}_{d+1} - \hat{y}_d} \right) \left(y - \hat{y}_d \right) \right) \tag{5-34}$$

$$z = \Omega\ \overline{y} \tag{5-35}$$

which we use in conjunction with (5-5) and (5-6).

Note that, again, we have the product of a binary variable (v_d) and a continuous variable (y). The linearization of equation (34) is the following:

$$\overline{y} \geq \sum_{d=1}^{D-1} \left(\left(\hat{y}_d\right)^{\alpha} v_d + \left(\frac{\left(\hat{y}_{d+1}\right)^{\alpha} - \left(\hat{y}_d\right)^{\alpha}}{\hat{y}_{d+1} - \hat{y}_d} \right) \left(\beta_d - \hat{y}_d\, v_d \right) \right) \tag{5-36}$$

$$y = \sum_{d=1}^{D-1} \beta_d \tag{5-37}$$

$$\beta_d \leq \hat{y}_{d+1}\, v_d \qquad \forall d = 1..D-1 \tag{5-38}$$

$$\beta_d \geq \hat{y}_d v_d \qquad \forall d = 1..D-1 \tag{5-39}$$

which is again used in conjunction with (5-5) and (5-6). When substituted in the original MINLP, they transform it into an MILP. Such MILP is a lower bound of the original problem if *z* only appears in the objective function as an additive term, together with the equation defining it (equation 5-33). Conversely, when *z* shows up in some constraint of the problem, but not in the objective as an additive term, then one would have to add an overestimator like the following:

$$\bar{y} \leq \sum_{d=1}^{D-1} v_d \left(\left(\frac{\hat{y}_d + \hat{y}_{d+1}}{2} \right)^{\alpha} + \alpha \left(\frac{\hat{y}_d + \hat{y}_{d+1}}{2} \right)^{\alpha-1} \left(y - \frac{\hat{y}_d + \hat{y}_{d+1}}{2} \right) \right) \tag{5-40}$$

which uses the tangent line at the middle of the interval as an upper bound.

5.2.3. Internal Elimination Strategy (Bound Contraction)

Once a problem has been linearized and solved, the solution from this LB is used to obtain good guesses for solving the upper bound problem (the original problem is used in most cases). Once a lower bound and an upper bound have been found there is a need to identify which intervals can be eliminated from consideration. The lower bound solution points at a set of intervals, one per variable. This solution is used to find an upper bound and also to guide the elimination of certain intervals. The procedure is as follows:

Step 1: Run the lower bound model with no forbidden intervals and re-discretized variables over the range that survived.

Step 2: Use the solution from the lower bound as an initial point to solve the full NLP or MINLP problem to obtain an Upper Bound.

Step 3: If the gap between the upper bound and the lower bound is lower than the tolerance, the solution was found. Otherwise go to Step 4.

Step 4: Run the lower bound model, this time forbidding the interval that contains the answer for the first discretized variable.

Step 5: If the new problem is infeasible, or if feasible and the objective function is higher than the current upper bound, then all the intervals of this variable, except the original one that was forbidden, are eliminated. The surviving feasible region between the new bounds is discretized again.

Step 6: Repeat the procedure for all the other variables, one at a time.

Step 7: Go back to Step 1.

Note that to guarantee the optimality, not all of the lower bound models need to be solved to zero gap. The only problems that need to have zero gap are the ones in which the lower bound of the problem (or sub-problems) are obtained, which is done in step 1. The lower bound models used to eliminate intervals (step 4) can be solved to feasibility between its lower bound and the current upper bound, which is always set as the upper bound of the whole procedure.

In some cases, a pre-processing step using bound arithmetic to reduce the initial bounds of certain variables can be performed. This issue is discussed together with the results.

The above is the standard version of the suggested interval elimination (bound contraction) procedure, which we call *One-pass with one forbidden interval elimination* because the elimination process takes place sequentially, only one variable at a time and only once for each variable.

Variations to the above elimination strategy are possible:

- Options related to the amount of times all variables are considered for bound contraction:
    - *One-Pass Elimination:* In Step 6, each variable is visited only once before a new lower bound of the whole problem is obtained.
    - *Cyclic Elimination:* In Step 6, once all variables are visited, the method returns to the first variable and starts the process again, as many times as needed, until no more bound contraction is achieved.
- Options related to the amount of times each variable is bound contracted:
    - *Exhaustive elimination:* In Step 6, once each variable is contracted, the process is repeated again for that same variable until no bound contraction takes place. Only then, the process moves to the next variable. Each variable is visited only once before a new lower
    - *Non-Exhaustive elimination:* In Step 6, once each variable is contracted once, the process moves to the next variable.
- Options related to the updating of the UB/LB:
    - *Active Upper Bounding:* Each time an elimination takes place, the upper bound is calculated again. This helps when the gap between lower and upper bound (feasible solution) improves too slowly.
    - *Active Lower Bounding*: Each time an elimination takes place, the lower bound solution calculated again. In such case, one would allow all surviving intervals, and rediscretize them. If the gap between LB

and UB is within tolerance one can terminate the entire procedure. This option could be really attractive if several variables are used.

- Options related to the the amount of intervals used for forbidding:
    - *Single interval forbidding*: This consists of forbidding only the interval that brackets the solution
    - *Extended interval forbidding*: This consists of forbidding the interval identified originally plus some number of adjacent ones. This is efficient when a large number of intervals are used to obtain lower bounds. Adjacent intervals, if left not forbidden, may render lower bounds that are not larger than the current upper bound. Thus, by forbidding them, other intervals are forced to be picked and those may render larger LB and lead to elimination.
- Options related to the the amount of variables that are forbidden:
    - *Single Variable Elimination*: This procedure is the one outlined above.
    - *Collective Elimination*: This procedure consists of forbidding the combination of the intervals identified in the lower bound. We anticipate having problems with this strategy when the size of the problem is large.

When no interval is eliminated and the lower bound-upper bound gap is still larger than the tolerance, one can resort to increase the number of intervals and start over. This procedure normally renders better lower bounds and more efficient eliminations when the *Extended interval forbidding is applied*. When the standard option, the *One-*

pass with one forbidden interval elimination, is used, an increase in the number of intervals will select a smaller part of the feasible range of each variable. If this smaller selected interval was part of the previously selected, no elimination occurs again. However, using the guided option, the interval selected by the more discretized lower bound may not be part of the larger one previously chosen. Then, in such a case, an elimination may be observed. Thus, increasing the number of intervals helps because it provides tighter lower bounds. However, a large number of intervals can also significantly increase the running time. A maximum number of intervals needs to be established, but one needs to recognize this maximum depends on the size of the problem.

5.2.4. Branch and Bound Procedure

It is possible that the above interval elimination procedure fails to reduce the gap that is even using the maximum number of intervals, no interval eliminations are possible. In such a situation, we resort to a branch bound procedure. In many methods addressing bilinear terms directly (Adhyla et al., 1999; Karuppiah and Grossmann, 2006a) or others like Zamora and Grossmann (1999), the branching is normally done in the variable that is being discretized. However one can branch on the other or on both. In our case, we branch on the continuous variables by splitting their interval from lower to upper bound in two intervals. As the non-discretized variables participate on the lower bound models and thus influence their tightness, the generation of sub-problems with different non-discretized variables bounds can speed up the procedure.

The following two criteria can be used on the branching and bound procedure:

- The new continuous variable that is split in two is the one that has the largest deviation between the value of $z_{i,j}^{LB}$ in the parent node and the product of the corresponding variables x_i^{LB} and y_j^{LB}, that is choose the variable i that satisfies the following.

$$Max_i \left\{ \left| z_{i,j}^{LB} - x_i^{LB} \, y_j^{LB} \right| \right\} \tag{5-41}$$

- Using information of the current upper bound solution: We do this by choosing the variable that contributes to the largest gap between z's from the lower and upper bound, that is, we choose the variable i that satisfies the following

$$Max_i \left\{ \left| z_{i,j}^{LB} - z_{i,j}^{UB} \right| \right\} \tag{5-42}$$

In addition to the B&B procedure, at each node we perform as many interval eliminations (bound contractions) as possible.

5.2.5. Similarities and Differences with other Methods

The presented methodology borrows and intersects several other previously presented discretization and underestimation methods that render lower bounds. For example, we are considering the use of direct discretization instead of McCormick (which is supposedly tighter). The advantages would be to verify if it runs faster and consequently is able to find the solution faster (even if using more iterations). However, the elimination procedure is different the ones used in previous methods.

5.2.6. Implementation issues

The complete method requires making several choices. These choices are:

- *Variables to be discretized*. In water management and pooling problems these could be concentrations, flowrates, or both.

- *Number of discrete intervals per variable*: It does not need to be the same for all variables.
- *LB model*: DDP1, DDP2, DDP3, MCP1, MCP2, or MCP3.
- *Variables chosen to perform Bound Contraction*: They need not be the same as the once chosen to be discretized. For example, one can discretize concentrations and build a DDP1-LB model based on these discretization, but perform bound contraction on flowrates. For this, one needs to discretize the flowrates as well. The LB-Model, however, would not consider other than continuous flowrates, only including equation (5-5) for flowrates to bracket the flowrate value and to be able to forbid it.
- *Elimination strategy*: The standard One-pass with one forbidden interval elimination, or the variants (One pass or Cyclic Elimination, Exhaustive or not Exhaustive Elimination, Active Upper/Lower Bounding or not, Single vs. Extended Intervals forbidding, or Collective elimination,).
- *Variables to partition in the Branch and bound procedure.*

With such a large amount of options, it is cumbersome to explore all of them. In the examples, some of the possibilities are reported. An effort was made to show some variant's success, even though they are less efficient. For the examples for which the method is not as quick and efficient, the best result obtained by the presented method is presented.

5.2.7. Results

Example 1: Illustration of the Interval Elimination procedure

The illustration of the elimination procedure is performed for the *One-pass with one forbidden interval elimination* procedure using a simple water network example from Wang and Smith (1994). This example optimizes only the *water-using subsystem*, which targets minimum freshwater consumption and has two water-using units and two contaminants. Table 5-1 presents the limiting data of this problem.

Table 5-1 – Limiting data of example 1.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	4	0	100
	B	2	25	75
2	A	5.6	80	240
	B	2.1	30	90

For the illustration of this example, the pure discrete concentration lower bound is used with two initial intervals (Figure 5.1) and the elimination procedure is applied on the outlet concentrations of the water-using units. The standard strategy (one-pass non-exhaustive elimination) is used.

In the upper part of Figure 5.2 the results of the lower bound using the pre-processed bounds, which corresponds to a value of 52.89 t/h, are depicted. Using the results from this lower bound as initial points, the full problem was run and the solution obtained (54 t/h) corresponds to the first upper bound of the problem.

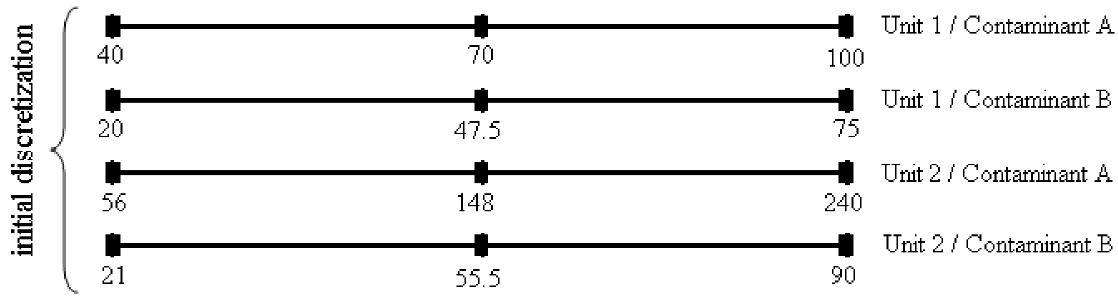


Figure 5.1 – Illustrative example of the discrete approach - initialization.

When the lower bound model is re-run forbidding the interval corresponding to Unit 1/Contaminant A, that is, the interval 70 to 100 ppm is forbidden, the interval from 40 to 70 ppm is eliminated because forcing the lower bound in this interval renders a value of the LB higher than 54 t/h. The remaining part (70ppm to 100ppm) is rediscretized in two new intervals. Then the lower bound model is run forbidding the interval corresponding to Unit 1/Contaminant B, which is the interval 47.5 to 75 ppm. The solution is again higher than 54 t/h. Thus, the interval between 20ppm and 47.5 ppm is eliminated and the remaining is rediscretized. Applying this procedure to the rest of the variables renders eliminating the intervals shown in Figure 5.2.

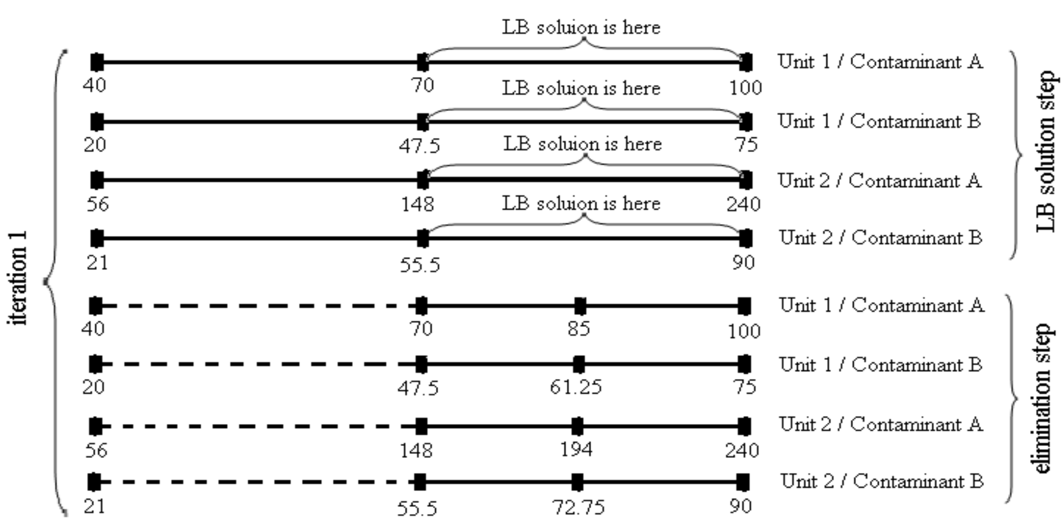


Figure 5.2 – Illustrative example of the discrete approach – 1^{st} iteration.

After the first iteration the lower and upper bound do not change (LB = 52.90 t/h and UB = 54 t/h). The second iteration of the illustrative example is shown in Figure 5.3. The elimination procedure is repeated again, one variable at a time, and in all cases, the solutions found are larger than the current upper bound. Therefore, each time the corresponding interval in each variable is eliminated, the selected interval is re-discretized and the procedure moves to the next variable.

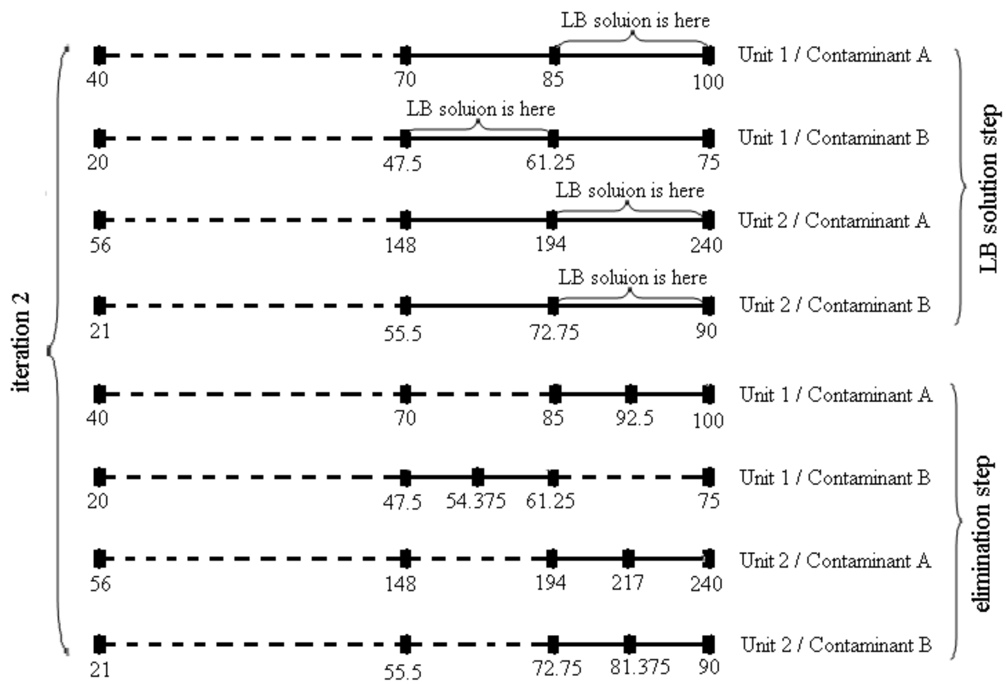


Figure 5.3 – Illustrative example of the discrete approach – 2^{nd} iteration.

This procedure is repeated until the lower bound solution is equal (or has a given tolerance difference) to the upper bound solution. This illustrative example, using the DDP3 and discretizing concentrations in two intervals, is solved in 3 iterations and 0.60 seconds using a relative tolerance of 1%. The actual solution reaches 0.65% gap. All the report solving times do not including pre-processing/compilation times.

Table 5-2 presents the progress of the solution through the iterations. The upper bound (54 t/h) is identified in the first iteration and is the global solution. The lower bound solution, however, does not improve until the third iteration. The optimum network of this example is presented in Figure 5.4.

The other option for the elimination step is cyclic non-exhaustive elimination. Table 5-3 and Table 5-4 show the progress of the solution when the cyclic non-exhaustive elimination is applied.

Table 5-2 – Solution progress of the illustrative example.

Iteration	Lower Bound	Upper Bound	Relative error	Intervals eliminated
0	52.90 t/h	54.00 t/h	2.02%	NA
1	52.90 t/h	54.00 t/h	2.02%	4
2	52.90 t/h	54.00 t/h	2.02%	4
3	53.65 t/h	54.00 t/h	0.65%	4

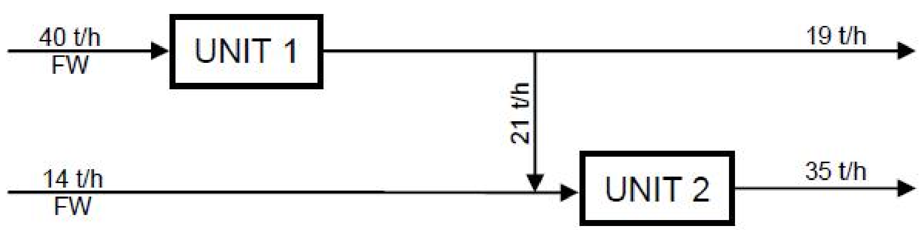


Figure 5.4 – Optimum network of example 1.

Table 5-3 – Solution progress of the illustrative example – using cyclic non-exhaustive elimination.

Iteration	Lower Bound	Upper Bound	Relative error	Number of cycles	Eliminations
0	52.90 t/h	54.00 t/h	2.02%	NA	NA
1	52.90 t/h	54.00 t/h	2.02%	4	10
2	53.67 t/h	54.00 t/h	0.62%	5	8

Table 5-4 – Number of elimination in each cycle – using cyclic non-exhaustive elimination.

Iteration	Cycle 1	Cycle 2	Cycle 3	Cycle 4	Cycle 5
1	4	3	2	1	NA
2	1	3	2	1	1

Despite the fact that this procedure takes a smaller number of iterations, the overall running time for this example was higher (2.26 s against 0.60 s using the one-pass elimination). This is expected because this is a small problem, in which the lower bounding (step 2) is not computationally expensive. Thus, unnecessary elimination (more than the needed to achieve the given tolerance gap) may occur if the lower bound is not often verified.

The solution using one-pass exhaustive elimination is also investigated. Table 5-5 shows the progress of the iterations and Table 5-6 shows which variable had its bounds contracted and how many eliminations existed in each iteration. This strategy took 1.30 seconds.

Table 5-5 – Solution progress of the illustrative example – using one-pass exhaustive elimination.

Iteration	Lower Bound	Upper Bound	Relative error	Eliminations
0	52.89 t/h	54.00 t/h	2.02%	NA
1	52.89 t/h	54.00 t/h	2.02%	10
2	53.67 t/h	54.00 t/h	0.62%	6

Table 5-6 – Exhaustive eliminations progress of the illustrative example – using one-pass exhaustive elimination.

Iteration	Cout			
	Unit 1 Contaminant A	Unit 1 Contaminant B	Unit 2 Contaminant A	Unit 2 Contaminant B
1	4	2	1	3
2	-	1	3	2

Effect of the Number of Intervals:

The number of initial intervals has also influence on the performance of the proposed methodology. Since it is known that a continuous variable can be substituted by discrete values when the number of discrete values goes to infinity, it is expected that less iterations are needed when more discrete intervals are added. On the other hand, this generates a higher number of integer variables (what means a lager MILP model), and might make the problem computationally very expensive (increase the overall time to run it).

This influence is analyzed only for the cases of one-pass non-exhaustive elimination, which have presented the best option when only 2 intervals are considered. Additionally, the influence of the *Extended interval forbidding* option is also verified. This option represents two main advantages: reduce the number of binary in the elimination step; and, facilitate eliminations. On the other hand, when only one interval is forbidden and an elimination takes place, the discharged portion of the variable is lager then if the *Extended interval forbidding* option was used and the stopping criteria is when the tolerance is satisfied. The results are shown in Figure 5.5 and Figure 5.6. The number of intervals is increased until twenty two intervals are reached.

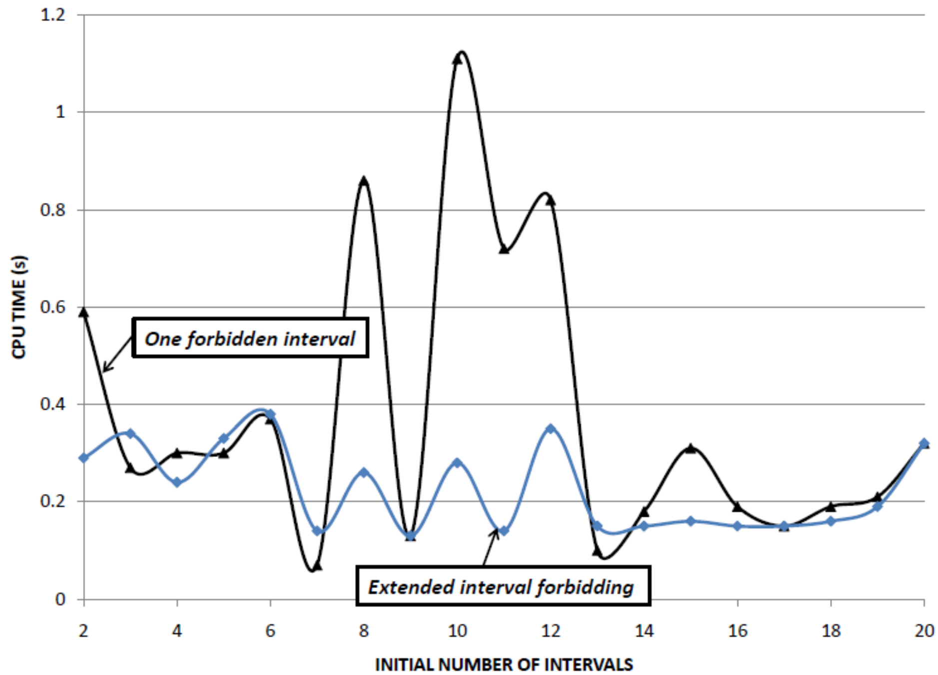


Figure 5.5 – Influence of the number of initial intervals and the use of *Extended interval forbidding* option – CPU time.

For the *One-pass with one forbidden interval elimination* option, the quickest solution (0.07s) is found when the procedure is initialized with 7 intervals. This is the point in which the solution is first found at the root node. For the *Extended interval forbidding* case, very similar CPU times are found for the cases in which the solution is found at the root node (7, 9, 11 and 13 to 18 intervals), that is, computational times of approximately 0.15 s.

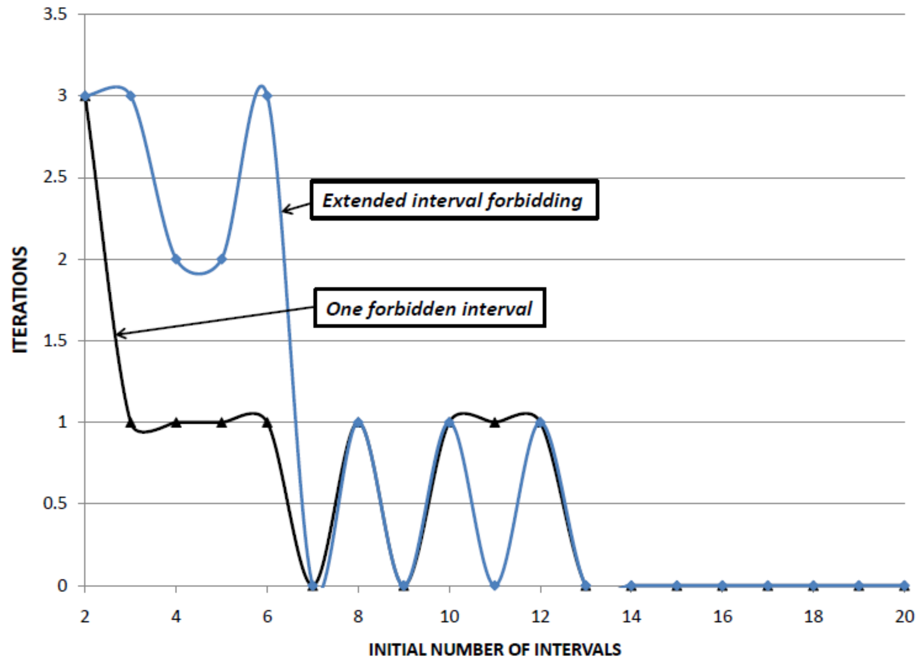


Figure 5.6 – Influence of the number of initial intervals and the use of *Extended interval forbidding* option - Iterations.

One of the decisions that have to be made is regarding the variable of that bilinear term that is being discretized. This decision strongly depends on the problem that is being approached. The bilinear terms generated by the splitters are formed by the following variables: Outlet concentration of the processes (water-using units and regeneration processes); and, flowrates. The choice of discretizing outlet concentrations of processes, the flowrates or both represents trade-offs among the tightness of the lower bound, the increase in number of binaries due to discretizations/linearizations and the efficiency of the MILP formulation. Table 5-7 show a comparison of the number of variables that need to be discretized in each case, comparing discretization of flowrates using *McCormick envelopes* and discretization of concentrations using the *direct discretization* method.

Table 5-7 – Comparison of number of discretized variables.

Number of units	Flows	C^{out} (number of contaminants)									
		1	2	3	4	5	6	7	8	9	10
2	4	2	4	6	8	10	12	14	16	18	20
3	9	3	6	9	12	15	18	21	24	27	30
4	16	4	8	12	16	20	24	28	32	36	40
5	25	5	10	15	20	25	30	35	40	45	50
6	36	6	12	18	24	30	36	42	48	54	60
7	49	7	14	21	28	35	42	49	56	63	70
8	64	8	16	24	32	40	48	56	64	72	80
9	81	9	18	27	36	45	54	63	72	81	90
10	100	10	20	30	40	50	60	70	80	90	100
11	121	11	22	33	44	55	66	77	88	99	110
12	144	12	24	36	48	60	72	84	96	108	120
13	169	13	26	39	52	65	78	91	104	117	130
14	196	14	28	42	56	70	84	98	112	126	140
15	225	15	30	45	60	75	90	105	120	135	150
16	256	16	32	48	64	80	96	112	128	144	160
17	289	17	34	51	68	85	102	119	136	153	170
18	324	18	36	54	72	90	108	126	144	162	180
19	361	19	38	57	76	95	114	133	152	171	190
20	400	20	40	60	80	100	120	140	160	180	200

Note that the number of flowrate variables is usually higher than the number of outlet concentrations variables (only the highlighted ones are not). Thus, depending on the problem one can applied more discretization in the concentration variables and obtain the same number of integers. For example, consider the problem with 20 units and 5 contaminants, which has 400 flow variables and 100 outlet concentration variables. If the flowrates are discretized in two intervals, we would need 800 binaries. In this case, keeping the same problem size, one can discretize the concentrations in 8 intervals instead of 2. A recursive formula to calculate the amount of binaries is $N_{intervals}(N_{units}+N_{regenerations})^2$ when flowrates are discretized and $N_{intervals}$ $N_{contaminants}(N_{units}+N_{regenerations})$ when concentrations are discretized.

Although the increase of number of binaries can suggest how the problem increases, the efficiency of the MILP formulations may show that the discretization of one of the variable is not a good option. This analysis can only be done when both formulations are investigated and compared.

Another characteristic of the suggested discrete method compared to the McCormick envelopes is its generality for monotonic functions and not specific for bilinear terms.

To evaluate the efficiency of the method several examples are presented. Examples 2, 3 and 4 are multicomponent refinery examples; the first and the second without regeneration processes and the third with regeneration units, all three solving for minimum freshwater. All these three examples do not require any elimination procedure because they find the solution at the first LB. Example 5 is added to compare the performance of the proposed method with that of Karuppiah and Grossmann (2006). In this case, the elimination procedure requires more than one iteration, so it is used to illustrate the performance of different options. Examples 6 to 8 are added to illustrate the performance of the method when cost is minimized. Example 9 shows the design of a complex wastewater treatment system, in which treatment processes should be selected among several options. Finally, example 10 presents an attempt of solving a challenging *total water system* problem, which considers several other aspects not consider in the previous examples.

Example 2: A Refinery Example

Example 2 is the classical small refinery example presented by Wang and Smith (1994). The objective is to minimize the freshwater consumption of a water system with three water-using units, three contaminants and one regeneration process. The limiting data of the water-using units used in this example is presented in Table 5-8. Note that these water-using units do not have fixed flowrate pre-defined by the problem.

Table 5-8 – Limiting data of example 2.

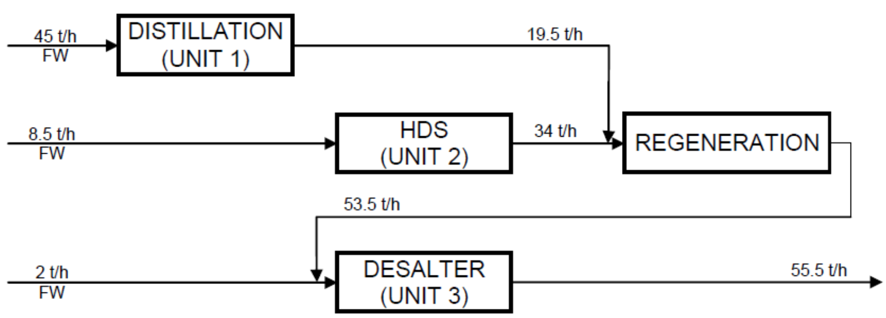
Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1 - Distillation	HC	0.675	0	15
	H_2S	18	0	400
	Salts	1.575	0	35
2 - HDS	HC	3.4	20	120
	H_2S	414.8	300	12,500
	Salts	4.59	45	180
3 - Desalter	HC	5.6	120	220
	H_2S	1.4	20	45
	Salts	520.8	200	9,500

The available freshwater source is free of contaminants and the available regeneration process is a foul water stripper with a rate of removal of 0.999 for H_2S.

Wang and Smith (1994) used a graphical approach to obtain the solution of this problem (55.5 t/h). Here concentrations are discretized concentrations and several different numbers of intervals are used, from 1 interval, to many more. In addition both types of discretization methods are applied: *Direct discretization* and *McCormick's envelopes*. The three different linearization procedures to linearize the product of continuous and binary variables of both lower bound models are attempted as well. Finally, discretized flowrates cases are run as well. All of these alternatives find the global optimum solution (55.47 t/h) at the root node.

In the case of 1 interval and direct discretization of flowrates using procedure 2 (DDP2) the model has 32 binary variables and 264 continuous variables. Conversely, in the case of 1 interval and direct discretization of concentration using DDP2, the model has 13 binary variables and 145 original continuous variables. Because there are no lower and upper bounds for the flows in this problem, the above counts do not consider the binaries corresponding to equations (4-11) through (4-26). The number of continuous variables is increased from the original value to a larger one because of the linearization procedure, which is different depending of which one is used.

Applying the suggested methodology using one interval, the optimum solution (55.47 t/h) is found in 0.10 s and 0.16 s, for discretized concentrations and discretized flowrates using DDP2, respectively. As stated above, in all these examples we only report the running time, not including the model pre-processing/generation time, which is about 1.6 sec and the solution reporting time, which is about 0.7 seconds (slightly larger for larger problems). The solution is actually obtained at the root node as the lower bound renders an objective function equal to the global minimum. In other words, there is no need for an interval elimination procedure. Although the solution value found is nearly the same (ours is slightly lower), the network is different. Figure 5.7compares both.



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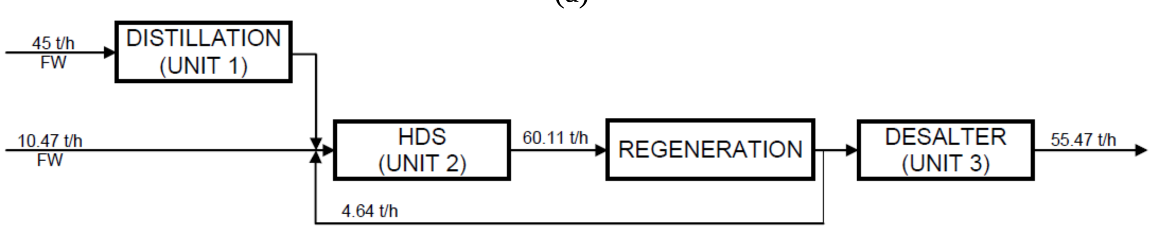

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Figure 5.7 – Optimum network of example 2. (a) Wang and Smith's (1994) solution and (b) Discretization Method.

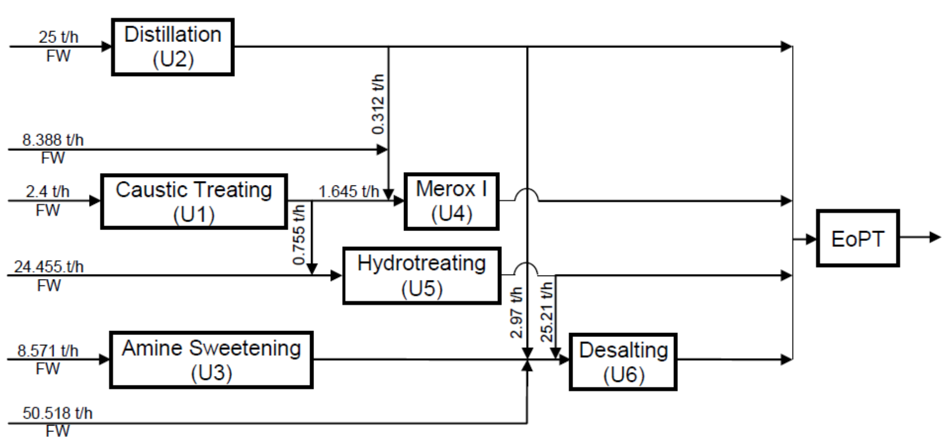
Example 3: Multicontaminant Water-using System without Regeneration - Freshwater minimization

This example is the refinery case presented by Koppol et al. (2003). This example has four key contaminants (salts, H2S, Organics and ammonia) and six water-using units. The limiting data of the water-using units are shown in Table 5-9. This network without reuse consumes 144.8 t/h of freshwater and the objective is to minimize freshwater consumption. The flowrate through the water-using units are not pre-defined and they can vary from the limiting low flowrate to a maximum allowed flowrate. The minimum freshwater consumption found by Koppol et al. (2003) is 119.33 t/h, which they did not solve to guaranteed global optimality.

In this problem, the same options of number of intervals, discretization methods and discretized variables as in example 2 were tried. A global optimum solution (119.33 t/h) is found in 0.14 s. The lower bound gives the optimum solution and thus it is found at the root node when *McCormick's envelopes* and when *Direct discretization* of concentrations are used. A LB that is different from the optimum solution is obtained when *Direct discretization* of flowrates are applied for less than 10 intervals. The minimum freshwater consumption is the same as that of Koppol et al. (2003), but the network obtained is different, which indicates that this problem is degenerate. Both networks are presented in Figure 5.8. The same comments regarding the time reported as in example 2 hold.

Table 5-9 – Limiting data of example 3.

Process	Contaminant	Mass Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1 - Caustic Treating	Salts	0.18	300	500
	Organics	1.2	50	500
	H2S	0.75	5000	11000
	Ammonia	0.1	1500	3000
2 - Distillation	Salts	3.61	10	200
	Organics	100	1	4000
	H2S	0.25	0	500
	Ammonia	0.8	0	1000
3 – Amine Sweetening	Salts	0.6	10	1000
	Organics	30	1	3500
	H2S	1.5	0	2000
	Ammonia	1	0	3500
4 - Merox-I Sweetening	Salts	2	100	400
	Organics	60	200	6000
	H2S	0.8	50	2000
	Ammonia	1	1000	3500
5 - Hydrotreating	Salts	3.8	85	350
	Organics	45	200	1800
	H2S	1.1	300	6500
	Ammonia	2	200	1000
6 - Desalting	Salts	120	1000	9500
	Organics	480	1000	6500
	H2S	1.5	150	450
	Ammonia	0	200	400



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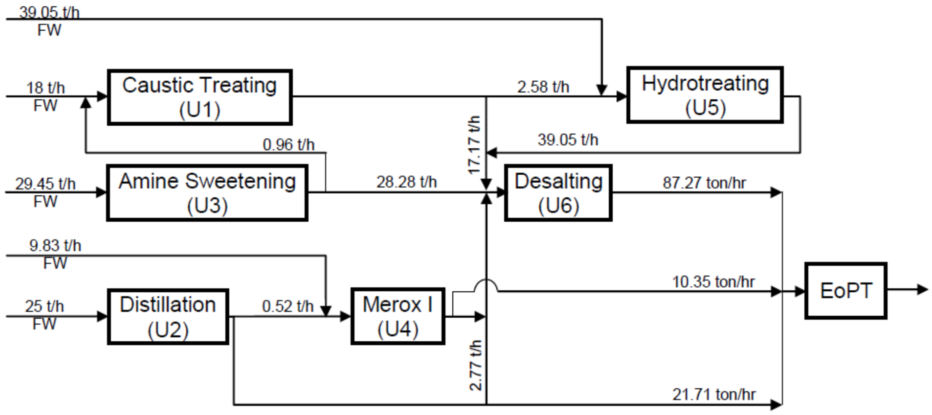

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Figure 5.8 – Optimum network of example 3. (a) Koppol et a. (2003) and (b) Discretization Method.

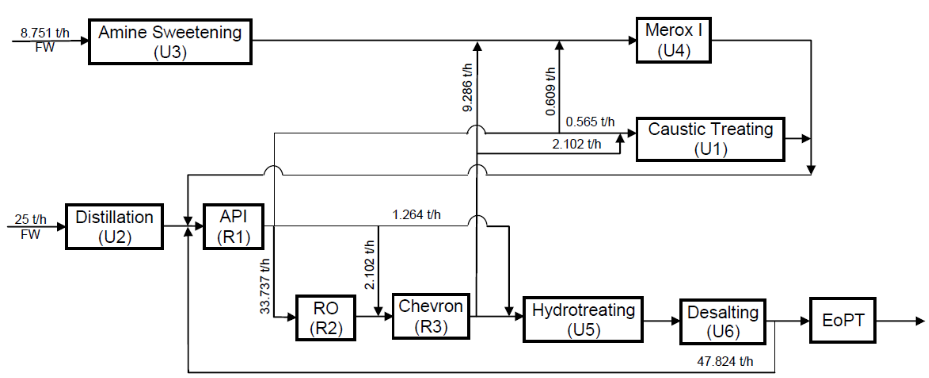
Example 4: Multicontaminant Water using System with Regeneration- Freshwater minimization

In this example the network presented in example 3 is solved with the addition of potential regeneration processes that are modeled as processes with fixed outlet concentrations. Three regeneration processes are available: Reverse osmosis, which reduces salts to 20 ppm; API separator followed by ACA, which reduces organics to 50 ppm; and, Chevron wastewater treatment, which reduces H_2S to 5 ppm and ammonia to 30 ppm. The optimum solution obtained by Koppol et al. (2003) reaches a minimum freshwater consumption of 33.571 t/h. As in the previous case, they did not solve guaranteeing global optimality.

Different options of number of intervals, discretization methods and discretized variables were tried. In all cases in which concentrations are discretized or flowrates are discretized using *McCormick's envelopes*, the same result was obtained: a lower bound solution of 33.571 t/h at the root node with only one interval. This solution corresponds to the global optimum solution of this problem. The best solution (fastest one) is found in approximately 0.56 s using MCP2 with discrete concentrations. The minimum freshwater consumption is the same as that of Koppol *et al*. (2003).

Although the minimum freshwater consumption is obtained, the found network presents very small flowrates such as 0.06 t/h. To avoid these small flowrates a minimum allowed flowrates of 1 t/h for the connections (equations 4-11 to 4-18) was added. In this case a lower bound equal to the global solution is also found at the root node, but the original model (upper bound model) does not find a feasible solution at the root node. Thus, the method has to keep looking for a solution and eliminating parts of the feasible region until the upper bound model finds the global optimum solution. Thus, the solution is found in 75.71 s using the standard elimination procedure with *active upper bounding* discretizing concentrations (2 intervals) through MCP2.

The networks obtained by Koppol et al. (2003) and ours are presented in Figure 5.9. The same comments regarding the time reported as in example 3 hold.



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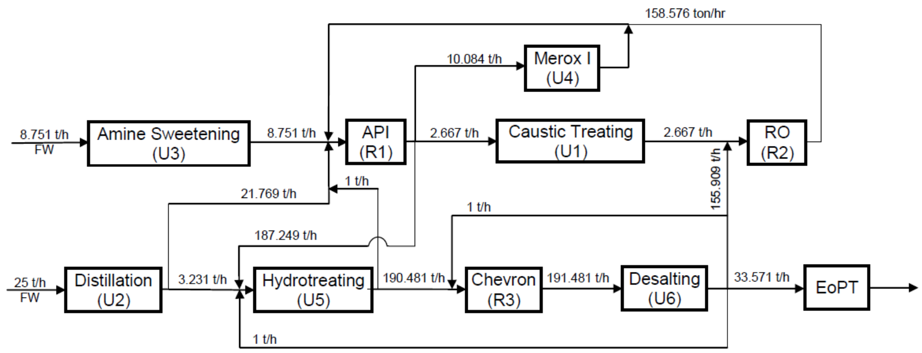

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Figure 5.9 – Optimum network of example 4. (a) Koppol et al. (2003) and (b) Discretization method.

When flowrates are discretized using *Direct discretization*, the lower bound is no longer equal to the global optimum solution and interval elimination is needed. In fact, the lower bound generated by this option is equal to zero. However, the lower bound can be further improved when a pre-processing step includes forbidden connections that cannot exist. In the WAP the following rule is used:

$$FUU_{u^*,u}^{Max} = 0 \qquad if \; C_{u,c}^{in,\max} < \bar{C}_c^{\min} \tag{5-43}$$

$$FRU_{r,u}^{Max} = 0 \qquad if \; C_{u,c}^{in,\max} < \bar{C}_c^{\min} \tag{5-44}$$

where $\bar{C}_c^{\min}$ is the minimum concentration of contaminant c in the system, which is defined by:

$$\bar{C}_c^{\min} = Min\left\{ Min_u \left\{ C_{u,c}^{out,\min} \right\}, Min_r \left\{ CR_{r,c}^{out,\min} \right\}, Min_w \left\{ CW_{w,c} \right\} \right\} \tag{5-45}$$

Now, adding the forbidden connections, the *Direct discretization* discretizing flowrates is tighter but still not as tight as the options that discretize flowrates or when flowrates are discretized using the *McCormick's envelopes*. Without a required minimum flowrates through the connections these lower bounds keep constant (16.1185 t/h) for up to 10 intervals.

Example 5: Multicontaminant Water using System without Regeneration - Freshwater + Regeneration flowrate Minimization

This example was proposed by Karuppiah and Grossmann (2006). It is a network involving two water using units, two treatment processes and two contaminants. Unlike the previous examples, in this case the water-using units have fixed flowrates, the treatment processes are modeled having a fixed efficiency and the objective is to minimize the summation of freshwater flowrate and the flowrate treated by the regeneration processes. The rationale for such an objective, according to the authors, is that the integrated system is being solved and a network with minimum freshwater consumption would have a higher combined freshwater and treated flowrate. There is a maximum discharge of the effluents to the sink (10ppm for both contaminant A and B). Tables Figure 5.10 and Figure 5.11 show the data of this example.

The global optimal solution (117.05 t/h) is found by Karuppiah and Grossmann (2006) in 37.72 s. In our case, the solution is not always found at the root node.

Table 5-10 – Water using units limiting data of example 5.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	

Table 5-11 – Regeneration processes data of example 5.

Process	Contaminant	Removal ratio (%)
1	A	95
	B	0
2	A	0
	B	95

Both lower bound models (*Direct discretization* and *McCormick's envelopes*) were analyzed discretizing concentrations and flowrates. The lower bound objectives as a function of the number of intervals used are presented in Figure 5.10. It is worth reminding here that the type of linearization used to represent the product of continuous and discrete variables does not alter the objective function.

Note that the lower bound models for discrete concentrations always give the same solution independent of whether one uses *Direct discretization* or *McCormick's envelopes*. Moreover, discretizing concentrations generates a tighter lower bound than discretizing flowrates for the same number of intervals. When flowrates are discretized, the choice of using *Direct discretization* or *McCormick's envelopes* makes a difference. This behavior was already observed in examples 3 and 4.

Additionally, as previously showed the lower bounds can be further improved when the pre-processing step includes forbidden connections that cannot exist. Figure 5.11 shows the lower bound obtained when the pre-exclusion of infeasible connections are added to the pre-processing step. Note that the lower bounds generated by the models that discretize concentration and *the McCormick's envelopes* with discrete flowrates are slightly improved, and the *Direct discretization* of flowrates keeps constant up to a certain level of discretization (7 intervals) before it starts to fell the influence of number of intervals.

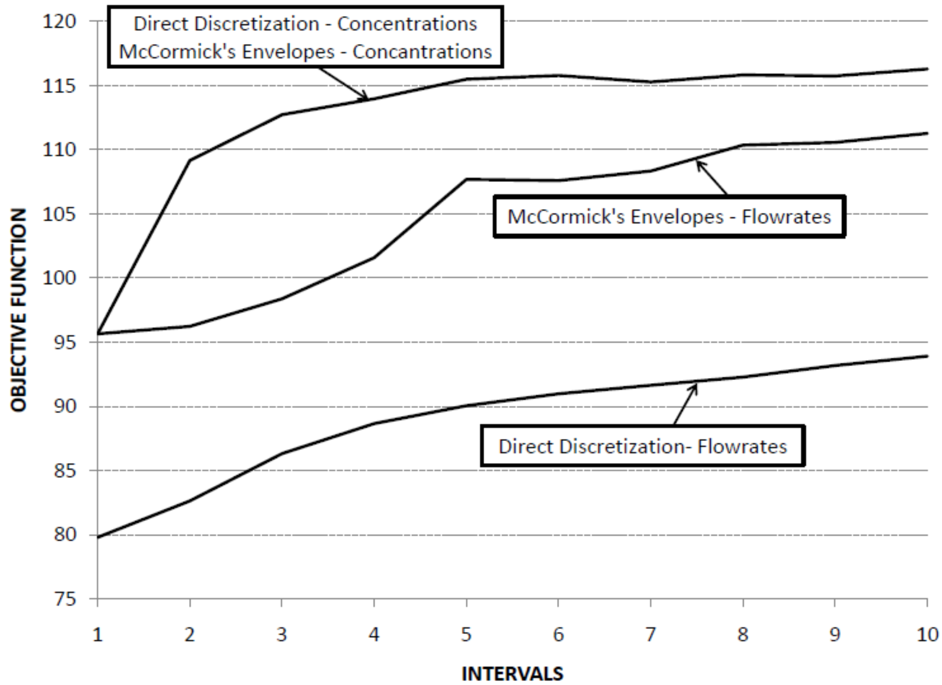


Figure 5.10 – Lower bound models objective function values as a function of the number of intervals.

In addition to the tightness of the lower bounds, the running time is an important issue to investigate. In this case it is not only the fact that we need to compare the *Direct discretization* model and *McCormick's envelopes* model (both for discrete concentration and discrete flowrates), but also the procedure used to linearize the product of the binary and continuous variables. Figure 5.12 and Figure 5.13 show the running times when forbidden connections are used or not, respectively.

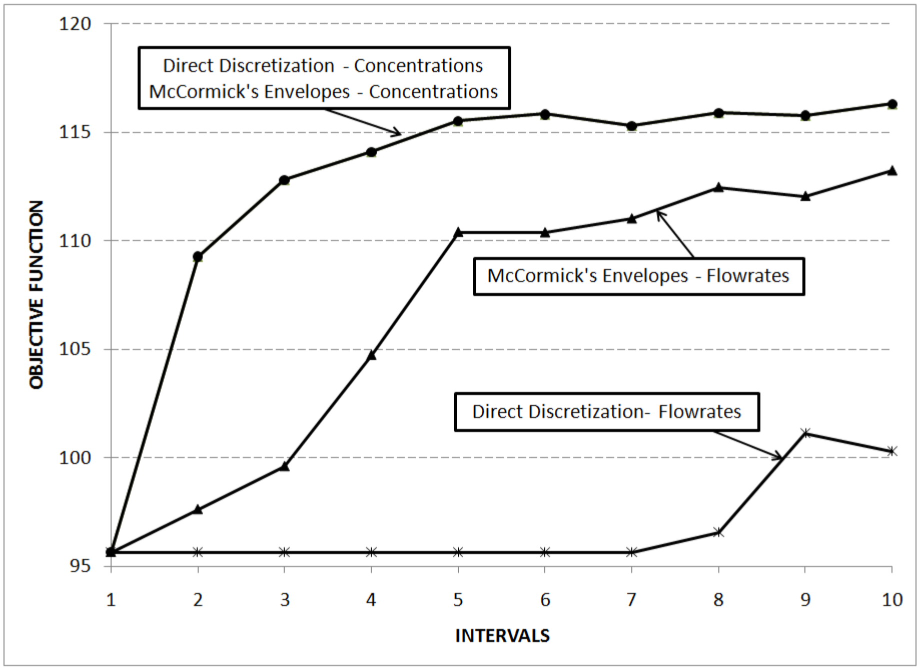


Figure 5.11 – Lower bound models objective function values as a function of the number of intervals – using pre-exclusion of infeasible connection.

The running times presented in Figure 5.12 and Figure 5.13 also reveal information about the different linearization procedures for the product of a binary and a continuous variable. Procedure DDP1-C presents much higher running time than the others. This procedure is no longer used in the rest of the paper for the different comparisons. Note that MCP3 is also less efficient when the pre-exclusion of connections is not applied (Figure 5.12).

In comparing procedures DDP2 and DDP3 in Figure 5.13, procedure DDP3 gives better results for this problem, but not significantly different. Thus, the use of procedure 2 is still considered in the following discussions.

Figure 5.14 shows the number of binary variables. The number of binary variables needed to discretize flowrate in this problem is always higher than the number of binary variables needed to discretize concentrations using the same number of intervals. This is a problem dependent characteristic as discussed above (in the *Effect of the Number of Intervals* section).

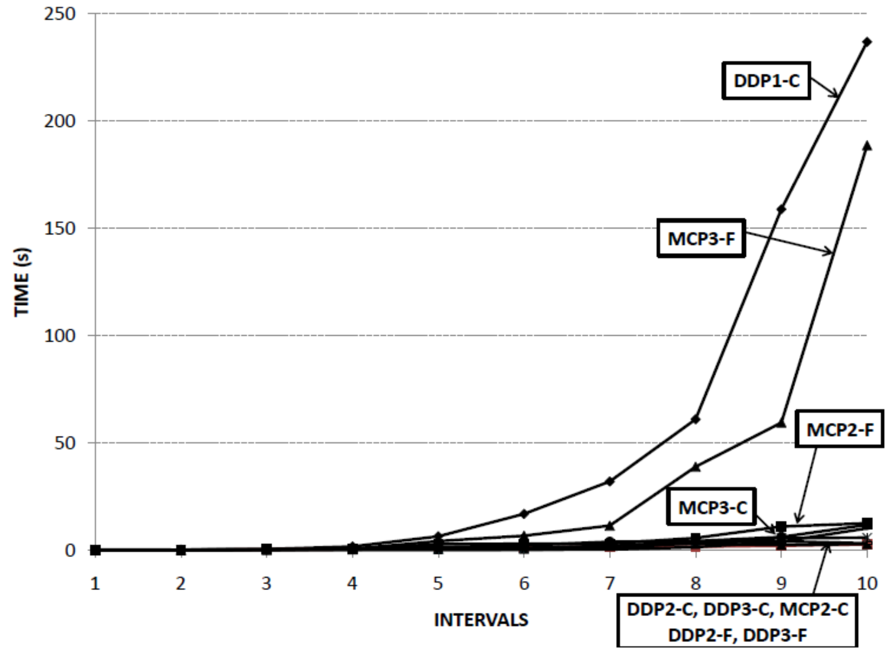


Figure 5.12 – Lower bound models computation time - no pre-exclusion of infeasible connection.

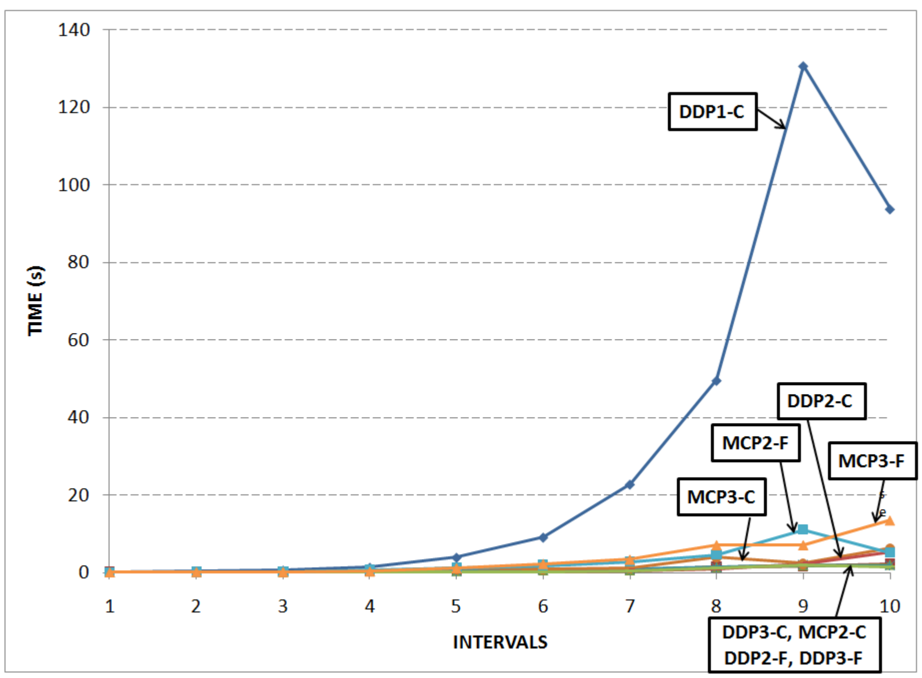


Figure 5.13 – Lower bound models computation time - using pre-exclusion of infeasible connection.

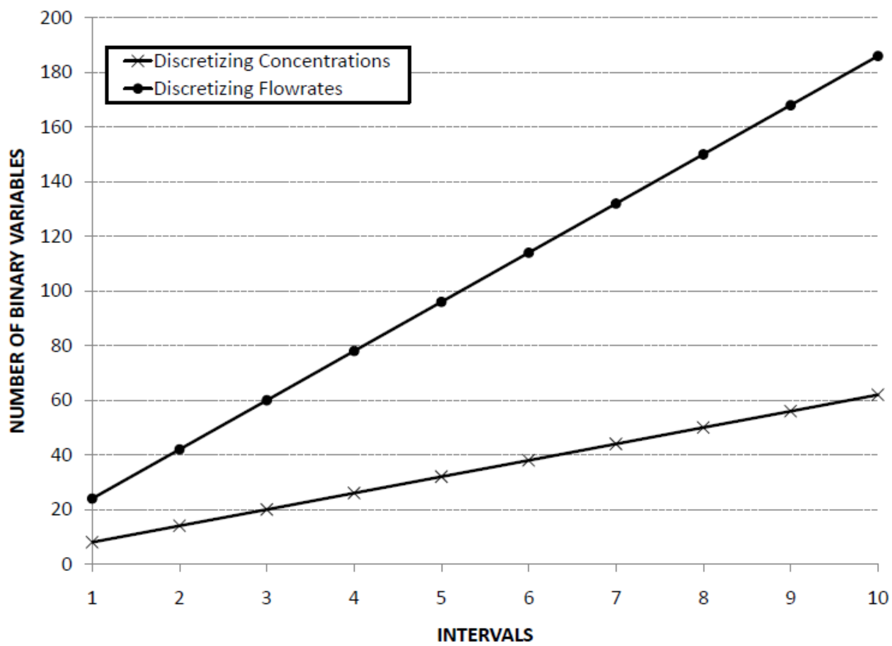
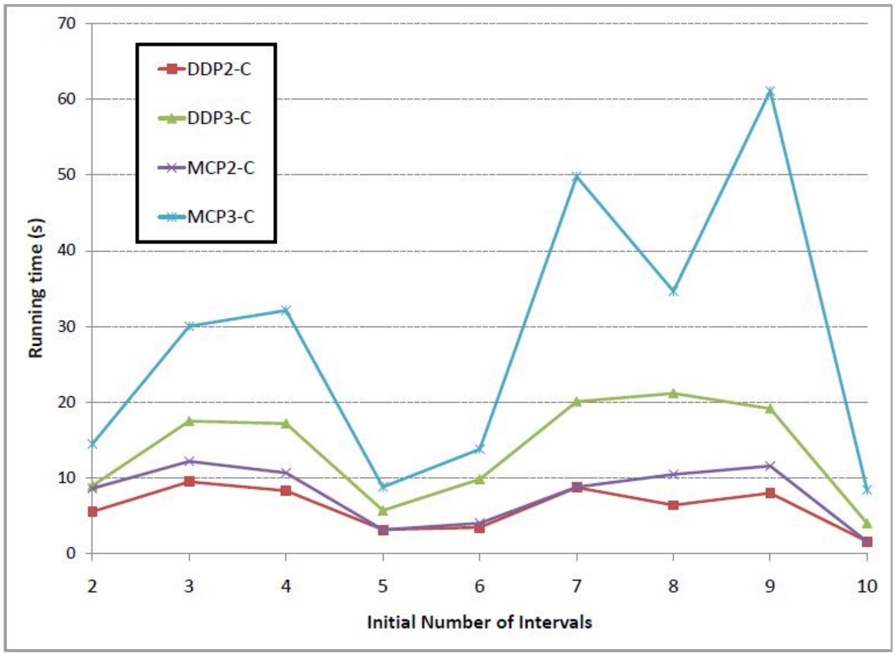


Figure 5.14 – Lower bound models analysis – Number of binary variables.

Because this is the first example that does not find the answer at the root node, the use of different elimination procedures is analyzed. *Direct discretization* of flowrates is not used here because the lower bounds generated by these models are significantly poorer than the *McCormick's envelopes* of flowrates (Figure 5.10 and Figure 5.11) although they have compatible computational time (Figure 5.12).

The problem is run using the *one-pass*, *non-exhaustive*, no *active upper bounding* and using the *extended interval forbidding*. Figure 5.15 shows the running time vs. the number of initial intervals chosen when the pre-exclusion of the infeasible connections are not used and when they are used. Note in Figure 5.15 that for most of the initial number of intervals, the pre-exclusion of infeasible connections improves the efficiency of the method. However, when the procedure starts with 10 intervals and the solution is found at the root node, the pre-exclusion of the infeasible connections does not favor the speed of the solution.



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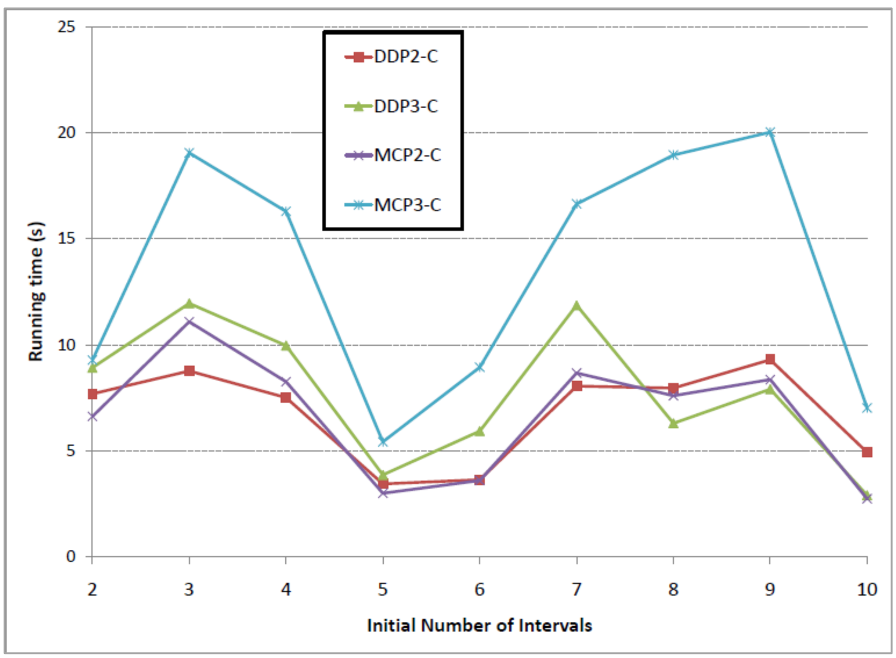

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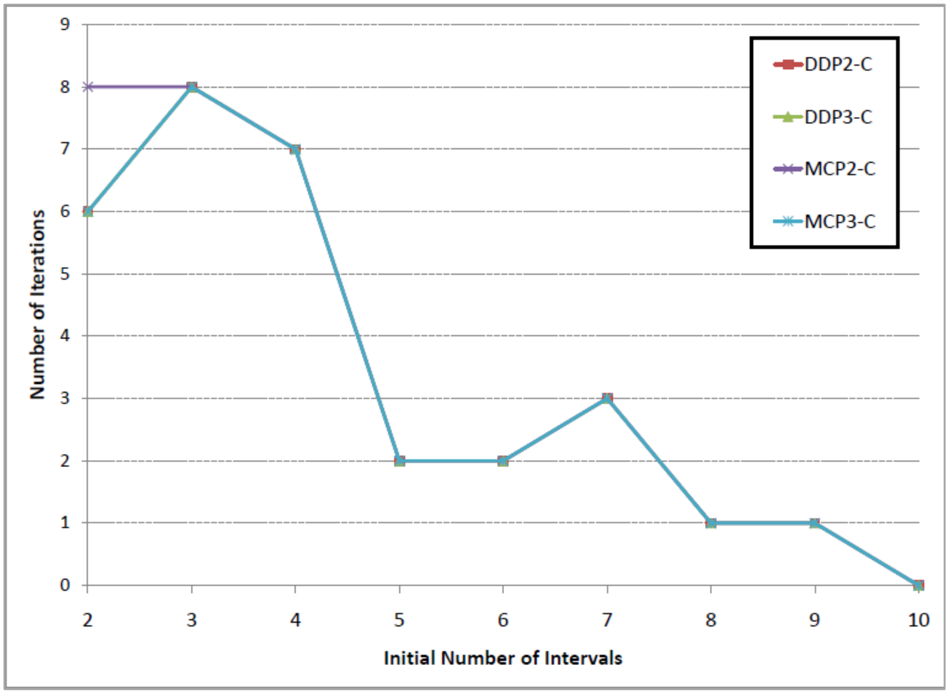
Figure 5.15 – GO procedure analysis – Running time – Discrete concentrations. a) Without pre-exclusion of infeasible connections; b) with pre-exclusion of infeasible connections.



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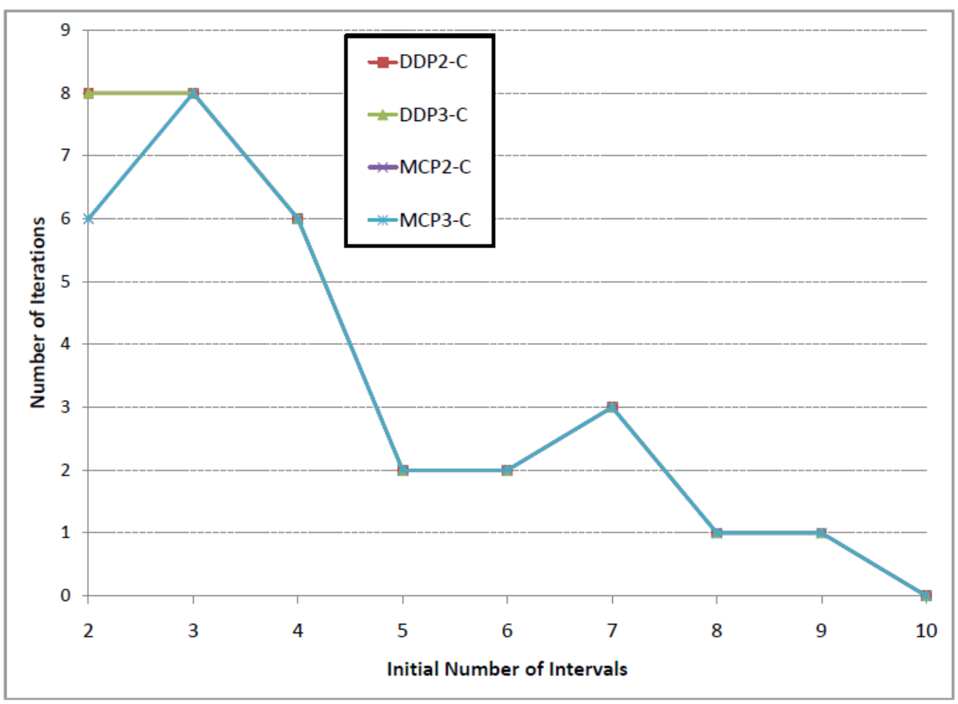

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Figure 5.16 – GO procedure analysis – Number of iterations – Discrete concentrations. a) Without pre-exclusion of infeasible connections; b) with pre-exclusion of infeasible connections.

Table 5-12 presents the solution of this problem using the different lower bound models when outlet concentrations are discretized. These solutions are the ones that give the lowest computational time.

Table 5-12 – Summary of results for discrete concentration of example 5.

LB Model	Discretized Variable	First LB	Initial # of intervals	Linearization procedure	Iterations	Time
Direct Discrete	Conc.	116.31 t/h	10	P2	0	1.59 s
McCormick envelopes	Conc.	116.31 t/h	10	P2	0	1.57 s

The solution discretizing flowrates in 2 intervals and using *McCormick's envelopes* took 11,795 s and 35 iterations when the standard procedure was used. The option of split the problem in sub-problems (branch-and-bound) after an elimination pass does not perform any elimination is now investigated. If one branches on concentrations (the non-discretized variables), the solution is found in 23.73 s, which investigates 4 sub-problems. Figure 5.17 shows an illustration of the procedure: At the root node an upper bound of 117.453 t/h is obtained and 3 eliminations iterations are performed; the lower bound is improved from 97.582 t/h to 100.027 t/h. In the first iteration 7 eliminations are performed and in the second 1 elimination takes place. As the third iteration does not make any elimination, the problem is divided in two sub-problems that are generated by splitting the outlet concentration of contaminant 1 in regeneration process 2:

Sub-problem 1 performs 6 elimination iterations and brings the lower bound from 108.133 t/h to 114.997 t/h. At this node the upper bound is still 117.453 t/h. Sub-problem 2 starts with a lower bound of 104.672 t/h and finds a better upper bound (117.053 t/h). After 4 iterations it reaches 116.316 t/h, which is less than 1% lower than the current upper bound. Thus, this node is no longer active.

The only active node (sub-problem 1) is further split in two other sub-problems through a bisection rule of the outlet concentration of contaminant 2 of regeneration process 1. As a result, sub-problem 3 is infeasible and sub-problem 4 has a lower bound value of 115.225 t/h, which is increased to 116.061 t/h after one iteration that performs 10 eliminations. This value is 0.85% lower than the current upper bound, which satisfies the given tolerance (1%) and consequently deactivated this node. As there are no more active nodes, the procedure stops and the global solution is equal to the current upper bound (117.053 t/h).

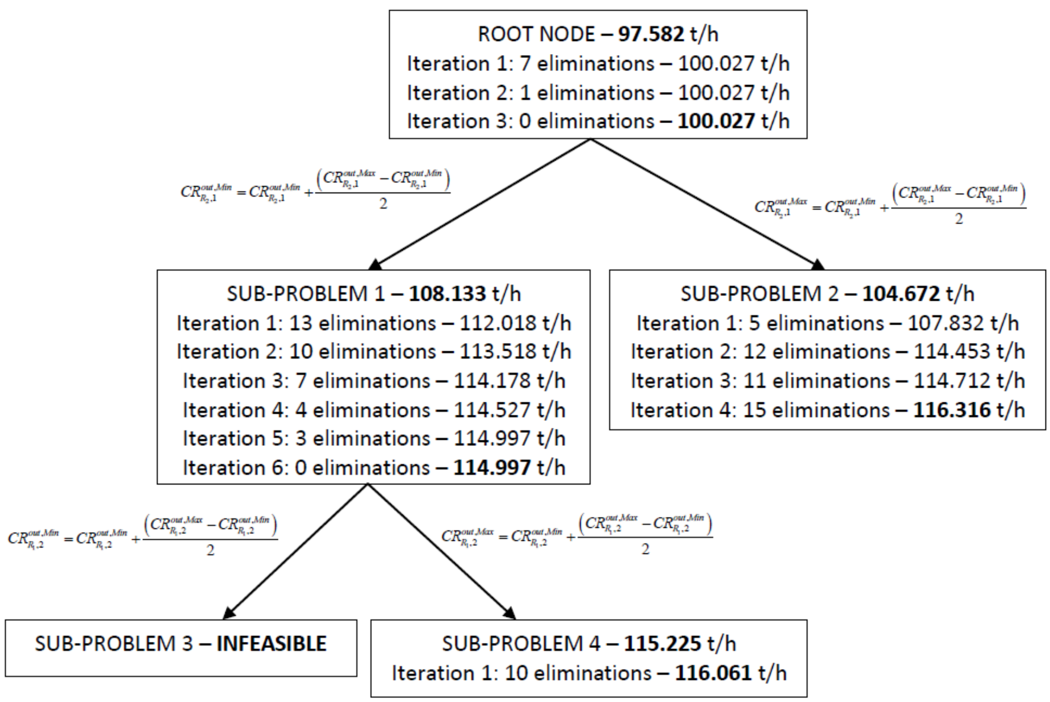

Figure 5.17 – illustration of the branch-and-bound procedure.

When the procedure branches on flowrates, it also investigates 4 sub-problems, but it takes 40.93 s. Table 5-13 presents the solution of this problem using the different branching variable when flowrates are discretized. The optimum network is presented in Figure 5.18.

Table 5-13 – Summary of results for discrete flowrates of example 5.

Branching Variable	Investigated sub-problems	Linearization procedure	Time
Outlet Concentrations	4	MCP2	23.73 s
Flowrates	4	MCP2	40.93 s

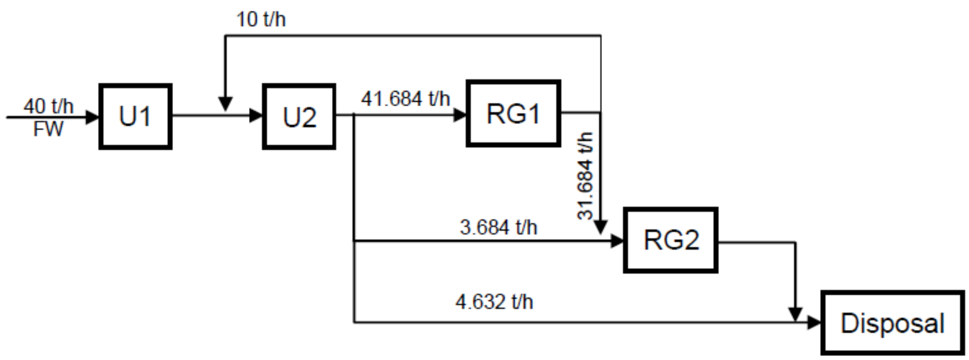

Figure 5.18 – Optimum network of example 5.

Example 6: Multicontaminant Water using System with Regeneration- Cost minimization

This example is a two contaminants, three water-using units and three regeneration processes problem proposed and solved by Karuppiah and Grossmann (2006). This problem minimizes total annual cost and assumes fixed flowrates through the water-using units and regeneration processes with fixed rate of removal. Maximum concentration at the disposal is 10 ppm for both contaminants. The data used for example 6 is presented in Table 5-14 and Table 5-15. The cost of freshwater is $1/t, the annualized factor is 0.1 and the plant runs 8000 h/year. The authors found the global optimal solution ($381,751.35/year) in 13.21 s. Later, Bergamini et al. (2008) solved the same problem to proven global optimality in 3.75 s.

Table 5-14 – Water using units limiting data of example 6.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	
3	A	1	50	60
	B	1	50	

Table 5-15 – Regeneration processes data of example 6.

Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16,800
	B	0		
2	A	80	0.003	24,000
	B	90		
3	A	0	0.0067	12,600
	B	95		

Here, outlet concentrations of the water using units and flowrates through the regeneration processes (due to the concave objective function) are discretized 4 intervals, resulting in a model (MCP2) that has 52 binary variables and 585 continuous variables. With the presented method pre-excluding the infeasible connections, the optimal solution is found in 0.41 s at the root node. This lower bound model (4 intervals) generates an objective function of $378,215.14 per year, which is 0.93% lower than the objective function and thus complies with the required tolerance (1%). If forbidding of infeasible connections is not used, the same lower bound model (MCP2 with discrete concentrations and 4 intervals) generates a value of $168,140.03 per year. The global solution is the same as that of Karuppiah and Grossmann (2006) and Bergamini et al. (2008). The obtained network is presented in Figure 5.19.

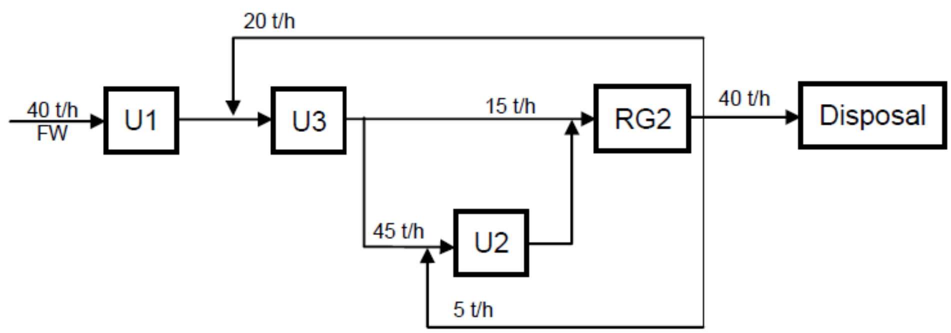

Figure 5.19 – Optimum network of example 6.

Example 7:

Example 7 is also taken from Karuppiah and Grossman (2006). It involves two contaminants and has four water-using units and two regeneration processes. Data related to the water-using units and regeneration processes are presented in Table 5-16 and Table 5-17. The same economic data and discharge limits (10 ppm) are applied for this problem.

Table 5-16 – Water using units limiting data of example 7.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	
3	A	1	50	50
	B	1	50	
4	A	2	50	50
	B	2	50	

Table 5-17 – Regeneration processes data of example 7.

Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16,800
	B	0		
2	A	0	0.0067	12,600
	B	90		

Concentrations and flowrates through the regeneration processes are discretized as in example 6 using 2 intervals. All the models (DDP2, DDP3, MCP2 and MCP3) that discretize concentrations in 2 intervals have a lower bound of $871,572.22 (wich is 0.28% lower than the global solution) and thus find the optimal solution ($874,057.37/year) in approximately 0.25 s at the root node. The resulting model has 24 binary variables and 408 continuous variables (DDP2 and MCP2) or 254 continuous variables (DDP3 and MCP3). The solution is presented in Figure 5.20.

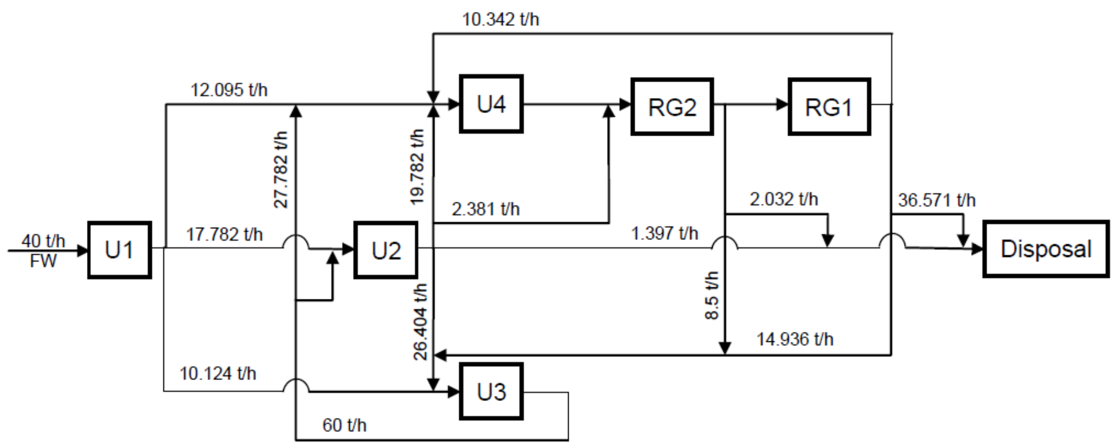

Figure 5.20 – Optimum network of example 7.

Example 8

This example is a large system presented by Karuppiah and Grossmann (2006). It involves three contaminants and has five water-using units with fixed flowrates and three regeneration processes. The data for this example is presented in Table 5-18 and Table 5-19. Additionally, the discharge limit of all the contaminants is 10 ppm.

Again, concentrations and flowrates through the regeneration processes are discretized and the interval elimination procedure is active for both sets of variables. Note that even without applying the reduction procedure in the flowrates through the connection, of their bounds may be influenced by the contraction of the regenerated flowrate's bounds due to the bounds arithmetic.

Table 5-18 – Water using units limiting data of example 8.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	F^{max} (t/h)
1	A	1	0	40
	B	1.5	0	
	C	1	0	
2	A	1	50	50
	B	1	50	
	C	1	50	
3	A	1	50	50
	B	1	50	
	C	1	50	
4	A	2	50	50
	B	2	50	
	C	2	50	
5	A	1	25	25
	B	1	25	
	C	0	25	

Table 5-19 – Regeneration processes data of example 8.

Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16,800
	B	0		
	C	0		
2	A	0	0.04	9,500
	B	0		
	C	95		
3	A	0	0.0067	12,600
	B	95		
	C	0		

Instead of using the standard procedure, the one-pass, extended interval forbidding, exhaustive elimination with active upper bounding is used in this example.

Karuppiah and Grossmann (2006) found the minimum TAC (global solution) of this of $1,033,810.95/year. Here, the same network was found in 30.15 s in the first iteration using the *McCormick's envelopes* model. This lower bound model (2 intervals) has 48 binary variables and 919 continuous variables. This network also has a small flowrate (0.04 t/h). Thus, the problem is solved using the MINLP formulation, which requires a minimum flowrate of 1 t/h through the connection. With this new constraint the found minimum TAC is $1,033,859.85, which is achieved in 73.79s after the first iteration. The network corresponding to this solution is presented in Figure 5.21. Although the small flowrates were eliminated, this network contains many recycles, which form the practical point of view could be rejected as too complex. However, if one also wants to avoid the complexity of networks, one could look for alternative solution, which could be degenerated or sub-optimum.

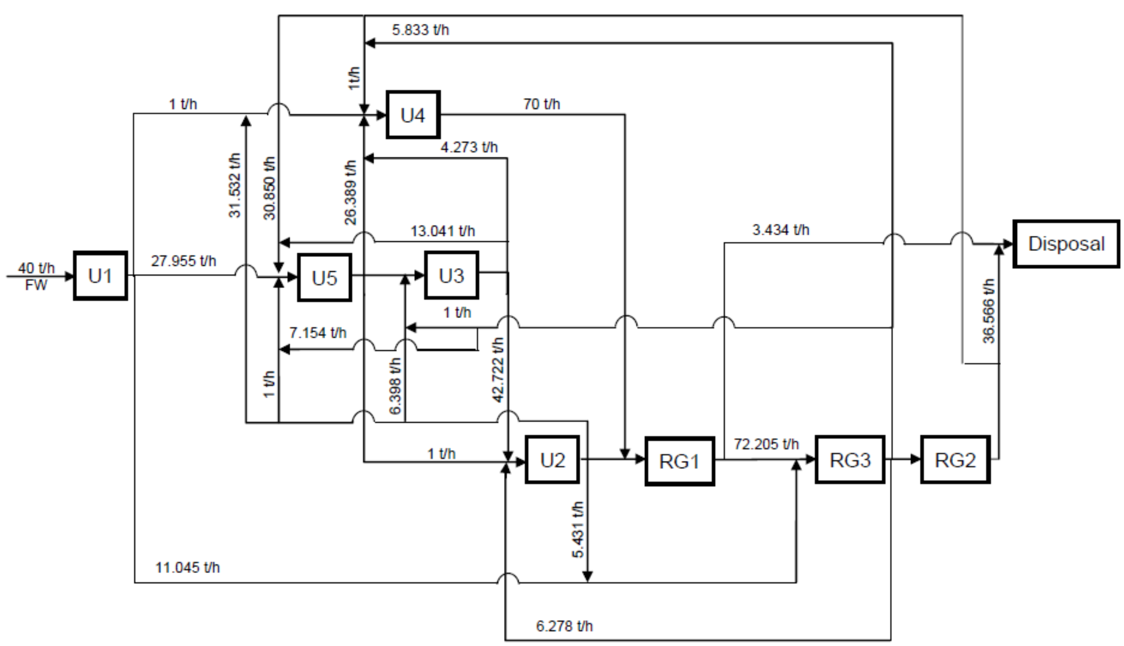

Figure 5.21 – Optimum network of example 8.

<u>*Example 9: Complex Wastewater Treatment Network*</u>

Example 9 is a complex wastewater treatment subsystem problem that was originally presented by Meyer and Floudas (2006) as a g generalized pooling problem.

The input data for this problem is slightly different from the ones presented so far, but it can also be solved using the model presented in chapter 4. A statement for this problem can be given by:

Given a set of wastewater sources w contaminated by different contaminants c that need to be removed, a set of regeneration processes r with given rate of removal for each contaminant, and a set of disposal sinks s with maximum allowed disposal concentration, one wants to minimize the cost of the wastewater system.

The data for this problem is presented in Table 5-20 to Table 5-22.

Table 5-20 – Sources data - example 9.

	W1	W2	W3	W4	W5	W6	W7
Flow	20	50	47.5	28	100	30	25
$CW_{w,c1}$	100	800	400	1200	500	50	1000
$CW_{w,c2}$	500	1750	80	1000	700	100	50
$CW_{w,c3}$	500	2000	100	400	250	50	150

Table 5-21 – Data of Regeneration processes - example 9.

	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
C1	90	87.5	99	0	90	0	0	99.5	10	70
C2	95	50	90	75	90	0	87	0	99	20
C3	0	50	95	75	20	95	90	0	0	30
FRC_r	48,901	36,676	13,972	48,901	48,901	48,901	36,676	36,676	13,972	13,972
VRC_r	3,860.3	2,895.2	1,102.9	3,860.3	3,860.3	3,860.3	2,895.2	2,895.2	1,102.9	1,102.9

Table 5-22 – Distances matrix for example 9.

$d_{i,j}$	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	S1
W1	40	65	75	100	120	110	150	210	280	245	150
W2	15	40	55	75	90	90	125	180	260	215	135
W3	40	35	30	65	100	85	115	170	240	220	100
W4	85	80	55	100	140	120	140	180	245	245	90
W5	95	70	55	45	75	45	40	75	150	150	40
W6	80	70	40	90	125	100	120	150	230	230	70
W7	70	45	30	40	75	50	60	100	175	165	45
R1	-	20	40	50	70	70	100	160	230	190	120
R2	20	-	30	30	60	50	80	140	215	180	95
R3	40	30	-	40	80	60	80	140	210	190	75
R4	50	30	40	-	40	15	50	110	180	150	85
R5	70	60	80	40	-	25	50	110	180	120	120
R6	70	50	60	15	25	-	30	100	170	130	90
R7	100	80	80	50	50	30	-	60	130	100	80
R8	160	140	140	110	110	100	60	-	70	100	95
R9	230	215	210	180	180	170	130	70	-	110	160
R10	190	180	190	150	120	130	100	100	110	-	190

The discharge limits of this system are 5 ppm, 5 ppm and 10 ppm for C1, C2 and C3 respectively. Table 5-22 shows the distances among processes.

Thus, the piping costs assuming a velocity of 1 m/s are given by:

$$FIJC_{i,j} = 124.6\ d_{i,j} \qquad \forall i \in \{W, U, R\},\ j \in \{W, U, R, S\} \tag{5-46}$$

$$VIJC_{i,j} = 1.001\ d_{i,j} \qquad \forall i \in \{W, U, R\},\ j \in \{W, U, R, S\} \tag{5-47}$$

The best known solution for was given by Meyer and Floudas as \$1.08643 × 10^6. They found a lower bound solution, which has a 1.2% gap from this given best known solution in 285,449 CPUs. Using the global optimization solver Baron, the optimum solutions is not found after 120 hours. The best solution found by BARON was \$1,107,905.

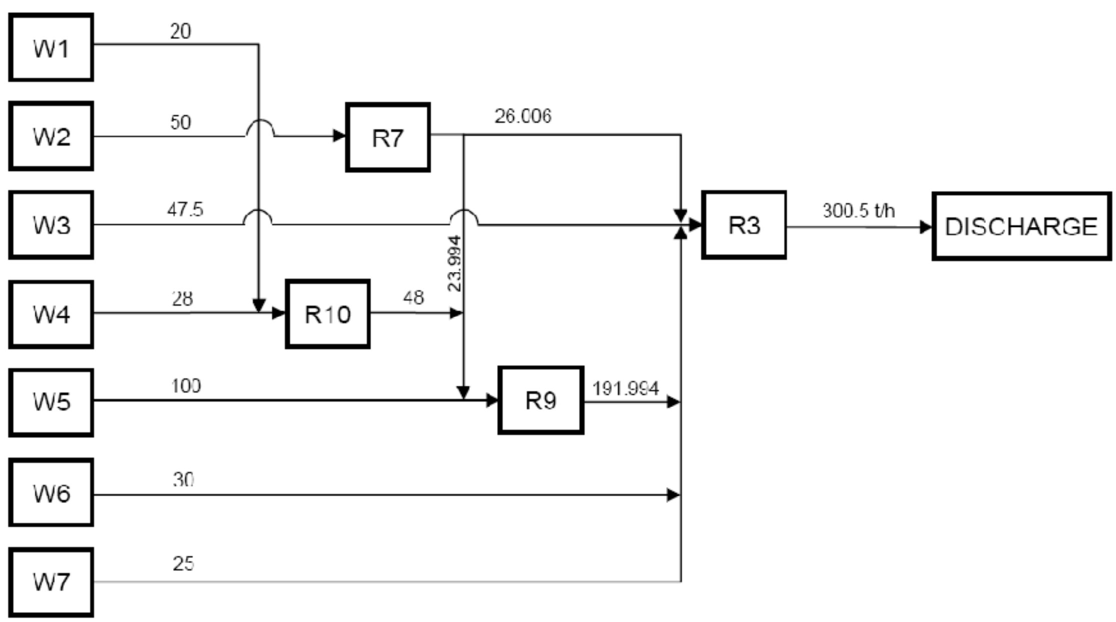

Figure 5.22 – Optimum network of example 9.

Minimizing the total cost using the presented method, the network presented in Figure 5.22, which has a total cost of \$1,086,187 was found in 16,336 CPUs. Table 5-23 shows the different procedures that were attempted. The lowest time that the solution was obtained is 16,336 CPUs.

Table 5-23 – Summary of the options tried in example 9.

Variable Discretized (Intervals)	**LB Model**	**Variables for Bound Contraction**	**BC settings**	**Variables for B&B**	**Time** ** **(CPUs)**	**Analyzed sub-problems**
Conc. (2 intervals)	MCP2	Concentrations (2 intervals) Reg. Flows (2 intervals)	Guided One pass Exhaustive UB updating	Connections Reg. Flows	16,336	16 (Optimum solution found in the 1st subproblem)
Conc. (2 intervals)	MCP2	Concentrations (2 intervals)	Guided One pass Exhaustive UB updating	Connections Reg. Flows	25,722	34 (Optimum solution found in the 8th subproblem)
Conc. (2 intervals)	MCP2	Concentrations (2 intervals) Reg. Flows (2 intervals)	Guided One pass Exhaustive UB updating LB updating	Connections Reg. Flows	21,420	16 (Optimum solution found in the 2nd subproblem)
Conc. (2 intervals)	MCP2	Concentrations (2 intervals)	Guided One pass Exhaustive UB updating LB updating	Connections Reg. Flows	28,590	34 (Optimum solution found in the 9th subproblem)
Flows (2 intervals)	MCP2	Connections flowrates (2 intervals) Reg. Flows (2 intervals)	Guided One pass Exhaustive UB updating	Connections Reg. Flows	28,930	28 (Optimum solution found at the root node)

Example 10: Refinery example

This problem was presented by Kuo and Smith (1997), which was solved using graphical approach for the design of effluent system and the cost evaluation considered freshwater cost and regeneration costs. Later, Gunaratnam et al. (2005) and Alva-Argaez et al. (2007) introduced piping costs and solved the problem using mathematical programming and minimizing the total annual cost considering freshwater cost, operating cost of regeneration processes and capital cost of regeneration processes and piping. The data is shown in Table 5-24 to Table 5-26.

Table 5-24 – Water using units limiting data of example 10.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
(1) Steam stripping	HC	0.75	0	15
	H_2S	20	0	400
	SS	1.75	0	35
(2) HDS-1	HC	3.4	20	120
	H_2S	414.8	300	12500
	SS	4.59	45	180
(3) Desalter	HC	5.6	120	220
	H_2S	1.4	20	45
	SS	520.8	200	9500
(4) VDU	HC	0.16	0	20
	H_2S	0.48	0	60
	SS	0.16	0	20
(5) HDS-2	HC	0.8	50	150
	H_2S	60.8	400	8000
	SS	0.48	60	120

Table 5-25 – Regeneration processes data of example 10.

Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
(1) Steam stripping	HC	0	1	16,800
	H_2S	99.9		
	SS	0		
(2) Biological treatment	HC	70	0.0067	12,600
	H_2S	90		
	SS	98		
(3) API separator	HC	95	0	4,800
	H_2S	0		
	SS	50		

The discharge limits of this system are 20 ppm for HC, 5 ppm for H_2S and 100 ppm for SS. The freshwater cost is \$0.2/t and the system operates 8600 hours per year. A 10% rate of discount is assumed. Table 5-26 shows the distances among processes. Thus, the piping costs are calculated as in equations (5-46) and (5-47).

The best solution for this problem minimizing TAC presented in the literature is \$616,824 (Alva-Argaez et al., 2007). This problem is included because it presents several challenges: fixed and variable cost for connection and minimum allowed flowrates through the connections, which makes it a MINLP problem; water-using units with variable flowrates; and, competing regeneration processes (more than one process is able to treat the same contaminant). The minimum allowed flowrate through connection and units is considered to be 5 t/h and the maximum 200 t/h.

Table 5-26 – Distances matrix for example 10.

$d_{i,j}$	WU 1	WU 2	WU 3	WU 4	WU 5	RG 1	RG 2	RG 3	Discharge
FW	30	25	70	50	90	200	500	600	2000
WU 1	0	30	80	150	400	90	150	200	1200
WU 2	30	0	60	100	165	100	150	150	1000
WU 3	80	60	0	50	75	120	90	350	800
WU 4	150	100	50	0	150	250	170	400	650
WU 5	400	165	75	150	0	300	120	200	300
RG 1	90	100	120	250	300	0	125	80	250
RG 2	150	150	90	170	120	125	0	35	100
RG 3	200	150	350	400	200	80	35	0	100

This problem can be solved to global optimality (1% gap) using BARON in 7 hours. The minimum TAC obtained id $574,155.

Using the GO method with elimination on discretized variable presented in this section, the lowest time achieved to guarantee the 1% tolerance solution was 25,293 CPUs. This procedure used MCP2 with 5 interval on concentrations and 2 on regeneration flows. Although the presented method takes longer than BARON to find the GO solution, it finds it at the root node. The optimum network found has a TAC of $578,183.

5.2.1. Summary of the results obtained by the discretization method

The results obtained above are summarized in Table 5-27 and Table 5.28. Table 5-27 summarizes the results of different option tried in each example. Note that among the solutions obtained using different options, most of the examples have their smallest

CUP time when the number of intervals is increased and the global solution is obtained at the root node.

Next, in Table 5-28, the solutions obtained with the discretization method are compared to previous work as well the iterations needed and the best time.

Table 5-27 – Summary of the options tried in each example using the discretization method

Example	Variable Discretized (Intervals)	LB Model	Variables for Bound Contraction	Strategy	Variables for B&B	Time** (CPUs)
1	Concent. 2 intervals	DDP3	Concent.	One-pass Non-exhaustive	Not needed	0.6
	Concent. 2 intervals	DDP3	Concent.	Cyclic Non-exhaustive	Not needed	2.26
	Concent. 2 interval	DDP3	Concent.	One-pass Exhaustive	Not needed	1.30
	Concent. 7 intervals	DDP3	Concent.	One-pass Non-exhaustive One. inter. Forbid	Not needed	0.07
	Concent. (9,11,13,18) intervals	DDP3	Concent.	One-pass Non-exhaustive Ext. inter. Forbid.	Not needed	0.15
2	Concent. 1 interval	DDP2	Not needed Solved at root node	Not needed	Not needed	0.10
	Flowrate 1 interval	DDP2	Not needed Solved at root node	Not needed	Not needed	0.16
3	Flowrates 2 intervals	DDP2	Not needed Solved at root node	One-pass Non-exhaustive	Not needed	10.67
	Flowrates 1 intervals	MCP2	Not needed Solved at root node	Not needed	Not needed	0.19
	Concent. 1 interval	DDP2	Not needed Solved at root node	Not needed	Not needed	0.17
	Concent. 1 interval	MCP2	Not needed Solved at root node	Not needed	Not needed	0.14
4 NLP	Flowrates 2 intervals	DDP2	Flowrates	One-pass Non-exhaustive	Not Needed	
	Flowrates 1 intervals	MCP2	Not needed Solved at root node	Not needed	Not needed	0.53
	Concent. 1 interval	DDP2	Not needed Solved at root node	Not needed	Not needed	0.57
	Concent. 1 interval	MCP2	Not needed Solved at root node	Not needed	Not needed	0.56
4 MINLP	Concent. 2 intervals	MCP2	Concent.	One-pass Non-exhaustive Active UB	Not Needed	75.71

5	Concent. 10 intervals	MCP2	Concent.	Not needed	Not Neede d	1.57
	Concent. 10 intervals	DDP2	Concent.	Not needed	Not Neede d	1.59
	Flowrates 2 intervals	MCP2	Flowrates	One-pass Non-exhaustive One inter. Forbid	Not Neede d	11,795
	Flowrates 2 intervals	MCP2	Flowrates	One-pass Non-exhaustive One inter. Forbid	Conc.	23.73
	Flowrates 2 intervals	MCP2	Flowrates	One-pass Non-exhaustive One inter. Forbid	Flows	40.93
6	Concent. 4 intervals	MCP2	Concent. Regeneration flowrates	Not needed	Not Neede d	0.41
7	Concent. 2 intervals	DDP2 DDP3 MCP2 MCP3	Concent.	Not needed	Not Neede d	0.25
8	Concent. 2 intervals	MCP2	Concent. Regeneration flowrates	One-pass Ext. inter. Forbid Exhaustive Active UB	Not Neede d	30.15
8 MINLP	Concent. 2 intervals	MCP2	Concent. Regeneration flowrates	One-pass Ext. inter. Forbid Exhaustive Active UB	Not Neede d	73.79
10	Concent. 5 intervals Reg. Flow 2 intervals	MCP2	Concent. Reg. Flows WU Flow	One-pass One inter. Forbid Exhaustive Active UB Active LB	Flows	25,293

** Only execution time.

Table 5-28 – Summary of the best results for the water networks.

Example	Original Solution	Our Global Solution	Iterations	Time***
1 – Wang and Smith (1994)	54.00 t/h	54.00 t/h	0	0.07 s
2 – Wang and Smith (1994)	55.50 t/h	55.47 t/h	0	0.1 s
3 – Koppol et al. (2003)	119.33 t/h	119.33 t/h	0	0.14 s
4 – Koppol et al. (2003) - NLP	33.57 t/h	33.57 t/h	0	0.56 s
4 – Koppol et al. (2003) - MINLP	33.57 t/h	33.57 t/h	1	75.71 s
5 – Karuppiah and Grossmann (2006)*	117.5 t/h (37.72 s)	117.05 t/h	0	1.57 s
6 – Karuppiah and Grossmann (2006)*	$381,751.35 (13.21 s/3.75 s**)	$381,751.35	0	0.41 s
7 – Karuppiah and Grossmann (2006)*	$874,057.37 (0.9 s)	$874,057.37	0	0.25 s
8 – Karuppiah and Grossmann (2006)*	$1,033,810.95 (231.37 s)	$1,033,810.95	1	30.15 s
8 – Karuppiah and Grossmann (2006) - MINLP	N/A	$1,033,859.85	1	73.79 s
9 – Meyer and Floudas (2006)	$\$1.08643 \times 10^6$ (285,449 s)****	$1,086,187	16 subproblems	16,336 s
10 – Alva-Argaez et. al (2007)	$616,824	$578,183	62 subproblems	25,293 s

* Problem originally solved for global optimality.

** The second time reported corresponds to Bergamini et al. (2008).

*** We show the Execution time only.

**** The solution was not found in the procedure, but compared to a lower bound that gives 1.2% gap from their best known solution.

In conclusion, it seems that using the larger number of intervals possible reduces the number of iterations when the problems are relatively small, which many times don't need any iteration because the solution can be found at the root node. This observation is not necessarily related to the size of the problem, but the tightness of the lower bound model. Note that example 8 and 9 have the same size, however the later showed to be much more difficult to solve for global optimality. The main difference can be attributed to the poor lower bound generated for the latter case.

Additionally, in some problems we observed that when concentration is discretized, the LB of the *Direct discretization* is as tight as the *McCormick's envelopes*, and discretization of concentrations normally generates tighter lower bounds than discretization of flowrates.

5.3. GO Method Using Interval Elimination on Non-Discretized Variables

An alternative method to obtain the global optimum solution of MINLP problems containing bilinearities is proposed here. The method can use a special relaxation to generate lower bounds or one of the relaxation previously discussed. The main difference of this method is related to the elimination procedure (bound contraction), which does not rely on discretization of any variable. Once the bound contraction procedure is finished, that is, no bounds can be contracted anymore, the method also follows the previous procedure of split the problem in subproblems using a branch and bound scheme at each node.

5.3.1. Relaxation Methodology

Consider z to be the product of two continuous variables x and y:

$$z_{ij} = x_i \; y_j \quad \forall i = 1,...,n; \forall j = 1,...,m \tag{5-48}$$

where both x_i and y_j are subject to certain bounds:

$$x_i^L \le x \le x_i^U \quad \forall i = 1,...,n \tag{5-49}$$

$$y_j^L \le y \le y_j^U \quad \forall j = 1,...,m \tag{5-50}$$

Then, equation (5-48) is replaced by the following two equations:

$$z_{ij} \geq \overline{x}_i^L y_j \quad \forall i = 1,...,n; \forall j = 1,...,m \tag{5-51}$$

$$z_{ij} \leq \overline{x}_i^U y_j \quad \forall i = 1,...,n; \forall j = 1,...,m \tag{5-52}$$

where updated bounds are used for x_i ($\overline{x}_i^L$ and $\overline{x}_i^U$). Note that (5-50) is still included in the problem.

Because equation (5-48) is replaced by the relaxation equations (5-51) and (5-52), the proposed problem is MILP and is also a lower bound of the original problem. The method updates the bounds of one variable at a time.

For reasons that will become clear later, reference values are introduced. These values are calculated after a lower bound is obtained using the relaxed model. Let $\hat{z}_{ij}$ and $\hat{x}_i$ be the results of running the lower bound problem. Then, reference values for x_i (x_i^{ref}) that represent the most likely value of x_i are obtained as follows:

$$x_i^{ref} = f_x^{(i)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{y}_1, \hat{y}_2, ..., \hat{y}_m) \quad \forall i = 1,...,n \tag{5-53}$$

The function $f_x^{(i)}$ (●) can have different forms, which are:

$$f_x^{(1)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{y}_1, \hat{y}_2, ..., \hat{y}_m) = \frac{\sum_{j=1,...m} \hat{z}_{ij}}{\sum_{j=1,...m} \hat{y}_j} \quad \forall i = 1,...,n \tag{5-54}$$

$$f_x^{(2)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{y}_1, \hat{y}_2, ..., \hat{y}_m) = \underset{\forall j=1,...m}{Max} \left\{ \frac{\hat{z}_{ij}}{\hat{y}_j} \right\} \quad \forall i = 1,...,n \tag{5-55}$$

$$f_x^{(3)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{y}_1, \hat{y}_2, ..., \hat{y}_m) = \underset{\forall j=1,...m}{Min} \left\{ \frac{\hat{z}_{ij}}{\hat{y}_j} \right\} \quad \forall i = 1,...,n \tag{5-56}$$

Distances to the bounds, called lower and upper departure, are also defined as follows:

$$d_i^L = x_i^{ref} - \overline{x}_i^L \qquad \forall i = 1,...,n \tag{5-57}$$

$$d_i^U = \overline{x}_i^U - x_i^{ref} \qquad \forall i = 1,...,n \tag{5-58}$$

5.3.2. Bound Contraction Procedure

The methodology is based on updating the bounds $\overline{x}_i^L$ and $\overline{x}_i^U$ for each variable one at a time. First, the Auxiliary Linear model ALB_r^L is defined as the one where the original bilinear constraint (5-48) for all variables is replaced by equations (5-51) and (5-52), with the exception of equation (5-48) for z_{rj}, which is replaced by equation (5-52) as above and a modified equation (5-51) as follows:

In turn, α_r^L is given by:

$$\alpha_r^L = x_r^{ref} + s\, d_r^U , \tag{5-59}$$

where s can vary from 0 to 0.99.

The variable to be analyzed r is defined by lowest departure is d_r^L, that is, x_r^{ref} is closer to $\overline{x}_r^L$ than to $\overline{x}_r^U$.

Thus, problem ALB_r^L is run for different incremental increasing values of s (Δs) until one reaches a point where the problem is infeasible or this lower bound is higher than the current upper bound for a certain $s=s^*$. This is illustrated in Figure 5.23.

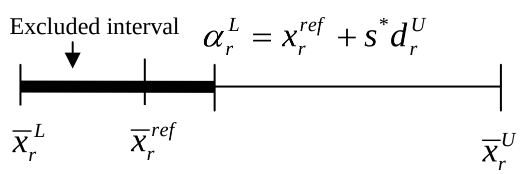

Figure 5.23 – Interval exclusion for bound contraction

Several different strategies can be implemented to determine s^*. One could start with s=0 and keep increasing s until s^* is identified or s is equal a pre-defined s^{max}. However, this strategy may take too many steps, especially when Δs is small. One alternative is to start with some value of *s, say* s=ε and x_r^{ref} equal to $f_x^{(2)}$. The reason for this is that $f_x^{(2)}$ is the best estimate of the largest reference value for x_i and therefore the excluded interval may contain all the possible solutions for x_i. Alternatively one can set x_r^{ref} equal to $f_x^{(1)}$ or $f_x^{(2)}$ but in this case some of the relaxed terms may have values on the non forbidden portion of x_i. Quite clearly, there is a compromise between the size of Δs ,or the chosen x_r^{ref} and the strategy to use. In the latter case the value of $x_r^{ref} = f_x^{(3)}$ may be too low and too many steps may be needed until an interval bound contraction is performed. However, if and contraction happens earlier, the procedure improves quickly because of the procedure is more efficient. In the former case, the chances of eliminations in earlier iterations are higher, but the improvement of the bound contraction is slower due to eliminations of smaller portions of the x_i. The simple case of starting with the suggested value of $x_r^{ref} = f_x^{(3)}$, starting with $s=\varepsilon$, and march forward if needed is chosen here. Note that x_r^{ref} must never be smaller than $f_x^{(3)}$.

Thus, at this point one can say that with all the current bounds in place for all variables, one can be certain that the solution of the problem does not contain a value of x_1 in the interval [$x_i^{ref} + s\, d_i^U , \overline{x}_r^U$] and therefore that portion of the feasible space can be eliminated. In other words one should update the upper bound as follows:

$\overline{x}_r^U \leftarrow x_i^{ref} + s\ d_i^U$.

When the lowest departure is d_r^U, that is, x_r^{ref} is closer to $\overline{x}_r^U$ than to $\overline{x}_r^L$, we define the Auxiliary Linear model ALB_r^U, where instead of modifying equation (5-52) for *i*=*r*, we modify equation (5-52) as follows:

$$z_{rj} \le \alpha_r^U y_j \quad \forall j = 1,...,m \tag{5-60}$$

Where $\alpha_r^U = x_r^{ref} - s\ d_r^L$ is used to improve the lower bound of x_r ($\overline{x}_r^L$). Again, in this equation *s* is a value between 0 and 1, and d_r^L is the distance paramenter previously defined. Thus, running ALB_1^U repeatedly until the problem is either infeasible of has a solution higher than the current upper bound for certain s^* one identifies new lower bound as follows $\overline{x}_r^L \leftarrow x_r^{ref} - s\ d_r^L$. In this case, one could start with *s*=0 or with a value of *s* such that $x_r^{ref} - s\ d_r^L < f_{x_r}^{(2)}$.

The algorithm then can proceed with this bound contraction until upper and lower bounds are close within a tolerance. If no further contraction can be made, the procedure needs to use a decomposition strategy of some sort where sub-problems are created. One such procedure could be a branch and bound scheme.

5.3.3. Global Optimization Algorithm

The bound contraction algorithm for contraction on one of the variables of the bilinear term is the following:

Assume that $\overline{x}_i^L = x_i^L$, $\overline{x}_i^U = x_i^U$

Run the LB model to get $\hat{z}_{ij}$, $\hat{x}_i$ and $\hat{y}_j$. Calculate x_i^{ref} and y_j^{ref} .

Use $\hat{z}_{ij}$, $\hat{x}_i$ and $\hat{y}_j$ as initial values to calculate the UB by running the original

MINLP. Alternatively, if this gives an infeasible answer, one can try some problem specific ad-hoc upper bound versions of the problem.

Calculate all the distances d_i^L and d_i^U. Determine the variable r that has the smallest distance. If $d_r^L < d_r^U$ go to step 5. Otherwise, go to step 6.

Run problem ALB$_r^L$ for different values of s until it is infeasible or it has an objective larger than the current upper bound of the problem. Set $\bar{x}_r^U \leftarrow \bar{x}_r^L + s^* \, d_r^U$. Go to step 7.

Run problem ALB$_r^U$ for different values of s until it is infeasible or it has an objective larger than the current upper bound of the problem. Set $\bar{x}_r^L \leftarrow \bar{x}_r^U - s^* \, d_r^L$. Go to step 7.

If $\bar{x}_i^U - \bar{x}_i^L < \varepsilon$ (the tolerance) for ALL $i \in I$ or (UB-LB)/UB<tolerance, then stop. Otherwise go to step 8.

If no variable was contracted in the previous pass, split the problem in sub-problems and repeat 1 to 7 for each sub-problem.

5.3.4. Extended Bound Contraction Procedure

The above bound contraction algorithm can also be run when both variables are involved in the procedure. We present now this extended bound contraction notion. In this case, for the lower bound, equation (5-48) is substituted by equations (5-51) and (5-52) as shown above plus the following two constraints.

$$z_{ij} \geq x_i \, \bar{y}_j^L \quad \forall i = 1,...,n; \forall j = 1,...,m \tag{5-61}$$

$$z_{ij} \leq x_i \, \bar{y}_j^U \quad \forall i = 1,...,n; \forall j = 1,...,m \tag{5-62}$$

where we use updated bounds for y_j ($\overline{y}_j^L$ and $\overline{y}_j^U$). Now, because both x_i and y_j are part of the model, we add the following constraints:

$$\overline{y}_j^L \le y_j \le \overline{y}_j^U \quad \forall j = 1,...,m \tag{5-63}$$

$$\overline{x}_i^L \le x_i \le \overline{x}_i^U \quad \forall i = 1,...,n \tag{5-64}$$

Once this LB model is solved we define reference values for x_i (x_i^{ref}) as above, and we also define distances for y_j (y_j^{ref}) as follows:

$$y_j^{ref} = f_y^{(i)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{x}_1, \hat{x}_2, ..., \hat{x}_n) \quad \forall j = 1,...,m \tag{5-65}$$

With the same options for f (●), namely:

$$f_y^{(1)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{x}_1, \hat{x}_2, ..., \hat{x}_n) = \frac{\sum_{i=1,...n} \hat{z}_{ij}}{\sum_{i=1,...n} \hat{x}_j} \quad \forall j = 1,...,m \tag{5-66}$$

$$f_y^{(2)}(\hat{z}_{i1}, \hat{z}_{i2}, ..., \hat{z}_{im}; \hat{x}_1, \hat{x}_2, ..., \hat{x}_n) = \underset{\forall i=1,...n}{Max} \left\{ \frac{\hat{z}_{ij}}{\hat{x}_i} \right\} \quad \forall j = 1,...,m \tag{5-67}$$

The same distances and bounds updates are applied here and the algorithm is run exactly as described above, except that all variables of the bilinear terms are considered for contraction. In addition, the presence of both variables as candidates for contraction may prompt the addition of some ad-hoc problem specific.

5.3.5. Results using interval elimination on non discretized variables

This method was applied to some of the problem presented earlier in this chapter. Problem that were solved at the root node were not test here.

The MINLP version of Koppol et al. (2003), which is example 4 from the previous section, was solved using the method of interval elimination on non discretized variables. The solving time for this problem was reduced from 75 CPUs to 32 CPUs.

The solving time of example 8 (NLP case) could be reduced from 30 CPUs to 7 CPUs. For that, the relaxed lower bound model presented in section 5.3.2 (no integers) was used and bound contraction (elimination procedure) was performed only on the flowrates through the regeneration processes and it was assumed an initial *s* equal 0.1, and $\Delta s = 0.45$. The procedure finds the solution after the first iteration, which significantly contracts the regeneration flowrates bounds and brings the lower bound of this problem from $1,016,955 to $1,023,546, which has a 0.99% gap from the optimum solution. The same network with small flowrates was with this method.

As previously discussed, these flowrates (0.042 t/h) are unpractical. The solution for the MINLP version of this problem was reduced from 73 CPUs to 39 CPUs. This solution used the relaxed model without discretization bound contracting the flowrates of regeneration processes using *s* equal 0.1 without increments option. The minimum TAC was found in the first iteration as being $1,033,870, which is slightly higher than the solution found using the method of elimination on discretized variables.

5.4. GO Method Using Subspace Analysis

The global optimization strategy using subspace analysis is based on the partition of the feasible region in boxed sub-spaces defined by the partition of specific variables into intervals. Using any valid lower bound model, a master problem is created. This master problem determines several sub-spaces where the global optimum may exist, disregarding the others. Each sub-space is then explored using any other global optimization methodology (one of the bound interval elimination methods previously presented, spatial B&B, among others).

5.4.1. Methodology

Consider the following MINLP problem:

$$\underset{x,y,Y}{Min}\; f(x,y,K) \tag{5-68}$$

s.t

$$g(x,y,K) \le 0 \tag{5-69}$$

$$x_i^L \le x_i \le x_i^U \quad \forall i \tag{5-70}$$

$$y_j^L \le y_j \le y_j^U \quad \forall i \tag{5-71}$$

$$(x,y) \in \mathbb{R}^2, K \in \{0,1\}^m \tag{5-72}$$

In this problem the continuous variables are separated in two sets, the set of "space partitioning variables" $X = \{x_i\}$ and the rest of the variables $Y = \{y_j\}$

The partitions variables X need to be divided following a given rule. Here they are divided in D^x*-1* identical intervals defined as follows:

$$\hat{x}_{i,d_i^x} = x_i^L + \left(d_i^x - 1\right)\frac{\left(x_i^U - x_i^L\right)}{D_i^x - 1} \qquad \forall x_i \in X, d_i^x = 1..D_i^x \tag{5-73}$$

Using the partition, the solution of the master problem need to be tracked to identify in which box the solution is located. Thus, a set of binary variables (λ_{i,d_i^x}) associated to each partition is needed together with the following equations:

$$\sum_{d_i^x=1}^{D_i^x-1} \hat{x}_{i,d_i^x}\,\lambda_{i,d_i^x} \le x_i \le \sum_{d=1}^{D_i^x-1} \hat{x}_{i,d_i^x+1}\,\lambda_{i,d_i^x} \qquad \forall x_i \in X \tag{5-74}$$

$$\sum_{d_i^x=1}^{D_i^x-1} \lambda_{i,d_i^x} = 1 \quad \forall x_i \in X \tag{5-75}$$

Consider now that a lower bound model of the original problem is constructed. Such a model is usually an MILP model obtained by performing certain relaxations of the different terms in the objective function and constraints. When constraints (5-74) and (5-75) are added to this LB model, the problem LB^0 is created.

Assume now that LB^0 is solved and a certain solution $((\bar{x}^0, \bar{y}^0, \bar{K}^0, \bar{\lambda}^0))$ is obtained. Thus, the first subspace $\Omega^{(0)}$ was identified. This subspace is then associated to a certain box defined by $\Omega_{i,d_i^x}^{(0)} = \lambda_{i,d_i^x}^0$. If one wants to identify another lower bound and its associated subspace $\Omega^{(1)}$ different from $\Omega^{(0)}$, the following integer cut is added:

$$\sum_{i|x_i \in X} \Omega_{i,d_i^x}^{(0)} \lambda_{i,d_i^x} \le \left(\sum_{i|x_i \in X} \Omega_{i,d_i^x}^{(0)} \right) - 1 \tag{5-76}$$

In turn, the addition of this integer cut creates the master problem (LB-MASTER$^{(1)}$). Generalizing, the LB-MASTER$^{(t)}$ is defined as the optimization problem defined by LB^0 and the following constraints:

$$\sum_{i|x_i \in X} \Omega_{i,d_i^x}^{(r)} \lambda_{i,d_i^x} \le \left(\sum_{i|x_i \in X} \Omega_{i,d_i^x}^{(r)} \right) - 1 \quad \forall r = 1, 2, \ldots, t-1 \tag{5-77}$$

where $\Omega_{i,d_{x,i}}^{(r)}$ is a vector of optimal values of λ_{i,d_i^x} for the rth problem.

Thus, if LB-MASTER$^{(r)}$ is run recursively one can construct a sequence of different subspaces of the partition variables, namely $\left\{ \left(\Omega_{1,d_1^y}^{(0)}, \ldots, \Omega_{r_y,d_{r_y}^y}^{(0)} \right) \middle| , \left(\Omega_{1,d_1^y}^{(1)}, \ldots, \Omega_{r_y,d_{r_y}^y}^{(1)} \right), \ldots, \left(\Omega_{1,d_1^y}^{(t)}, \ldots, \Omega_{r_y,d_{r_y}^y}^{(t)} \right) \right\}$. This sequence stops at iteration t, when the gap between the LB and any known UB becomes negative (that is, LB>UB).

Consider a very simple problem of two partition variables. Figure 5.24 shows 4 boxes corresponding to the partition variables.

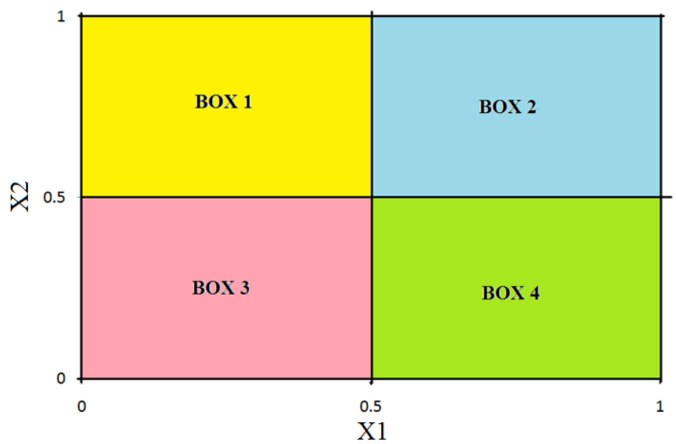

Figure 5.24 – Sub-space of the partition variable.

Assume, now that the lower bound model is run, and box 2 is identified as optimal. Assume further that box 3 is identified as the second lower bound. Finally assume that the third problem gives a solution with negative gap. Thus only two subspaces have been identifies as potentially containing the global optimum. This is shown in Figure 5.25.

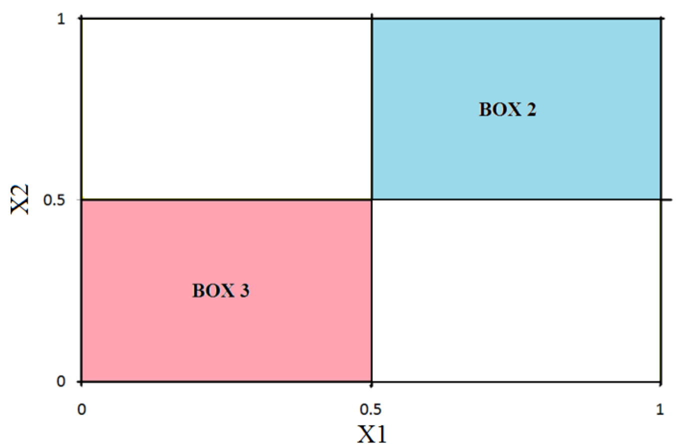

Figure 5.25 – Illustration of surviving sub-spaces

Suppose now that after running this problem, instead of box 2 and 3, only boxes 2 and 4 are identified. This means that boxes 1 and 3 fathom and one can perform a bound contraction on variable x_1. This procedure is named "bound contraction through sub-space fathoming".

Therefore, several variants of this procedure can be proposed:

Sub-space enumeration first: In this procedure, all boxes are identified, one after another. The procedure is the following:

Step 1 - (Optional) Run a bound contraction procedure using the solution as starting point for the original model.

Step 2 - Set r=0

Step 3 - Run the LB-MASTER$^{(r)}$ model.

Step 4 - If the LB is higher than the current global UB, go to step 10.

Step 5 - Use the solution of the LB model as a starting point of the upper bound model, thus (eventually) obtaining a new updated global UB.

Step 6 - Run the LB model again confining the partition variables to the current selected box. We call this LB_r. If LB_r is larger than the current global UB, fathom the present box. Likewise, fathom all previous boxes for which LB_r is larger than the current updated global upper bound.

Step 7 - (Optional) Run the UB model confining all variables to the box found. At this point one can use the box for partition variables only, or even add the box for the discretized variables. The aim here is to obtain a better upper bound when step 4 failed to produce a feasible solution. If the UB model is too time consuming, one can omit this step, if step 4 produced a feasible point.

Step 8 - Add an integer cut to remove the current sub-space from consideration. Go to step 2.

Step 9 - Fathom all boxes for which LB_r is higher than the new UB. Go to step. Perform bound contraction through sub-space fathoming. If bound contraction is possible, update the bounds, partition the space again, set r=r+1 and go to step 3. Otherwise go to step 10.

Step 10 - Pick the box with the smallest LB_r. Attempt global optimization inside this box, considering the current global UB when the UB is updated. The search should stop when the local LB is higher that the global UB.

Step 11 - If no new box is available, stop. The the Global Optimum was found

Global Optimization inside each Sub-space first: In this procedure, boxes are identified and the global optimum (or infeasibility for the current UB) in each box is found before proceed to the next box. The procedure is:

Step 1 - (Optional) Run bound contraction procedure using the solution as starting point for the original model.

Step 2 - Set r=0

Step 3 - Run the LB-MASTER$^{(r)}$ model.

Step 4 - If the LB is higher than the current global UB, Stop.

Step 5 - Use the solution of the LB model as a starting point of the upper bound model, thus (eventually) obtaining a new updated global UB.

Step 6 - Obtain the global optimum inside the current box. Update the global UB if needed. In this step, any global optimization method can be used with on small variant. Any update of the UB should consider the current global UB.

Step 7 - Set r=r+1 and go to step 3.

The choice of what variable should be partitioned is related to the improvement of the objective function of the LB-MASTER$^{(r)}$ when sub-spaces are forbidden. This can be heuristically done choosing different alternatives and analyzing the improvement.

5.4.2. The special Case of Bilinear MINLP Problems

This section addresses in more detail how to apply the above method to the case of bilinear MINLP problems. For completeness, let us define the set Y as a union of three sets: $X \cup Y = V \cup W \cup Z \cup R$. Here $V = \{v_j\}$, $W = \{w_k\}$, $Z = \{z_{j,k}\}$,and $R = \{r_l\}$. Thus, all variables participating in bilinear terms are included in V, W and Z, and the rest, in R. Thus,

$$z_{j,k} = v_j\, w_k \quad \forall j,k \tag{5-78}$$

The use of discrete models to generate valid lower bounds is a common practice in global optimization. In the previous sections, different discretization methods were discussed and bound contraction procedures were presented. Thus it is common practice to discretize one of the variables, say $v_{j.}$ In turn, the lower bound model LB^0 can be constructed partitioning X and discretizing V.

It is important to notice that X and V do not need to have an empty intersection. In fact, all variants for X can be chosen as completely separate from Y. As presented above, that is $X \cap Y = \varnothing$, or X=R or a subset of R, X=V or a subset of V, X=W or a subset of W or any combination thereof.

Some variations of this method were investigated for the two larger problems solved in section 5.2.

Table 5-29 shows the results obtained for the wastewater subsystem problem from Meyer and Floudas (2006), which is the example 9 in section 5.2. This problem was run by picking the concentrations of the pools as discretization variables and the flow of the pools as partition variables using the following options: guided, one interval forbidden exhaustive elimination and active upper bound updating. The solving time could be reduced from 16,336 CPUs to 14,498 CPUs. Only one option was tried for Alva-Argaez et al. (2007) problem. The solution was presented in Table 5-30. The method did not show improvement in the solving time found using the elimination procedure on discretized variables.

Table 5-29 – Summary of the options tried for the generalized pooling problem (Meyer and Floudas, 2006).

LB Model	Boxes variables	Variables for Bound Contraction	Variables for Branch and Bound	Time** (CPUs)
MCP2-C Concentrations (2 intervals) Reg. Flows (2 intervals)	Reg. Flows (2 intervals)	Concentrations Reg. Flow	All Flowrates	14,498
MCP2-C Concentrations (2 intervals) Reg. Flows (2 intervals)	Reg. Flows (2 intervals)	Concentrations Reg. Flow	Concentrations	22,224
MCP2-C Concentrations (2 intervals) Reg. Flows (2 intervals)	Reg. Flows (3 intervals)	Concentrations Reg. Flow	All Flowrates	17,071

Table 5-30 – Summary of the options tried for the generalized pooling problem (Alva-Argaez et al., 2007).

LB Model	Boxes variables	Variables for Bound Contraction	Variables for Branch and Bound	Time** (CPUs)
MCP2-C Concentrations (5 intervals) Reg. Flows (2 intervals)	Reg. Flows (2 intervals)	Concentrations WU Flow Reg. Flow	All Flowrates	36,394

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6. DEGENERACY OF WATER ALLOCATION PROBLEMS

Degeneracy is an important issue to be analyzed in optimization problems for several reasons. From the modeling point of view they can be caused by the lack of details addressed in the model, and thus some solutions can be in reality unpractical. On the other side, degeneracy generates alternative solutions in which opportunities related to other objectives or constraints may be sought allowing a better evaluation of different options.

6.1. Overview

Putra and Amminudin (2008) approached the existence of what they call "class of good solutions". These solutions are different design options that find the same optimum (or near optimum solutions), but show different perspectives concerning cost, layout (complexity) or efficiency of the regeneration processes. They find the "class of good solutions" by fixing the maximum number of connection to an operation or existence of regeneration-recycling, and then minimizing the freshwater consumption. They find four "good solutions" and compare them with three others found by previous works (Kuo, 1996; Alva-Argaéz, 1999; Gunaratnam, 2003).

As in Putra and Amminudin (2008), several other methodologies for designing water systems in process plants are based on minimizing freshwater consumption. The objective makes sense, even on its own because in several situations water scarcity suggests minimizing water regarding of costs. In other cases, freshwater consumption is used as a substitute for the cost function in the belief that water costs overwhelm other fixed capital costs. Some of these methods are graphical and algorithmic; others are based on mathematical programming. Among the first, there is the popular “Pinch Technology”-based procedure, whose early proponents and contemporary advocates consider and defend as a good method to provide “insights” into the right answer.

6.2. Degeneracy and Sub-Optimal Solutions

With the exception of Putra and Amminudin (2008), who present an approach to generate what they call “class of good solutions”, no other work has presented a methodology to find degenerate and sub-optimum solutions of water allocation problems. Putra and Amminudin (2008) proposed a two-step approach to find the multiple solutions. In the first step the structure of the network is defined using an MILP model, and then a NLP model is used to find the conditions for the found structure. They claim this strategy renders a global optimum, but they offer no proof of this assertion. Because of the two step strategy proposed, we doubt it is. The “class of good solutions” is found fixing the piping connections, which can be related to the number of water reuse streams, maximum number of connection to an operation or existence of regeneration-recycling, and minimizing the freshwater consumption. Even if degeneracy and sub-optimum solutions can be found using this procedure, there can still exist other alternative solutions for the same piping network.

To ameliorate the above problems, an automatic method to find a significant higher number of options, if not all of them, is proposed. The search for alternative solutions is done in a matter in which a new network configuration (connections among freshwater source, water using units, regeneration processes and sink) is successively found with respect to a certain objective function. At each new search the previous found network are excluded from the feasible solution. In a problem with high degeneracy, the optimum solution (objective function value) will be repeated for many of the found structures and the alternative solutions provide a more flexible scope in the decision making process. On the other hand, when the problem is not highly degenerated, the alternative solutions can provide non optimum solutions in which present other advantages such as much lower investment costs, easier operability, etc. The alternative solutions are found as follows:

Step 1: Run the model presented in section 3.

Step 2: Forbid the networks previously found.

Step 3: Go back to Step 1.

To forbid the networks, the following constraint is added to the model:

$$\sum_{(i,j)\in\left\{\begin{matrix}(w,u),(u,u^*),(u,r),\\(u,s),(r,u),(r,r^*),(r,s)\end{matrix}\right\}} NYIJ_{n,i,j}YIJ_{i,j}+\left(1-NYIJ_{n,i,j}\right)\left(1-YIJ_{i,j}\right)\leq CARD(NYIJ)-1 \quad \forall n<n_{found} \tag{6-79}$$

where n corresponds to the n^{th} network previously found. n_{found} is the number of networks previously found and $NYIJ_{n,i,j}$ are the values of the binary variables obtained in run n, which define the configuration of each network. In turn, $CARD(NYIJ)$ is the cardinality of the set of binary variables $NYIJ$. Thus, the network exclusion constraints forbid combinations of possible connections found all previous iterations. The left hand side of the equation is used to account for existing (first term) and non-existing connections (second term) in the n^{th} solution. In other words, all the previously found combinations will have the summation equal to *CARD(NYIJ)* and therefore cannot be repeated. Thus, to generate a new network, at least one of the connections needs to be included or excluded.

6.3. Results

Results have showed that for some problems present a significant number of degenerate solutions regarding minimum freshwater consumption. On the other hand, there are problems in which degeneracy is not present or is very small. A single contaminant case is analyzed first and then multiple contaminant cases are analyzed.

6.3.1. Example 1

This example corresponds to the *water-using subsystem* example presented by Wang and Smith (1994), which has four water-using units. The data for this problem is shown in Table 6-1.

Table 6-1 – Limiting data of example 1.

Process	Mass Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	2	0	100
2	5	25	75
3	30	80	240
4	40	30	90

The problem minimizing freshwater consumption is solved to global optimality to find the 100 first networks. A minimum flowrate of 1 t/h is required for all connections. Here, the minimum flowrate is not only related to practical issues, but also to avoid the existence of combinations of networks that, in reality, have zero flowrate through the connections. To solve this problem, the global optimization approach presented in section 5.2 with a 1% tolerance was used.

Figure 6.1 illustrates the freshwater consumption and the number of connections for the first 100 solutions, the first 96 featuring the minimum consumption of 90 t/h and the last four exhibiting a slightly higher value. All solutions were obtained minimizing freshwater adding the corresponding connections exclusion constraint (30). Note that all the 100 solutions were found using an Intel Xeon 2.67 GHz and 2.5 GB of RAM in 1 hour (wall clock time).

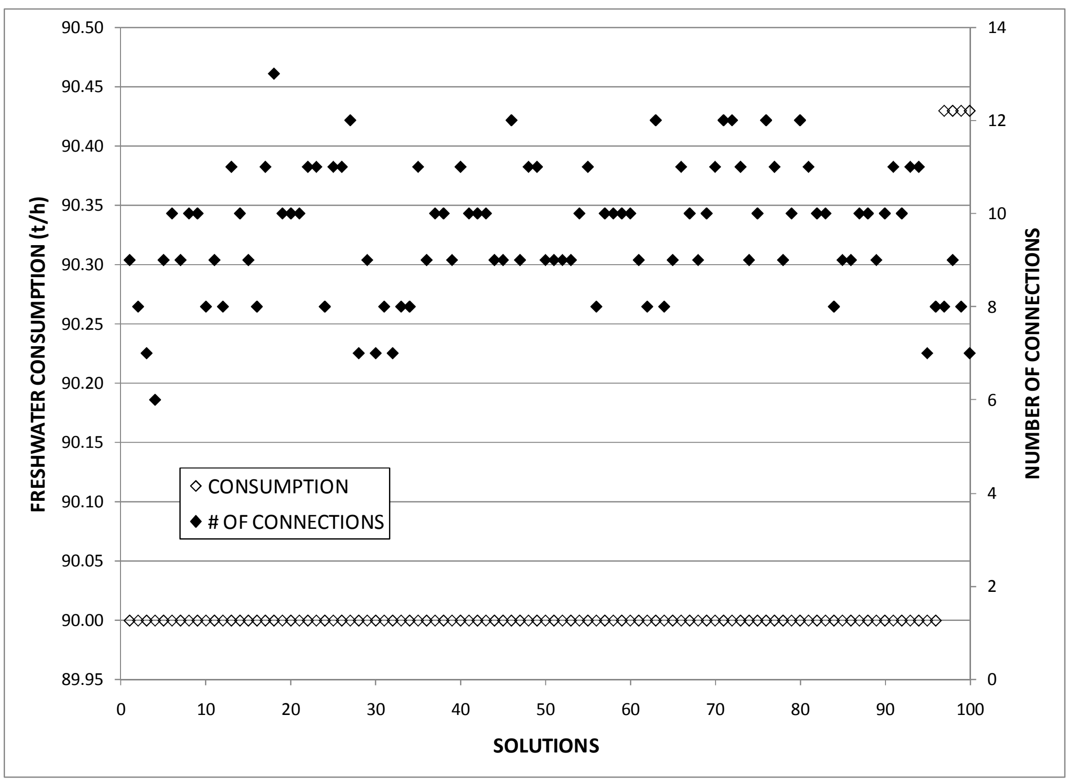

Figure 6.1 – Hundred first solutions for minimum freshwater consumption of the water-using subsystem single contaminant example from Wang and Smith (1994).

To determine what the right network is, one needs to add cost. This can be done by:

- Making an assessment of the cost of each network after they are found, a strategy that may work well if the number of networks is small.
- Solving the problem again, fixing the flowrate to its minimum and minimizing capital cost, or cost of regeneration, or both.

Note that only in the case where the effluent from the end-of-pipe treatment is not recycled and totally disposed of, the cost of regeneration is proportional to the cost of freshwater and therefore treatment costs cannot be used as an economical objective (see Faria and Bagajewicz, 2009).

These results show that pinch-technology-based methods as well as other graphical and algorithmic procedures are in principle incapable of performing the above proposed sorting and therefore they fail to provide proper insights beyond identifying the value of minimum consumption, something that mathematical programming can also easily determine.

6.3.2. Example 2

This is the case of *water-using subsystem* optimization presented by Wang and Smith (1994), which involves two water-using units and two contaminants and minimizes freshwater.

Table 6-2 presents the limiting data of this problem. The minimum freshwater consumption of this network without reuse is 63.33 ton/h.

Table 6-2 – Limiting data of example 1.

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	4	0	100
	B	2	25	75
2	A	5.6	80	240
	B	2.1	30	90

As no regeneration process is used in this example, only two cases are analyzed:

- No recycle of the end-of-pipe treatment (optimization of *water-using subsystem*);
- The effluent stream from the end-of-pipe treatment can be reused by the water-using units (*total water system*).

For the end-of-pipe treatment, it is assumed that an outlet concentration of 10 ppm for both contaminants, which are in agreement with the maximum allowed to disposal.

In the first case (no recycle of end-of-pipe treatment allowed) the minimum freshwater consumption can be reduced to 54 t/h, which is approximately 15% less than the current consumption obtained when no water reuse is considered. When alternative solutions are investigated, it indicates the existence of a unique solution (no-degeneracy) at 54 t/h, that is, no degeneracy. The next possible solution identified when the first is excluded features 63.33 t/h, which is the network without reuse and is not degenerate either.

If for some reason (cost for example, as it was explored previous chapters) one would want to explore higher consumptions, 3 possible networks consuming 66.67 ton/h are found. Note that if one wants to minimize number of connection, the optimum network is network 5, which is a network in series and has the largest consumption. All these networks are presented in Table 6-3.

Table 6-3 – Alternative network configurations for the *water-using subsystem* of the multiple contaminants example from Wang and Smith (1994).

		Unit 1	Unit 2	EOP
Network 1 54 ton/h	Freshwater	40	14 t/h	-
	Unit 1	-	21 t/h	19 t/h
	Unit 2	-	-	35 t/h
Network 2 63.33 ton/h	Freshwater	40 t/h	23.33 t/h	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	23.33 t/h
Network 3 66.67 ton/h	Freshwater	57.143 t/h	9.524 t/h	-
	Unit 1	-	57.143 t/h	-
	Unit 2	-	-	66.667 t/h
Network 4 66.67 ton/h	Freshwater	66.667 t/h	-	-
	Unit 1	-	44.094 t/h	22.572 t/h
	Unit 2	-	-	44.094 t/h
Network 5 66.67 ton/h	Freshwater	66.667 t/h	-	-
	Unit 1	-	66.667 t/h	-
	Unit 2	-	-	66.667 t/h

*A minimum flowrate of 1 t/h was used.

Next, the case in which the recycle of the effluent stream from the end-of-pipe treatment is allowed is analyzed. In such case, the minimum freshwater consumption can be further reduced to 40 ton/h freshwater consumption network. This is 26% lower than the previous case (and 36.8% lower than the consumption without reuse).

Eleven feasible alternative networks were found in this case, in which the first three solutions obtained consume 40 t/h of freshwater and the next three 41 t/h. The eleven feasible solutions are summarized in Figure 6.2. The 3 solutions at minimum consumption and the subsequent 3 slightly higher are presented in Table 6-4. Quite clearly, in this case, the networks use a very small flowrate in some connections and will not be even considered. Others, like network 3, exhibit independent cycles, which are usually avoided.

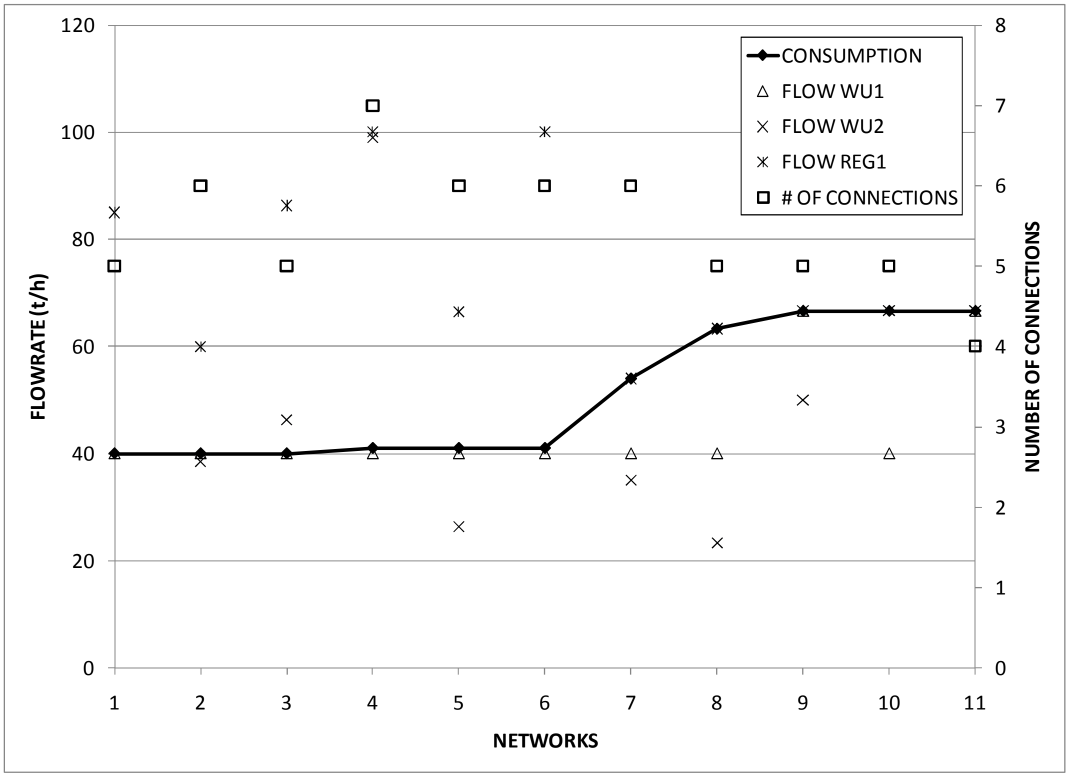

Figure 6.2 – Feasible networks for the *total water system* of the multiple contaminants from Wang and Smith (1994).

At the risk of stating the obvious, the inability or difficulty of methods other than mathematical programming to solve for cost is reiterated. That pinch technology is not designed to look for cost, and moreover, has large difficulties handling multicomponent cases, is known, but we also want to mention that this class of methods cannot perform the above exercise either.

Table 6-4 – Alternative solutions at minimum consumptions for the *total water system* of the multiple contaminants from Wang and Smith (1994).

		Unit 1	Unit 2	EOP
Network 1 40 ton/h	Freshwater	40 t/h	-	-
	Unit 1	-	40 t/h	-
	Unit 2	-	-	85 t/h
	EOP	-	45 t/h	-
Network 2 40 ton/h	Freshwater	40 t/h	-	-
	Unit 1	-	18.56 t/h	21.44 t/h
	Unit 2	-	-	38.56 t/h
	EOP	-	20 t/h	-
Network 3 40 ton/h	Freshwater	40 t/h	-	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	46.33 t/h
	EOP	-	46.33 t/h	-
Network 4 41 ton/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	39 t/h	1 t/h
	Unit 2	-	-	99 t/h
	EOP	-	59 t/h	-
Network 5 41 ton/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	-	40 t/h
	Unit 2	-	-	26.418 t/h
	EOP	-	25.418 t/h	-
Network 6 41 ton/h	Freshwater	40 t/h	1 t/h	-
	Unit 1	-	40 t/h	40 t/h
	Unit 2	-	-	100 t/h
	EOP	-	59 t/h	-

*A minimum flowrate of 1 ton/h was used.

6.3.3. Example 3

This example discuses larger degeneracy and cost issues in the example analyzed by Putra and Amminudin (2008). This example is a larger refinery problem, which was originally presented by Kuo and Smith (1996, 1998) and later also investigated by Gunaratman et al. (2003, 2005) and Alva-Argaez et al. (1998, 1999, 2007). This is a *total water system problem* that has five water-using units, three regeneration processes and considers three contaminants. Putra and Amminudin (2008) showed four alternative solutions for this problem and compared them with the results previously obtained by others. Guanaratman et al. (2006) and Alva-Argaez et al. (2007) solved for total annualized cost, including piping cost. Table 6-5 to Table 6-7 show the data used in this example. The discharge limits of this system are 20 ppm for HC, 5 ppm for H_2S and 100 ppm for suspended solids (SS). The freshwater cost is \$0.2/t and the system operates 8600 hours per year. A 10% rate of discount is assumed. The minimum flowrate allowed through the connection is 5 t/h and a maximum through the connection and processes is 200 t/h.

Table 6-5 – Water using units limiting data of example 3.

Water units	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
(U1) Steam stripping	HC	0.75	0	15
	H_2S	20	0	400
	SS	1.75	0	35
(U2) HDS-1	HC	3.4	20	120
	H_2S	414.8	300	12500
	SS	4.59	45	180
(U3) Desalter	HC	5.6	120	220
	H_2S	1.4	20	45
	SS	520.8	200	9500
(U4) VDU	HC	0.16	0	20
	H_2S	0.48	0	60
	SS	0.16	0	20
(U5) HDS-2	HC	0.8	50	150
	H_2S	60.8	400	8000
	SS	0.48	60	120

Table 6-6 – Regeneration processes data of example 3.

Regeneration Process	Contaminant	Removal ratio (%)	OPN_r	VRC_r
(R1) Steam stripping	HC	0	1	16,800
	H_2S	99.9		
	SS	0		
(R2) Biological treatment	HC	70	0.0067	12,600
	H_2S	90		
	SS	98		
(R3) API separator	HC	95	0	4,800
	H_2S	0		
	SS	50		

Table 6-7 – Distances for example 3.

$d_{i,j}$	WU 1	WU 2	WU 3	WU 4	WU 5	RG 1	RG 2	RG 3	Discharge
FW	30	25	70	50	90	200	500	600	2000
WU 1	0	30	80	150	400	90	150	200	1200
WU 2	30	0	60	100	165	100	150	150	1000
WU 3	80	60	0	50	75	120	90	350	800
WU 4	150	100	50	0	150	250	170	400	650
WU 5	400	165	75	150	0	300	120	200	300
RG 1	90	100	120	250	300	0	125	80	250
RG 2	150	150	90	170	120	125	0	35	100
RG 3	200	150	350	400	200	80	35	0	100

Using the distances given in Table 6-7 and assuming a velocity of 1 m/s, the piping costs are given by:

$$FIJC_{i,j} = 124.6\ d_{i,j} \qquad \forall i \in \{W,U,R\},\ j \in \{W,U,R,S\} \qquad (6\text{-}1)$$

$$VIJC_{i,j} = 1.001\ d_{i,j} \qquad \forall i \in \{W,U,R\},\ j \in \{W,U,R,S\} \qquad (6\text{-}2)$$

The best known solution for this problem minimizing TAC is \$616,824 (Alva-Argaez et al., 2007). In the suggested procedure, the minimum consumption (58 t/h) is identifiefd by solving the problem without costs. The minimum total annual cost (without fixing the freshwater flowrate) was also found to global optimality using Baron and specifying 1% tolerance. The run took 7 hours and 5 minutes and rendered a network featuring a minimum total annual cost of $574,155, which happens to feature the previously identified minimum consumption of 58 t/h.

To analyze the degeneracy of this problem at the minimum consumption, the consumption is fixed at its minimum (58 t/h) and 100 feasible solutions networks were sought. This was done by using a minimum cost objective function, and a 99% gap for the global method presented in chapter 5. This is different from what was done in Example 1 and 2. Here we are having the explicit purpose of saving computational time. Indeed, if one runs minimizing freshwater and forbids previously foud networks, the computational time is higher. Finally, one could try to run only once in order to identify the network with lowest cost. Such a run takes much longer than the presented alternative (7 hours vs. 1 hour and 40 minutes to find100 feasible networks). Note that the minimum cost network that one would identify if one runs to 0% gap features a set of connections that is eventually identified later, as long as all degenerate solutions are explored and one does not stop earlier. That said, one can be certain that the optimum network is found, but not necessarily the optimum flows.

This method does not guarante that the global solution featuring minimum cost is obtained when a maximum number of network is previously set. The main objective here is simply obtain alternative networks featuring the same freshwater consumption.

The results for the netwoks identified in example 3 are presented in Figure 6.3. They are presenetd in a increasing cost order of total annualized cost, which is not necessarily the order they are found. In addition, operating cost, annualized capital cost and number of connections are shown for completeness. The overall running time of this method to find the hundred degenerate solutions is 2,525 CPUs. It is worth pointing out that the first 20 are fast and then, because of the network exclusion constraints, the running time per run increases for some of them.

Note that the lowest TAC found among these 100 solutions is $572,767, which is lower than the one found by BARON using 1% global optimality tolerance. This best solution, which was found among the 100 options, was the 5th network to be found, which took 76 CPUs. The flows through the water-using units and regeneration processes corresponding to these solutions are presented in Figure 6.4 and Figure 6.5 respectively.

Even is the procedure does not guarantee global optimality of costs, it identifies good solutions when we compare to the ONLY solution one can find using a global optimization approach.

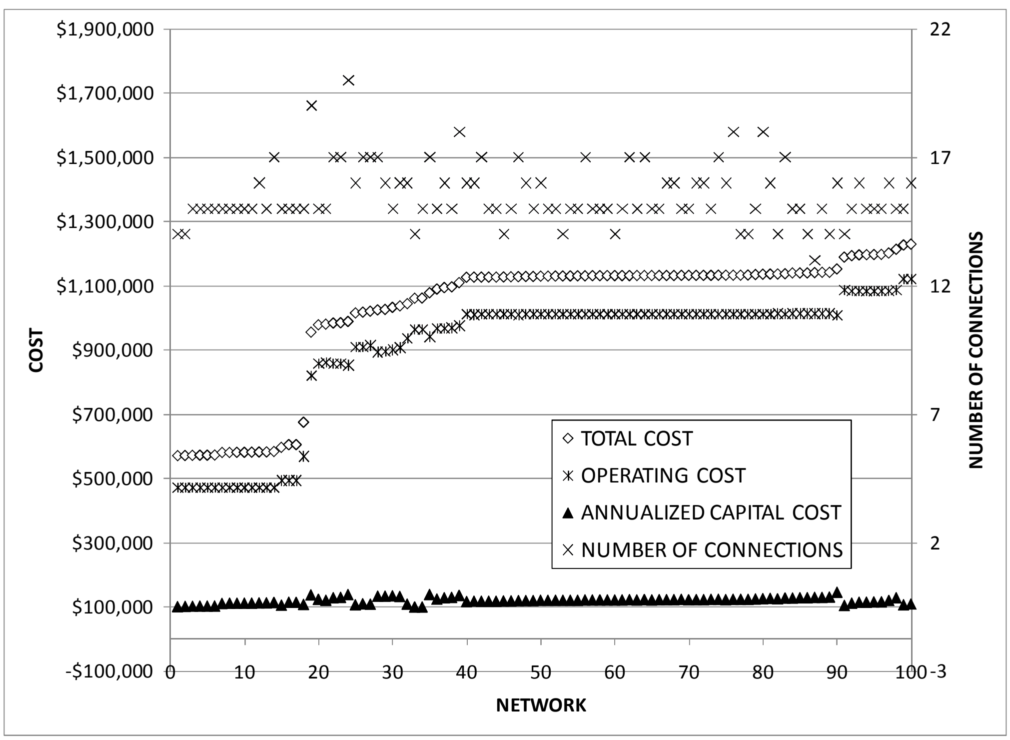

Figure 6.3 – Hundred minimum consumption (58 t/h) alternative network configurations of refinery example from Kuo and Smith (1994).

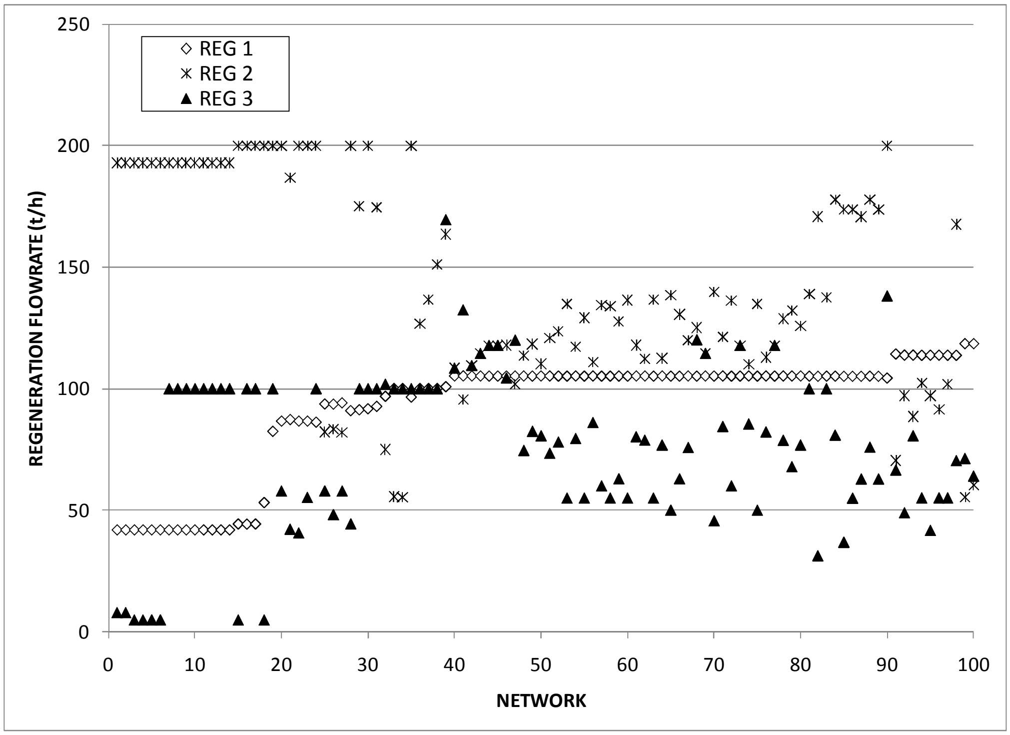

Figure 6.4 – Water-using unit flowrates - Hundred alternative network configurations at minimum consumption (58 t/h) for the refinery example from Kuo and Smith (1994).

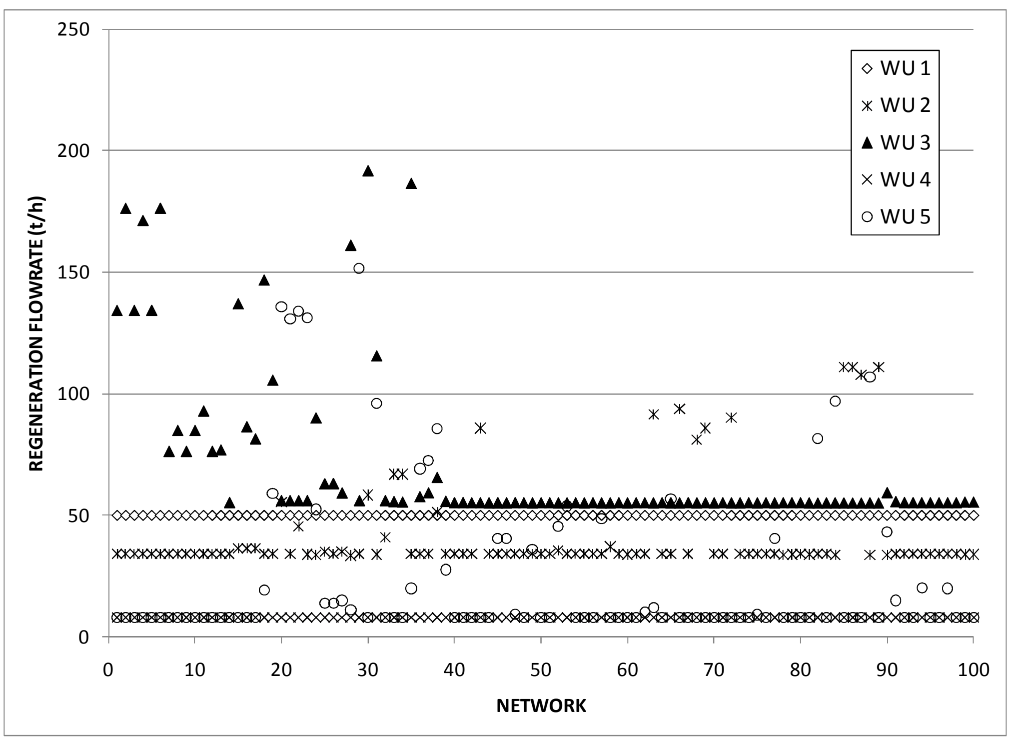

Figure 6.5 – Regeneration processes flowrates - Hundred alternative network configurations at minimum consumption (58 t/h) for the refinery example from Kuo and Smith (1994).

Additionally, if one wants to look at different criteria (always operating at minimum consumption), one can chose the network with minimum TAC, or minimum operating cost, minimum capital cost or smaller complexity (here identified as the number of connections). Table 6-8 compares these options (the bold numbers are the ones corresponding to the minimum value of the optimization). Note that the network with minimum TAC has also the minimum operating cost. However, among the 100 found solutions there are other 14 networks that have the same operating costs. Figure 6.6 to Figure 6.8 show the three networks presented in Table 6-8.

Table 6-8 – Networks with best criteria.

Criteria	TAC ($/year)	Operating cost ($/year)	Capital cost ($)	Number of connections
TAC	572,767	472,073	1,006,944	14
Operating cost	572,767	472,073	1,006,944	14
Capital cost	1,062,126	962,963	991,626	14
Number of connections	1,141,479	1,012,617	1,288,623	13

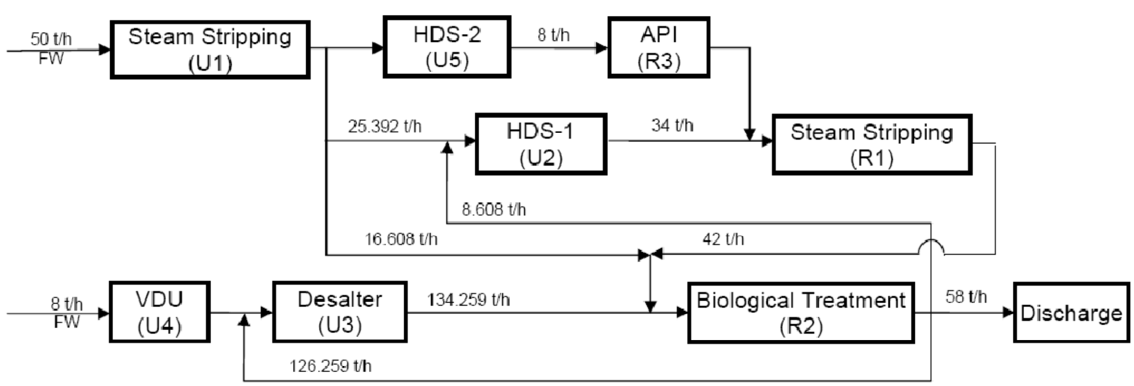

Figure 6.6 – Network with minimum TAC (and minimum operating cost).

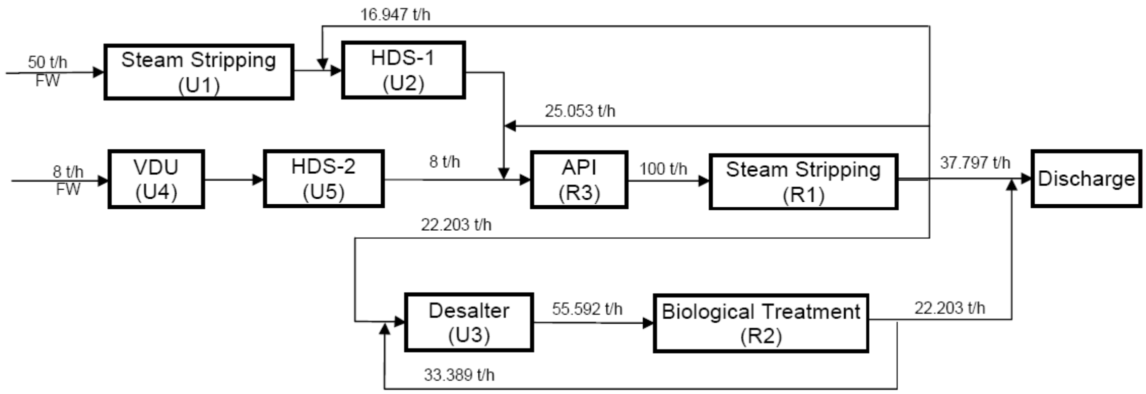

Figure 6.7 – Network with minimum capital cost.

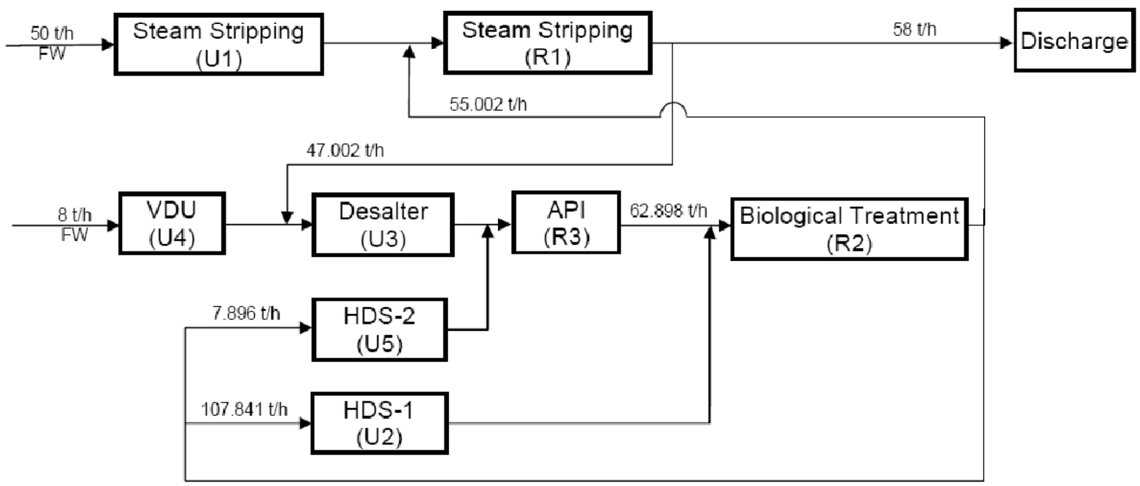

Figure 6.8 – Network with minimum number of connections.

The results presented so far do not considered structural constraints or practical considerations other than the ones given by the input data. Putra and Amminudin (2008) discuss some of these issues. Their concerns were regarding the following two practical issues:

- The API separator should be placed in the upstream of biological treatment due to increase in performance (higher inlet concentration) and to guarantee that oil is not sent to the biological treatment;
- Regeneration recycling shouldn't be allowed to avoid accumulation of certain

contaminants. In other words, the regeneration process cannot send treated water back to the units that sent wastewater to it.

Applying these criteria, they eliminate 2 of the 4 alternative solutions found by their procedure. Here, these issues are included in the model. For the first one, a maximum inlet concentration of 66 ppm of HC is added to the biological treatment. This value corresponds to the maximum value that makes the biological treatment able to bring the concentration down to the HC environmental limit (20 ppm). For the second issue, a constraint to forbid all direct recycles, reuse recycling and regeneration recycling is added. This constraint is presented next:

$$YIJ_{i,j} + YJI_{j,i} \leq 1 \quad \forall\left(i,j\right) \in \left\{(u,u^{*}),(u,r),(r,u),(r,r^{*})\right\} \tag{6-3}$$

The minimum freshwater consumption obtained using this modified problem is also 58 t/h. As before, the consumption is fixed and the first 100 alternative solutions are found. The costs are presented in Figure 6.9 and the minimum TAC found among the 100 solution is $592,573. This optimum network is presented in Figure 6.10.

Note that incorporating this constraint forced the network to avoid a direct recycle to the same regeneration process, but it found a recycle through another unit. In reality additional constraints should be added to avoid any kind of recycle. Although this might be unwanted due to possible accumulation, it is not necessarily the correct way to approach this issue. To keep the design under desired operating conditions one can add more contaminants and stricter inlet limitations, not only for the units but also to regeneration processes.

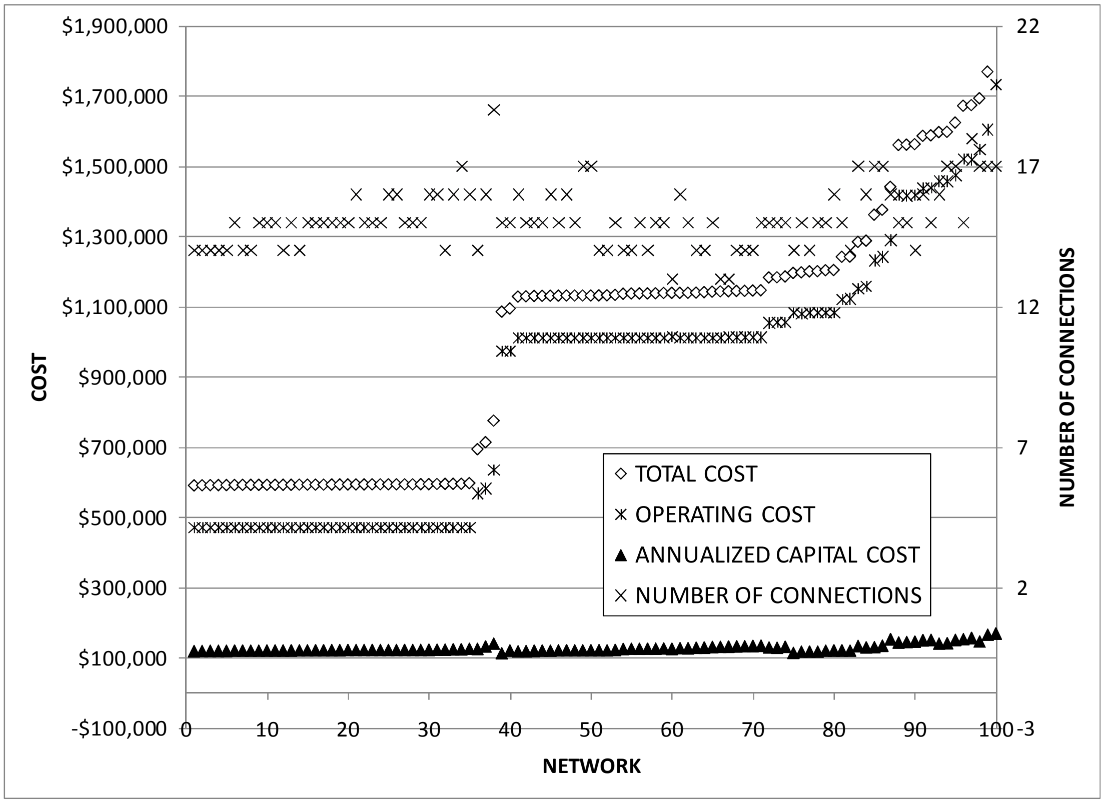

Figure 6.9 – Hundred minimum consumption (58 t/h) alternative network configurations of refinery example from Kuo and Smith (1994) including the practical issues pointed out by Putra and Amminudin (2008).

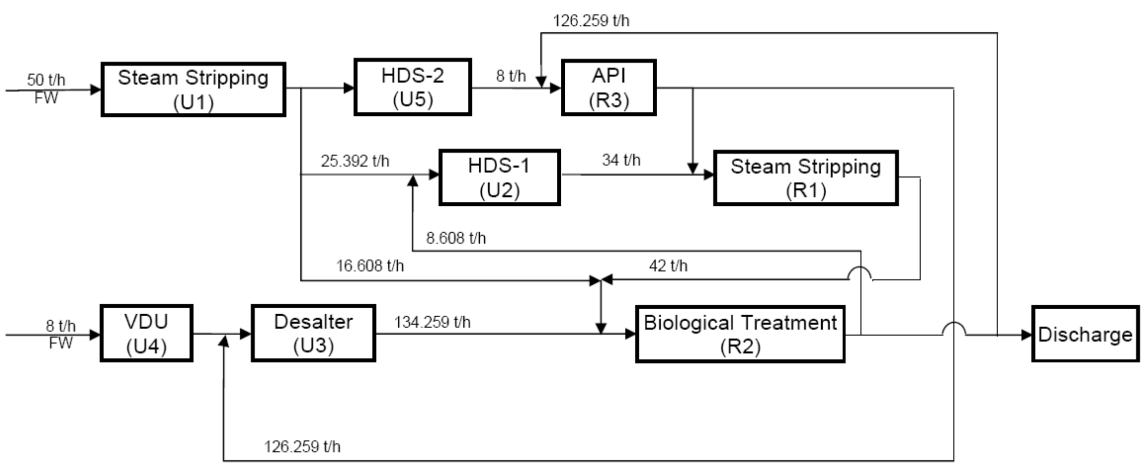

Figure 6.10 – Network with minimum TAC of Example 3 considering practical issues.

6.3.4. Example 4

In this example we want to find the first 50 solutions minimizing TAC without fixing the freshwater consumption at its minimum. The example is the *total water system* presented as example 4 by Karuppiah and Grossmann (2006), which was previously presented in chapter 5 as example 8. The data for this example is presented in Table 5-18 and Table 5-19.

Karuppiah and Grossmann (2006) solved the problem as an NLP problem. However, setting aside the fact that the NLP model for this problem renders a solution with unpractical small flowrates, to consistently forbid networks we need to impose a minimum allowed flowrate through the connection so the connection only exists if there is a flowrate different than zero. Thus, our problem becomes an MINLP.

The optimum solution (within 1% tolerance) of this MINLP problem was presented in chapter 4 and it features a cost of $1,033,859.85 when the minimum flowrate through connections is set as 1 ton/h. In turn, Baron found a minimum TAC of $1,036,384 in 287 s using a 1% tolerance. The lowest TAC found using the proposed procedure is $1,033,832, which is also slightly lower than both 1% tolerance global solution found here and Baron. The reason for this is that the network with TAC of $1,033,832 is not the first network found with 1% tolerance. In reality it is found in after forbidden the 4 first networks found for 1% tolerance. At this exact cost there are other 7 alternatives and the 50th largest TAC is $1,035,288. Note that this high degeneracy in TAC can be attributed to the absence of connection costs. In this problem the only variables that account for the TAC are the freshwater consumption and flowrates through regeneration processes.

Figure 6.11 and Figure 6.12 show the costs and regeneration flowrates for the 50 lowest TAC solution obtained for this problem. Because this procedure was done to find the global solutions every time a network is forbidden, it takes much longer than the previous one (20 hrs). However, when this problem is run with 99% gap with the purpose of only find feasible networks, identify 500 networks are identified in 12 hours and 30 min. Note that the first 50 alternative networks were found in 25 minutes.

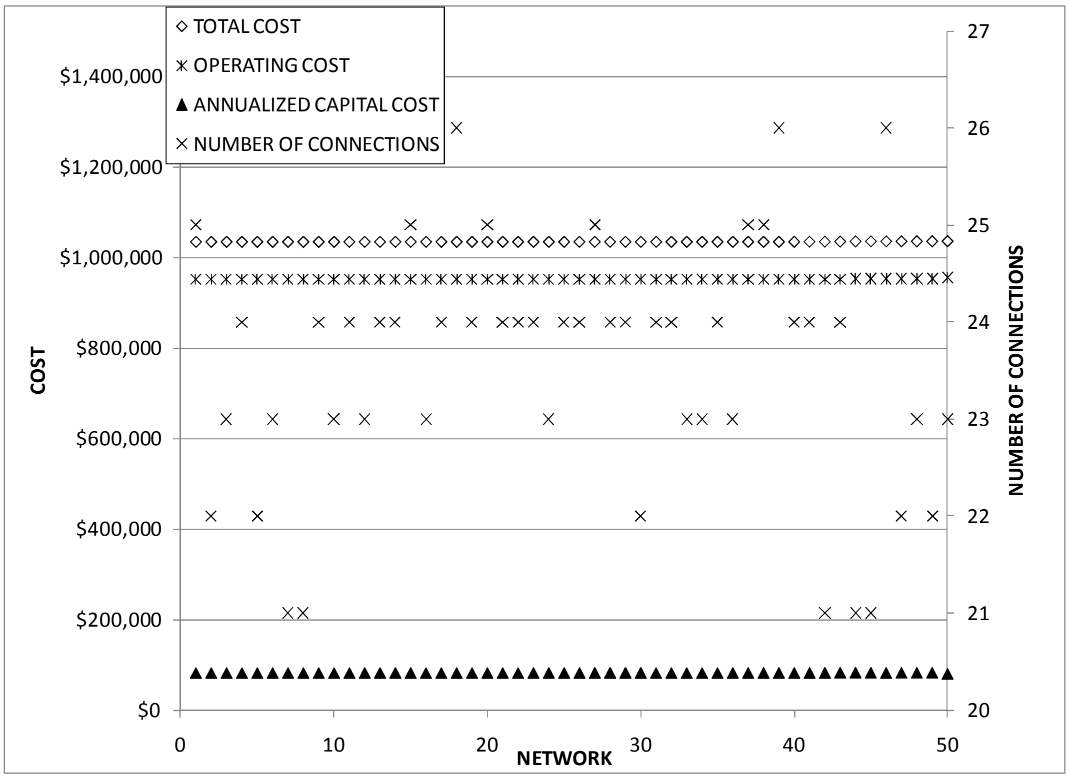

Figure 6.11 – Costs - Fifty alternative network configurations at minimum TAC for the modified example 4 from Karuppiah and Grossmann (2006).

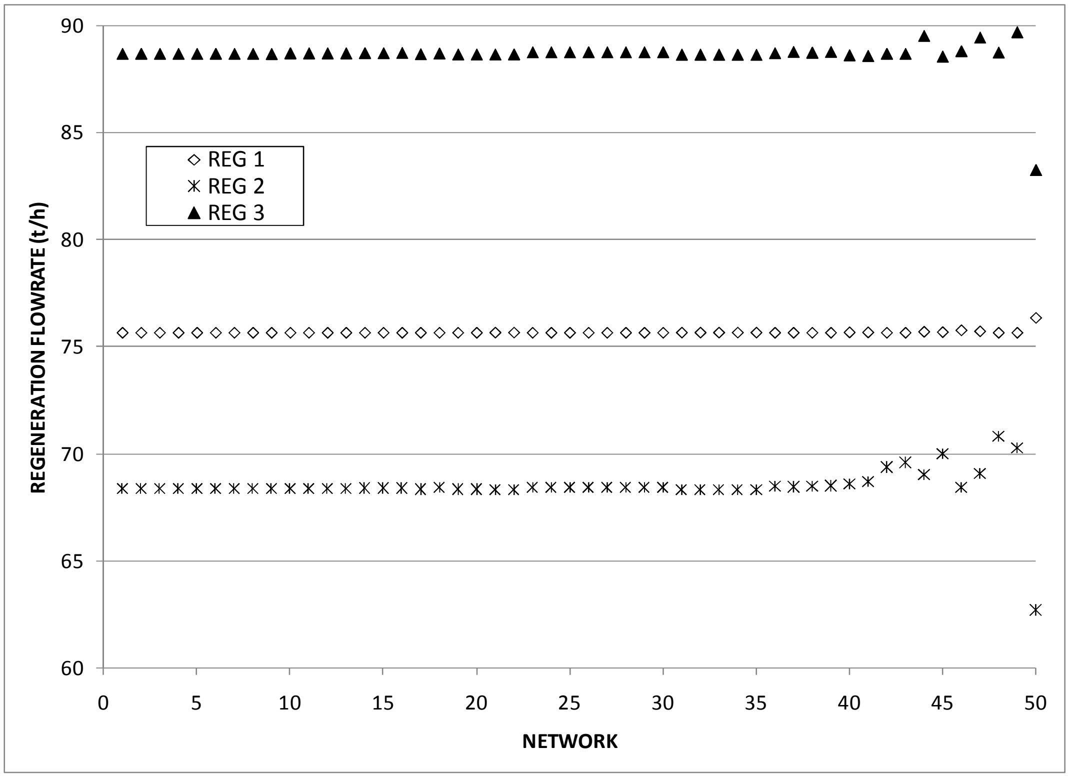

Figure 6.12 – Regeneration processes flowrates - Fifty alternative network configurations at minimum TAC for the modified example 4 from Karuppiah and Grossmann (2006).

6.4. Conclusions

This chapter points out the fact that minimum freshwater solutions of water management problems in process plants sometimes exhibit a large degeneracy. These results confirm that even for single contaminant cases, pinch-technology based methods as well as other algorithmic ones cannot provide the insights they claim they can provide and are unable to deal effectively with the identification of all the degenerate solutions, not even show whether the degeneracy is small or large. It is also shown that degeneracy happens not only on minimum freshwater consumption problems, but also in cases where cost is minimized.

Finally, it seems that these degeneracies are close related to modeling assumption and should disappear with more detailed modeling. For example, the efficiency of regeneration processes are considers the same independent of what are the inlet conditions. If more detailed relations are imposed to the model, some of these alternative solutions will become infeasible.

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7. PLANNING MODEL FOR INDUSTRIAL WATER SYSTEMS

Planning models for industrial water systems are needed to address future environmental regulations, increasing costs of freshwater, variability on the quality of the available freshwater source, bottlenecks caused by expansion of the capacity plant, etc. This chapter presents the case of retrofit to address increase in plant capacity associated to new water-using units planned to be added through time and/or an increase on the mass load of existing water-using units. The model can be used for both grassroots designs and retrofits.

7.1. Overview

Retrofit designs in water systems become important to be addressed systematically in many situations, such as: adjusting the system to new environmental regulation, increased costs of freshwater, variability and/or changes on the quality of the available freshwater source, bottlenecks caused by expansion of the capacity plant, etc. Because these plants many times have already a water system installed, a model to find the best retrofit solution should consider its operability and economic aspects as well. In addition, a timeline that takes into account when new constraints and requirements will take place needs to be considered, so that one can consider and decide upon actions that anticipate to those, or simply actions that respond to these changes.

Although many methodologies dealing with grassroots of water systems have been proposed (see Bagajewicz, 2000 for articles up to 2000; Savelski and Bagajewicz, 2001; Koppol et al., 2003; Gunaratnam et al., 2005; Karuppiah and Grossmann, 2006;

Alva-Argaez et al., 2007; among others), only few presented a methodology for the retrofit design of existing water networks (Fraser and Hallale, 2000; Bagajewicz et al., 2000; Jodicke et al.,2001; Nourai et al.,2001; Tan and Manan, 2006; Dvarioniene and Stasiskiene, 2007; Tan et al.,2008; Faria and Bagajewicz, 2006, 2009).

Here only the case of retrofit due to an increase in plant capacity is presented. Specifically, the installation of new water-using units and/or the increase on the mass load of existing water-using units is addressed, which is usually caused by modifications of process conditions for economic reasons, different production plans or for changes in raw materials processed. However, the presented model does not loss its generality and can be easily extended to the other cases.

7.2. Problem Statement

The planning model is concerned with future expansions and environmental regulations.

This problem can be stated as follows: *Given a system with different situations in time, it is desired to determine where, when and what capacity of connections are needed; which, when and what capacity of treatment processes (if any) need to be installed to obtain an optimum network.*

The planning model is based on the water allocation problem model presented in chapter 4, but it includes the time dimension. For different points in time, one may have different instances that can be caused by an increase in mass loads, a planned addition of water-using units in the future, a future reduction of discharge limits, etc. Certainly this problem could be solved without the need of a planning model, but the optimum solution could be missed. Without a planning model, one could solve the problem first for the current needs and then solve a retrofit problem for the next point in time. Another option would be to solve the problem with consideration of this specific future situation (worst case scenario). In both cases, better solutions may be found if the different instances are simultaneously solved.

7.3. Mathematical Model

Water balance at the water-using units: the water balance through the units has to be done for every analyzed period of time.

$$\sum_{w} FWU_{w,u,t} + \sum_{u^*} FUU_{u^*,u,t} + \sum_{r} FRU_{r,u,t} = \sum_{s} FUS_{u,s,t} + \sum_{u^*} FUU_{u,u^*,t} + \sum_{r} FUR_{u,r,t} \quad \forall u,t \tag{7-4}$$

In this balance, $FWU_{w,u,t}$ is the flowrate from water source *w* to water-using unit *u* for period *t*; $FUU_{u,u^*,t}$ is the flowrate from water-using unit *u* to water-using unit *u** at time *t;* $FRU_{r,u,t}$ is the flowrate from regeneration process *r* to water-using unit *u* at time *t;* $FUS_{u,s,t}$ is the flowrate from water-using unit *u* to wastewater discharge *s* at time *t;* and, $FUR_{u,r,t}$ is the flowrate from water-using unit *u* to regeneration process *r* at time *t*.

Water balance at the regeneration processes: the water balance through the regeneration processes for every time is also needed:

$$\sum_{w} FWR_{w,r,t} + \sum_{u} FUR_{u,r,t} + \sum_{r^*} FRR_{r^*,r,t} = \sum_{u} FRU_{r,u,t} + \sum_{r^*} FRR_{r,r^*,t} + \sum_{s} FRS_{r,s,t} + FL_{r,t} \qquad \forall r,t \tag{7-5}$$

In this balance, $FWR_{w,r,t}$ is the flowrate from water source *w* to regeneration process *r* for period *t* and $FL_{r,t}$ are the water losses in regeneration *r*.

Contaminant balance at the water-using units:

$$\sum_{w}\left(CW_{w,c}\ FWU_{w,u,t}\right)+\sum_{u^*} ZUU_{u^*,u,c,t}+\sum_{r} ZRU_{r,u,c,t}+\Delta M_{u,c,t} = \sum_{u^*} ZUU_{u,u^*,c,t}+\sum_{s} ZUS_{u,s,c,t}+\sum_{r} ZUR_{u,r,c,t} \qquad \forall u,c,t \tag{7-6}$$

Here, $CW_{w,c}$ is concentration of contaminant *c* in water source *w*; $ZUU_{u,u^*,c,t}$ is the mass flow of contaminant *c* from water-using unit *u* to water-using unit *u** at time *t;* $ZRU_{r,u,c,t}$ is the mass flow of contaminant *c* from regeneration process *r* to water-using unit *u* at time *t;* $ZUS_{u,s,c,t}$ is the mass flow of contaminant *c* from water-using unit *u* to wastewater discharge *s* at time *t;* and, $ZUR_{u,r,c,t}$ is the mass flow of contaminant *c* from water-using unit *u* to regeneration process *r* for period *t*.

Maximum inlet concentration at the water-using units: Aside from driving force restrictions, this constraint is also used to limit the total flowrate through the unit to be larger than a certain minimum.

$$\sum_{w}\left(CW_{w,c}\ FWU_{w,u,t}\right)+\sum_{u^*} ZUU_{u^*,u,c,t}+\sum_{r} ZRU_{r,u,c,t} \le C_{u,c,t}^{in,max}\left(\sum_{w} FUW_{w,u,t}+\sum_{u^*} FUU_{u^*,u,t}+\sum_{r} FRU_{r,u,t}\right) \qquad \forall u,c,t \tag{7-7}$$

Here $C_{u,c,t}^{in,max}$ is the maximum allowed inlet concentration of contaminant *c* in water-using unit *u* for period *t*.

<u>*Maximum outlet concentration at the water-using units:*</u> This is established by mass transfer driving force considerations.

$$\sum_{w}\left(CW_{w,c}\ FWU_{w,u,t}\right)+\sum_{u^*} ZUU_{u^*,u,c,t}+\sum_{r} ZRU_{r,u,c,t}+\Delta M_{u,c,t}$$
$$\leq C_{u,c,t}^{out,max}\left(\sum_{u^*} FUU_{u,u^*,t}+\sum_{r} FUR_{u,r,t}+\sum_{u^*} FUU_{u,u^*,t}+\sum_{s} FUS_{u,s,t}\right)\quad \forall u,c,t \tag{7-8}$$

Here $C_{u,c,t}^{out,max}$ is the maximum allowed outlet concentration of contaminant *c* in water-using unit *u* for period *t*.

<u>*Treated flowrate and capacity of the regeneration processes:*</u> the flowrate treated by the regeneration processes is computed using equation (7-6) and (7-7) for every period. Equation (7-8) gives the capacity of the installed regeneration process, which consequently constraints the flowrates of every time after the regeneration process is installed. Equation (7-9) gives the time in which the regeneration process is installed and equation (7-10) controls the maximum allowed number of regeneration process *r* to be installed.

$$FR_{r,t}^{in}=\sum_{w} FWR_{w,r,t}+\sum_{u} FUR_{u,r,t}+\sum_{r^*} FRR_{r^*,r,t}\qquad \forall r,t \tag{7-9}$$

$$FR_{r,t}^{out}=\sum_{u} FRU_{r,u,t}+\sum_{r^*} FRR_{r,r^*,t}+\sum_{s} FRS_{r,s,t}\qquad \forall r,t \tag{7-10}$$

$$FR_{r,t}^{in}\leq \sum_{t^*\leq t} RegCap_{r,t^*}+ECap_{r}\qquad \forall r,t \tag{7-11}$$

$$RegCap_{r,t}\leq RegCap_{r}^{MAX}\ YR_{r,t}\qquad \forall r,t \tag{7-12}$$

$$\sum_{t} YR_{r,t}\leq MaxYR_{r}\qquad \forall r \tag{7-13}$$

In these equations, $FR_{r,t}^{in}$ and $FR_{r,t}^{out}$ are respectively the inlet and outlet flowrate through regeneration process r for period t, $RegCap_{r,t}$ is the capacity of regeneration process r installed for period t, $RegCap_r^{MAX}$ is the maximum capacity of regeneration process r at every installation; $ECap_r$ is the existing capacity of regeneration r (retrofit case); $YR_{r,t}$ is the binary variable related to the existence and installation timing of regeneration process r, and $MaxYR_r$ is maximum number of expansion of regeneration process r.

Contaminant balance at the regeneration processes mixer: The mass flows of contaminants feeding the regeneration unit $ZR_{r,c,t}^{in}$ are computed in equation (7-11) using also contaminants mass flows from other units ($ZUR_{u,r,c,t}$) and from other regeneration processes ($ZRR_{r^*,r,c,t}$). These contaminant mass flows are defined later. In turn, equation (12) also establishes a balance between the flow of contaminant coming out of the regeneration unit ($ZR_{r,c,t}^{out}$) and the mass flows to units ($ZRU_{r,u,c,t}$), the mass flows to other regeneration units ($ZRR_{r,r^*,c,t}$) and the discharged water ($ZRS_{r,s,c,t}$).

$$ZR_{r,c,t}^{in} = \sum_{w} \left(FWR_{w,r,t} CW_{w,c} \right) + \sum_{u} ZUR_{u,r,c,t} + \sum_{r^*} ZRR_{r^*,r,c,t} \quad \forall r,c,t \tag{7-14}$$

$$ZR_{r,c,t}^{out} = \sum_{u} ZRU_{r,u,c,t} + \sum_{r^*} ZRR_{r,r^*,c,t} + \sum_{s} ZRS_{r,s,c,t} \qquad \forall r,c,t \tag{7-15}$$

Performance of the regeneration processes: we include two classes of regeneration processes: Those that have defined (and fixed) outlet concentration and those that are based on a removal efficiency. Equation (7-13) and (7-14) are used to represent both cases by introducing a binary variable $XCR_{r,c}$ that defines when regeneration process *r* has its performance defined by a fixed outlet concentration ($XCR_{r,c} = 1$) or by efficiency ($XCR_{r,c} = 0$).

$$CR^{out}_{r,c,t} = CR^{in}_{r,c,t}\, \varphi_{r,c,t} \left(XCR_{r,c} - 1 \right) + CRF^{out}_{r,c}\ XCR_{r,c} \qquad \forall r,c,t \tag{7-16}$$

$$\varphi_{r,c,t} = f(CR^{in}_{r,c,t}, FR^{in}_{r,t}) \qquad \forall r,c,t \tag{7-17}$$

In equation (7-13), $CR^{out}_{r,c,t}$ is the outlet concentration of regeneration process *r* for period *t*, $CR^{in}_{r,c,t}$ is the inlet concentration of regeneration process *r* for period *t*, and $\varphi_{r,c,t}$ is the efficiency of regeneration process *r* for period *t*. In equation (13), $f(CR^{in}_{r,c,t}, FR^{in}_{r,t})$ defines the efficiency. In some cases, this efficiency can be defined as a constant, which is the option used in this paper.

Maximum allowed discharge concentration:

$$\sum_u ZUS_{u,s,c,t} + \sum_r ZRS_{r,s,c,t} \le CS^{max}_{s,c,t} \left(\sum_u FUS_{u,s,t} + \sum_r FRS_{r,s,t} \right) \quad \forall s,c,t \tag{7-18}$$

Here, $CS^{max}_{s,c,t}$ is the maximum discharge concentration of disposal *s* at time *t*.

Minimum and maximum flowrates:

$$FIJ_{i,j,t} \ge FIJ^{Min}_{i,j} \sum_{t^* \le t} YIJ_{i,j,t^*} \quad \forall (i,j) \in \left\{ \begin{matrix} (w,u),(w,r),(u,u^*),(u,r), \\ (u,s),(r,u),(r,r^*),(r,s) \end{matrix} \right\}, t \tag{7-19}$$

$$FIJ_{i,j,t} \le \sum_{t^* \le t} CapFIJ_{i,j,t^*} + ECapFIJ_{i,j} \qquad \forall (i,j) \in \left\{ \begin{matrix} (w,u),(w,r),(u,u^*),(u,r), \\ (u,s),(r,u),(r,r^*),(r,s) \end{matrix} \right\}, t \tag{7-20}$$

Where $ECapFIJ_{i,j}$ is the existing capacity of the connection between process *I* and process *j*; and $CapFIJ_{i,j,t^*}$ is the capacity of the connection between process *I* and process *j* to be installed in time *t*.

Capacity of connections:

$$CapFIJ_{i,j,t} \le FIJ_{i,j}^{Max}\, YIJ_{i,j,t} \quad \forall (i,j) \in \left\{ \begin{matrix} (w,u),(w,r),(u,u^*),(u,r), \\ (u,s),(r,u),(r,r^*),(r,s) \end{matrix} \right\}, c, t \tag{7-21}$$

Contaminant mass loads:

$$ZIJ_{i,j,c,t} = FIJ_{i,j,t} * Cout_{i,j,t} \quad \forall i \in \{U,R\},\ j \in \{U,R,S\}, c, t \tag{7-22}$$

$$ZR_{r,c,t}^{in} = FR_{r,t}^{in} CR_{r,c,t}^{in} \qquad \forall r, c, t \tag{7-23}$$

$$ZR_{r,c,t}^{out} = FR_{r,t}^{out} CR_{r,c,t}^{out} \qquad \forall r, c, t \tag{7-24}$$

<u>*Objective functions:*</u> we have 4 different objective functions. Equation (7-22) represents freshwater consumption, equation (7-23) represents operating cost, equation (7-24) computes capital costs and equation (7-25) computes net present cost.

$$FW_t = \sum_w \sum_u FWU_{w,u,t} \tag{7-25}$$

$$OpCost_t = \left(\sum_w \alpha_w FW_{w,t} + \sum_r OPN_{r,t} * FR_{r,t}^{in} \right) \tag{7-26}$$

$$FCI_t = \left(\sum_{(i,j) \in \left\{ \begin{matrix} (w,u),(u,u^*),(u,r), \\ (u,s),(r,u),(r,r^*),(r,s) \end{matrix} \right\}} YIJ_{i,j,t} FCC_{i,j} + CapFIJ_{i,j,t} VCC_{i,j} \right) + \sum_r YR_{r,t} FCRP_r + VCRP_r * \left(RegCap_{r,t} \right)^{0.7} \tag{7-27}$$

$$NPC = \sum_t DF_t * (OpCost_t + FCI_t) \tag{7-28}$$

7.4. Results

To illustrate the methodology the refinery example from Wang and Smith (1994) with the addition of the pre-treatment system is used. Table 7-1 presents the limiting data for the base case, which represents the first period of time analyzed.

Table 7-1 – Limiting data – Planning problem.

Process	Contaminant	Mass load	C_{in} (ppm)	C_{out} (ppm)
1 - Distillation	HC	0.675 kg/h	0	15
	H_2S	180 kg/h	0	400
	Salts	1.575 kg/h	0	35
2 - HDS	HC	4.08 kg/hr	20	120
	H_2S	425 kg/hr	300	12500
	Salts	6.12 kg/h	45	180
3 - Desalter	HC	12.32 kg/hr	120	220
	H_2S	2.52 kg/hr	20	45
	Salts	532 kg/hr	200	9500

One external freshwater source with 200 ppm of HC, 3 ppm of H_2S and 150 ppm is considered to feed this system. Besides the regeneration process (foulwater stripper) and end-of-pipe treatment included by Wang and Smith, there also available two water pre-treatment units. The end-of-pipe treatment is able to bring the concentration down to environmental limits (10 ppm for all contaminant) and is allowed to recycle. The data for these regeneration processes are presented in Table 7-2.

The system operates 8600 hours/year and we assume an interest rate of 10%. The cost of connection are $FCC_{i,j}$=\$125 and $VCC_{i,j}$=\$1/t.

Table 7-2 – Regeneration processes data – Planning problem.

Process	Contaminant	*CR* (ppm) or RR (%)	$C^{in,max}$ (ppm)	OPN_r (\$/t)	$VCRP_r$(\$/$t^{0.7}$)
WPT 1	HC	10 ppm	500	0.30	8,500
	H_2S	NA	200		
	Salts	NA	200		
WPT 2	HC	0 ppm	20	0.50	10,500
	H_2S	0 ppm	200		
	Salts	0 ppm	200		
Regenerative foulwater stripper	HC	0 %	NA	1.00	16,800
	H_2S	0.999 %	NA		
	Salts	0 %	NA		
EOPT	HC	10	NA	1.0067	34,200
	H_2S	10	NA		
	Salts	10	NA		

7.4.1. *Increasing in mass load of existing units*

In this first case it is considered that due to future changes in production planning, the mass loads of hydrocarbon will increase in every water-using units as shown in Table 7-3.

Table 7-3 – Increasing in the mass load of hydrocarbons.

Process	1 - Distillation	2 - HDS	3 - Desalter
Mass load	1.467 kg/h	10.08 kg/h	18.32 kg/h

It is considered that the changes will happen after 5 years and we want to determine which regeneration processes should be installed and when. To solve this problem one could use alternatives other than building a planning model:

Solve the problem for the "worst case", that is, the one with the largest mass loads, or;

Solve the problem for the first period and the retrofit the plant after 5 years, which is, solve for the first period, fix the decided connections and set their cost as zero, and then run for the latter case.

To compare the advantages of the planning model, both alternatives were solved. The first one gives a total cost of $3,777,798, which can be split as $1,644,939 of capital cost and $2,132,859 of operating cost. This solution is presented in Figure 7.1 and was found to global optimality in 1.5 CPUs. Note that assuming the design using the worst case, one would consider that this found network would be build at the beginning of the operation. Thus, in addition to this cost, we still need to compute the operating cost of the periods before the changes. Minimizing this operating cost considering the given design, we found it to be $1,162,048. This solution was found to global optimality in 1.6 CPUs. Thus, adding up the cost to calculate the net present cost, we found a NPC of $4,129,360.

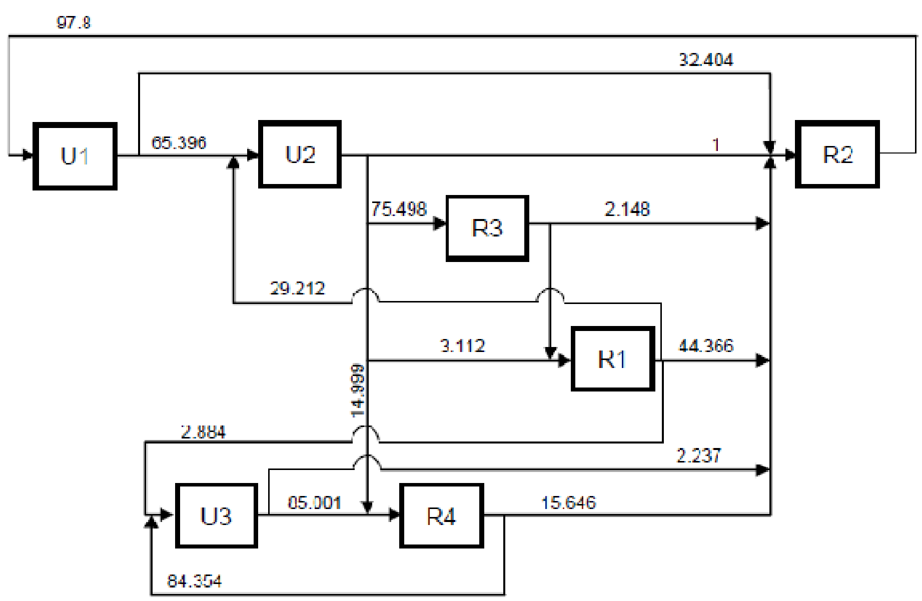


Figure 7.1 – Solution using the first alternative procedure – design using the worst case.

In the second alternative the problem minimizing total cost for the first periods is solved first. This network is presented in Figure 7.2 and has a total cost of $2,251,176 in which is $1,072,004 of capital cost and $1,179,173 of operating cost. This solution was found to global optimality in 39.3 CPUs.

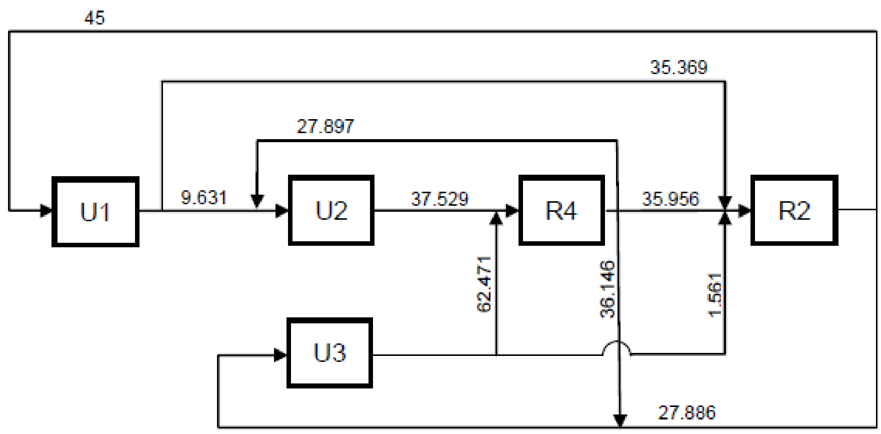


Figure 7.2 – Solution using the second alternative procedure – before expansion.

However, due to the future increase in mass load, this network will need to be retrofitted in 5 years. Thus, the retrofit model is run. The cost of existing connection and regeneration processes are set to zero. In addition to the two available processes that were not used at the beginning of the operations, the existing regeneration processes were also allowed to be expanded. The minimum total cost found for the retrofitted network is $ 2,748,213, which is $622,409 of capital cost and $ 2,125,804 of operating cost. Summing up these costs, a net present cost of $3,955,068 is found. Note that regenerations 1 and 3 were added and regeneration 2 had an expansion of 24.914 t/h. The retrofitted network is presented in Figure 7.3. The ticker lines are connection that already existed. However, they may have been expanded when needed.

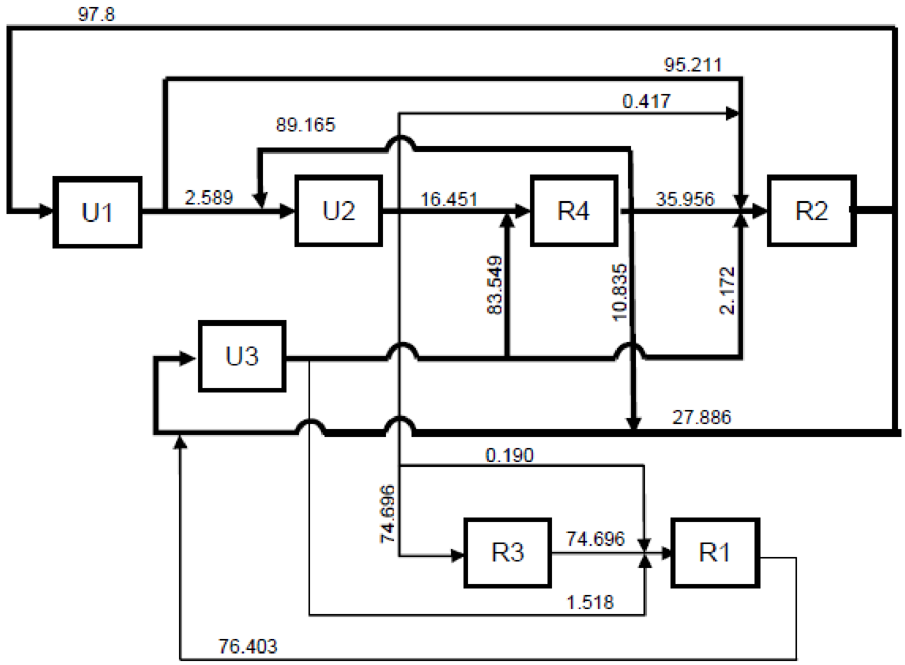
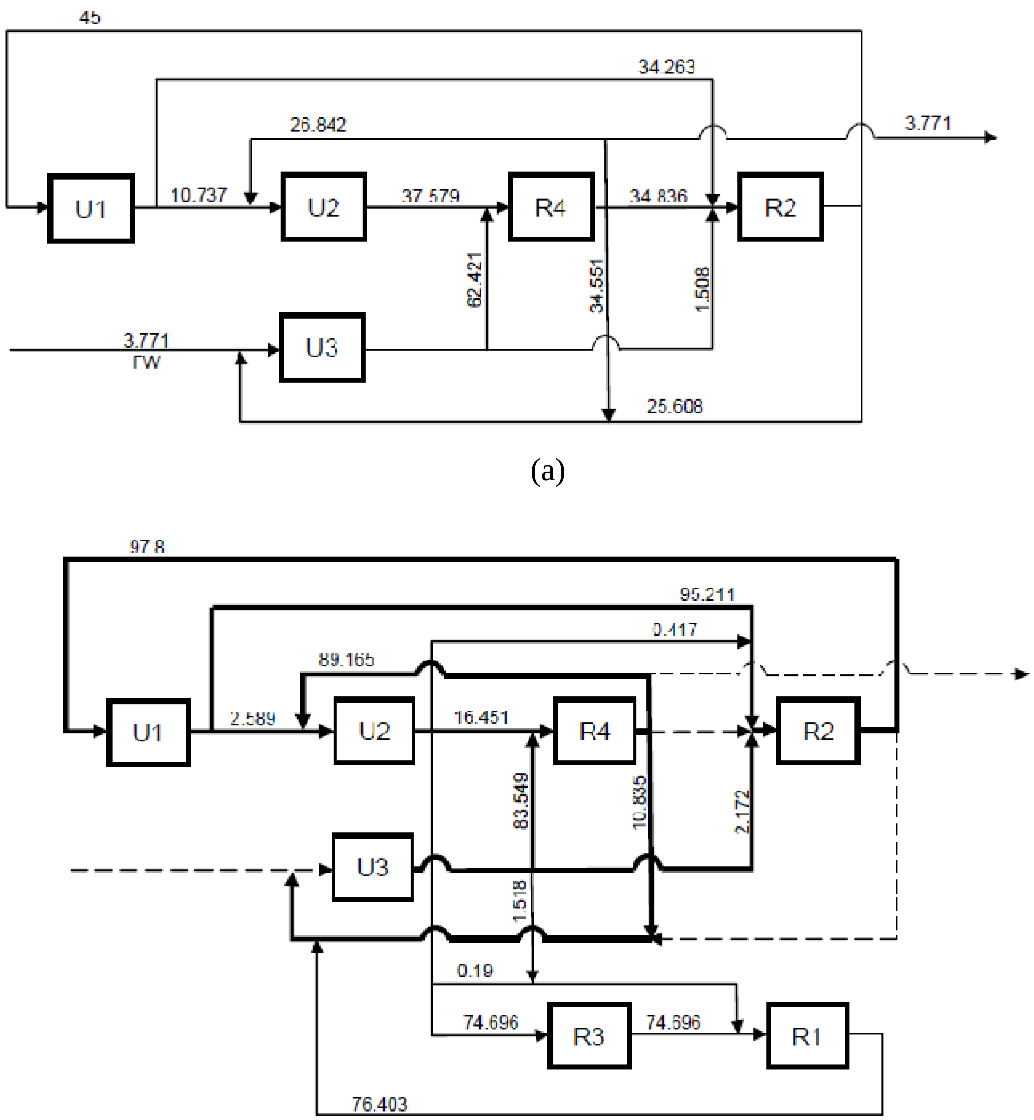


Figure 7.3 – Solution using the second alternative procedure – retrofitted network.

Finally the problem is solved using the planning model. The best found solution has a NPC of $3,939,928. The planning model chooses to install regenerations 2 (capacity of 97.8 t/h) and 4 (capacity of 100 t/h) at the beginning of operation. After 5 years the plant is expanded and regenerations 1 (capacity of 76.403 t/h) and 3 (capacity of 74.696 t/h) are installed together with few new connections. In Figure 7.4b the ticker lines represent connections that already existed and the dotted lines connections that are no longer used. The other lines are connection installed during the expansion.



(a)

(b)

Figure 7.4 – Solution using the planning model – a) First period. b) Future Expansion.

7.5. Conclusions

The planning model showed the importance of considering expected future changes in the system before it is design, even if changes are not implemented when the plant starts operations. A wrong decision at the beginning of operation many generate a significant cost when changes have to be made.

7.6. References

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8. CONCLUSIONS AND FUTURE WORK

This work discussed and presented several intricacies of optimization of process plants water networks using mathematical programming.

First, assumptions that could eventually make these models less complex to solve were investigated. In turn, it was showed that those assumptions have limitations and therefore cannot be used to general cases of WAP.

Also, the objective function choices were analyzed and a methodology to find most profitable solutions was presented in chapter 3. Besides the intrinsic value of the presented method, few conclusions could be made from the results:

- Minimum freshwater consumption is not always the best target
- Different measurements of profitability may lead to different optimum networks
- It is extremely important to also look at alternative solutions in a costs-benefits type of analysis

Next, conceptual changes on the definition of WAP were proposed and compared with the existing definitions. These changes are based on the inclusion of the water pre-treatment subsystem, which has been left out of the WAP definition for almost three decades. With the new WAP definition, it was shown that several consumption targets were in reality overestimated and, including the water pre-treatment, these targets can actually achieve zero-liquid discharge cycles.

Several optimization methods to solve WAP were presented in chapter 5. Although the main objective of all of them was to find a robust method to solve the WAP to global optimality, the wanted robustness was not achieved. However, the methods showed good results for all examples of WAP solved to global optimality in the literature. Additionally, they were able to find better solution than the best solution presented in the literature within the first iterations.

Alternatively, a method to find several alternative solutions was presented in chapter 6. The method showed that it is not only able to find the optimum solution (and sometimes a better one found for 1% global optimality tolerance), but also to given innumerous suboptimum options. Some of the conclusions made from these results can be highlighted:

- Graphical methods cannot handle this amount of information and so mathematical programming is definitely the right route to solve the WAP;
- The minimum consumption WAP can be extremely degenerate and a single solution may not capture some interesting alternatives given by other solutions;
- Depending on how the minimum cost WAP is approached, it can also be very degenerate;
- Problems in which are difficult to find the global solution presented degenerate solutions (or sub-optimum solutions) for many different operating conditions. This issue is directly related to the bound contraction step of GO methods.
- More details need to be used to narrow down the amount of these degenerate solutions.

Using the optimization methods presented, a planning model could be solved. The results showed the importance of considering expected future changes in the system before it is design, even if changes are not implemented when the plant starts operations. A wrong decision at the beginning of operation many generate a significant cost when changes have to be made.

Although the WAP has being studied for three decades and it considered completely solved by many authors, the biggest challenges at the present moment are related to a robust global optimization method, the simplified assumption used for the water-using units and regeneration processes and analysis of flexibility and uncertainty.

As in the conceptual analysis of the WAP definition presented in chapter 4, the simplified modeling assumption of water-using units and regeneration process in current WAP models may be putting in risk the reliability of these solutions. In turn, the two last issues, flexibility and uncertainty, are very important analysis to be performed in any design of process plants. However, they should be sought after these detail models are included in WAP.

APPENDIX – Summary of the optimality conditions

(Savelski and Bagajewicz, 2000)

Definitions:

Head Processes: Water-using units that receive only freshwater.

Intermediate Processes: Water-using units that receive water previously used by other(s) water-using unit(s) and also sent their used water to other(s) water-using unit(s)

Terminal Processes: Water-using units that receive water previously used by other(s) water-using unit(s) and also sent their used water to only to treatment

Partial Wastewater Provider: Water-using units that send part or their used water to other(s) water-using unit(s) and another part to treatment.

Theorem 1: (Necessary condition of concentration monotonicity). *If a solution to the WAP is optimal*, *then at every Partial Wastewater Provider, the outlet concentrations are not lower than the concentration of the combined wastewater stream coming from all the precursors*.

Theorem 2 (Necessary condition of maximum concentration for head processes). *If a solution of the WAP problem is optimal*, *then the outlet concentration of a Head Process is equal to its maximum or an equivalent solution with the same overall freshwater consumption exists in which the concentration is at its maximum.*

Theorem 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 or an equivalent solution with the same overall freshwater consumption exists where the concentration is at its maximum.*

Theorem 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 or an equivalent solution with the same overall freshwater consumption exists*.