An Optimization-Based Computational Procedure for Retrofit of Refinery Water Network Systems Incorporating Water Reuse, Regeneration, and Recycle

by
Leong Pei Chie

Dissertation submitted in partial fulfilment of
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Universiti Teknologi PETRONAS
Bandar Seri Iskandar
31750 Tronoh
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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Approved by,

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(KHOR CHENG SEONG)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

APRIL 2009

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

LEONG PEI CHIE

ABSTRACT

Water is a key element for the normal functioning of refineries and petrochemical plants in the hydrocarbon processing industry. Scarcities in freshwater supply and increasingly stringent rules on wastewater discharges have emerged as issues of major concern in our time. Water has become an increasingly crucial resource to industrial plants due to increased requirements in operating efficiency and optimization, to avoid high demand of water, and the drive for sustainable development that may result in plants being vulnerable to interruptions in water supply and to water shortages in the future. It is a well-acknowledged fact that cost of water is low but its value is high, and that there is increased regulatory requirements for zero discharge from process plants. In line with these developments, this work has been undertaken with the goal of formulating and solving a mathematical optimization model for the optimal design of an integrated water network system for a typical oil refinery via combined knowledge of engineering heuristics and mathematical programming. The integrated model explicitly considers the incorporation of water minimization approaches and strategies that consist of the potential for water reuse, regeneration, and recycle (W3R), with the objective of minimizing freshwater consumption and wastewater flows while complying to the maximum allowable contaminant concentrations where it is concerned. The stipulated objective directly corresponds to minimizing the associated capital and operating costs of the facility, although cost is not explicitly considered in this work. The methodology includes data collection on flowrates and contaminant concentrations and the subsequent step of data reconciliation on the water balances. Next, a superstructure embedding all feasible alternatives for the implementation of the potential W3R opportunities are developed. A nonlinear programming (NLP) model is then formulated based on the superstructure with the addition of constraints on the maximum allowable contaminant concentrations to meet regulatory discharge requirements as well as for the evaluation of W3R opportunities. Computational studies are performed on the NLP model using GAMS algebraic modeling platform on an industrially-significant problem representative of industrial scale with six contaminants considered. The satisfactory numerical results show that our proposed approach is a promising tool to aid decision-making in the retrofit of refinery water network systems.

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CHAPTER 1

INTRODUCTION

1.1 Background Study

The concepts of water minimization and water reuse were previously less attractive due to limited technologies and cost restrictions. However, with the advancement in water management and treatment technologies, these concepts have received significant attention in recent years. More industries and companies are investigating the viability of the concepts as worthy alternatives in addressing environmental concerns and water supply problems.

The drive for seeking an alternative approach in managing water consumption can be attributed among others to the more stringent regulations on discharges, increased environmental awareness, limited freshwater resources, higher costs for freshwater supply and wastewater treatment, and increased requirements for plant efficiency and optimization. These are among the major issues that plant managers worldwide need to address in their daily plant operations. Consequently, it is timely to build know how on the potential adoption and implementation of water minimization and water reuse approaches and strategies.

Despite the various advanced technologies available for water reuse, it is essential that a thorough evaluation is made to identify the most suitable approaches and systems structure for implementation. This case study is carried out to study on retrofit of refinery water network systems via water minimization through water reuse, regeneration, and recycle initiatives considering the challenges facing now with water utilization. It aims to formulate a mathematical model with optimization procedure that describes the freshwater consumption and wastewater flows (Yoo et al., 2007; Bagajewicz, 2000). This research project utilized mathematical programming as the optimization tool because:

- it enables automated optimal solution provided formulation is correct;
- ease of incorporating various constraints,

  e.g., concentration limits (can accurately model real-world situation in reality);
- simultaneous considerations of multiple alternatives/options for water reuse, regeneration, & recycle;
- can easily accommodate large number of variables (flowrates & concentrations)/multiple contaminants

1.2 Problem Statement

Data given in the case study includes a set of water using and water treatment units, and a supply source of freshwater to satisfy the demand in the water using processes. It is known that a certain number of contaminants are picked up in the water using processes, which are then removed in the treatment units. Mass balances in these units, as well as in the mixers and splitters, which help to connect the process units and treatment units into a network, have to hold. Other constraints that have to be satisfied are that the contaminant concentrations of certain streams must not exceed specified values, and the contaminant concentrations have to be reduced to environmental limits before discharge.

The goal of the design problem is to determine optimal flowrates amd contaminant compositions of the streams identified for potential reuse, regeneration & recycle (W3R) and the optimal flowrates and contaminant compositions of the streams that have been identified for potential reuse, regeneration, and recycle for the retrofit of the existing network of water using and wastewater treating units. In this work, we use the term water network system to refer to the overall system comprising the water-using and water-treatment units. The optimization model is carried with the assumption show below in the following section.

1.2.1 Model assumptions

In this work, certain assumptions are adopted in modelling the system:

- can easily accommodate large number of variables (flowrates & concentrations)/multiple contaminants;
- the total flowrate of a stream is taken to be constant and equal to that of pure water in that stream because the level of individual contaminant flows is so slow and is therefore negligible (that is, the contaminants are at the concentration level of parts per million) (Karuppiah and Grossmann, 2006; Bagajewicz et al., 2002);
- the treatment units are treated simply with fixed recoveries;
- water flow demands of the utility units are assumed to be fixed (for systems all data for the limiting water profiles is available and is certain (Argaez et al., 1998);
- the number of water using and water treatment operations is fixed (Argaez et al., 1998);
- the removal ratios for each treatment unit are independent of the inlet concentration to the particular unit (Argaez et al., 1998);
- heat integration is not allowed, hence isothermal network operation is assumed (Argaez et al., 1998);
- the network operates under constant pressure (Argaez et al., 1998);
- the contaminant load is fixed and is independent of the flowrate; although this assumption can be challenged conceptually and even practically in some cases, it has been considered adequate for most of the systems analyzed (Bagajewicz et al., 2002)

1.3 Research Motivations

The rapid growth in petroleum refinery industry has created a very competitive environment for this industry. To be competitive in this industry, the process has to be in optimal condition whereby the production cost is minimized and the profit is to be maximized. Plant utility optimization is one of the methods to be considered to enlarge the profit margin. Optimization is the use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process. Fresh water consumption and wastewater generated by the plant have been the main concern nowadays due to:

- increasingly stringent environmental regulations;
- scarcity of water resources;
- high demand of water may make the plant vulnerable to:
  - interruptions in the water supply
  - water shortages in the future
- increased requirement in operating efficiency and optimization
- sustainable development in terms of maintenance and enhancement of environmental, social and economic resources

It should be kept in mind that the cost of water is low but the value is high and the world's practice has been moving towards zero discharge which will remain as a challenge to the researchers and engineers in future.

1.4 Research Objectives and Scope of Work

1.4.1 Objectives

The objective of the study is to formulate and solve a mathematical optimization model that determines the optimal freshwater and wastewater flows of the utility side of a refinery plant with the incorporation of water minimization approaches and strategies consisting of water reuse, regeneration, and recycle. The questions that we are interested to answer in this work relates to the retrofit decisions of the optimal retrofit of the water use. The optimization model which incorporates W3R techniques is formulated with the aims for minimum freshwater import, minimum wastewater generation, and allowable contaminant concentrations.

Originality of this research project is to enhance the identification in potential feasible alternative for W3R and the repeated treatment units. This is done via the combination of heuristic and mathematical optimization approaches with the understanding on plant and knowledge on physics of the problem. Heuristic or the physical insights on the water network system is enable to provide guidelines in determining the feasible alternatives in retrofit of water network systems and the potential of repeated treatment units to obtain freshwater quality for the treated water. Apart from that, this research project also incorporates large number of variables on flows and contaminant concentrations, which makes it a multidimensional optimization and nonlinear programming (NLP) problem.

1.4.2 Scope of work

The completed work includes, among other activities, qualitative and quantitative studies on assessing the water consumption areas of a refinery plant and development of the preliminary site water balance (i.e., the water supply and demand).

The scope of work in this project is detailed as follows:

- development of water balance based on a refinery plant;
- data reconciliation on the balance developed;
- development of a superstructure that includes feasible alternative structures for potential water reuse, regeneration, and recycle for the retrofit of the existing network of water using and wastewater treating units based on the *utility section* of a refinery plant
- formulation of a mathematical model with nonlinear programming (NLP) method by way of optimization procedure based on the developed superstructure that incorporates the following major elements (as the model constraints):
    - the validated water balance developed, which describes the freshwater and wastewater flows in the existing water network of the site's utility section;

  - potential for water reuse, regeneration, and recycle;
  - water treatment options with related data on the performance efficiency (typically in percentage) of a treatment unit (fixed removal ratio)
  - constraints stipulating that the contaminant concentrations of certain streams must not exceed particular specified values;
- solution of the resulting optimization model to determine the optimal flowrates and contaminant compositions of the streams that have been identified for potential reuse, regeneration, and recycle, with the aim of minimizing the flowrate processed by each treatment unit and the total flowrate of all units

CHAPTER 2

LITERATURE REVIEW AND THEORY

2.1 Water Network Systems

Water is vital for the normal functioning of the process industry. It has been assumed to be limitless low cost natural resource in the past. The predicted scarcities of industrial water over the next few decades and the increasingly stringent environmental regulations for wastewater disposal will require efficient and responsible utilization of water in industry (Karuppiah and Grossmann, 2006). Furthermore, there is increasing awareness of the danger to the environment caused by the discharge water nowadays. Besides, the imposition of even-stricter discharge regulations has driven up effluent treatment costs, requiring capital expenditure with little or no productive return.

Traditionally, fresh water has been used for process purposes, and wastewater generated in these processes has been sent to a central treatment unit for contaminants removal to meet regulatory specifications for the wastewater disposal. It is normally being discharged to the environment. For example, fresh water is used in evaporative cooling systems to make up for the evaporative losses and blow down from the cooling water circuit. All of the effluents tend to be mixed together, along with contaminated storm water, treated centrally in a wastewater treatment system and discharge to the environment. If the use of water can be reduced, it will directly reduce the cost of water supplied and the effluent treatment. There is thus considerable incentive to reduce both freshwater consumption and waster water generation (Smith, 2005).

2.2 Techniques for Freshwater and Wastewater Minimization

The three basic techniques for water network optimizations are reuse, regeneration and recycle. Wang and Smith (1994a) have proposed water reuse, regeneration-reuse, and regeneration-recycling as an approach for fresh water minimization. The enhanced water network system depends on the contaminants contained in each outlet of the process unit and the quality of the inlet water required for the subsequent process units (McLaughin & Groff, 1992). Figure 1 below showing a simple configuration of which fresh water is used in all operations.

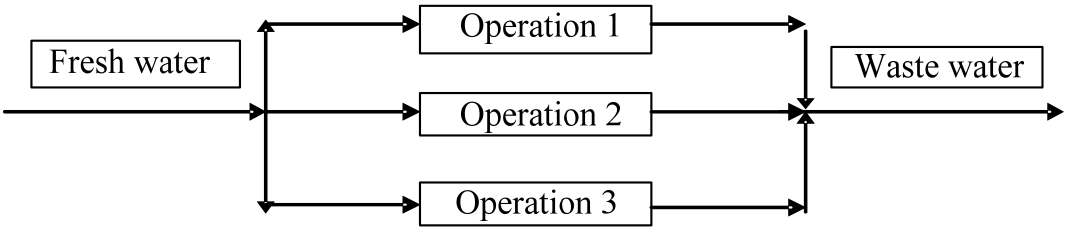

Figure 2.1 Freshwater used in all operations

2.2.1 *Water reuse*

Water reuse means that the used water is fed into another process unit provided that the contamination level of the discharge water is acceptable at the inlet of the other process unit. Reusing water reduces both the volume of the freshwater and the volume of wastewater, as the same water is used twice. Multistage washing operation: low quality water could be used in initial stages, and high-quality water used in the final stages (Smith, 2005). Figure 2 shows the implementation of water reuse in a simple water network.

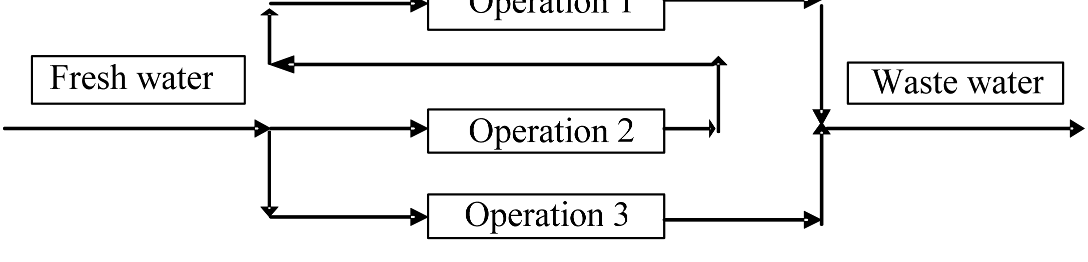

Figure 2.2 Water Reuse

2.2.2 Water regeneration reuse

The used water is fed into a treatment unit to regenerate water of which the quality is acceptable for further use. Regeneration reuse reduces both the volume of the freshwater and wastewater, and also removes part of the effluent load before reuse to prevent contaminants build up throughout the entire process cycle. In addition, regeneration removes part of the contaminant load that would have to be otherwise removed in the final effluent treatment (Smith, 2005). The regeneration reuse technique is illustrated in Figure 3.

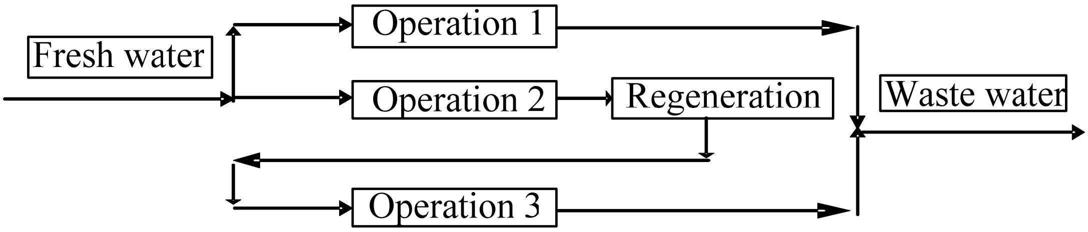

Figure 2.3 Regeneration Reuse

2.2.3 Water regeneration recycle

The used water is fed into a treatment unit before being recycled back to the same or other process units due to the high contents of contaminants which exceeds the allowable level, as shown in Figure 4. Regeneration recycling reduces both the volume of the freshwater and the volume of wastewater, besides reduces the effluent load by virtue of the regeneration process taking up part of the required effluent treatment load to avoid contaminants build up in the subsequent process unit (Smith, 2005).

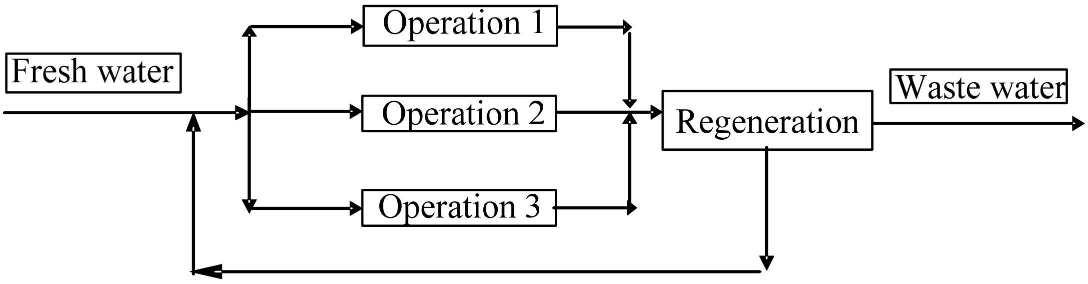

Figure 2.4 Regeneration Recycle

In water network optimization, regenerate reuse and regenerate recycling are similar in terms of their outcomes. The distinction between the regeneration reuse and regeneration recycle is that in regeneration reuse the water only goes through any given operation once, which in regeneration recycle the water can go through the same operation many times. Regeneration recycling allows larger reductions in the freshwater use and wastewater generation than in the regeneration reuse. However problems can be encountered in the regeneration recycling, recycling allowed the build up of undesired contaminants in the recycle, such as micro-organisms or products of corrosion. These contaminants not removed in the regeneration might build up to the extent creating problems to the process (Smith, 2005).

2.3 Treatment Systems

There are two significant reasons why water contamination needs to be considered. The first is that aqueous effluent must comply with environmental regulations before discharge. The concentration, and perhaps load, of contamination of various specified contaminants must be less than the regulatory requirements. The second reason is that contaminant levels will affect the feasibility of reuse and recycling of water. If water is to be reused or recycled; the level of inlet contamination to the operation receiving the reused or recycled water must be acceptable (Smith, 2005). Lists of contaminants and respective units are shown in Table 1.

Table 2.1 List of contaminants and respective units

Contaminant	**Unit**
Oil and Grease (O&G)	mg/L
Total dissolved solid (TSS)	mg/L
pH	-
Chemical Oxygen Demand (COD)	mg/L
Total Phenol	mg/L
Iron (Fe)	mg/L

Table 2.2 List of treatment units with respective removal ratio

Treatment units	Abbreviation	Contaminants Removed or Treated	Removal Ratio
Mud trap / Corrugated plate interceptor	MT/CPI	Oil and Grease	99%
Dissolved air flotation	DAF	Oil and Grease	81.5%
Effluent treatment system	ETS	Oil and Grease, TSS, COD,	84%, 68%, 88%, respectively
Sand filtration	SF	TSS, Fe	70%, 45%
Ultrafiltration	UF	TSS, COD	80%, 80%
Reverse osmosis	RO	TSS, COD	97.5%, 90%
Multimedia filtration	MMF	TSS, Fe	70%, 45%
Carbon filtration	CF	TSS, Fe	70%, 45%

Treatment units utilized in refinery water network systems is show in Table 2.2. Instead of end-of-pipe water treatment, another way of dealing with the effluent treatment is distributed effluent treatment or segregated effluent treatment. Local treatment can take place on the outlet of any operation unit before being reuse or regeneration or going to final waste water treatment and discharge.

Wastewater from different water-using operations may contain different types of contaminants. For instance, if two streams require different treatment operations, it makes no sense to mix them up before the treatment which will increase both capital and operating costs. The capital costs of waste water treatment is generally proportional to the total flow of waste water treated and the operating cost increases with decreasing concentration for a given mass of contaminant to be removed (Smith, 2005). Wang and Smith (1994a) have proposed a methodology for designing effluent treatment systems where wastewater is treated in a distributed manner. Treating wastewater in a distributed manner, in which effluent streams are treated separately instead of bringing them into a single stream prior to treatment, reduces treatment cost since the capital cost and operating cost of a treatment operation are directly proportional to the water flowrate through the treatment units, which is smaller in the case of distributed systems.

The concept of distributed effluent treatment is one that tends to treat effluents before they are mixed together. Treatment is made specific to individual (or small numbers if) contaminants while still concentrated. The benefit is that, by avoiding mixing, this increases the potential to recover material, leading to less waste and lower cost of raw materials. However, the overriding benefit is usually that the effluent volume to be treated is reduced significantly, leading to lower effluent treatment costs overall.

2.4 Review on the Earlier Work in Freshwater and Wastewater Minimization Techniques in Water Network Systems

Most of the studies published in literature have dealt with the issue of minimizing the freshwater generation in water-using processes separately from the design of effluent treatment systems. There are very few studies on the integration of water using and treating processes into a single system. The seminal paper in this area was by Takama et al. (1980), who solved the problem of optimal water allocation in a petroleum refinery. This paper presented a petroleum refinery case study to produce an optimal water allocation for water-using operations and wastewater treatment units by utilizing mathematical programming. A superstructure of all water-using operations and cleanup processes was set up and an optimization was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. The authors made an important contribution by addressing the problem of water management as a combination of water: wastewater allocation among processes and wastewater distribution to cleanup units. The paper has successfully provided a basic concept and approach for solving water/wastewater problem in chemical process plants. Their works has been improved by many researchers for the subsequent years.

Wang and Smith (1994) propose a limiting water profile and pinch point concept to find the target of minimum freshwater consumption and design the associated water-using operations network. They consider both single and multiple contaminants and also put consideration a practical constraint of not allowing local recycling without regeneration to avoid accumulation of certain contaminants. This is the first application of water reuse, regeneration, and recycle concept (W3Rs) in water-using operations network by using a graphical method. However, their method has major drawback due to its capability of modeling water-using operations as mass transfer-based operations. Furthermore, it is pointed out that no systematic and reproducible algorithm is given in the explanation, leaving the design to the hands of experienced professionals. This paper also approached the design of distributed effluent treatment as mentioned in section 2.3; the model proposed assumes no merging of the streams which are from different sources and can be sent to different treatment unit. The treatment units are assumed to have fixed pollutant removal ratio. (Bagajewicz, 2000)

Doyle and Smith (1997) formulate a superstructure model connecting every possible connection among water-using operations for multiple contaminants in water reuse problems. They construct the formulations by assuming that all contaminants reach their maximum outlet concentrations for all units, propose relaxation in component balance relationships, and then solve the formulation by Linear Programming (LP) to obtain water network corresponds to minimum freshwater consumption. Then, with the obtained water network, they reformulate the problem back into Non Linear Programming (NLP) and optimize it to get the exact value. This method addressed new design problems, in which all possible piping connections can be formulated to get optimum solution of total freshwater consumption. However, the obtained solution may not be a practical solution due to its complexity towards having the optimum solution and other practical constraints that are not addressed such as forbidden or compulsory piping connections and geographical constraints.

Galan and Grossmann (1998) develop nonconvex NLP and MINLP models for the design of distributed wastewater treatment plants, utilizing the network superstructure presented by Wang and Smith (1994). This paper deals with the optimum design of a distributed wastewater network where multicomponent streams are considered that are to be processed by units for reducing the concentration of several contaminants. The proposed model gives rise to a nonconvex nonlinear problem which often exhibits local minima and causes convergence difficulties. The authors proposed a multistart heuristic procedure for the global optimization of the formulated nonconvex models; a search procedure is proposed in this paper that is based on the successive solution of a relaxed linear model which provides initialization points for the solution of the original NLP problem. Their algorithm is based on the generation of multiple starting points through a convex underestimation problem. The model is also extended for selecting different treatment technologies and for handling membrane separation modules.

Alva Argaez (1999) uses the insights of water-using operations given by Kuo (1996) and proposes an iterative method of optimizing the mathematical programming involving MINLP formulations. This approach was intended to seek for minimum total annual investment and operating cost of water-using operations network by applying water reuse scheme. However, the method is complex and involves too many variables to be optimized iteratively. Argaez et al., (1998) have used a mathematical programming approach to optimize a superstructure, which includes possibilities for water treatment and reuse. They have presented a Mixed Integer Non-Linear Programming (MINLP) model, which is decomposed into a sequence of Mixed Integer Linear Programming (MILP) problems to approximate the optimal solution.

Savelski and Bagajewicz (2000) attempted to construct water reuse networks for single contaminant problem by fulfilling necessary conditions of optimality, maximum outlet concentrations, and concentration monotonicity. They formulate mass transfer-based operation into Linear Programming (LP) and then optimize the formulation. In their extended studies regarding multiple contaminants problem (Savelski and Bagajewicz, 2003), they set up quite similar necessary conditions of optimality of at least one contaminant reaches its maximum outlet concentration and monotonicity of key contaminant, and then solve the problem with a proposed algorithmic procedure that is guaranteed to achieve a global optimum. However, the obtained global solution suffers a setback where a very low flowrate is produced, which in practical, it is assumed to be a zero flowrate.

It is observed that the earlier studies only focused on the design issues concerning either one of these two subsystems to avoid handling the complex interactions between water using and wastewater-treatment networks. An integrated approach for the overall system design remained a challenge until a general nonlinear programming (NLP) model was developed by Huang et al. Although the above NLP model has been proven to be useful in creating optimal water-system designs on the basis of given objective functions, the resulting network structures may still be less than desirable in practical applications. This is due to the fact that it was not formulated to produce the structural features needed for effective operation of the overall water systems. It is therefore necessary to improve the present optimization strategies to meet this demand for obtaining the optimum solution while controlling the network configuration.

Huang et al. (1999), had presented a theoretical model for constructing an optimal Water Usage and Treatment Network (WUTN) in a chemical plant. The paper proposed a systematic approach in determining the optimal water usage and treatment network (WUTN) in any chemical plant, which features the least amount of fresh water consumption and/or minimum wastewater treatment capacity via mathematical programming model. In particular, because design equations of all wastewater treatment facilities and all units which utilize either process or utility water are included in the model, more comprehensive integration on a plantwide scale can be achieved. The proposed method is more reliable, more accurate, and much faster in synthesizing the WUTNs. Furthermore, more cost-efficient alternatives may be identified in certain design cases.

Wang et al. (2003) propose a design methodology for multiple contaminants problem with single internal water main. The method shows that the solution gives lower freshwater consumption in term of global solution. The networks obtained provide simpler water networks, easy to design, operate and control, for plants involving many unit processes. However, mixing wastewater from many water-using operations in the internal water main can give mixing of certain unwanted contaminants that are not allowed to be reused in practical term.

Karuppiah and Grossman (2006) has generalize the synthesis problem by proposing a superstructure, similar to that by Takama et al. (1980) for the design of integrated water systems, that combines the water using and water treating units in a single network. The optimization of the superstructure incorporates all the feasible design alternatives for water treatment, reuse and recycle is formulated as Non-Linear Programming (NLP) problem which is then reformulated as a MINLP problem. The superstructure optimization models are non-convex due to the presence of bilinearities in the constraints and so the local NLP algorithms often fail to converge to a solution, or else lead to sub-optimal solution.

Chang and Li (2005) presented a design procedure to generate practical structures for the water-usage and -treatment networks. The optimization strategies used are developed on the basis of a modified version of the existing nonlinear programming model, particularly used to incorporate additional design options and a fixed number of repeated treatment units into the superstructure. The inequality constraints on their concentrations are added in the revised model formulation to account for the possible existence of unrecoverable solutes. A reliable method is developed to produce a good initial guess for enhancement in convergence efficiency. It is produced in three steps, which are construct an initial network structure, select the feasible flow rate of every branch in the initial structure to satisfy water balances, and solve a set of linear equations for the inlet and outlet concentrations of each unit in the initial structure via linear programming solver. This paper relaxed the constraints on self-looping around a water-using or wastewater-treatment unit, addressed the issue of repeated treatment unit systematically and included the performance index reflecting structure simplicity in the objective function.

The two-step optimization approach consists of two steps, namely structural targeting and parametric optimization. The first step is performed to obtain several water networks that take into account all the common practical considerations and the second step is used to optimized variables for each of the optimized water network structure. The results produce ‘a class of good solutions’, where the users are able to select which particular option will be relevant to be applied. Those common practical considerations includes keeping low level of piping complexity, forbidden/compulsory piping connections, geographical constraints or plant layout limitations, satisfying the quantity and the quality of water supplied, safety considerations, and even company preferences. (Putra and Amminudin, 2008).

All of the above methods of reducing total freshwater consumption using water reuse, regeneration, and recycle concept (the W3Rs concept) have their own advantages and disadvantages, respectively. Graphical approaches are based on the application of single contaminant and focused on targeting. Practical considerations and its complexity are not taken into account, which the lead to unrealistic designs as this does not reflect what is really happening in the real scenarios. Complex problems utilizing multiple contaminants are successfully solved with mathematical approaches. In this way, common practical considerations can be considered. Nonetheless, the problem complexity requires advanced computational efforts as well as iterative procedures to produce a single optimum solution. It does not give another optimum solution unless more efforts and times are provided so.

Engineers are more willingly to have more than one optimum solution as well as to have manual control over the optimization process. They would like to see how their views and thoughts considered during the optimization progress. Thus, by having these advantages, at the end of optimization, engineers will have many solutions to be chosen

2.5 Advantages of the Mathematical Programming Approach

The benefits of solving optimization problem for retrofit of refinery water network system through mathematical programming approach include its reliability in generating solution because potential human errors can be avoided in solving large-scale multicontaminant water usage and treatment network (WUTN) design problems (Huang et al., 1999). It enables us to model the real-world situation accurately and less hassle compare to having to conduct experiments. Furthermore, it is versatile because the proposed mathematical program can be easily adapted for a wide range of revamp and grassroots design applications (Huang et al., 1999). It is comprehensive because more alternatives and in certain cases, more appropriate designs can be identified when compared with the manual approach of water pinch analysis. Some of the alternatives may even be overlooked (or possible neglected) by experienced engineers. In addition, the effects of incorporating multiple passes through a water treatment unit can be easily studied within a mathematical program by considering the presence of repeated water treatment units.

2.6 Modeling Software for Water Network Optimization: GAMS

The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. It consists of a language compiler and a stable of integrated high-performance solvers. GAMS is tailored for complex, large scale modeling applications, and allows to build large maintainable models that can be adapted quickly to new situations. The design of GAMS has incorporated ideas drawn from relational database theory and mathematical programming and has attempted to merge these ideas to suit the needs of strategic modelers. Relational database theory provides a structured framework for developing general data organization and transformation capabilities. Mathematical programming provides a way of describing a problem and a variety of methods for solving it. Linear, nonlinear, mixed integer, mixed integer nonlinear optimizations and mixed complementarity problems can currently be accommodated.

GAMS has been developed to improve on this situation by:

- providing a high-level language for the compact representation of large and complex models
- allowing changes to be made in model specifications simply and safely
- allowing unambiguous statements of algebraic relationships
- permitting model descriptions that are independent of solution algorithms

CHAPTER 3
METHODOLOGY

3.1 Methodology

In general, the mathematical programming approach to process synthesis and design activities and problems consists of the following four major steps (Grossmann, 1990; Floudas, 1995, pp. 233.234; Novak et al., 1996) as in Figure 3.1 with the following descriptions:

1. Development of the superstructure to represent the space of topological alternatives of the naphtha flow to petrochemical plant configuration;
2. Establishment of the general solution strategy to determine the optimal topology from the superstructure representation of candidates;
3. Formulation or modeling of the postulated superstructure in a mathematical form that involves discrete and continuous variables for the selection of the configuration and operating levels, respectively; and
4. Solution of the corresponding mathematical form, i.e., the optimization model from which the optimal topology is determined.

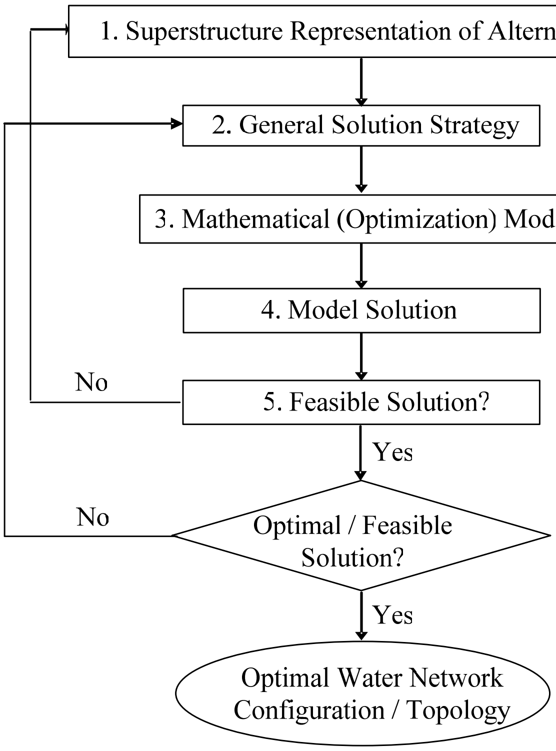

Figure 3.1 Major steps in the mathematical programming approach to process synthesis and design problems

As indicated in Figure 3.2, the suggested procedure for the retrofit design of the optimal refinery water network structure (or configuration or topology) comprises the following main steps, as adapted from Floudas (1987):

1. A superstructure includes all possible and feasible flowsheets showing the interconnections of the process units and material streams.
2. General solution strategy is to be determined for the optimization problem.
3. The overall superstructure is formulated as a nonlinear programming (NLP) optimization model with its objective functions and material balances applied to each alternative retrofit structure as its constraints.
4. The solution to the NLP problem of step 3 will provide the optimal retrofitted water network structure with the flowrates of the corresponding optimally-selected streams along with the concentrations (or compositions) of the components for each stream.
5. It will be evaluated and compared to the current practice to check for the feasibility of the solution.

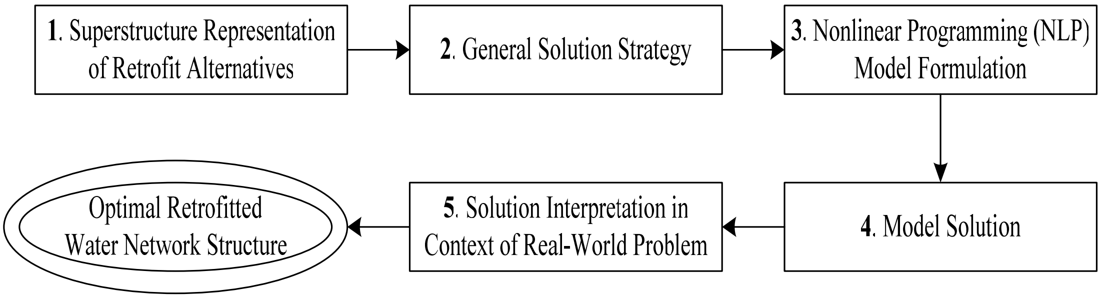

Figure 3.2 Outline of the general retrofit design strategy (Floudas, 1987)

With reference to the two diagrams above for general mathematical programming approach and for general retrofit design strategy, steps implemented in the mathematical programming approach for refinery water network system in this research project are slightly different, as shown in Figure 3.3. Data reconciliation is crucial and necessary to be carried with the given input before proceed to constructing the optimization model. This is an important step to make sure the superstructure of refinery water network system can be modeled accurately in GAMS and to enhance the solution's feasibility.

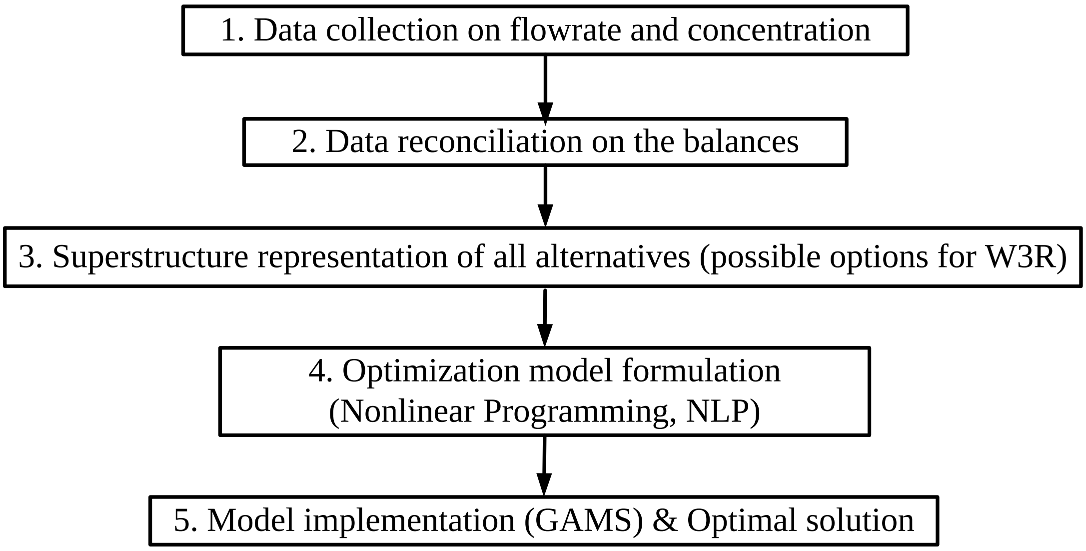

Figure 3.3 Necessary steps in the mathematical programming approach for refinery water network system

Note: Please refer Appendix C for the Gantt chart of this research project.

CHAPTER 4

OPTIMIZATION MODEL FORMULATION

4.1 The existing flowsheet of the refinery water network systems

The basic idea of superstructure representation is that it includes the current existing water network systems as well as the potential feasible alternatives. Figure 4.1 depicts the superstructure representation of the current existing water-using and water-treatment units. The simplified superstructure representation of current existing water-using and water-treatment units of a refinery plant is shown in Figure 4.2. Generally refinery water network systems consists of process units (PU) which is known as water-using units and treatment units (TU).

The current practice involves the supply of freshwater resource from external supplier and the treated water is for discharge provided that the contaminants concentrations are complied with the environmental discharge regulation, which is within the maximum allowable limits. Based on Figure 4.1, it is observed that centralized treatment systems is employed where all the wastewater generated from different operation units are mixed together before going through the same treatment units. The subsequent section elaborates on the procedures and deliberations involved in developing the alternatives or options for W3R.

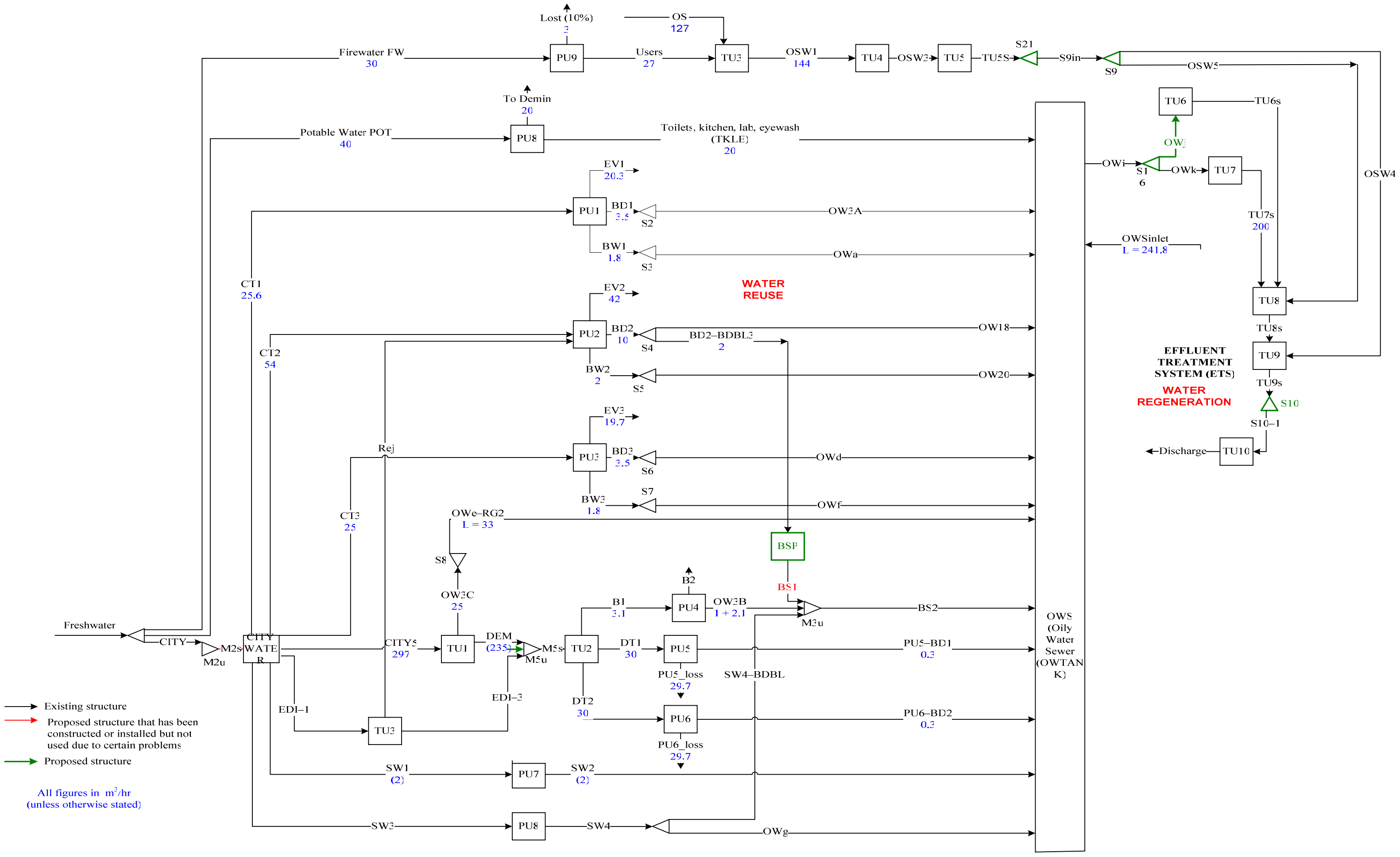

Figure 4.1 Flowsheet of current existing water-using and water-treatment units

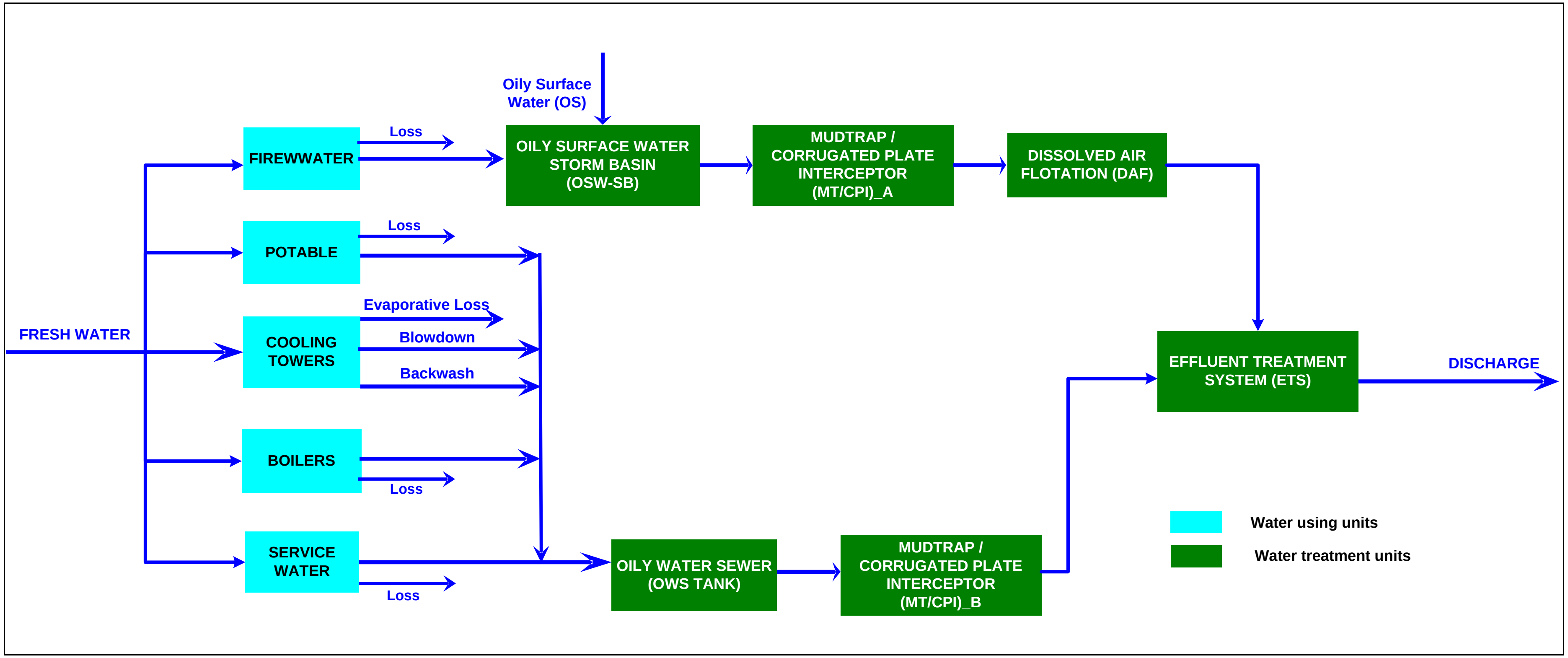

Figure 4.2 Simplified superstructure representation of current existing water-using and water-treatment units

4.1.1 Identification of potential feasible alternatives for water reuse, recycle, and regeneration (W3R)

Heuristics or more specifically the understanding of the plant itself is very important in identifying the potential opportunities of options to perform/undertake water reuse, regeneration, and recycle. As mentioned in the previous section, centralized effluent treatment system was utilized in the current refinery water network systems. This system tends to mix all cleaner and dirtier wastewater together of which the author identified a weakness in this practice. There is potential for retrofit and by implementing decentralized treatment systems which is also know as distributed treatment systems is able to fill this gap. Distributed treatment systems allow local treatment takes place to avoid merging of two different levels of wastewater from different types of operations units. Cleaner wastewater requires simpler and less costly treatment units. Moreover the operating cost of treatment units is proportional to the volume of the wastewater. It is unnecessary to employ the highest quality of treatment units for cleaner wastewater and only for those that needs advanced treatment. Two areas of mixing have been identified for potential W3R together with the most straightforward approach has formed three case studies for this research project.

Base case which is the current existing water network systems provides the base against which comparisons are made for the other alternatives, mainly in terms of the amount or percentage of freshwater recovery (that is, amount of further reduction in freshwater import), as well as (but to a lesser extent) the reduction in wastewater generated. The basis for Case A and C stipulates that all blowdown and backwash streams from the cooling towers are reused to cool down the blowdown streams from the heat recovery steam generator boilers and from the auxiliary boilers. In the current operation, service water (that is) taken from the freshwater source/main water source is used to perform this cooling task. Thus, the aim/objective is to reduce usage of freshwater through supplying less service water as required for this operation.

Case A is typically the most straightforward and easiest (design-wise/from a design point-of-view) retrofitting option. As depicted in Figure 4.3, it considers the conventional centralized wastewater (or effluent) treatment system with the addition of a “polishing” step that is accomplished through the installation of a cartridge (carbon) filter (CF), followed by an ultrafiltration (UF) unit, and finally treatment via reverse osmosis (RO), for the ultimate aim of recycling to the main water source (City Water) or for other usage. Carbon Filter is required as a polishing step because the incoming/its inlet stream may have hydrocarbons. It is meant to be used only when its inlet stream has a high contaminant load (and is thus deemed to be off-specifications).

Case B is formed with the aim of segregating cleaner wastewater from the utilities, (i.e., the blowdown and backwash streams from cooling tower) from mixing with the dirtier wastewater produced from the process units inside the Oily Surface Water (OSW) tank. In contrast to Case A, Case B implemented decentralized effluent treatment system which considers the treatment of the cooling tower blowdown streams using a sequence of UF and RO systems for recycle to the main water tank (City Water). It is infeasible with only UF and RO unless with additional pretreatment for O&G removal which is the corrugated plate interceptor before recycle. This alternative may be undesirable due to relatively small flowrates. However Case B serves as a guide in identifying potential W3R and the volume is depends on the respective plants to be retrofitted and whether worthwhile or not is depends on the reuse or recycle purposes after regeneration.

Case C serves to asses the possibility of recycling to the main water source by segregating dirtier wastewater from the operation units in refinery plant from the cleaner wastewater generated/produced from the utilities, which are currently fed into OWS, by mixing the utility wastewater with the oily surface water, in OSW Storm Basin; followed by additional regeneration of multimedia filtration, UF and RO and then cycle to City Water. Multimedia filtration is employed to remove total dissolved solids.

Figure 4.3 and 4.4 depict the superstructure representation of the current existing water-using and water-treatment units with the inclusion of the possible options for water reuse, recycle, and regeneration (W3R).

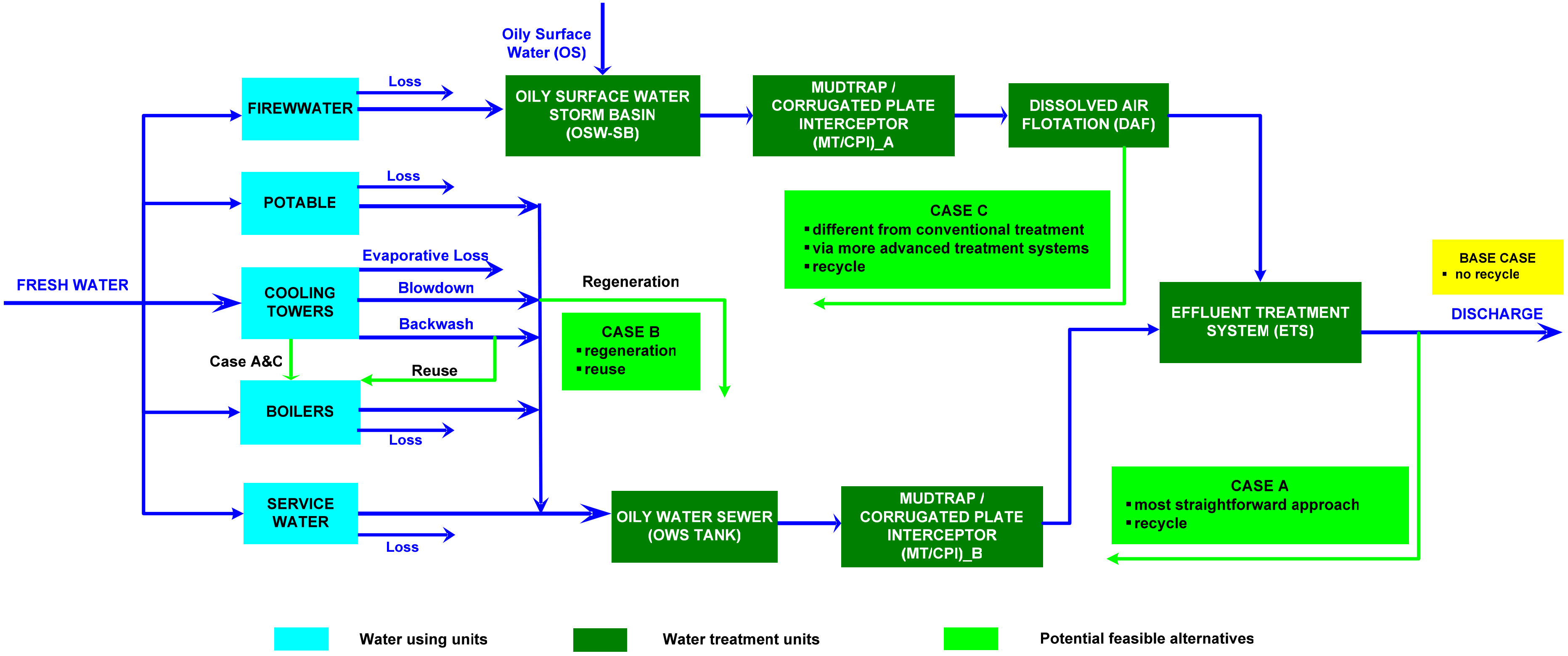

Figure 4.3 Simplified superstructure representation of current existing water-using and water-treatment units all feasible flowsheet structures

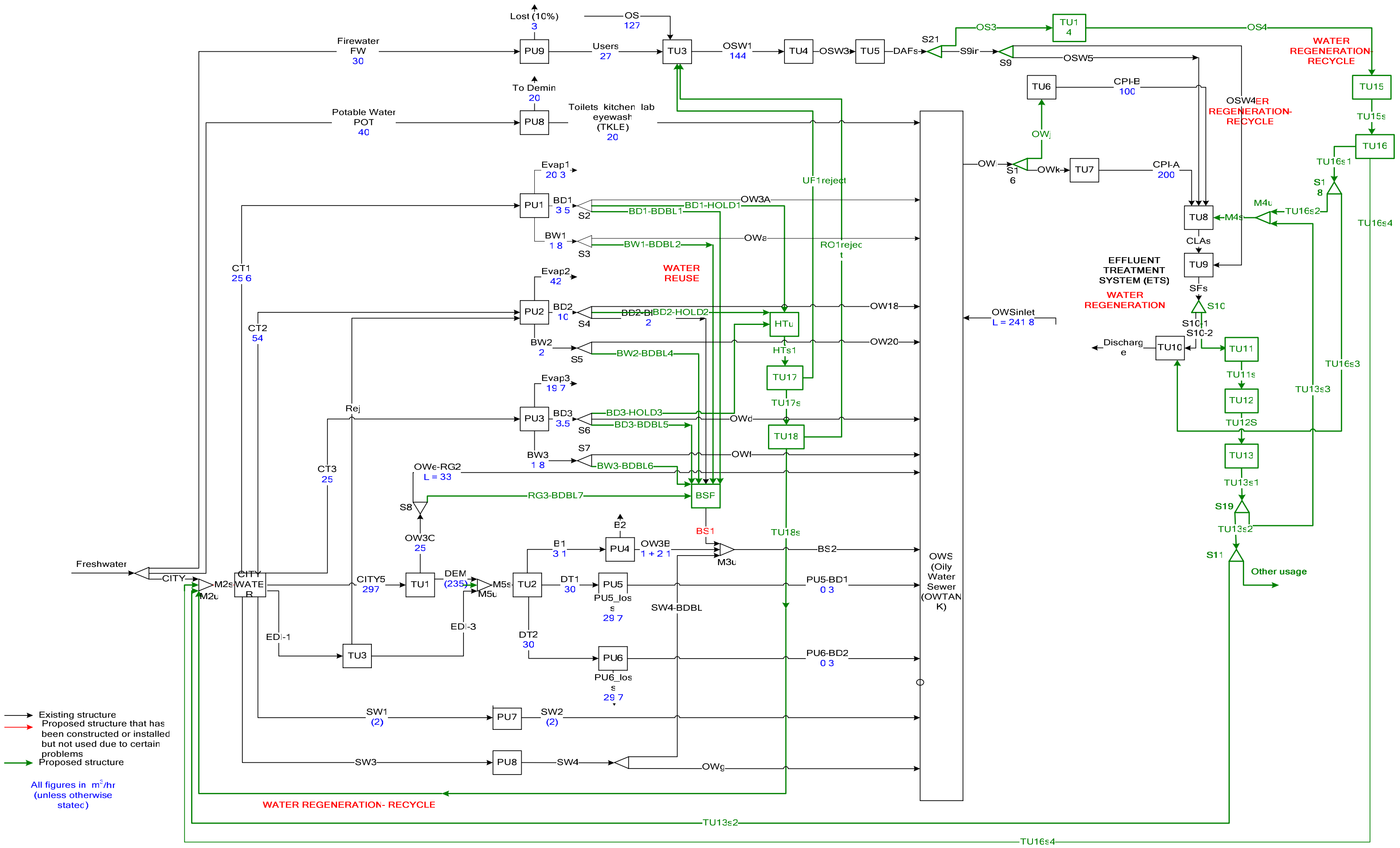

Figure 4.4 Modified state–task network (STN)-based superstructure representation of the refinery water network system with W3R options

4.2 Model Formulation

MATERIAL BALANCE CONSTRAINTS

In general, there are two forms of material balances that hold, and they account for:
(1) the total stream flows (or flowrates) and compositions of a stream, and
(2) the individual component flows of a stream.

The second form is given by the multiplication of a total stream flow with the composition of a certain component. In the case of water systems, the composition of a component is typically represented as its contaminant. It should be noted that we cannot use flows and compositions on one part and component flows on the other. We can either use one form or the other but not partially. This is because if component flows are used together with total flows and compositions, then the component flows have to be related to compositions, which will introduce new nonlinearities that will increase the complexities of the model formulation. Besides, we will not be able to carry forward the information if certain flows are modelled in terms of total flows while others are expressed in terms of individual flows.

4.2.1 Modeling with compositions and individual flows

It is known that a certain number of contaminants are picked up in the water using processes, which are then removed in the treatment units. Mass balances in these units, as well as in the mixers and splitters, which help to connect the process units and treatment units into a network, have to hold. Other constraints that have to be satisfied are that the contaminant concentrations of certain streams must not exceed specified values, and the contaminant concentrations have to be reduced to environmental limits before discharge. All the flows F_i and contaminant concentrations $C_{i,j}$ in the system are non-negative and they are the unknown decision variables in the optimization model whose values need to be determined. It should be noted, however, that this superstructure is restricted to having fixed flows in each of the potential branches.

The optimization problem consists of selecting the flows and compositions of the stream in order to optimize a given objective function which can be expressed in terms of flows and/or compositions. The problem corresponds to a continuous nonlinear programming problem in which nonconvexities arise in the mass balance equation (I. Quesada and I.E. Grossmann, 19954). In this case study, binary variables involved in the modeling would be the concentration data that is required as constraints for the model optimization process. A water network system can be modeled to consist of mixers, splitters, treatment, and process units.

4.2.1.1 Convergent-Flow-Path Units

A convergent-flow-path unit, typically a mixer, mx ∈ MX consists of a set of inlet streams *s* that are specified in the index set $\mathrm{MX_{in}}$ and an outlet stream $s_1 \in \mathrm{MX_{out}}$, as depicted in Figure 4.5.

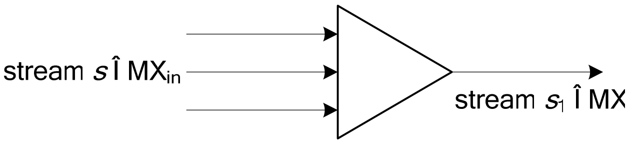

Figure 4.5 Graphical representation of convergent-flow-path unit or mixer in the superstructure

Material balance on total flowrates:

The overall material balance on total stream mass flowrates for the mixer mx is given by:

$$\sum_{s \in \mathrm{MX_{in}}} F_s = F_{s_1} \quad \forall s_1 \in \mathrm{MX_{out}} \tag{1}$$

Component material balance (using individual component flowrates):

The material balance for each contaminant *j* is expressed as:

$$\sum_{s \in \mathrm{MX_{in}}} F_s C_{j,s} = F_{s_1} C_{j,s_1} \qquad \forall s_1 \in \mathrm{MX_{out}}, \in j \in J \tag{2}$$

Note that the above material balance contains bilinear terms that are nonconvex, which will require the implementation of global optimization techniques. The bilinear terms can be avoided by representing them in terms of individual component flowrates:

$$\sum_{s\in \mathrm{MX}_{\mathrm{in}}} f_{j,s} = f_{j,s_1} \qquad \forall s_1 \in \mathrm{MX}_{\mathrm{out}}, \in j \in J \tag{3}$$

However, as mentioned, in this work, we employ the use of total flows and compositions. Hence, the formulation using component flows such as in equation **(3)** is not used and will not be discussed for the rest of the model presented here.

4.2.1.2 Divergent-Flow-Path Units

A divergent-flow-path unit, typically a splitter, sp ∈ MX consists of a set of inlet streams *s* that are specified in the index set $\mathrm{SP}_{\mathrm{in}}$ and a set of outlet streams $s_1 \in \mathrm{SP}_{\mathrm{out}}$, as depicted in Figure 4.6.

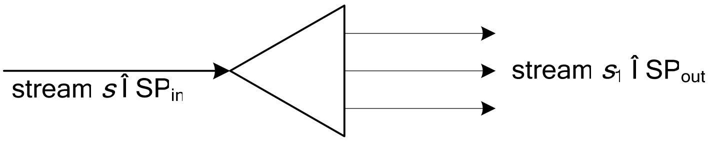

Figure 4.6 Graphical representation of divergent-flow-path unit or splitter in the superstructure

Material balance on total flowrates:

$$F_s = \sum_{s_1\in \mathrm{SP}_{\mathrm{out}}} F_{s_1} \quad \forall s \in \mathrm{SP}_{\mathrm{in}} \tag{4}$$

Component material balance

Note that it is necessary to enforce that the components maintain the same composition in each of the streams leaving the splitter. In other words, we assume that all outlet streams have the same compositions as the feed stream or inlet stream. Thus, the contaminant concentration of the streams leaving the splitter is equal to the concentration of the inlet stream. For the case of unknown concentrations, the stream compositions variables for each component *j* in stream *s* $C_{j,s}$ (or $x_{j,i}$ or ξ_i^j or ξ_i) can be defined and assumed to be set equal to each other for the input stream and the output streams, as given by the following contaminant concentration balance:

$$C_{j,s} = C_{j,s_1} \qquad \forall j \in J, \forall s \in \mathrm{SP}_{\mathrm{in}}, \forall s_1 \in \mathrm{SP}_{\mathrm{out}} \tag{5}$$

Individual component flow balances

The material balance for each component *j* is given by:

$$f_{j,s} = \sum_{s_1 \in \mathrm{SP_{out}}} f_{j,s_1} \qquad \forall j \in J, \forall s \in \mathrm{SP_{in}} \tag{6}$$

4.2.1.3 Treatment Units

We consider a treatment unit $t \in$ TU with an inlet stream $s \in \mathrm{TU_{in}}$ and an outlet stream $s_1 \in \mathrm{TU_{out}}$ as depicted in Figure 4.7.

Figure 4.7 Treatment Unit

Material balance on total flowrates:

The inlet and outlet flows for a treatment unit are equal as given by the following:

$$F_s = F_{s_1} \qquad \forall s \in \mathrm{TU_{in}}, \forall s_1 \in \mathrm{TU_{out}} \tag{7}$$

Component material balance

The individual contaminant flows in the outlet stream s_1 can be expressed as a linear function of the individual contaminant flows in the inlet stream *s* in terms of the coefficient of removal ratio for contaminant *j* in unit *t* (in percentage) $R_{j,t}$. Therefore, because the inlet and outlet flows for a treatment unit are equal from equation **(7)**, the material balance equation for each contaminant *j* inside the treatment unit *t* becomes linear and is thus given by the following:

$$C_{j,s_1} = \left(1 - R_{j,t}\right) C_{j,s} \qquad \forall j \in J, \forall s \in \mathrm{TU_{in}}, \forall s_1 \in \mathrm{TU_{out}}, \forall t \in \mathrm{TU} \tag{8}$$

where $R_{j,t}$ = fixed removal ratio (in percentage) in treatment unit *t* for contaminant *j*

The detailed material balance constraints can be found in the complete model formulation provided in Appendix A.

BOUNDS ON VARIABLES

Lower and upper bounds are stipulated for the variable flows and concentrations to facilitate the numerical computation of the optimization algorithm that is employed:

$$F_s^{\mathrm{L}} \le F_s \le F_s^{\mathrm{U}} \qquad \forall s \in S \tag{9}$$

$$C_{j,s}^{\mathrm{L}} \le C_{j,s} \le C_{j,s}^{\mathrm{U}} \qquad \forall j \in J, \forall s \in S \tag{10}$$

NON-NEGATIVITY CONSTRAINTS

Nonnegativity constraints are enforced on the decision variables of flows and concentrations:

$$F_s, C_{j,s} \ge 0 \qquad \forall j \in J, \forall s \in S \tag{11}$$

Remarks on the model formulation

In this problem, certain contaminant concentrations can be measured and are obtained from available plant data; hence they are known fixed values (and not variables).

Table 4.1 Lists of fixed contaminants concentration of wastewater from different operation units

	OnG (mg/L)	TSS (mg/L)	pH	COD (mg/L)	Total Phenol (mg/L)	Fe (mg/L)
SAMB	-	10	7	22.2	-	2.0
CITY	-	10	7	22.2	-	2.0
CT1	-	10	7	22.2	-	2.0
CT2	-	10	7	22.2	-	2.0
CT3	-	10	7	22.2	-	2.0
CITY5	-	10	7	22.2	-	2.0
SW1	-	10	7	22.2	-	2.0
SW3	-	10	7	22.2	-	2.0
FW	-	10	7	22.2	-	2.0
POT	-	10	7	22.2	-	2.0
BD1	1	37	7.32	81	-	1.08
OW3A	1	37	7.32	81	-	1.08
BD2	3	5	6	30	-	0.54
BD3	3.60	1.00	7.78	48.00	-	0.89
BW1	1	37	7.32:	81	-	1.08
OWa	1	37	7.32:	81	-	1.08
OW3B	-	3	8	116	-	-
OS8	2	40	8	52	3	-
RG3–BDBL7	-	12	5	47	-	-
CPI–A & B	1	30	0	242	1.23	-

ENERGY BALANCE CONSTRAINTS

An energy balance constraint is enforced on the water reuse to cool the blowdown stream from the boiler. We employ the following assumptions in formulating the energy constraint:

- heat capacity of water is constant (that is, it is not temperature-dependent) since we are referring only to the heat content of water flows;
- ambient temperature for water is taken to be 30°C;
- the outlets of the blowdown and backwash streams are isothermally mixed (that is, the outlet streams are mixed at the same temperature).

Thus, the general formulation of the energy constraint is given by:

$$Q_{\mathrm{supply}} = Q_{\mathrm{target}}$$

$$F_{s,\mathrm{supply}}\, \cancel{C_{p,\mathrm{W}}}\, \Delta T_{u,\mathrm{supply}} = \sum_{s} F_{s,\mathrm{target}}\, \cancel{C_{p,\mathrm{W}}}\, \Delta T_{u,\mathrm{target}}$$

$$F_{s_1}\left(T_{u,s_1}^{\mathrm{in}} - T_{u,s_1}^{\mathrm{out}}\right) = \sum_{s} F_{s}\left(T_{u,s}^{\mathrm{out}} - T_{u,s}^{\mathrm{in}}\right) \qquad \forall s \in S_{\mathrm{cold}}, \forall s_1 \in S_{\mathrm{hot}} \qquad \textbf{(12)}$$

CHAPTER 5

COMPUTATIONAL EXPERIMENTS AND NUMERICAL RESULTS

5.1 Solution Strategy

The governing principle of our solution strategy for determining, synthesizing, and analyzing the optimal W3R strategies for the retrofit of an existing refinery water network system is to develop an automated optimization framework with explicit consideration for heuristics, rules-of-thumb, physical insights, and engineering experience. This framework is used at the stage of developing and evaluating the feasible W3R alternatives as well as at the post-optimality stage of evaluating the feasible solutions or even the optimal solution computed by our preferred optimization model solver.

The major heuristics considered in our optimization framework involve the concept of distributed wastewater treatment (Wang and Smith, 1994) and the novel approach of repeated treatment units proposed by Chang and Li (2005). We proposed approach for this work in a slightly different manner in order to generate decisions on the number of repeated treatment units to handle the presence of remaining contaminants that need to be removed/eliminated to meet requirements for reuse/recycle or the less stringent requirements for discharge to the environment

5.1.1 Concept of Repeated Treatment Units

The operating conditions of all water-using units are determined by the process requirements while the water-treatment units in a superstructure can be viewed as the offline equipment available for possible installation. On the other hand, contaminant levels in the treated water for potential reuse or recycle must always fall within the permissible limits or comply to regulatory requirements. Thus, to achieve this necessary condition for the optimal solution, we have adopted the concept of repeated treatment units introduced by Chang and Li (2005), which rely on the following three rules:

Rule 1. For a treatment unit characterized by the constant outlet concentration of a single contaminant, the number of repeated units is set as 1 if there is no upper throughput limit. Otherwise, the number of repeated units, n_j^{unit} unit, should be the same as the number of units to process all wastewaters, the smallest positive integer.

Rule 2. For a treatment unit characterized by the removal ratio *Rj* of a single solute, a simple hand calculation procedure can be devised on the basis of equation 13 to determine the number of stages, *nj* stage, needed to reduce the solute concentration from its highest possible value, *C*source max, to the lower bound, *C*sink min. Specifically, *nj* stage should be the smallest positive integer.

$$\left(1 - R_{j,t}\right)^{n_{j,\text{stage}}} \leq \frac{C_{\text{min,sink}}}{C_{\text{max,source}}} \qquad \forall t \in T \qquad \textbf{(13)}$$

Rule 3. For a multiple-solute treatment unit, different unit numbers may be obtained by following either rule 1 or rule 2 on the basis of the process data of different solutes. To avoid incorporating an unnecessarily large number of repeated units in the superstructure, a heuristic is adopted in this work to select one of these computed numbers; i.e., the chosen value of n_j unit should be the largest one among those that are not more than 3 times the smallest number.

In this work, we have adopted a modified approach based on Chang and Lee (2005) in determining the number of repeated treatment units which is by applying heuristics together with equation **(13)** shown above. All the wastewater will complete one treatment cycle and the results obtained is to be evaluated to solve for the number of repeated treatment units for a particular contaminant(s) that does not meet the stipulated concentration requirements after one treatment cycle. This is to identify key contaminants that determine the quality of the treated water. For example, if oil and grease is the sole contaminant that is beyond the allowable limit, the number of repeated treatment units for the oil and grease removal unit will then be evaluated. The treated water with oil and grease level higher than required will go through the particular treatment units for the number of removal cycles determined; instead of going through the entire water treatment system. Our suggested approach could be more economically attractive with the expected reduction in flowrates due to not considering treatment units that do not require repeated units, as explained further in the next section.

5.2 Computational Results

The results of all cases which include the flowrates and contaminants concentrations with their respective number of repeated treatment units are show in Table 5.1 and 5.2, for all the cases. Table of comparison of computational statistics for each case is shown in Table 5.3. Instead of looping the treated water through the entire treatment system, this method is apparently more economic as it reduces the flowrate passing through each treatment units; the operating cost of treatment unit is proportional to the inlet flowrate. The rule of thumb in deciding which treatment unit(s) is to be repeated is to choose the one with the highest removal ratio for the removal of the contaminant(s) of which the concentration is higher than the allowable; if there is more than one treatment unit which is able to remove that particular contaminant. For instance, in Case B, the only contaminant that is higher than freshwater quality is oil and grease. The treatment units for oil and grease are dissolved air flotation (DAF) and corrugated plate interceptor (CPI). The latter unit has higher removal ratio and thus be selected for the repeated treatment units.

As shown in Table 5.1, Case A produces low water quality with large flowrate, which is for reuse below max inlet concentration of process units. In the case of treating the water to be as good as fresh water, it requires 3 treatment cycles for O&G removal which is by CPI, 2 treatment cycles for Total phenol removal by ETS and Fe removal by multiple stages of sand and carbon filtration. Case B produces very high water quality with small flowrate, which is for reuse in operations with strict tolerance on allowable contaminant concentrations. It requires two repeated treatment units for O&G removal by CPI with the aims of recycle with freshwater quality. Case C produces high water quality with medium flowrate, which is for reuse below max inlet concentration of process units. It requires three repeated treatment units for Total phenol & Fe removal by multimedia filtration to achieve freshwater quality recycle.

Table 5.1 Treatment units with respective removal ratio

Parameters	Base Case	Case A	Case B	Case C
Freshwater	513.2	513.2	513.4	510.4
Discharge	444	-	444	300
Reuse	-	39.6	77.46	39.6
Potential Recycle	-	440.6	15	96

Table 5.2 Contaminants concentration after one treatment cycle and the number of repeated units required indicated in parentheses

Contaminants	Freshwater	Discharge	Case A	Case B	Case C
Oil & Grease	0	10	25.10 (3)	1.826 (2)	21.36 (3)
TSS	10	10	8.386	0.32	4.885
pH	7	5.5 -9.0	7.833	4.45	73.917
COD	22.2	100	169.4	2.33	1.988
Total phenol	0	1.0	3.418 (2)	0	0.479
Fe	2.0	5.0	19.02 (2)	0.54	9.507 (3)

Table 5.3 Model and computational statistics

Computational Statistics	Base Case	Case A	Case B	Case C
Type of model	Nonlinear program (NLP)			
Solver	GAMS/CONOPT3			
No. of continuous variables	978	986	990	996
No. of constraints	418	432	454	420
No. of iterations				
CPU time (s)	trivial			

In general, our computational results could be summarized in the following simplified representation of the optimal flowsheet structure of the proposed retrofit to the refinery water network system, Figure 4.7 and 4.8. The options are not evaluated simultaneously and the water quality to be generated is depends on the potential reuse and recycle purposes. The engineers have flexibility in determining the quality of treated water, in terms of determining the number of repeated treatment units required with the respective concentration required; as well as the potential for water reuse in terms of the amount (flowrate) of water that can be reused and where it is suitable for.

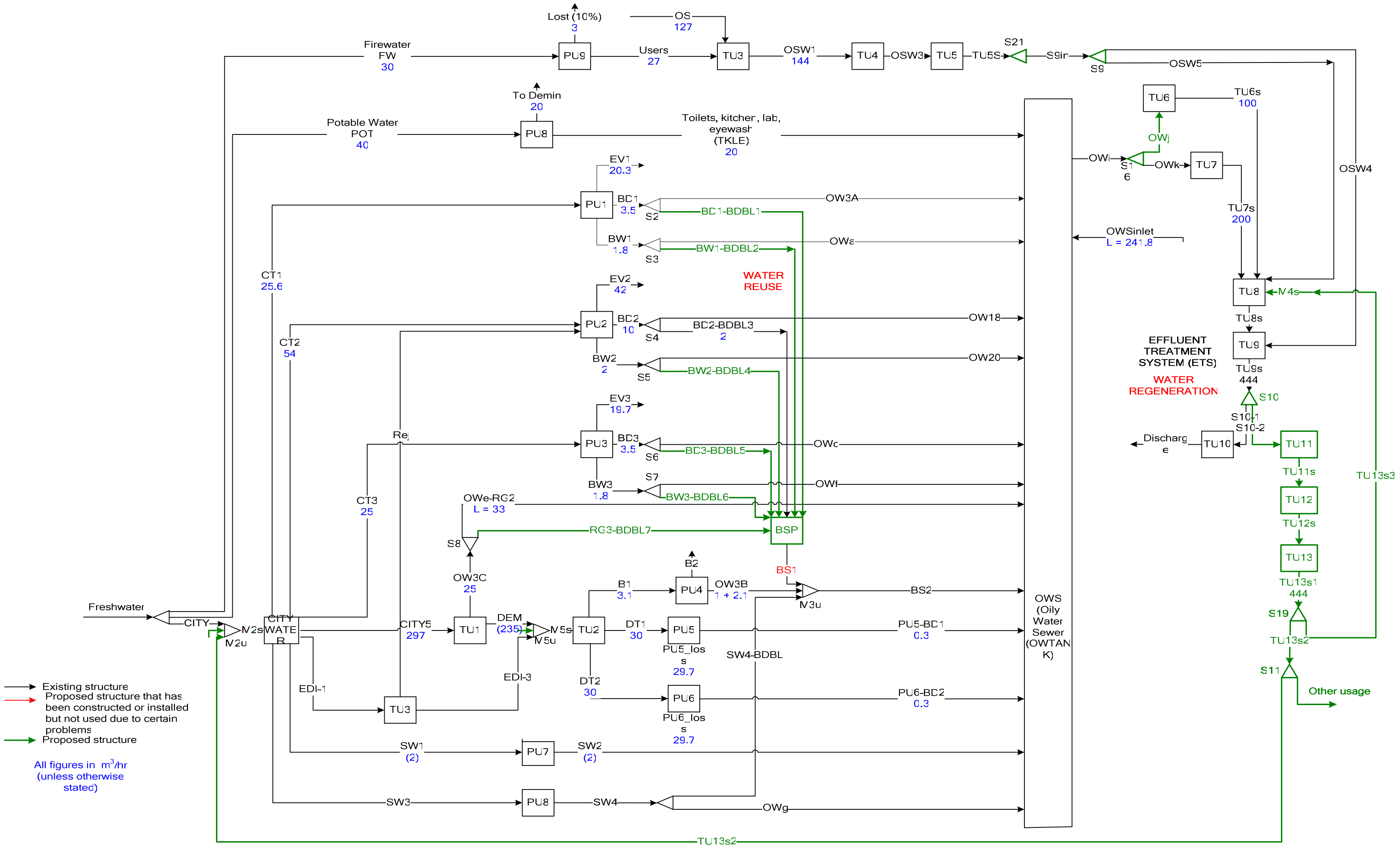

Figure 5.1 Flowsheet for Case A

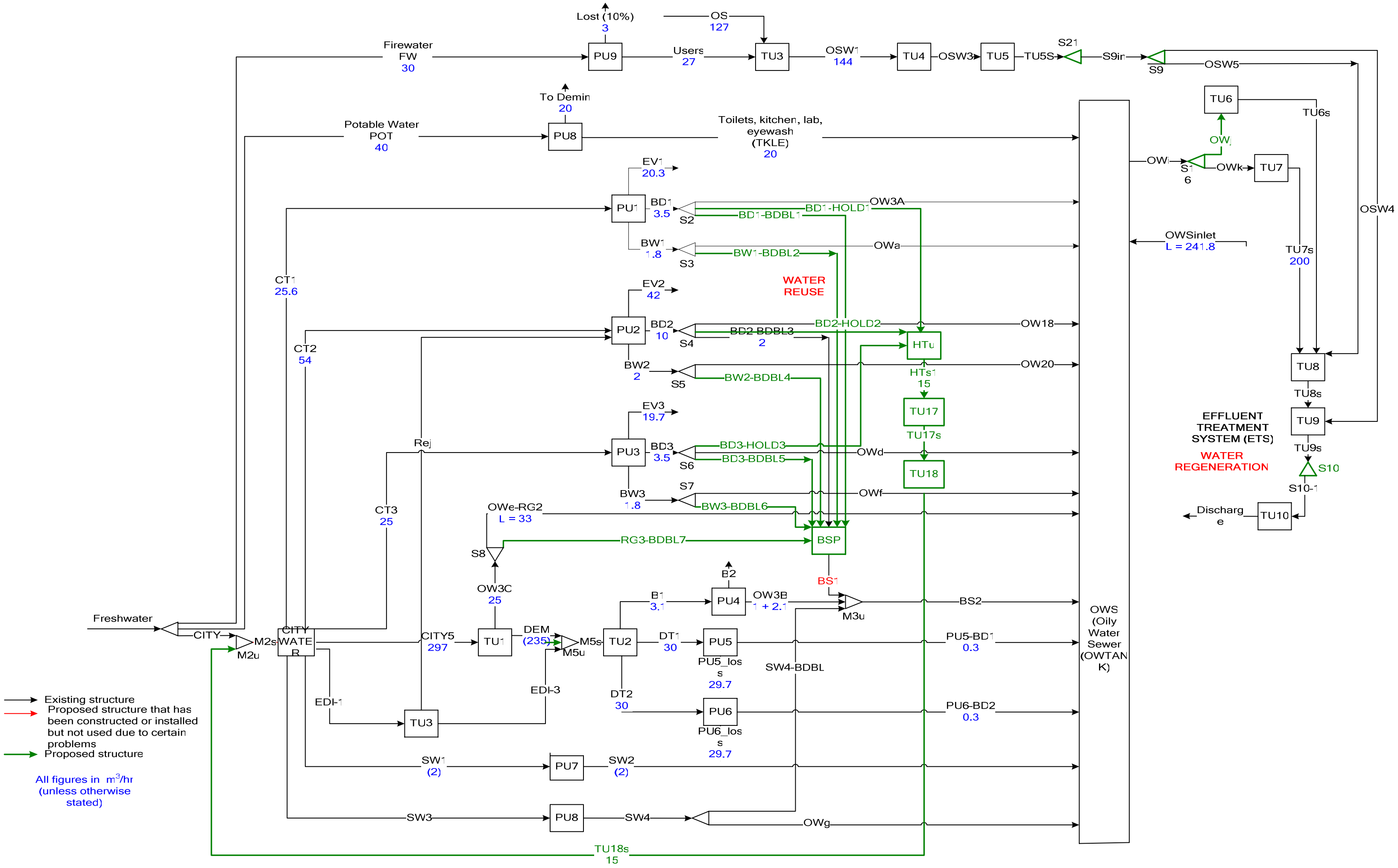

Figure 5.2 Flowsheet for Case B

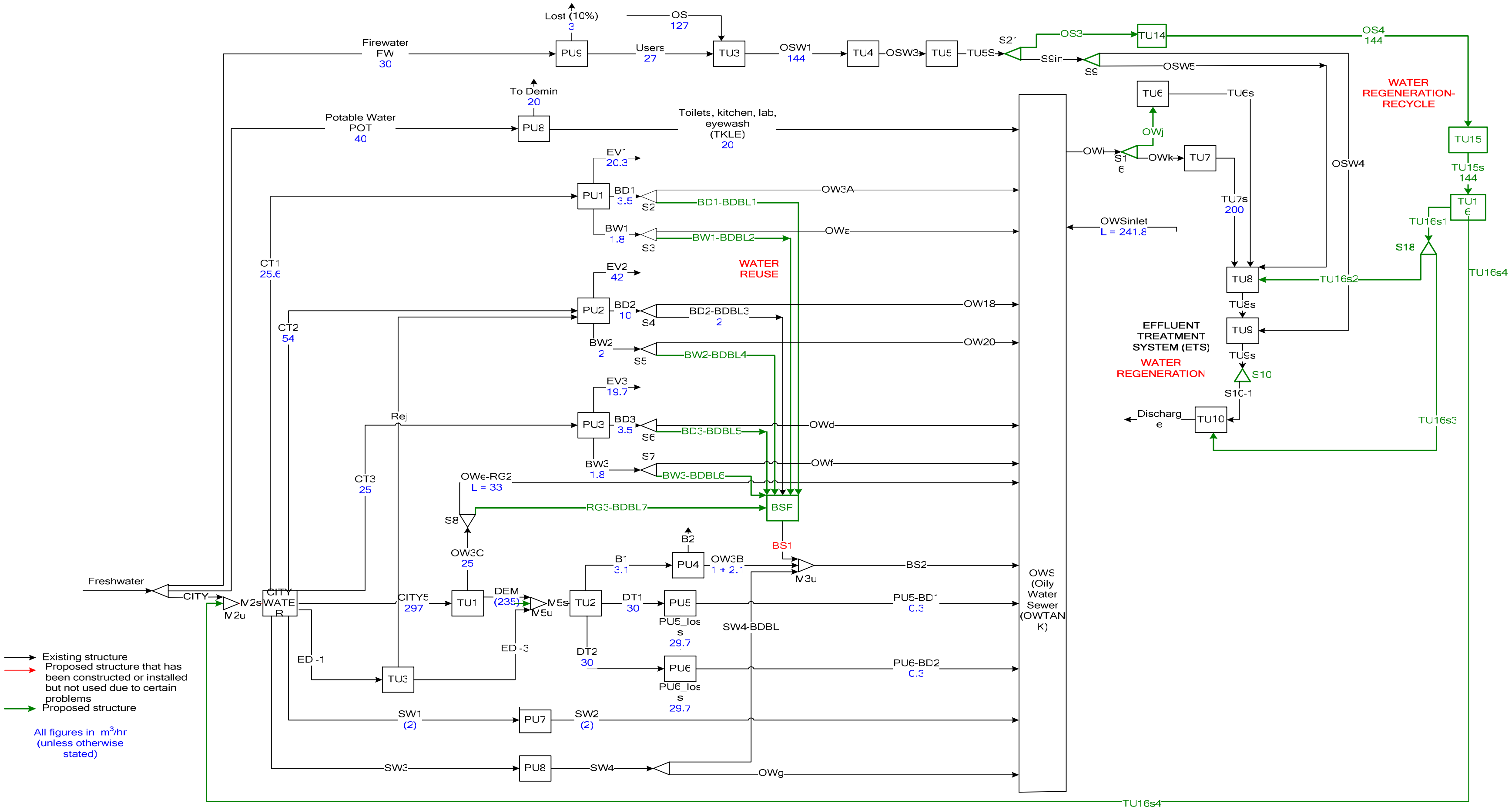

Figure 5.3 Flowsheet for Case C

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

Superstructure embedding all feasible alternatives of the refinery water network has been constructed. Utility-water consumption and wastewater treatment are analyzed under the same framework; therefore the resulting designs should be more comprehensive. Besides, nonlinear programming (NLP) optimization model has been developed with the incorporation of engineering heuristics and physical insight on the refinery water network systems.

This work has taken into consideration of a large, industrial-scale project (as reflected by the number of continuous variables involved). A total of six contaminants, which is industrially-significant and representative of industrial scale problems, are considered in the computational study of this work. (In comparison, the largest problem in the highly-cited study of Karuppiah and Grossmann (2006), and which is represented as having industrial scale by them, involves (only) three contaminants.)

The suggested optimization model developed with the combined knowledge of mathematical programming and heuristic is able to aid decision-making in determining optimal retrofit of refinery water network systems (for economic and commercialization potential).

Recommendations

Further development is required to optimize and improve the reliability of the mathematical model. For instance:

- Further improvement on the coding for the data interface between GAMS and Microsoft Excel
  - To enhance the automation in data transfer with external source of data in order to increase the efficiency of data extraction and avoid human error
- To incorporate economics optimization by formulating objective function that explicitly considers capital & operating costs
- Practical limit on the repeated treatment units based on cost considerations
- To incorporate consideration for level of piping complexity especially for application of proposed model to complicated or large refinery water network systems

Based on our findings in this work, an immediate recommendation would be to improve the cost efficiency in water usage at the plant.

- For medium-to-long term measures, we would suggest the refinery to consider housekeeping and management initiatives for water conservation before actually proceeding to implementation of W3R initiatives.

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APPENDIX

A. Material Balance in GAMS

A.1 Material balance for mixers

INLET_MIX(U,S) unit.(input stream)	OUTLET_MIX(U,S) unit.(output stream)
M1u.(UF1bypass, RO1permeate) M2u.(CITY, CITY3) M3u.(BDBLs1, OW3B, SW4-BDBL) M4u.(RO3reject3, RO2reject2) M5u.(DEM, EDI-3) BDBLu.(BD1-BDBL1, BW1-BDBL2, BD2-BDBL3, BW2-BDBL4, BD3-BDBL5, BW3-BDBL6, RG3-BDBL7) OWS.(TKLE, BDBLs2, SW2, OWg, OWSinlet, WHB-BD1, WHB-BD2) HTu.(BD1-HOLD1, BD2-HOLD2, BD3-HOLD3) OSW-SB.(USERS, OS7, OS13, OS8, OS5)	M1u.(RO1permeate2) M2u.M2s M3u.(BDBLs2) BDBLu.(BDBLs1) OWS.(OWi) M4u.(M4s) M5u.M5s HTu.(HTs1) OSW-SB.(OSW1)

A.2 Material balance for splitters

INLET_SPLIT(U,S) unit.(input stream)	OUTLET_SPLIT(U,S) unit.(output stream)
SPLIT1.SAMB SPLIT2.(BD1) SPLIT3.(BW1) SPLIT4.(BD2) SPLIT5.(BW2) SPLIT6.(BD3) SPLIT7.(BW3) SPLIT8.(OW3C) SPLIT9.(DAFs) SPLIT10.(SFs) SPLIT11.(RO3permeate) SPLIT12.(RO11s) SPLIT13.(SW4) SPLIT15.(EDI-1) SPLIT16.(OWi) SPLIT17.(GBs) SPLIT18.(RO2reject1) SPLIT19.(RO3reject1) SPLIT20.(RO1permeate2) HPU1.(DT1) HPU2.(DT2) PSR1_SW.(SW1) PSR2_SW.(SW3) FIREWATER.(FW) POTABLE.(POT) BOILER.(BOILER1) CITYWATER.M2s DEMIN_TANK.M5s	SPLIT1.(FW,POT,CITY) SPLIT2.(OW3A, BD1-BDBL1) SPLIT3.(OWa, BW1-BDBL2) SPLIT4.(OW18, BD2-BDBL3, BD2-HOLD2) SPLIT5.(OW20, BW2-BDBL4) SPLIT6.(OWd, BD3-BDBL5) SPLIT7.(OWf, BW3-BDBL6) SPLIT8.(OWe-RG2, RG3-BDBL7) SPLIT9.(OSW4, OSW5) SPLIT10.(S10-1, S10-2) SPLIT10.(S10-1) SPLIT11.(CITY3) SPLIT12.(RO13s) SPLIT13.(OWg, SW4-BDBL) SPLIT15.(EDI3, RejRO-EDI) SPLIT16.(OWj, OWk) SPLIT17.(GBrecycle, DISCHARGE) SPLIT18.(RO2reject2, RO2reject3) SPLIT19.(RO3reject2, RO3reject3) SPLIT20.(RO11s, RO1discharge) HPU1.(WHB-BD1,HPU1_loss) HPU2.(WHB-BD2,HPU2_loss) PSR1_SW.(SW2) PSR2_SW.(SW4) FIREWATER.(USERS, FW_LOST) POTABLE.(TKLE, TO_DEMIN) BOILER.(OW3B,BOILER_steam) CITYWATER.(CT1, CT2, CT3, SW1, SW3, CITY5, EDI-1) DEMIN_TANK.(BOILER1, DT1, DT2)

A.3 Material balance for treatment units

INLET_TREATMENT(U,S) unit.(input stream)	OUTLET_TREATMENT(U,S) unit.(output stream)
RO1.UF1permeate	RO1.(RO1permeate, RO1reject)
RO2.UF2permeate	RO2.(RO2permeate, RO2reject1)
RO3.UF3permeate	RO3.(RO3permeate, RO3reject1)
UF1.HTs1	UF1.(UF1permeate, UF1reject)
UF2.OS4	UF2.UF2permeate
UF3.(CFs)	UF3.UF3permeate
DEMIN_TANK.(DEM, MB-EDIs, EDI3)	DEMIN_TANK.(BOILER1, DT1, DT2)
IX.(CITY5)	IX.(OW3C, DEM)
MB-EDIu.(RO12s)	MB-EDIu.(MB-EDIs)
MT-CPI-A.(OWk)	MT-CPI-A.(CPI-A)
MT-CPI-B.(OWj)	MT-CPI-B.(CPI-B)
MT-CPI-C.(OSW1)	MT-CPI-C.(OSW3)
DAFu.(OSW3)	DAFu.(DAFs, OS3)
MMF.(OS3)	MMF.(OS4)
CFu.(S10-2, SFs)	CFu.(CFs)
RO-EDI.(EDI-1)	RO-EDI.(EDI-3, RejRO-EDI)
ETS.(GBrecycle, CPI-A, CPI-B, OSW5)	EQBu.(EQBs)
SFu.(CLAs, OSW4)	ETS.(CLAs)
GBu.(S10-1, RO3reject2)	SFu.(SFs)
OSW-SB.(USERS, OS7, OS13, OS8, OS5)	GBu.(GBs)
	OSW-SB.(OSW1)

OUTLET_TREATMENT_CLEAN(U,S)		OUTLET_TREATMENT_REJECT (U,S)
RO1.(RO1permeate) RO2.(RO2permeate) RO3.(RO3permeate) UF1.(UF1permeate, UF1reject) UF1.(UF1permeate, UF1reject, UF1bypass) UF2.UF2permeate UF3.UF3permeate DEMIN_TANK.(BOILER1, DT1, DT2) IX.(DEM, OW3C) MB-EDIu.(MB-EDIs)	UF1.(UF1reject) RO1.RO1reject RO2.RO2reject1 RO3.RO3reject1 RO3.(RO3reject2, RO3reject3) RO-EDI.(RejRO-EDI)	UF1.(UF1reject) RO1.RO1reject RO2.RO2reject1 RO3.RO3reject1 RO3.(RO3reject2, RO3reject3) RO-EDI.(RejRO-EDI)

B. NOTATIONS

Sets and Indices

S	set of material streams s
J	set of contaminants j
U	set of all units or tasks u
MX	set of convergent-flow-path units (mixers) mx
SP	set of divergent-flow-path units (splitters) sp
TU	set of treatment unit t
$\mathrm{MX}_{\mathrm{in}}$	set of inlet streams into mixer mx
$\mathrm{MX}_{\mathrm{out}}$	set of outlet streams from a mixer mx
$\mathrm{SP}_{\mathrm{in}}$	set of inlet streams into splitter sp
$\mathrm{SP}_{\mathrm{out}}$	set of outlet streams from a splitter sp
S_{hot}	set of hot streams that requires cooling
S_{cold}	set of cold streams that requires heating

Parameters/Constants

$R_{j,t}$	removal ratio of contaminant j in treatment unit t
F_i^{L}	lower bound on flowrate in stream i
F_i^{U}	upper bound on flowrate in stream i
$C_{j,i}^{\mathrm{L}}$	lower bound on contaminant concentration j in stream i
$C_{j,i}^{\mathrm{U}}$	upper bound on contaminant concentration j in stream i
$T_{u,s}^{\mathrm{in}}$	temperature of unit u from which a stream s is entering
$T_{u,s}^{\mathrm{out}}$	temperature of unit u from which a stream s is leaving

Continuous Decision Variables

F_i	flowrate of inlet stream s
F_k	flowrate of outlet stream s_1
$f_{j,s}$	flowrate of contaminant j in stream s
$C_{j,s}$	concentration of contaminant j in stream s

C. GANTT Chart

FYP I

No	Detail	Week													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of Project Topic	■	■												
2	Preliminary Research Work • Literature Review • Possible process routes		■	■	■	■	■	■	■						
3	Superstructure construction						■	■	■						
4	Model formulation						■	■	■	■	■	■	■		
5	Modeling in GAMS								■	■	■	■	■	■	
6	Interim Report Preparation													■	■

FYP II

No.	Detail/ Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Project Work Continue	■	■	■												
2	Submission of Progress Report 1				■											
3	Project Work Continue				■	■	■	■								
4	Submission of Progress Report 2								■							
5	Seminar (compulsory)									■	■	■				
5	Project work continue								■	■	■	■	■			
6	Poster Exhibition										■					
7	Submission of Dissertation													■		
	(Soft bound)															
8	Oral Presentation														■	
9	Submission of Project Dissertation															■
	(Hard bound)															■