Optimization of Water Network Retrofit Design for Petroleum Refineries with Water Reuse, Regeneration, and Recycle Strategies (W3R)

by

Foo Ngai Yoong

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

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Universiti Teknologi PETRONAS

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CERTIFICATION OF APPROVAL

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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.

FOO NGAI YOONG

ABSTRACT

Water is a key element in the operation of petroleum refineries. In the past, wastewater was typically piped to a centralized treatment plant and research efforts were focused mainly on improving treatment technologies. It was later recognized that distributed wastewater treatment networks in which wastewater streams are treated separately may be preferable to the centralized approach. Moreover, scarcities in freshwater supply and increasingly stringent rules on wastewater discharge have emerges as issues of major concerns to plant operators, along with an increased awareness in the need to support sustainable development initiatives and minimization of water footprint. In line with these development, there are increased interests to incorporate water reuse, regeneration (i.e, treatment), and recycle (W3R) approaches in the design of refinery water network systems, with the aim of minimizing freshwater consumption and wastewater generation. This work presents an optimization model to determine the optimal design of refinery water network systems. The integrated model explicitly considers the incorporation of water minimization strategies by first postulating a source–interceptor–sink superstructure that embeds many possible feasible flowsheet alternatives for the implementation of potential W3R approaches. Subsequently, a mixed-integer nonlinear programming (MINLP) model is formulated based on the superstructure to determine the optimal water network structure in terms of the continuous variables of total stream flowrates, contaminant concentrations and the 0–1 binary variables of stream interconnections in the piping network. The superstructure and the MINLP model explicitly handles the membrane-based interceptors (primarily ultrafiltration and reverse osmosis units) and the non-membrane-based interceptors, in which in the former, the feed, permeate, and reject streams are assumed as an individual process units. The objective of the model is to minimize the fixed capital costs of installing piping interconnections and the variable cost of operating all stream interconnections while reducing the pollutants level to within limits by environmental regulations under all the associated material balances of flows and concentrations. The proposed modeling approach is implemented on an industrially-significant numerical example using the GAMS/BARON global optimization platform to obtain a globally cost-optimal water network topology.

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NOMENCLATURE

Sets and Indices

I	set of sources i
J	set of sinks j
K	set of all types of interceptors k
K_G	set of general non-membrane-based interceptors k_G
K_P	set of permeate streams of membrane-based interceptors k_P
K_R	set of reject streams of membrane-based interceptors k_R
Q	set of contaminants q

Continuous variables on water flowrates for stream connections:

$F_a(i,j)$	stream connecting source i to sink j
$F_{b,G}(k_G,j)$	stream connecting general non-membrane-based interceptor k_G to sink j
$F_{b,P}(k_P,j)$	stream connecting permeate stream of membrane-based interceptor k_P to sink j
$F_{b,R}(k_R,j)$	stream connecting reject stream of membrane-based interceptor k_R to sink j
$F_{c,G}(k_G, k_G')$	stream connecting general non-membrane-based interceptor k_G to other interceptor k_G'
$F_{c,P}(k_P, k_P')$	stream connecting permeate stream of membrane-based interceptor k_P to other interceptor k_P'
$F_{c,R}(k_R, k_R')$	stream connecting reject stream of membrane-based interceptor k_R to other interceptor k_R'
$F_{cc,G}(k'_G,k_G)$	stream connecting other general non-membrane-based interceptor k'_G to interceptor k_G
$F_{cc,P}(k_P',k_P)$	stream connecting permeate stream of other membrane-based interceptor k_P' to interceptor k_P

$F_{cc,R}(k_R{'},k_R)$ stream connecting reject stream of other membrane-based interceptor k'_R to interceptor k_R

$F_d(i,k)$ stream connecting source i to interceptor k

Continuous variables on concentrations of contaminants for:

$C_{SO}(q,i)$ contaminant q in source i

$C_G(q,k_G)$ contaminant q in general non-membrane-based interceptor k_G

$C_P(q,k_P)$ contaminant q in permeate stream of membrane-based interceptor k_P

$C_R(q,k_R)$ contaminant q in reject stream of membrane-based interceptor k_R

Binary variables on existence of stream piping connections:

$y_a(i,j)$ stream connecting source i to sink j

$y_{b,G}(k_G,j)$ stream connecting general non-membrane-based interceptor k_G to sink j

$y_{b,P}(k_P,j)$ stream connecting permeate stream of membrane-based interceptor k_P to sink j

$y_{b,R}(k_R,j)$ stream connecting reject stream of membrane-based interceptor k_R to sink j

$y_{c,G}(k_G, k_G{'})$ stream connecting general non-membrane-based interceptor k_G to other interceptor $k_G{'}$

$y_{c,P}(k_P, k_P{'})$ stream connecting permeate stream of membrane-based interceptor k_P to other interceptor $k_P{'}$

$y_{c,R}(k_R, k_R{'})$ stream connecting reject stream of membrane-based interceptor k_R to other interceptor $k_R{'}$

$y_{cc,G}(k'_G,k_G)$ stream connecting other general non-membrane-based interceptor k'_G to interceptor k_G

$y_{cc,P}(k_P{'},k_P)$ stream connecting permeate stream of other membrane-based interceptor $k_P{'}$ to interceptor k_P

$y_{cc,R}(k_R{'},k_R)$ stream connecting reject stream of other membrane-based interceptor k'_R to interceptor k_R

$y_d(i,k)$ stream connecting source i to interceptor k

Parameters

RR(q,k) removal ratio of contaminant q in interceptors k

α liquid recovery factor

$C_{\max}(q,j)$ maximum concentration of contaminant q at inlet to sink j

Parameters on operating cost of stream connections:

$c_a(i,j)$ operating cost of stream connecting source i to sink j

$c_{b,\mathrm{G}}(k_\mathrm{G},j)$ operating cost of stream connecting general non-membrane-based interceptor k_G to sink j

$c_{b,\mathrm{P}}(k_\mathrm{P},j)$ operating cost of stream connecting permeate stream of membrane-based interceptor k_P to sink j

$c_{b,\mathrm{R}}(k_\mathrm{R},j)$ operating cost of stream connecting reject stream of membrane-based interceptor k_R to sink j

$c_{c,\mathrm{G}}(k_\mathrm{G}, k_\mathrm{G}')$ operating cost of stream connecting general non-membrane-based interceptor k_G to other interceptor k'_G

$c_{c,\mathrm{P}}(k_\mathrm{P}, k_\mathrm{P}')$ operating cost of stream connecting permeate stream of membrane-based interceptor k_P to other interceptor k_P'

$c_{c,\mathrm{R}}(k_\mathrm{R}, k_\mathrm{R}')$ operating cost of stream connecting reject stream of membrane-based interceptor k_R to other interceptor k_R'

$c_{cc,\mathrm{G}}(k'_\mathrm{G},k_\mathrm{G})$ operating cost of stream connecting other general non-membrane-based interceptor k'_G to interceptor k_G

$c_{cc,\mathrm{P}}(k_\mathrm{P}',k_\mathrm{P})$ operating cost of stream connecting permeate stream of other membrane-based interceptor k_P' to interceptor k_P

$c_{cc,\mathrm{R}}(k_\mathrm{R}',k_\mathrm{R})$ operating cost of stream connecting reject stream of other membrane-based interceptor k'_R to interceptor k_R

$c_d(i, k)$ operating cost of stream connecting source i to interceptor k

Parameters on capital cost of stream piping connections:

$c_{ay}(i,j)$	capital cost of stream connecting source i to sink j
$c_{by,\mathrm{G}}(k_{\mathrm{G}},j)$	capital cost of stream connecting general non-membrane-based interceptor k_{G} to sink j
$c_{by,\mathrm{P}}(k_{\mathrm{P}},j)$	capital cost of stream connecting permeate stream of membrane-based interceptor k_{P} to sink j
$c_{by,\mathrm{R}}(k_{\mathrm{R}},j)$	capital cost of stream connecting reject stream of membrane-based interceptor k_{R} to sink j
$c_{cy,\mathrm{G}}(k_{\mathrm{G}}, k'_{\mathrm{G}})$	capital cost of stream connecting general non-membrane-based interceptor k_{G} to other interceptor k'_{G}
$c_{cy,\mathrm{P}}(k_{\mathrm{P}}, k'_{\mathrm{P}})$	capital cost of stream connecting permeate stream of membrane-based interceptor k_{P} to other interceptor k_{P}'
$c_{cy,\mathrm{R}}(k_{\mathrm{R}}, k'_{\mathrm{R}})$	capital cost of stream connecting reject stream of membrane-based interceptor k_{R} to other interceptor k_{R}'
$c_{ccy,\mathrm{G}}(k'_{\mathrm{G}},k_{\mathrm{G}})$	capital cost of stream connecting other general non-membrane-based interceptor k'_{G} to interceptor k_{G}
$c_{ccy,\mathrm{P}}(k'_{\mathrm{P}}, k_{\mathrm{P}})$	capital cost of stream connecting permeate stream of other membrane-based interceptor k_{P}' to interceptor k_{P}
$c_{ccy,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}})$	capital cost of stream connecting reject stream of other membrane-based interceptor k'_{R} to interceptor k_{R}
$c_{dy}(i, k)$	capital cost of stream connecting source i to interceptor k

Upper bounds on continuous variables on water flowrates for stream connections:

$F_a^{\mathrm{U}}(i,j)$	stream connecting source i to sink j
$F_{b,\mathrm{G}}^{\mathrm{U}}(k_{\mathrm{G}},j)$	stream connecting general non-membrane-based interceptor k_{G} to sink j
$F_{b,\mathrm{P}}^{\mathrm{U}}(k_{\mathrm{P}},j)$	stream connecting permeate stream of membrane-based interceptor k_{P} to sink j
$F_{b,\mathrm{R}}^{\mathrm{U}}(k_{\mathrm{R}},j)$	stream connecting reject stream of membrane-based interceptor k_{R} to

sink j

$F_{c,\mathrm{G}}^{\mathrm{U}}(k_{\mathrm{G}},k_{\mathrm{G}}')$ stream connecting general non-membrane-based interceptor k_{G} to other interceptor k_{G}'

$F_{c,\mathrm{P}}^{\mathrm{U}}(k_{\mathrm{p}},k_{\mathrm{p}}')$ stream connecting permeate stream of membrane-based interceptor k_{P} to other interceptor k_{P}'

$F_{c,\mathrm{R}}^{\mathrm{U}}(k_{\mathrm{R}},k_{\mathrm{R}}')$ stream connecting reject stream of membrane-based interceptor k_{R} to other interceptor k_{R}'

$F_{cc,\mathrm{G}}^{\mathrm{U}}(k_{\mathrm{G}}',k_{\mathrm{G}})$ stream connecting other general non-membrane-based interceptor k'_{G} to interceptor k_{G}

$F_{cc,\mathrm{P}}^{\mathrm{U}}(k_{\mathrm{p}}',k_{\mathrm{p}})$ stream connecting permeate stream of other membrane-based interceptor k_{P}' to interceptor k_{P}

$F_{cc,\mathrm{R}}^{\mathrm{U}}(k_{\mathrm{R}}',k_{\mathrm{R}})$ stream connecting reject stream of other membrane-based interceptor k'_{R} to interceptor k_{R}

$F_{d}^{\mathrm{U}}(i,k)$ stream connecting source i to interceptor k

Lower bounds on continuous variables on water flowrates for stream connections:

$F_{a}^{\mathrm{L}}(i,j)$ stream connecting source i to sink j

$F_{b,\mathrm{G}}^{\mathrm{L}}(k_{\mathrm{G}},j)$ stream connecting general non-membrane-based interceptor k_{G} to sink j

$F_{b,\mathrm{P}}^{\mathrm{L}}(k_{\mathrm{P}},j)$ stream connecting permeate stream of membrane-based interceptor k_{P} to sink j

$F_{b,\mathrm{R}}^{\mathrm{L}}(k_{\mathrm{R}},j)$ stream connecting reject stream of membrane-based interceptor k_{R} to sink j

$F_{c,\mathrm{G}}^{\mathrm{L}}(k_{\mathrm{G}},k_{\mathrm{G}}')$ stream connecting general non-membrane-based interceptor k_{G} to other interceptor k_{G}'

$F_{c,\mathrm{P}}^{\mathrm{L}}(k_{\mathrm{p}},k_{\mathrm{p}}')$ stream connecting permeate stream of membrane-based interceptor k_{P} to other interceptor k_{P}'

$F_{c,\mathrm{R}}^{\mathrm{L}}(k_{\mathrm{R}},k_{\mathrm{R}}')$ stream connecting reject stream of membrane-based interceptor k_{R} to other interceptor k_{R}'

$F^{\mathrm{L}}_{cc,\mathrm{G}}(k_{\mathrm{G}}',k_{\mathrm{G}})$ stream connecting other general non-membrane-based interceptor k'_{G} to interceptor k_{G}

$F^{\mathrm{L}}_{cc,\mathrm{P}}(k_{\mathrm{p}}',k_{\mathrm{p}})$ stream connecting permeate stream of other membrane-based interceptor k_{P}' to interceptor k_{P}

$F^{\mathrm{L}}_{cc,\mathrm{R}}(k_{\mathrm{R}}',k_{\mathrm{R}})$ stream connecting reject stream of other membrane-based interceptor k'_{R} to interceptor k_{R}

$F^{\mathrm{L}}_{d}(i,k)$ stream connecting source i to interceptor k

CHAPTER 1
INTRODUCTION

1.1 Background

As the world moves towards sustainable progress, a new and improved water network design to optimize the usage of water is critical. In facing the current challenges with water utilization, this consultancy work is carried out to study possible retrofit alternatives for the refinery water network systems through water minimization approaches and strategies that consist of water reuse, regeneration, and recycle initiative subsequently referred to as W3R in the rest of the report. A high level conceptual study is required to identify the feasibility of the W3R options with the quantitative analysis mathematical modeling enables a quantitative analysis on the feasibility of the W3R options to be carried out. The modeling tool GAMS is software which is the computation engine is running in the background to generate the optimal solution. It is user-friendly software and allows the user to focus on the model formulation.

In this paper, the minimization of water consumption that incorporates all feasible design alternatives for water treatment, reuse, recycle and regeneration is represented in a graphical targeting approach and then followed by a mathematical programming framework formulated as a mixed-integer nonlinear programming (MINLP) and require to solve this mathematical optimization model using GAMS modeling software.

A local Malaysian refinery is interest in the minimization of fresh water consumption resulted from the high demand of water consumption needs. Thus, in facing the current challenges with water utilization, this consultancy work is carried out to study possible retrofit alternatives for the water network systems of the petroleum refinery plant through water minimization approaches and strategies that consist of water reuse, regeneration, and recycle initiatives, subsequently referred to as W3R in the rest of the report.

1.2 Problem Statement

The problem addressed in this work can be stated as follows. Given a set of water supply streams – outlet of process units and a supply source of freshwater (sources), a set of water treatment units (interceptors), and a set of water using units (sinks) to satisfy demand in water using processes, determine the optimal flowrates and contaminant concentrations of streams for all potential alternatives with reuse, regeneration, and recycle (W3R), and the stream piping interconnections with the aim of minimizing the total operating cost and capital cost processed by all units. Thus, a high-level conceptual study is required to identify and assess the feasibility of the W3R options. In this regard, mathematical modeling enables a quantitative analysis on the feasibility of the W3R options to be carried out.

1.3 Model Assumptions

The proposed model is based on the following assumptions: the number of water sources is fixed, the number of sinks and interceptors is fixed, the flowrates of sources are fixed, the flowrates through the sinks are fixed, removal ratios for each interceptor unit are independent of the inlet concentration to the particular unit and the interceptor are treated simply with fixed recoveries. We also considered single contaminant which is oil and grease (O&G) exist in the water network. Besides that, 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 slow and is therefore negligible (that is, the contaminants are at the concentration level of parts per million). 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. Heat integration is not allowed and hence the network operation is assumed under isothermal condition and isobaric condition.

1.4 Research Objective

In this paper, the objective is to find the optimal water network configuration with structural representation of the solution alternatives presented in superstructure of source–interceptor–sink framework. This superstructure consists of a prespecified number of modules that are interconnected in all possible ways in order to account for all potential design configurations. The selection of the optimal design from this superstructure is formulated as a mixed-integer nonlinear programming (MINLP) that require solving this nonlinear mathematical optimization model using GAMS modeling language platform. The MINLP model determines the decision variables of water flowrates and contaminant concentrations with the objective of minimizing freshwater import for consumption and wastewater generation through the incorporation of W3R alternatives options. The contaminant concentrations must within the permissible limits of operations and regulatory discharge requirements.

1.5 Basic Conceptual of Models

The mathematical model of integrated process water network consists of mass balance equations for water and contaminants for every unit in the network. The model is formulated as a nonconvex mixed-integer nonlinear programming (MINLP) for the case when 0–1 variables are included to the model of the cost of piping and selection of interceptors. The nonlinearities in the models appear in the mass balance equations in the form of bilinear terms (concentration times flowrate). The nonlinearities appear in the objective function as concave term of the cost functions. Hence, the water network models are nonconvex and lead to difficulties in obtaining the global optimal solution.

CHAPTER 2
LITERATURE REVIEW AND THEORY

2.1 Water Network Systems

Traditionally, freshwater 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, freshwater 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 wastewater generation (Smith, 2005).

2.2 Techniques for Freshwater and Wastewater Minimization through Reuse, Regeneration, and Recycle

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 freshwater is 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 1 shows the implementation of water reuse in a simple water network.

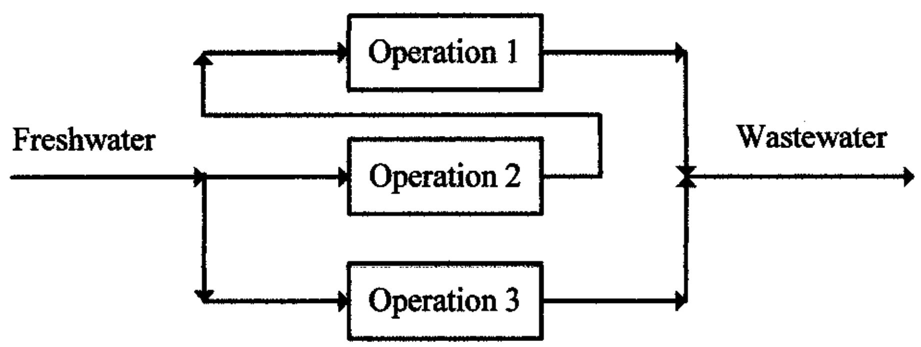

Figure 1: Water reuse scheme

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 2.

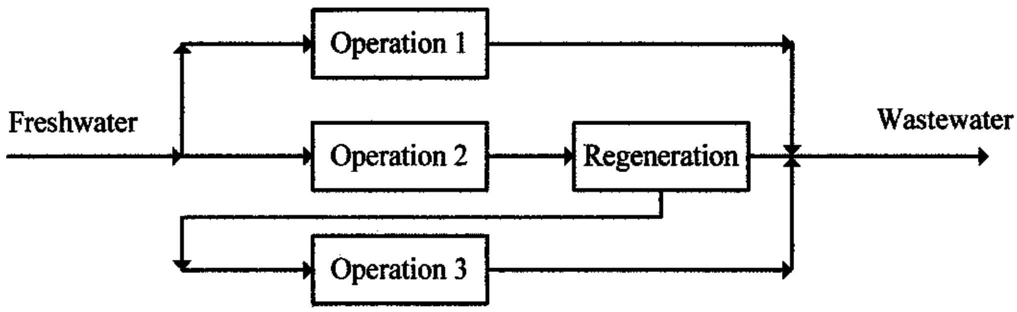

Figure 2: Water regeneration reuse scheme

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 3. 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).

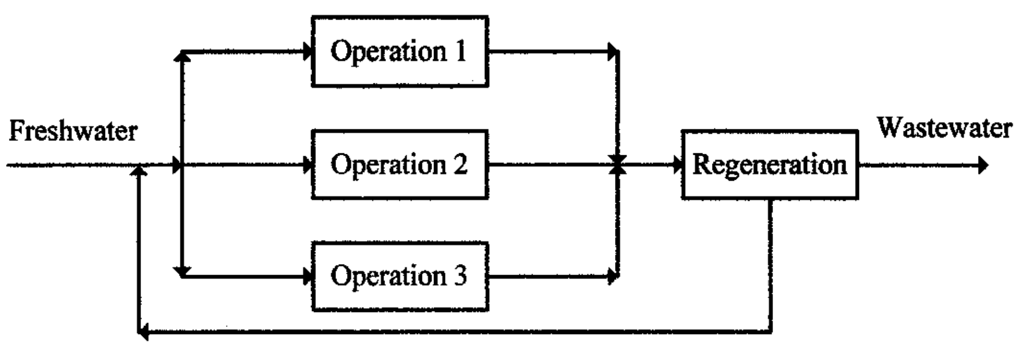

Figure 3: Water regeneration and recycle scheme

In water network optimization, regeneration reuse and regeneration recycle 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, while 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 regeneration reuse. However problems can be encountered in the regeneration recycling, recycling allowed the build up of undesired contaminants in the recycle, such as microorganisms 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 Literature Review on Past Work in Water Network Systems Design and Retrofit Design

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).

Frederico B. Gabriel and El-Halwagi (2005) present a structural representation of the solution alternatives for material reuse and recycle using a source-interceptor-sink framework. Then, an applicable mathematical formulation is developed. The authors invoke a number of simplifying assumptions to facilitate reformulation of the problem into a linear program.

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.

Before the 1980s, wastewater was typically piped to a centralized treatment plant and research efforts were focused mainly on improving treatment technologies. It was later recognized that distributed wastewater treatment networks in which wastewater streams are treated separately may be preferable to the centralized approach. It is because technologies well suited to decontaminate specific streams and it can be used to process of require smaller volumes of water. The authors proposed an algorithm to find global solution using the principles of the reformulation-linearization technique (RLT) and applied to the class of generalized pooling problems (Clifford & Christodoulos, 2005).

Raymond R. Tan, Denny K.S. Ng, Dominic C.Y. Foo and Kathleen (2009) present a novel superstructure-based optimization model of single-contaminant for industrial water networks with partitioning regenerators. A membrane separation-based regenerator (e.g ultrafiltration, reverse osmosis) function by splitting a contaminated water stream into a regenerated lean stream and a low quality reject stream. The optimization model presented in this work is integrates a single, centralized partitioning regenerator with a source-sink superstructure under assumption of fixed flowrate type processes are within the plant. The global optimal solutions can be found using commercial software. Note that there is design flexibility for both the lean and reject streams to be as inlet of the regenerator to be reuse/recycle within the plant.

A convex hull discretization approach to the global optimization of pooling problems proposed by Viet Pham, Carl Laird and El-Halwagi, 2009 is to ensure the global optimal solution of bilinear optimization problem. Because of the presence of bilinear terms, the traditional formulation is nonconvex. There is a need to develop computationally efficient and easy-to-implement global-optimization techniques. In this paper, a new approach is proposed based on three concepts: linearization by discretizing nonlinear variables, preprocessing using implicit enumeration of the discretization to form a convex-hull which limits the size of the search space, and application of integer cuts to ensure compatibility between the original problem and the discretized formulation.

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.

CHAPTER 3

METHODOLOGY / PROJECT WORK

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 4 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.

The general mathematical programming approach proposed by Grossman and Floudas can be modified to use in the water network design for petroleum refinery plant. The methodology is represented in Figure 4 as below:

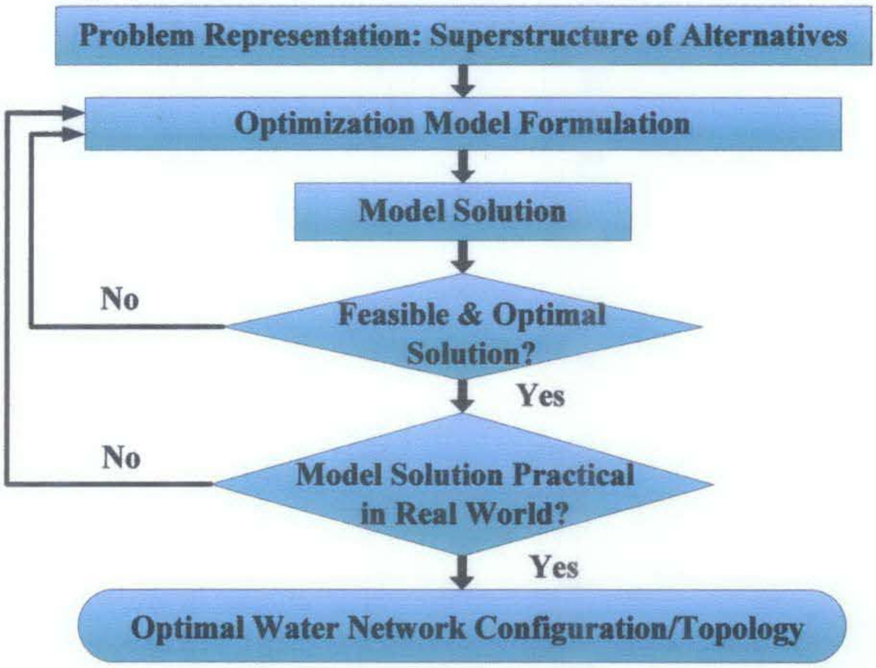

Figure 4: Major steps in the mathematical programming approach to process synthesis and design problems

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. 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. The procedures for the retrofit design of the optimal refinery water network structure (or configuration or topology) comprises the following main steps are shown as below:

1. Data collection of flowrate and concentration from refinery plant.
2. Data reconciliation on the balances.
3. A superstructure of source-interceptor-sink model (as in Figure 5) includes all possible and feasible flowsheets showing the interconnections of the process units and material streams.

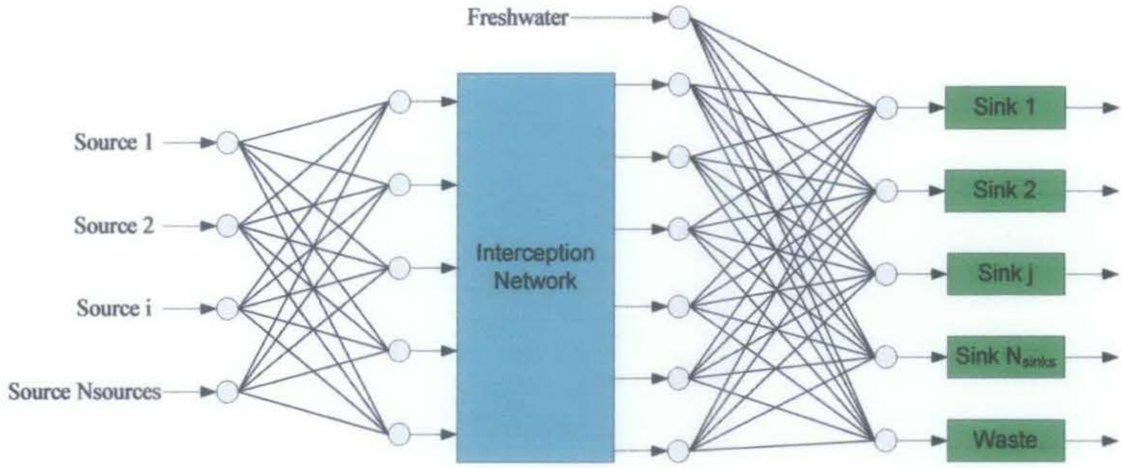

Figure 5: Simplified superstructure representation of the refinery water network system (Frederico B. Gabriel and Mahmoud M. El-Halwagi, 2005).

4. The overall superstructure is formulated as a mixed-integer nonlinear programming (MINLP) optimization model with its objective functions and material balances applied to each alternative retrofit structure as its constraints.
5. General solution strategy is to be determined for the optimization problem using GAMS modeling. The solution to the MINLP problem 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.
6. It will be evaluated and compared to the current practice to check for the feasibility of the solution.

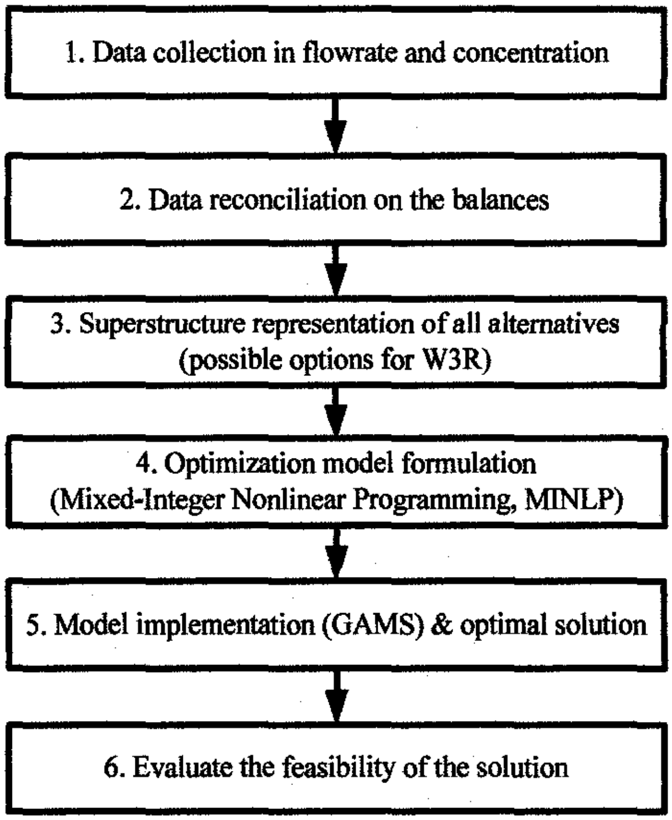

Figure 6: Procedure in the mathematical programming approach for the retrofit of refinery water network systems.

3.2 GAMS Modeling Platform

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 complementarily 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 4

OPTIMIZATION MODEL FORMULATION

4.1 Superstructure Representation of Alternatives for Petroleum Refinery Water Network Systems

In order to minimize the overall water consumption of petroleum refinery plant, a superstructure representation that accounts for all alternatives configurations has drawn. The superstructure representation encompasses the current existing water network systems as well as all the potential feasible alternatives. Generally refinery water network systems consist of process units which are known as water-using units and treatment units. For the superstructure of source–interceptor–sink mapping, the sources of water streams are denoted as source nodes i. The treatment units are denoted as interceptor (or regenerator) k. The final destinations of water, which are the water using units, are denoted as sink nodes j.

In this work, the wastewater streams are treated separately. Distributed wastewater treatment network is preferable to the centralized approach because this technology well suited to decontaminate specific streams and it can be used to process of require smaller volumes of water. There are two types of interceptor which are general non-membrane based interceptor and membrane based interceptor. For the membrane based interceptor, we have permeate and reject stream as the outlet.

A contribution of this work is to develop a general superstructure and the corresponding MINLP model formulation that explicitly handles the modeling of the mass balances for the membrane-based interceptors, primarily the treatment technologies of ultrafiltration and reverse osmosis, and the non-membrane-based interceptors. For the former, the permeate and reject streams of a membrane-based interceptor are assumed as imaginary individual interceptors.

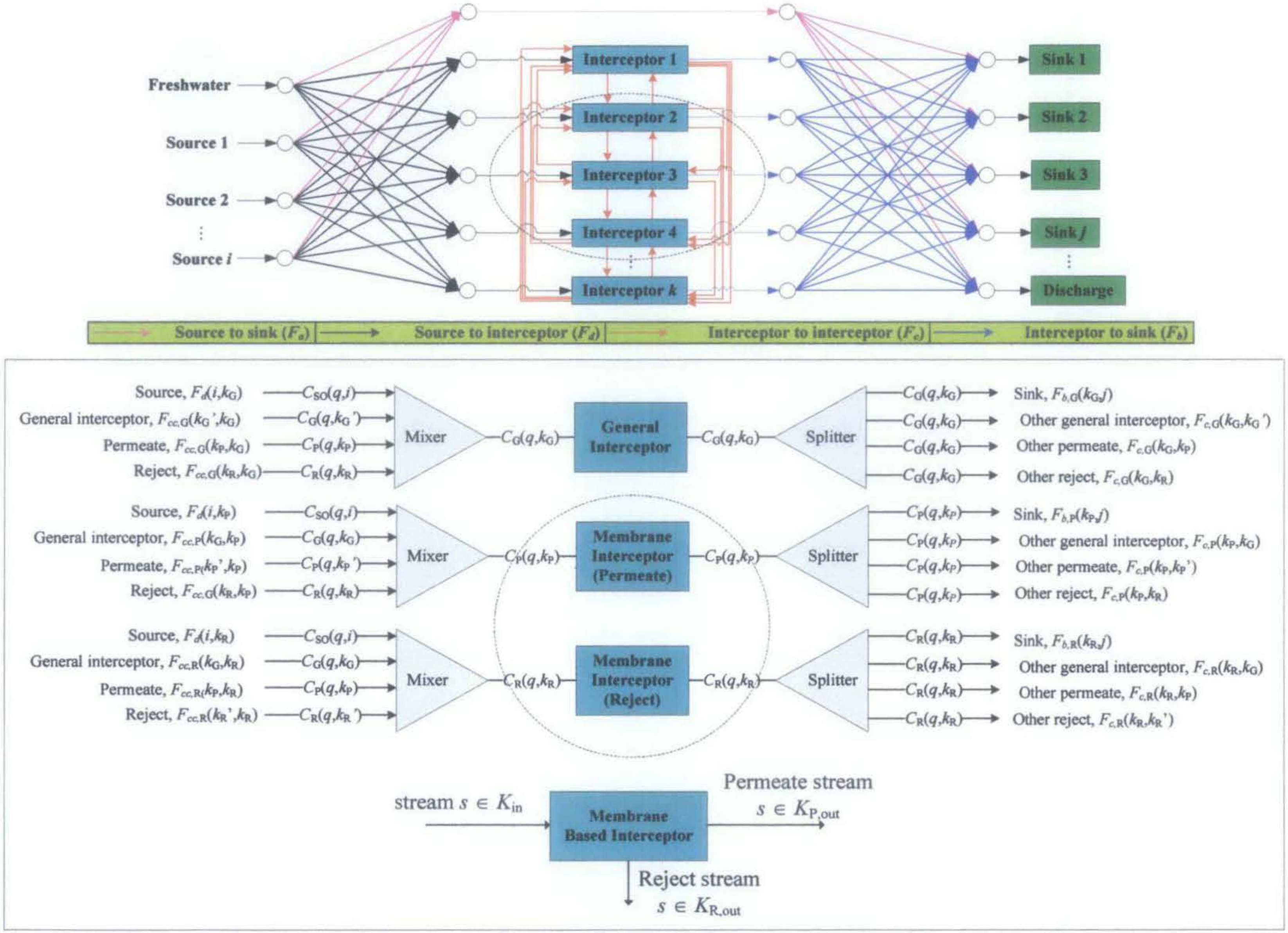

Figure 7: Superstructure representation of alternatives for a refinery water network structure

4.2 Optimization Model Formulation

Based on Mathematical Formulation proposed by Meyer and Floudas (2006), constraints are the limitation of the process. Constraints can be in term of equality, inequality, linear, or non-linear. The constraints in the research project include non-linear material balances with bilinear term and process specification and treatment unit specification. For this research project, the programming problem involved is mixed integer non-linear programming problem (MINLP). There are 4 types of constraints proposed by Meyer and Floudas, which are:

1. Material balances:
   a) Water flow balances around source
   b) Contaminant flow balances around source
   c) Water flow balances around treatment unit (interceptor)
      i general non-membrane based interceptor
      ii permeate and reject stream of membrane based interceptor
   d) Contaminant flow balances around treatment units (interceptor)
      i general non-membrane based interceptor
      ii permeate and reject stream of membrane based interceptor
   e) Water flow balances around sink
   f) Contaminant flow balances around sink
2. Variables' bounds
3. Integrating constraints
4. Big–*M* logical constraints

The mathematical formulations of minimizing the overall operating cost and capital cost for sources, interceptors and sinks are shown as below:

4.3 Material Balances for Sources

In many processes there is loss of water that cannot be reused in a water operation. This unit represent water sink. Cooling towers are typical process units where water is lost by evaporation. For the material balances for a source, it consists of a set of streams from sources equal to a set of streams directed from sources to interceptors and a set of streams directed from sources to sinks. The water flow balances and the concentration balances for source node is given by **(1)**. The concentration balance for a source is not needed because it is the same as the water flow balance.

4.3.1 Water flow balances for a source node

$$F(i) = \sum_{k \in K} F_d(i,k) + \sum_{j \in J} F_a(i,j) \qquad \forall i \in I \tag{1}$$

4.4 Material Balances for Interceptor

As highlighted, we formulate a model on the material balances for the interceptor that explicitly treats a membrane-based interceptor separately from a general non-membrane-based interceptor. A general non- membrane-based interceptor is modeled to have a single outlet stream that is possibly splitted to each sink, whereas the permeate and reject streams of a membrane-based interceptor are assumed as imaginary individual interceptors modeled with their own unique flow balances and concentration balances, as developed in the following.

4.4.1 Water flow balances for general non-membrane based interceptor

The flow balance for a general non-membrane based interceptor equates the flow from all the mixed streams entering the mixer at the inlet of the interceptor to all the stream splits from the splitter at the outlet (or exit) of the interceptor:

$$\sum_{i \in I} F_d(i,k_G) + \sum_{\substack{k'_G \in K_G \\ k'_G \neq k_G}} F_{cc,G}(k'_G,k_G) + \sum_{k_P \in K_P} F_{cc,G}(k_P,k_G) + \sum_{k_R \in K_R} F_{cc,G}(k_R,k_G)$$

$$= \sum_{j \in J} F_{b,G}(k_G,j) + \sum_{\substack{k'_G \in K_G \\ k'_G \neq k_G}} F_{c,G}(k_G,k'_G) + \sum_{k_P \in K_P} F_{c,G}(k_G,k_P) + \sum_{k_R \in K_R} F_{c,G}(k_G,k_R)$$

$$\forall k_G \in K_G$$

(2)

It is noteworthy that for the directed flowrate term of $F_{c,G}$ (and the corresponding directed reverse flow of $F_{cc,G}$) from a general interceptor to another general interceptor (for instance, the flow from a mud trap corrugated plate interceptor to a dissolved flotation unit), we have been careful not to account for the flowrate between two units that are actually representing the same unit.

4.4.2 Contaminant concentration balances for general non-membrane based interceptor

$$\left(1-\mathrm{RR}(q,k_G)\right)\left(\begin{array}{l}\sum_{i \in I} F_d(i,k_G)\cdot C_{SO}(q,i) + \sum_{\substack{k'_G \in K_G \\ k'_G \neq k_G}} F_{cc,G}(k'_G,k_G)\cdot C_G(q,k'_G) \\ + \sum_{k_P \in K_P} F_{cc,G}(k_P,k_G)\cdot C_P(q,k_P) + \sum_{k_R \in K_R} F_{cc,G}(k_R,k_G)\cdot C_R(q,k_R)\end{array}\right)$$

$$= \left(C_G(q,k_G)\right)\left(\begin{array}{l}\sum_{j \in J} F_{b,G}(k_G,j) + \sum_{\substack{k'_G \in K_G \\ k'_G \neq k_G}} F_{c,G}(k_G,k'_G) \\ + \sum_{k_P \in K_P} F_{c,G}(k_G,k_P) + \sum_{k_R \in K_R} F_{c,G}(k_G,k_R)\end{array}\right) \quad \forall k_G \in K_G, \forall q \in Q$$

(3)

4.4.3 Water flow balances for permeate stream of membrane based interceptor

$$\sum_{i\in I} F_d(i,k_\mathrm{P}) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} F_{cc,\mathrm{P}}(k_\mathrm{G},k_\mathrm{P}) + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} F_{cc,\mathrm{P}}(k'_\mathrm{P},k_\mathrm{P}) + \sum_{k_\mathrm{R}\neq k_\mathrm{P}} F_{cc,\mathrm{P}}(k_\mathrm{R},k_\mathrm{P})$$
$$= \sum_{j\in J} F_{b,\mathrm{P}}(k_\mathrm{P},j) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{G}) + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} F_{c,\mathrm{P}}(k_\mathrm{P},k'_\mathrm{P}) + \sum_{\substack{k_\mathrm{R}\in K_\mathrm{R}\\ k_\mathrm{R}\neq k_\mathrm{P}}} F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{R})$$
$$\forall k_\mathrm{P}\in K_\mathrm{P}$$

(4)

Similar to the water flow balance in **(2)**, we have been careful not to account for the directed flow from one permeate unit to another permeate unit that are actually representing the same permeate stream.

4.4.4 Contaminant concentration balances for permeate stream of membrane-based interceptor

$$\left(1-\mathrm{RR}(q,k_\mathrm{G})\right)\left(\begin{array}{l}\sum_{i\in I} F_d(i,k_\mathrm{P})\cdot C_\mathrm{SO}(q,i) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} F_{cc,\mathrm{P}}(k_\mathrm{G},k_\mathrm{P})\cdot C_\mathrm{G}(q,k_\mathrm{G})\\ + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} F_{cc,\mathrm{P}}(k'_\mathrm{P},k_\mathrm{P})\cdot C_\mathrm{P}(q,k'_\mathrm{P}) + \sum_{k_\mathrm{R}\neq k_\mathrm{P}} F_{cc,\mathrm{P}}(k_\mathrm{R},k_\mathrm{P})\cdot C_\mathrm{R}(q,k_\mathrm{R})\end{array}\right)$$
$$= C_\mathrm{P}(q,k_\mathrm{P})\left(\begin{array}{l}\sum_{j\in J} F_{b,\mathrm{P}}(k_\mathrm{P},j) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{G})\\ + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} F_{c,\mathrm{P}}(k_\mathrm{P},k'_\mathrm{P}) + \sum_{\substack{k_\mathrm{R}\in K_\mathrm{R}\\ k_\mathrm{R}\neq k_\mathrm{P}}} F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{R})\end{array}\right)$$
$$\forall k_\mathrm{P}\in K_\mathrm{P}, \forall q\in Q$$

(5)

4.4.5 Split ratio on flow based on liquid phase recovery for permeate stream of membrane-based interceptor

$$\alpha\left(\begin{array}{l}\sum_{i\in I} F_d(i,k_{\mathrm{P}}) + \sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{cc,\mathrm{P}}(k_{\mathrm{G}},k_{\mathrm{P}}) + \sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{P}}}} F_{cc,\mathrm{P}}(k'_{\mathrm{P}},k_{\mathrm{P}}) + \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{P}}}} F_{cc,\mathrm{P}}(k'_{\mathrm{R}},k_{\mathrm{P}})\\ +\sum_{i\in I} F_d(i,k_{\mathrm{R}}) + \sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{cc,\mathrm{R}}(k_{\mathrm{G}},k_{\mathrm{R}}) + \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}}) + \sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k'_{\mathrm{P}},k_{\mathrm{R}})\end{array}\right)$$

$$= \sum_{j\in J} F_{b,\mathrm{P}}(k_{\mathrm{P}},j) + \sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{c,\mathrm{P}}(k_{\mathrm{P}},k_{\mathrm{G}}) + \sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{P}}}} F_{c,\mathrm{P}}(k_{\mathrm{P}},k'_{\mathrm{P}}) + \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{P}}}} F_{c,\mathrm{P}}(k_{\mathrm{P}},k'_{\mathrm{R}})$$

$$\forall (k_{\mathrm{P}},k_{\mathrm{R}})\in K_{\mathrm{P}},K_{\mathrm{R}} \tag{6}$$

4.4.6 Water flow balances for reject stream of membrane based interceptor

$$\sum_{i\in I} F_d(i,k_{\mathrm{R}}) + \sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{cc,\mathrm{R}}(k_{\mathrm{G}},k_{\mathrm{R}}) + \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}}) + \sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k_{\mathrm{P}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k_{\mathrm{P}},k_{\mathrm{R}})$$

$$= \sum_{j\in J} F_{b,\mathrm{R}}(k_{\mathrm{R}},j) + \sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{G}}) + \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k'_{\mathrm{R}}) + \sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{R}}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k'_{\mathrm{P}})$$

$$\forall k_{\mathrm{R}}\in K_{\mathrm{R}} \tag{7}$$

Again, here we have been careful not to account for the directed flow from one reject unit to another reject unit that are actually representing the same reject stream.

4.4.7 Contaminant concentration balances for reject stream of membrane-based interceptor

$$\mathrm{RR}(q,k_{\mathrm{R}})\left(\begin{array}{l}\sum_{i\in I} F_d(i,k_{\mathrm{R}})\cdot C_{\mathrm{SO}}(q,i)+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{cc,\mathrm{R}}(k_{\mathrm{G}},k_{\mathrm{R}})\cdot C_{\mathrm{G}}(q,k_{\mathrm{G}})+\\ \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}})\cdot C_{\mathrm{R}}(q,k'_{\mathrm{R}})+\sum_{\substack{k_{\mathrm{P}}\in K_{\mathrm{P}}\\ k_{\mathrm{P}}\neq k_{\mathrm{R}}}} F_{cc,\mathrm{R}}(k_{\mathrm{P}},k_{\mathrm{R}})\cdot C_{\mathrm{P}}(q,k_{\mathrm{P}})\end{array}\right)$$

$$=\left(C_{\mathrm{R}}(q,k_{\mathrm{R}})\right)\left(\begin{array}{l}\sum_{j\in J} F_{b,\mathrm{R}}(k_{\mathrm{R}},j)+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{G}})+\\ \sum_{\substack{k'_{\mathrm{R}}\in K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k'_{\mathrm{R}})+\sum_{\substack{k_{\mathrm{P}}\in K_{\mathrm{P}}\\ k_{\mathrm{P}}\neq k_{\mathrm{R}}}} F_{c,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{P}})\end{array}\right)\quad \forall k_{\mathrm{R}}\in K_{\mathrm{R}},\forall q\in Q$$

(8)

The contaminant concentration balances can be determined under the condition of fixed removal ratio, RR. The parameter RR denoted the fraction of contaminant entering the reject stream of interceptor and the fraction of (1–RR) for the permeate stream of interceptor according to Foo (2009). Fixed removal ratio, $R_{j,t}$ represent the amount of contaminants being removed by the treatment unit. As a result, the term $(1–R_{j,t})$ is the amount of contaminants left after treatment. The value of $R_{j,t}$ is always between 0 and 1. From the equation above, it shows that the level of contaminant is less (has decreased) after the treatment unit. The value of contaminant of the outlet stream of treatment unit is always lesser than the inlet stream of treatment unit. The assumption for this constraint is that the removal ratio, $R_{j,t}$ is assumed to be constant, independent of the level of contaminant in the inlet flow.

The parameter α denotes as liquid recovery factor (a fixed fraction) of the interceptor inlet flow rate that exits in permeate stream, which yields the water balances across the interceptor. The equation further implies that the fraction (1–α) of the inlet water is discharged as the interceptor reject stream.

On the other hand, the water balance can be determined under conditions of fixed removal ratio, RR. The parameter RR is denoted as a fraction of the solute entering the interceptor that exits in reject stream. Note that $1-\mathrm{RR}<\alpha$ since the interceptor achieves purification by partitioning the solvent (water) and contaminant (oil and grease) differently between two streams.

4.4.8 Split ratio on flow based on liquid phase recovery for reject stream of membrane based interceptor

$$(1-\alpha)\left(\begin{array}{l}\sum_{i\in I} F_d(i,k_R)+\sum_{k_G\in K_G} F_{cc,R}(k_G,k_R)+\sum_{\substack{k'_R\in K_R\\ k'_R\neq k_R}} F_{cc,R}(k'_R,k_R)+\sum_{\substack{k'_P\in K_P\\ k_P\neq k_R}} F_{cc,R}(k_P,k_R)+\\ \sum_{i\in I} F_d(i,k_P)+\sum_{k_G\in K_G} F_{cc,P}(k_G,k_P)+\sum_{\substack{k'_P\in K_P\\ k'_P\neq k_P}} F_{cc,P}(k'_P,k_P)+\sum_{\substack{k'_R\in K_R\\ k'_R\neq k_P}} F_{cc,P}(k'_R,k_P)\end{array}\right)$$
$$=\sum_{j\in J} F_{b,R}(k_R,j)+\sum_{k_G\in K_G} F_{c,R}(k_R,k_G)+\sum_{\substack{k'_R\in K_R\\ k'_R\neq k_R}} F_{c,R}(k_R,k'_R)+\sum_{\substack{k'_P\in K_P\\ k'_P\neq k_R}} F_{c,R}(k_R,k'_P)$$
$$\forall k_R\in K_R$$

(9)

4.5 Material Balances for Sink

4.5.1 Water flow balances for sink

$$F_2(j)=\sum_{i\in I} F_a(i,j)+\sum_{k_G\in K_G} F_{b,G}(k_G,j)+\sum_{k_P\in K_P} F_{b,P}(k_P,j)+\sum_{k_R\in K_R} F_{b,R}(k_R,j)\qquad \forall j\in J$$

(10)

Flow balance for a sink is needed because total flowrate into a sink is fixed (but the individual flowrates of streams going into a sink is not fixed, e.g., with more reuse into a sink, less freshwater is required). It is noteworthy that the above flow balance for a sink is not included in the model by Meyer and Floudas (2006). But it is considered in our model to specify the inlet flowrate to a sink, which represents the water flow required for the normal operation of a sink (which in most cases is a process unit). We want to specify the (minimum) amount of water required to operate a sink, which is usually a unit operation. For example, a sink maybe a reactor, and there is a certain flowrate of water that is required for the normal operation of the reactor. Water can also a reactant in the reactor, thus, certain amount of water flowrate is required to operate the reactor.

4.5.2 Contaminant concentration balances for sink

$$F_2(j)\cdot C_{\max}(q,j) \geq \sum_{i\in I} F_a(i,j)\cdot C_{SO}(q,i) + \sum_{k_G\in K_G} F_{b,G}(k_G,j)\cdot C_G(q,k_G) + \sum_{k_P\in K_P} F_{b,P}(k_P,j)\cdot C_P(q,k_P) + \sum_{k_R\in K_R} F_{b,R}(k_R,j)\cdot C_R(q,k_R) \quad \forall j\in J, \forall q\in Q$$

(11)

For water reuse/recycle, the contaminant concentrations for the inlet stream to a sink cannot exceed its maximum inlet concentrations (for example, for the sink of cooling tower PSR-1 CT, maximum contaminant concentration for oil and grease, O&G cannot be greater than 50 ppm). In other words, the concentration balance for a sink does not have to hold (that is, does not have to obey an equality) to be equal to $C(i,j)$. As long as $C(i,j)$ is less than the maximum inlet concentration for a contaminant $C_{max}(i,j)$ for a sink, then the water can be reused or recycled.

4.6 Variables' bounds

$$F_a^L(i,j) \leq F_a(i,j) \leq F_a^U(i,j)$$

(12)

4.7 Integral constraints defining binary zero–one variables

$$y^a(i,j) \in \{0,1\} \ldots \text{for all } i \in I,\ k \in K$$

(13)

4.8 Big-*M* logical constraints

We employ big-*M* logical constraints to enforce the lower and upper bounds on the flowrate variables that relate them to the 0–1 variables representing the existence of the associated stream interconnections:

$$F_a(i,j) \le F_a^{\mathrm{U}}(i,j) \cdot y_a(i,j)$$

$$F_a(i,j) \ge F_a^{\mathrm{L}}(i,j) \cdot y_a(i,j)$$

(14)

Big-*M* reformulation is used to convert a logic or nonconvex constraint to a set of constraints describing the same feasible set, using auxiliary binary variables and additional constraints. The big-*M* reformulations will feature terrible numerical behavior, and the relaxations that are used in the mixed integer solver will be very weak, leading to excessive branching and thus increased computation time.

4.9 Forbidden mixing of the permeate and reject streams of an interceptor in a sink, in another interceptor, and from another interceptor

$$\begin{aligned} &F_{b,\mathrm{P}}(k_{\mathrm{P}},j) \cdot F_{b,\mathrm{R}}(k_{\mathrm{R}},j) = 0 \quad && \forall j \in J \\ &F_{b,\mathrm{P}}(k_{\mathrm{P}},k') \cdot F_{b,\mathrm{R}}(k_{\mathrm{R}},k') = 0 \quad && k \ne k', \forall k \in K \\ &F_{b,\mathrm{P}}(k,k_{\mathrm{P}}) \cdot F_{b,\mathrm{R}}(k,k_{\mathrm{R}}) = 0 \quad && \forall k \in K \end{aligned}$$

(15)

The equations above are to ensure that all permeate and reject streams from the same interceptor would not mix again in the sink. The permeate stream of an interceptor is a lean stream. It should send to sinks. It also restricts the matching of a permeate and reject streams from the same interceptor, *k* in another interceptor, *k'*. The equations forbid permeate and reject streams from different interceptor to mix in the same interceptor.

4.10 Forbidden cycling between two interceptors

Cycling or looping between two interceptors is disallowed because a pipe cannot have flows in two directions:

$$y_c(k,k') + y_{cc}(k',k) \le 1, \quad k \ne k', \forall k \in K$$

(16)

An associated constraint related to forbidden cycling is to stipulate that the corresponding flowrates of cycling between two interceptors have to be of the same value:

$$F_c(k,k') = F_{cc}(k',k), \quad k \ne k', \forall k \in K$$

(17)

4.11 Logical constraint on existence of permeate and reject streams of the same interceptor

Based on the physical configuration of a membrane separation unit, it is also physically feasible to have both the permeate and reject streams of the same interceptor existing together:

$$y_e(k_{\mathrm{P}}) = y_e(k_{\mathrm{R}}), \quad (k_{\mathrm{P}}, k_{\mathrm{R}}) \in \mathbf{K_P K_R}$$

(18)

where set $\mathbf{K_P K_R}$ is the set that maps the permeate stream of an interceptor to the reject stream of the same interceptor (for example, the mapping of permeate and reject streams of UF1).

4.12 Objective function

$$\min \sum(\text{operating cost}) \cdot F + \sum(\text{capital cost}) \cdot y \qquad (19)$$

The objective of this work is to minimize the fixed capital costs of installing piping interconnections and the variable cost of operating all stream interconnections. Thus, the mathematical formulation for the objective function is the multiplication of cost of each treatment of a set of wastewater streams to the flowrates of each stream. The optimal global solution is the minimum of overall cost of treatment of a set of wastewater streams while reducing the pollutants level to within limits by environmental regulations.

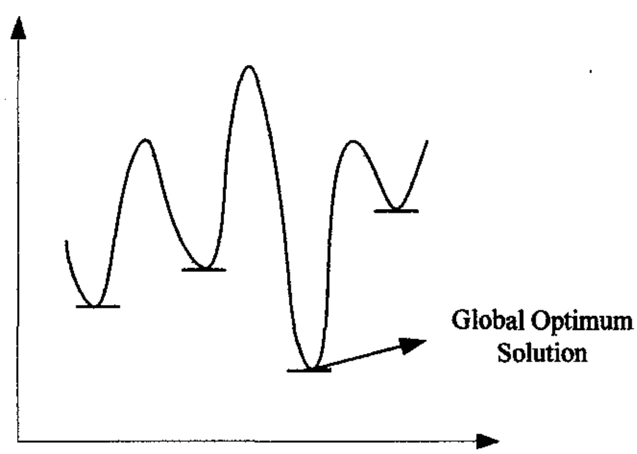

Figure 8: Global optimum solution for nonlinear non-convex programming model.

The complete formulation of the objective functions given by the summation of the components of variable operating cost times flowrate (F) and fixed capital cost times binary variable (y)

1. source to sink
2. general non-membrane-based interceptor to sink
3. permeate stream of membrane-based interceptor to sink

4. reject stream of membrane-based interceptor to sink

5. general non-membrane-based interceptor to interceptor

6. permeate stream of membrane-based interceptor to interceptor

7. reject stream of membrane-based interceptor to interceptor

8. source to interceptor

$$
\left.
\begin{aligned}
\text{total cost} = {} & \sum_{\substack{i\in I\\ j\in J}} c_a(i,j)\cdot F_a(i,j) + \sum_{j\in J} c_{b,\mathrm{G}}(k_\mathrm{G},j)\cdot F_{b,\mathrm{G}}(k_\mathrm{G},j) \\
& + \sum_{j\in J} c_{b,\mathrm{P}}(k_\mathrm{P},j)\cdot F_{b,\mathrm{P}}(k_\mathrm{P},j) + \sum_{j\in J} c_{b,\mathrm{R}}(k_\mathrm{R},j)\cdot F_{b,\mathrm{R}}(k_\mathrm{R},j) \\
& + \sum_{\substack{k\in K\\ k'\in K\setminus\{k\}}} c_{c,\mathrm{G}}(k_\mathrm{G},k'_\mathrm{G})\cdot F_{c,\mathrm{G}}(k_\mathrm{G},k'_\mathrm{G}) + \sum_{k_\mathrm{P}\in K_\mathrm{P}} c_{c,\mathrm{G}}(k_\mathrm{G},k_\mathrm{P})\cdot F_{c,\mathrm{G}}(k_\mathrm{G},k_\mathrm{P}) \\
& + \sum_{k_\mathrm{R}\in K_\mathrm{R}} c_{c,\mathrm{G}}(k_\mathrm{G},k_\mathrm{R})\cdot F_{c,\mathrm{G}}(k_\mathrm{G},k_\mathrm{R}) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} c_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{G})\cdot F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{G}) \\
& + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} c_{c,\mathrm{P}}(k_\mathrm{P},k'_\mathrm{P})\cdot F_{c,\mathrm{P}}(k_\mathrm{P},k'_\mathrm{P}) + \sum_{\substack{k_\mathrm{R}\in K_\mathrm{R}\\ k_\mathrm{R}\neq k_\mathrm{P}}} c_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{R})\cdot F_{c,\mathrm{P}}(k_\mathrm{P},k_\mathrm{R}) \\
& + \sum_{k_\mathrm{G}\in K_\mathrm{G}} c_{c,\mathrm{R}}(k_\mathrm{R},k_\mathrm{G})\cdot F_{c,\mathrm{R}}(k_\mathrm{R},k_\mathrm{G}) + \sum_{k_\mathrm{P}\in K_\mathrm{P}} c_{c,\mathrm{R}}(k_\mathrm{R},k_\mathrm{P})\cdot F_{c,\mathrm{R}}(k_\mathrm{R},k_\mathrm{P}) \\
& + \sum_{\substack{k'_\mathrm{R}\neq K_\mathrm{R}\\ k'_\mathrm{R}\neq k_\mathrm{R}}} c_{c,\mathrm{R}}(k_\mathrm{R},k'_\mathrm{R})\cdot F_{c,\mathrm{R}}(k_\mathrm{R},k'_\mathrm{R}) + \sum_{\substack{k\in K\\ k'\in K\setminus\{k\}}} c_{cc,\mathrm{G}}(k'_\mathrm{G},k_\mathrm{G})\cdot F_{cc,\mathrm{G}}(k_\mathrm{G},k'_\mathrm{G}) \\
& + \sum_{k_\mathrm{P}\in K_\mathrm{P}} c_{cc,\mathrm{G}}(k_\mathrm{P},k_\mathrm{G})\cdot F_{cc,\mathrm{G}}(k_\mathrm{P},k_\mathrm{G}) + \sum_{k_\mathrm{R}\in K_\mathrm{R}} c_{cc,\mathrm{G}}(k_\mathrm{R},k_\mathrm{G})\cdot F_{c,\mathrm{G}}(k_\mathrm{R},k_\mathrm{G}) \\
& + \sum_{k_\mathrm{G}\in K_\mathrm{G}} c_{cc,\mathrm{P}}(k_\mathrm{G},k_\mathrm{P})\cdot F_{cc,\mathrm{P}}(k_\mathrm{G},k_\mathrm{P}) + \sum_{\substack{k'_\mathrm{P}\in K_\mathrm{P}\\ k'_\mathrm{P}\neq k_\mathrm{P}}} c_{cc,\mathrm{P}}(k'_\mathrm{P},k_\mathrm{P})\cdot F_{cc,\mathrm{P}}(k'_\mathrm{P},k_\mathrm{P}) \\
& + \sum_{\substack{k_\mathrm{R}\in K_\mathrm{R}\\ k_\mathrm{R}\neq k_\mathrm{P}}} c_{cc,\mathrm{P}}(k_\mathrm{R},k_\mathrm{P})\cdot F_{cc,\mathrm{P}}(k_\mathrm{R},k_\mathrm{P}) + \sum_{k_\mathrm{G}\in K_\mathrm{G}} c_{cc,\mathrm{R}}(k_\mathrm{G},k_\mathrm{R})\cdot F_{cc,\mathrm{R}}(k_\mathrm{G},k_\mathrm{R}) \\
& + \sum_{k_\mathrm{P}\in K_\mathrm{P}} c_{cc,\mathrm{R}}(k_\mathrm{P},k_\mathrm{R})\cdot F_{cc,\mathrm{R}}(k_\mathrm{P},k_\mathrm{R}) + \sum_{\substack{k'_\mathrm{R}\neq K_\mathrm{R}\\ k'_\mathrm{R}\neq k_\mathrm{R}}} c_{cc,\mathrm{R}}(k'_\mathrm{R},k_\mathrm{R})\cdot F_{cc,\mathrm{R}}(k'_\mathrm{R},k_\mathrm{R}) \\
& + \sum_{\substack{i\in I\\ k\in K}} c_d(i,k)\cdot F_d(i,k)
\end{aligned}
\right\} \text{operating cost}
$$

$$
\left.
\begin{aligned}
&+\sum_{\substack{i\in I\\ j\in J}} c_{ay}(i,j)\cdot y_a(i,j)+\sum_{j\in J} c_{by,\mathrm{G}}(k_{\mathrm{G}},j)\cdot y_{b,\mathrm{G}}(k_{\mathrm{G}},j)\\
&+\sum_{j\in J} c_{by,\mathrm{P}}(k_{\mathrm{P}},j)\cdot y_{b,\mathrm{P}}(k_{\mathrm{P}},j)+\sum_{j\in J} c_{by,\mathrm{R}}(k_{\mathrm{R}},j)\cdot y_{b,\mathrm{R}}(k_{\mathrm{R}},j)\\
&+\sum_{\substack{k\in K\\ k'\in K\setminus\{k\}}} c_{cy,\mathrm{G}}(k_{\mathrm{G}},k'_{\mathrm{G}})\cdot y_{c,\mathrm{G}}(k_{\mathrm{G}},k'_{\mathrm{G}})+\sum_{k_{\mathrm{P}}\in K_{\mathrm{P}}} c_{cy,\mathrm{G}}(k_{\mathrm{G}},k_{\mathrm{P}})\cdot y_{c,\mathrm{G}}(k_{\mathrm{G}},k_{\mathrm{P}})\\
&+\sum_{k_{\mathrm{R}}\in K_{\mathrm{R}}} c_{cy,\mathrm{G}}(k_{\mathrm{G}},k_{\mathrm{R}})\cdot y_{c,\mathrm{G}}(k_{\mathrm{G}},k_{\mathrm{R}})+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} c_{cy,\mathrm{P}}(k_{\mathrm{P}},k_{\mathrm{G}})\cdot y_{c,\mathrm{P}}(k_{\mathrm{P}},k_{\mathrm{G}})\\
&+\sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{P}}}} c_{cy,\mathrm{P}}(k_{\mathrm{P}},k'_{\mathrm{P}})\cdot y_{c,\mathrm{P}}(k_{\mathrm{P}},k'_{\mathrm{P}})+\sum_{\substack{k_{\mathrm{R}}\in K_{\mathrm{R}}\\ k_{\mathrm{R}}\neq k_{\mathrm{P}}}} c_{cy,\mathrm{P}}(k_{\mathrm{P}},k_{\mathrm{R}})\cdot y_{c,\mathrm{P}}(k_{\mathrm{P}},k_{\mathrm{R}})\\
&+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} c_{cy,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{G}})\cdot y_{c,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{G}})+\sum_{k_{\mathrm{P}}\in K_{\mathrm{P}}} c_{cy,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{P}})\cdot y_{c,\mathrm{R}}(k_{\mathrm{R}},k_{\mathrm{P}})\\
&+\sum_{\substack{k'_{\mathrm{R}}\neq K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} c_{cy,\mathrm{R}}(k_{\mathrm{R}},k'_{\mathrm{R}})\cdot y_{c,\mathrm{R}}(k_{\mathrm{R}},k'_{\mathrm{R}})+\sum_{\substack{k\in K\\ k'\in K\setminus\{k\}}} c_{ccy,\mathrm{G}}(k'_{\mathrm{G}},k_{\mathrm{G}})\cdot y_{cc,\mathrm{G}}(k_{\mathrm{G}},k'_{\mathrm{G}})\\
&+\sum_{k_{\mathrm{P}}\in K_{\mathrm{P}}} c_{ccy,\mathrm{G}}(k_{\mathrm{P}},k_{\mathrm{G}})\cdot y_{cc,\mathrm{G}}(k_{\mathrm{P}},k_{\mathrm{G}})+\sum_{k_{\mathrm{R}}\in K_{\mathrm{R}}} c_{ccy,\mathrm{G}}(k_{\mathrm{R}},k_{\mathrm{G}})\cdot y_{c,\mathrm{G}}(k_{\mathrm{R}},k_{\mathrm{G}})\\
&+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} c_{ccy,\mathrm{P}}(k_{\mathrm{G}},k_{\mathrm{P}})\cdot y_{cc,\mathrm{P}}(k_{\mathrm{G}},k_{\mathrm{P}})+\sum_{\substack{k'_{\mathrm{P}}\in K_{\mathrm{P}}\\ k'_{\mathrm{P}}\neq k_{\mathrm{P}}}} c_{ccy,\mathrm{P}}(k'_{\mathrm{P}},k_{\mathrm{P}})\cdot y_{cc,\mathrm{P}}(k'_{\mathrm{P}},k_{\mathrm{P}})\\
&+\sum_{\substack{k_{\mathrm{R}}\in K_{\mathrm{R}}\\ k_{\mathrm{R}}\neq k_{\mathrm{P}}}} c_{ccy,\mathrm{P}}(k_{\mathrm{R}},k_{\mathrm{P}})\cdot y_{cc,\mathrm{P}}(k_{\mathrm{R}},k_{\mathrm{P}})+\sum_{k_{\mathrm{G}}\in K_{\mathrm{G}}} c_{ccy,\mathrm{R}}(k_{\mathrm{G}},k_{\mathrm{R}})\cdot y_{cc,\mathrm{R}}(k_{\mathrm{G}},k_{\mathrm{R}})\\
&+\sum_{k_{\mathrm{P}}\in K_{\mathrm{P}}} c_{ccy,\mathrm{R}}(k_{\mathrm{P}},k_{\mathrm{R}})\cdot y_{cc,\mathrm{R}}(k_{\mathrm{P}},k_{\mathrm{R}})+\sum_{\substack{k'_{\mathrm{R}}\neq K_{\mathrm{R}}\\ k'_{\mathrm{R}}\neq k_{\mathrm{R}}}} c_{ccy,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}})\cdot y_{cc,\mathrm{R}}(k'_{\mathrm{R}},k_{\mathrm{R}})\\
&+\sum_{\substack{i\in I\\ k\in K}} c_{dy}(i,k)\cdot y_d(i,k)
\end{aligned}
\right\}\text{capital cost}
\qquad \textbf{(20)}
$$

The flowrate of a water-using unit designated as a water sink should be equals to the water flowrate requirement constant a given flowrate. The concentration of undesirable species in the permeate stream should not exceed a certain limit as typically imposed by the environmental regulations. The concentration limits of wastewater effluents are according to the Standard B of Environmental Quality Act 1974 in the Constitution of Malaysia.

CHAPTER 5

COMPUTATIONAL EXPERIMENTS AND NUMERICAL RESULTS

5.1 Numerical Data

To illustrate the application of our proposed modeling approach, we consider an industrial-scale case study based on an actual operating oil refinery comprising 29 water sources including a single source of freshwater, 16 interceptors or regenerators, and 13 sinks including the discharge. The simplified superstructure representation for the case study is shown in Figure 9.

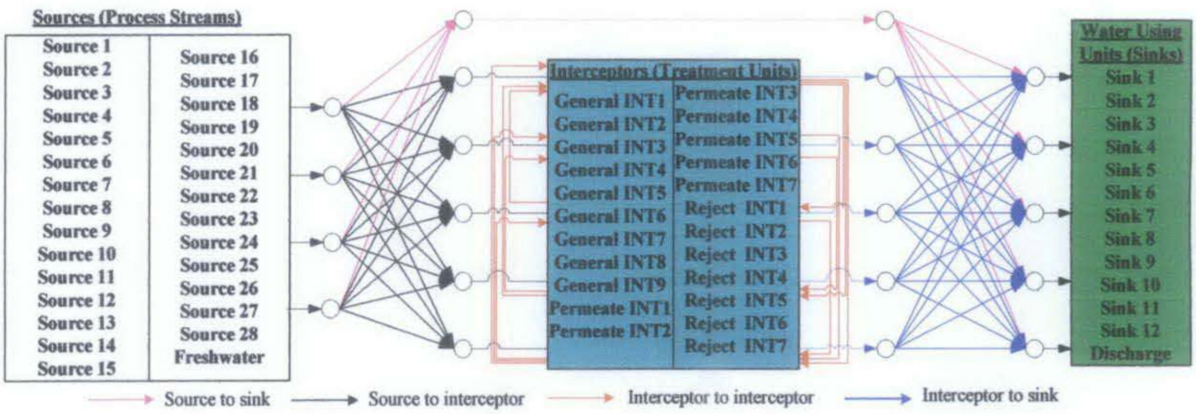

Figure 9: The proposed source-interceptor-sink representation of refinery water network based on industrial case study.

To illustrate the implementation of our modeling approach, we consider a case study involving a total number of twenty nine process units (or source nodes), sixteen potential treatment units (or interceptor nodes) and thirteen numbers of water using units (or sink nodes). Here are the list of sources, interceptors and sinks that are involved in this project.

Table 1: List of process units (or source nodes)

Source	Name	Description
Source 1	Coke-RunOff	coke run off unit
Source 2	PSR1-ProcessArea	process area 1
Source 3	Sulfur-RunOff	sulfur run off unit
Source 4	Lift-Station-4	lift station 4
Source 5	Users	user
Source 6	TKLE	toilet, kitchen, laboratory, equipment
Source 7	PSR1-Desalter	desalter unit 1 to remove salt from crude oil
Source 8	PSR2-Desalter	desalter unit 2 to remove salt from crude oil
Source 9	SWTU-Train	service water train
Source 10	PSR2-Process	process units in PSR 2
Source 11	PSR1-Flare-KO-Drum	flare drum in PSR 1
Source 12	PSR1-Crude-Tank-Drain	crude tank drain in PSR 1
Source 13	PSR2-Crude-Tank-Drain	crude tank drain in PSR 2
Source 14	Intermediate-Condensate-Tank	intermediate condensate tank
Source 15	BD1	cooling water blowdown unit 1
Source 16	BW1	backwash operation of cooling tower 1
Source 17	BD2	cooling water blowdown unit 2
Source 18	BW2	backwash operation of cooling tower 2
Source 19	BD3	cooling water blowdown unit 3
Source 20	BW3	backwash operation of cooling tower 3
Source 21	OWe-RG2	-
Source 22	BDBLs2	blowdown to boiler
Source 23	WHB-BD1	blowdown 1 from waste heat boiler, WHB
Source 24	WHB-BD2	blowdown 2 from waste heat boiler, WHB
Source 25	SW2	service water to PSR-2 (seawater/DCU/offsites)
Source 26	OWg	-
Source 27	SW4-BDBL	service water–blowdown to boiler

Source	Name	Description
Source 28	OW3b	oily surface water storm basin
Source 29	FRESHWATER	freshwater

Note:

- An em-dash ("–") indicates negligible.

Table 2: List of treatment units (or interceptor nodes)

Interceptor	Name	Description
Interceptor 1	MT-CPI-A	mud trap corrugated plate interceptor Basin A
Interceptor 2	MT-CPI-B	mud trap corrugated plate interceptor Basin B
Interceptor 3	MT-CPI-C	mud trap corrugated plate interceptor Basin C
Interceptor 4	DAFu	dissolved air floatation unit
Interceptor 5	SFu	sand filtration unit
Interceptor 6	ETS	effluent treatment system
Interceptor 7	MMF	multimedia filtration unit
Interceptor 8	IX	ion exchange unit
Interceptor 9	CFu	carbon filtration unit
Interceptor 10	RO-EDIperm	permeate stream of reverse osmosis
	RO-EDIrej	reject stream of reverse osmosis
Interceptor 11	RO1perm	permeate stream of reverse osmosis unit 1
	RO1rej	reject stream of reverse osmosis unit 1
Interceptor 12	RO2perm	permeate stream of reverse osmosis unit 2
	RO2rej	reject stream of reverse osmosis unit 2
Interceptor 13	RO3perm	permeate stream of reverse osmosis unit 3
	RO3rej	reject stream of reverse osmosis unit 3
Interceptor 14	UF1perm	permeate stream of ultrafiltration unit 1
	UF1rej	reject stream of ultrafiltration unit 1

Interceptor	Name	Description
Interceptor 15	UF2perm	permeate stream of ultrafiltration unit 2
	UF2rej	reject stream of ultrafiltration unit 2
Interceptor 16	UF3perm	permeate stream of ultrafiltration unit 3
	UF3rej	reject stream of ultrafiltration unit 3

Table 3: List of water using units (or sink nodes)

Sink	Name	Description
Sink 1	FIREWATER	firewater
Sink 2	OSW-SB	oily surface water storm basin
Sink 3	POTABLE	potable water
Sink 4	PSR1-CT	PSR1–cooling tower
Sink 5	Cogen-CT	Cogen–cooling tower
Sink 6	MG3-CT	MG3 - cooling tower 3
Sink 7	BOILER	boiler system
Sink 8	HPU1	hydrogen production unit 1
Sink 9	HPU2	hydrogen production unit 2
Sink 10	PSR1-SW	service water to PSR–1 header
Sink 11	PSR2-SW	service water to PSR–2 header
Sink 12	BDBLu	blowdown to boiler unit
Sink 13	Discharge	the amount of water flowing in a channel

The contaminant considered in this study is oil and grease (O&G) with the unit in mg/L. The data on flowrates and contaminant concentrations for sources and sinks that declared as fixed values in the computational study are listed in the table as below. The removal ratio of the interceptors that obtained from literature review and the initial values for flowrates and the upper bound values of Big-*M* logical constraints are listed in table as below.

Table 4: Contaminant considered in this study and their measurement

Contaminant	Unit
Oil and Grease (O&G)	mg/L

Table 5: Data on fixed values of flowrates and contaminant concentrations based on plant data for sources

Number	Source	Flowrate (m^3/h)	OnG (mg/L)
1	Coke-RunOff	5	2
2	PSR1-ProcessArea	23	2
3	Sulfur-RunOff	20	0
4	Lift-Station4	69	24100
5	Users	27	0
6	TKLE	20	0
7	PSR1-Desalter	30	1430
8	PSR2-Desalter	45	0
9	SWTU-Train	100	0
10	PSR2-Process	2	0
11	PSR1-Flare-KO-Drum	17	0
12	PSR1-Crude-Tank-Drain	1	439
13	PSR2-Crude-Tank-Drain	6	0
14	Intermediate-Condensate-Tank	1	544
15	BD1	3.5	1
16	BW1	1.8	1
17	BD2	10	3
18	BW2	2	3
19	BD3	3.5	3.6
20	BW3	1.8	3.6
21	OWe-RG2	25	1
22	BDBLs2	72.3	72.3

Number	Source	Flowrate (m^3/h)	OnG (mg/L)
23	WHB-BD1	0.3	0.3
24	WHB-BD2	0.3	0.3
25	SW2	2	2
26	OWg	0	20
27	SW4-BDBL	67.2	1
28	OW3b	3.1	4
29	FRESHWATER	– (decision variable)	0

Table 6: Data on fixed values of flowrates and maximum inlet contaminant concentrations (C_{max}) on GAMS modeling software for sinks

Number	Sink	Flowrate (m^3/h)	C_{max} for OnG (mg/L)
1	FIREWATER	3	90
2	OSW-SB	27	80
3	POTABLE	20	70
4	PSR1-CT	25.6	50
5	Cogen-CT	54	50
16	MG3-CT	25	50
7	BOILER	208.9	10
8	HPU1	29.7	50
9	HPU2	29.7	50
10	PSR1-SW	2	70
11	PSR2-SW	36.96	70
12	BDBLu	56.33	90
13	Discharge	403.006	10

Table 7: Data on removal ratio of the interceptor

Interceptor	Name	Removal ratio
Interceptor 1	MT-CPI-A	0.5
Interceptor 2	MT-CPI-B	0.5
Interceptor 3	MT-CPI-C	0.99
Interceptor 4	DAFu	0.815
Interceptor 5	SFu	0
Interceptor 6	ETS	0.84
Interceptor 7	MMF	0
Interceptor 8	IX	0.5
Interceptor 9	CFu	0
Interceptor 10	RO-EDIperm	0
	RO-EDIrej	0
Interceptor 11	RO1perm	0
	RO1rej	0
Interceptor 12	RO2perm	0
	RO2rej	0
Interceptor 13	RO3perm	0
	RO3rej	0
Interceptor 14	UF1perm	0
	UF1rej	0
Interceptor 15	UF2perm	0
	UF2rej	0
Interceptor 16	UF3perm	0
	UF3rej	0

Table 8: Initial values of flowrates (in unit m^3/h)

Number	Continuous Variable	Initial Value
1	F_a (Coke-RunOff, OSW-SB)	5
2	F_a (PSR1-ProcessArea, OSW-SB)	23
3	F_a (Sulfur-RunOff, OSW-SB)	20
4	F_a (Lift-Station4, OSW-SB)	69
5	F_a (Users, OSW-SB)	27
6	F_a (SW4-BDBL, BDBLu)	67.2
7	F_a (OW3b, BDBLu)	3.1
8	F_d (TKLE, MT-CPI-A)	10
9	F_d (TKLE, MT-CPI-B)	10

Table 9: Variable upper bounds in Big-M logical constraints (in unit m^3/h)

$$F_a^{\mathrm{U}}(i,j) = 200$$

$$F_a^{\mathrm{U}}(\text{freshwater}, \text{OSW-SB}) = 200$$

$$F_d^{\mathrm{U}}(i,k) = 513.2$$

$$F_{b,\mathrm{G}}^{\mathrm{U}}(k_{\mathrm{G}}, j) = 513.2$$

$$F_{b,\mathrm{P}}^{\mathrm{U}}(k_{\mathrm{P}}, j) = 513.2$$

$$F_{b,\mathrm{R}}^{\mathrm{U}}(k_{\mathrm{R}}, j) = 513.2$$

$$F_{b,\mathrm{G}}^{\mathrm{U}}(\text{RO1rej}, \text{PSR1-CT}) = 200$$

$$F_{c,\mathrm{G}}^{\mathrm{U}}(k_{\mathrm{G}}, k_{\mathrm{G}}') = 513.2$$

$F^{U}_{c,P}(k_p, k_p') = 513.2$
$F^{U}_{c,R}(k_R, k_R') = 513.2$
$F^{U}_{cc,G}(k_G', k_G) = 513.2$
$F^{U}_{cc,P}(k_p', k_p) = 513.2$
$F^{U}_{cc,R}(k_R', k_R) = 513.2$

Table 10: Operating cost data of streams interconnection.

Pipeline	Cost (RM)	Pipeline	Cost (RM)
c_a	10	$c_{c,R}$	10
$c_{b,G}$	10	$c_{cc,G}$	10
$c_{b,P}$	10	$c_{cc,P}$	10
$c_{b,R}$	10	$c_{cc,R}$	10
$c_{c,G}$	10	c_d	10
$c_{c,P}$	10		

Table 11: Capital cost data of streams interconnection.

Pipeline	Cost (RM)	Pipeline	Cost (RM)
c_{ay}	10	$c_{cy,R}$	10
$c_{by,G}$	10	$c_{ccy,G}$	10
$c_{by,P}$	10	$c_{ccy,P}$	10
$c_{by,R}$	10	$c_{ccy,R}$	10
$c_{cy,G}$	10	c_{dy}	10
$c_{cy,P}$	10		

5.2 Computational Results

Table 12: Model sizes and computational statistics

Type of model	Mixed-integer nonlinear programming (MINLP)
Solver	GAMS 23.2.1/BARON
Computer specifications	Compaq notebook PC, 0.99 GB RAM memory, Intel® Core™ 2 Duo 900 MHz processor
No. of continuous variables	4,920
No. of discrete variables	2,423
No. of bilinear variables	34,990
No. of constraints	4,556
No. of iterations	449
Computational time (s)	3923

The optimal water network structure with reuse for the data tabulated in Tables 1–11 is shown in Figure 10.

The optimization is executed using the global optimization solver GAMS/BARON with an absolute optimality tolerance of 0.5 and a relative optimality tolerance of 0.7.

Based on the current freshwater consumption of 705 m^3/h for the refinery considered in this case study, our proposed new water network design after integration with W3R yields a reduction in freshwater consumption reduce to 513.2 m^3/h which is about 27%

The obtained optimal water network structure does not require the use of the treatment units of MT-CPI-A, MT-CPI-B, MT-CPI-C, DAFu, ETS, MMF, and IX, hence leading to lower capital costs.

Freshwater directed to an interceptor is not an ideal configuration because contaminant inside the freshwater stream is very low and more capital cost may required for that particular stream connection. On the other hand, freshwater can be directly sent to an interceptor to dilute other inlet sources to the interceptor in order to facilitate the treatment process/achieve higher treatment quality.

Certain sinks such as boilers require operations with very high water quality (i.e., very low contaminant concentrations or very clean water)—to meet this requirement, may use freshwater treated in ion exchange

If total source flowrate is greater than total sink flowrate, the difference will go to discharge. If total sink flowrate is greater than total source flowrate, the difference is met by freshwater requirements. If the sink flowrates and concentrations requirements are not met, then the optimal solution requires more freshwater and treatment operations depending on their relative costs, i.e., if freshwater cost is lower than treatment cost, more freshwater is needed, while if treatment cost is lower, more treatment operations are required

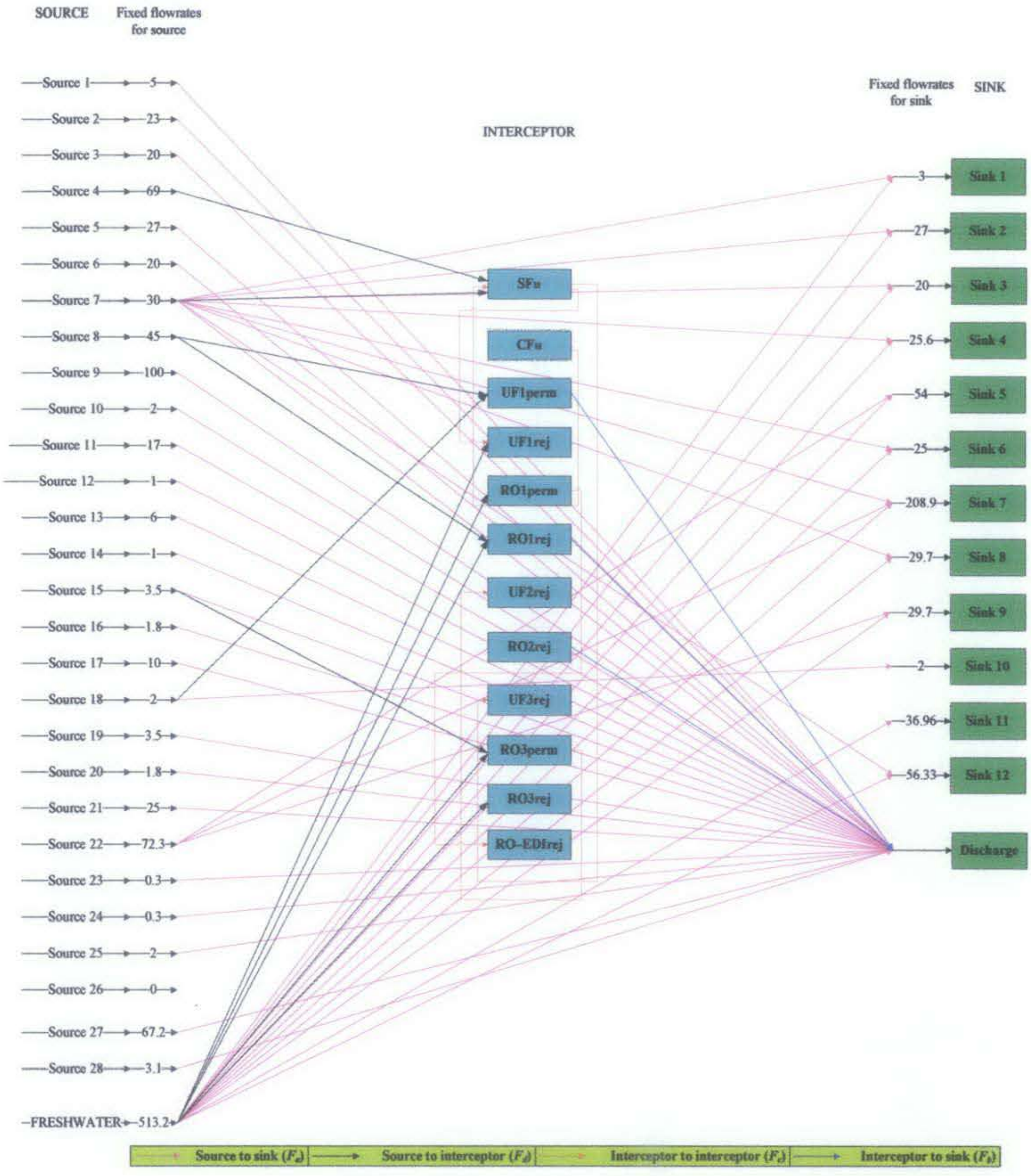

Figure 10: Optimal water network representation based on GAMS results

CHAPTER 6
CONCLUSION

In conclusion, the mathematical optimization of mixed-integer nonlinear programming, MINLP which includes the economic evaluation can be solved simultaneously using GAMS modeling language platform. The modeling approach of mathematical optimization is suitable in the undertaking of this work because it allows the simultaneous determination of two important decision variables of flowrates and contaminant concentrations. The modeling tool GAMS is software which is the computation engine is running in the background to generate the optimal solution suitable. It is user-friendly software and allows the user to focus on the model formulation. The study focused on model formulation of an industrial case study with twenty nine sources, sixteen potential treatment technologies and thirteen sinks. A MINLP optimization model for the synthesis of single contaminant petroleum refinery water network with distributed wastewater treatment network has been developed. The model formulation is developed differently for non-membrane based interceptor and membrane based interceptor with the parameter of liquid recovery factor, α and removal ratio, RR. A large number of feasible network configurations were found using the MINLP software GAMS/BARON. The proposed MINLP model can achieve the following objectives: (i) minimize freshwater consumption, (ii) minimize wastewater generation, and (iii) minimize the operating and capital cost within the permissible contaminant concentrations limit and regulatory discharge requirements.

CHAPTER 7
RECOMMENDATIONS

In the future work, a rigorous cost data of operating cost and capital cost for each stream shall be used. The single contaminant system (oil and grease) in this paper can be improved considering a system with multiple contaminants. The example of contaminants existing in the streams are total suspended solid (TTS), iron (Fe), chemical oxygen demand (COD), pH and total phenol. The relaxations that are used in the mixed-integer nonlinear programming, MINLP is very week, leading to excessive branching and thus increased computation time. It is recommended to apply convexification techniques to reduce the computation time using a suitable solution strategy to handle the bilinearities. Besides that, the further validation of optimal refinery water network structure with compared to real-world practical features shall be improved. This optimization model can be improved to make applicable in all the water network system of petroleum refinery and petrochemical plant.

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APPENDICES

Appendix 1: GAMS results

Continuous Variable	Optimal flowrate
F_a (PSR1-Desalter, FIREWATER)	0.189
F_a (PSR1-Desalter, OSW_SB)	1.510
F_a (PSR1-Desalter, POTABLE)	0.979
F_a (PSR1-Desalter, PSR1-CT)	0.895
F_a (PSR1-Desalter, MG3-CT)	0.874
F_a (PSR1-Desalter, BOILER)	0.732
F_a (PSR1-Desalter, HPU1)	1.038
F_a (PSR1-Desalter, BDBLu)	3.545
F_a (BDBLs2, Cogen-CT)	37.344
F_a (BDBLs2, BOILER)	14.416
F_a (BDBLs2, HPU2)	20.539
F_a (BW2, PSR1-SW)	2.000
F_a (FRESHWATER, FIREWATER)	2.811
F_a (FRESHWATER, OSW-SB)	25.490
F_a (FRESHWATER, POTABLE)	19.021
F_a (FRESHWATER, PSR1-CT)	24.705
F_a (FRESHWATER, Cogen-CT)	16.656
F_a (FRESHWATER, MG3-CT)	24.126
F_a (FRESHWATER, BOILER)	193.752
F_a (FRESHWATER, HPU1)	28.662

Continuous Variable	Optimal flowrate
F_a(FRESHWATER, HPU2)	9.161
F_a(FRESHWATER, PRS2-SW)	36.960
F_a(FRESHWATER, BDBLu)	52.785
F_a(Coke-RunOff, Discharge)	5.000
F_a(PSR1-ProcessArea,Discharge)	23.000
F_a(Sulfur-RunOff, Discharge)	20.000
F_a(Users, Discharge)	27.000
F_a(TKLE, Discharge)	20.000
F_a(PSR1-Desalter, Discharge)	1.978
F_a(PSR1-Crude-Tank-Drain, Discharge)	1.000
F_a(PSR2-Crude-Tank-Drain, Discharge)	6.000
F_a(PSR1-Flare-KO-Drum, Discharge)	17.000
F_a(PSR2-Process, Discharge)	2.000
F_a(SWTU-Train, Discharge)	100.000
F_a(Intermediate-Condensate-Tank, Discharge)	1.000
F_a(BD1, Discharge)	3.500
F_a(BD2, Discharge)	10.000
F_a(BD3, Discharge)	3.500
F_a(BW1, Discharge)	1.800
F_a(BW3, Discharge)	1.800
F_a(Owe-RG2, Discharge)	25.000
F_a(WHB-BD1, Discharge)	0.300
F_a(WHB-BD2, Discharge)	0.300
F_a(SW2, Discharge)	2.000

Continuous Variable	Optimal flowrate
F_a(SW4-BDBL, Discharge)	67.200
F_a(OW3b, Discharge)	3.100
$F_{b,P}$(UF1perm, Discharge)	40.787
$F_{b,R}$(RO1rej, Discharge)	6.502
$F_{b,R}$(RO3rej, Discharge)	13.240
$F_{c,G}$(SFu, UF3rej)	152.369
$F_{c,P}$(RO1perm, RO-EDIrej)	15.170
$F_{c,P}$(RO3perm, UF2rej)	30.894
$F_{c,R}$(UF1rej, SFu)	17.480
$F_{cc,G}$(CFu, SFu)	65.110
F_d(Lift-Station4, SFu)	69.000
F_d(PSR1-Desalter, SFu)	18.259
F_d(PSR2-Desalter, RO1rej)	4.213
F_d(PSR2-Desalter, UF1perm)	40.787
F_d(BD1, RO3perm)	7.340927×10^{-7}
F_d(BW2, UF1perm)	2.446976×10^{-7}
F_d(FRESHWATER, RO1perm)	15.170
F_d(FRESHWATER, RO1rej)	2.289
F_d(FRESHWATER, RO3perm)	30.894
F_d(FRESHWATER, RO3rej)	13.240
F_d(FRESHWATER, UF1rej)	17.480

Appendix 2: Gantt chart and project key milestone

No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14	15	16	17	18	19
1	Solve GAMS Modeling	■	■	■	■	■	■	■		■	■	■	■	■	■						
2	Evaluate the solution's feasibility											■	■	■	■						
3	Submission of Progress Report 1					X															
4	Prepare poster exhibition																				
5	Submission of Progress Report 2 (Draft of Final Report)								**Mid Term Break**				X								
6	Poster Exhibition / Pre-EDX												X								
7	Submission of Final Report															X					
8	Final Oral Presentation																			X	
9	Submission Final Report (hardbound)																				X

X	Suggested milestone
■	Process