OPTIMIZATION OF REFINERY WATER NETWORK RETROFIT WITH OPPORTUNITIES FOR WATER REUSE, REGENERATION AND RECYCLE (W3R)

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CHEMICAL ENGINEERING
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Optimization of Refinery Water Network Retrofit with Opportunities for Water Reuse, Regeneration and Recycle (W3R)

by

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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.

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ABSTRACT

Water is a key element for the stable and reliable operation of petroleum refineries. However, it has now become a major concern in the industry because of multiple reasons that include increasingly stringent environmental regulations on wastewater discharges, giving rise to higher requirements for operating efficiency and optimization. In addition, scarcities in clean water resources and freshwater supply have sparked the drive for implementing sustainable development efforts. In line with this situation, this work has been undertaken with the ultimate **objective** of developing a mathematical optimization model for the optimal retrofit of an integrated water management network system for a petroleum refinery. The **problem statement** can be briefly stated as follows: given a set of water-using and water-treatment units and a freshwater supply source with known compositions, we wish to determine the optimal interconnections of the water network systems structure and their corresponding flowrates and compositions that satisfy the following three criteria as stipulated in the objective function of the optimization model: (1) minimum freshwater import for consumption; (2) minimum wastewater generation; and (3) contaminant concentrations that are within the allowable limits of the associated operations and the legislative regulatory requirements for discharges to the environment. The **scopes of study involves the formulation and solution of a nonlinear programming (NLP) optimization model that explicitly considers the incorporation of the potential for water reuse, regeneration, and recycle** (W3R). The **methodology** begins with the construction of a superstructure representation, which is amenable to tighter model formulation, embedding all feasible alternatives for potential W3R opportunities. Subsequently, an NLP model is formulated based on the superstructure, and the model is solved to optimality with the implementation of efficient algorithms that are available in the open literature. To illustrate the proposed modeling approach, computational studies on industrial-scale problems have been performed using the GAMS algebraic modeling platform, with **findings** resulting in an optimal retrofit structure of the water network that satisfies real-world practical requirements.

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NOMENCLATURE & NOTATIONS

Fixed-Load Model Formulation

(a) Sets and Indices

MU	mixer unit
SU	splitter unit
PU	process unit
TU	treatment unit
S	inlet streams into mixer unit (MU)
S_1	single outlet stream of mixer units (MU)
T	set of plant t
C	set of contaminant c

(b) Parameters

$L_{j,p}$	Mass load for process unit
F_k, F_i, P_p	Throughput for process unit
$R_{j,t}$	Removal ratio for treatment unit

(c) Continuous Variables

F_s	Inlet flow to mixer unit, splitter unit and treatment unit
F_{s_1}	Outlet flow to mixer unit, splitter unit and treatment unit
$C_{j,s}$	Inlet concentration to mixer unit, splitter unit and treatment unit

C_{j,s_1} Outlet concentration to mixer unit, splitter unit and treatment unit

$C_{j,i}$ Inlet concentration to process unit

$C_{j,k}$ Outlet concentration to process unit

Fixed-Flow Model Formulation

(a) Sets and Indices

SO set of source

INT set of interceptor

SI set of sink

CO set of contaminant

(b) Parameters

$F(\text{so})$ flow rate of source

$C_{\text{co}}(\text{so})$ Concentration for source

RR Removal ratio for treatment unit

$C_{\text{co,max}}(\text{si})$ Maximum allowable inlet concentration for sink

(c) Continuous Variables

Fa(so,si) stream connecting source *s* to sink *e*

*F*b(int,sink) stream connecting plant *t* to sink *e*

Fc(int,int') stream connecting plant t to plant t'

Fd(so,int) stream connecting source to plant t

$C_{\text{co}}(\text{so,si})$ Concentration from source to sink

$C_{\text{co}}(\text{so, int})$ Concentration from source to interceptor

(d) Binary Variables

y_a(s,e)	Stream connecting source *s* to sink *e*
y_b(t,e)	Stream connecting plant *t* to sink *e*
y_c(t,t')	Directed stream connecting plant *t* to plant *t'*
y_d(s,t)	Stream connecting source *s* to plant *t*
y_e(t)	Plant *t* effluent

CHAPTER 1
INTRODUCTION

1.1 Background

In the past, the concepts of water minimization and water recovery were previously less attractive due to cost restrictions, limited technologies and lack of environmental awareness. 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 higher costs for freshwater supply and wastewater treatment, stringent regulations on discharges, limited freshwater resources, increased of environmental awareness, and lastly increased requirements for plant efficiency and optimization. However, the scarcity of freshwater is the critical problem that draws most people's attention.

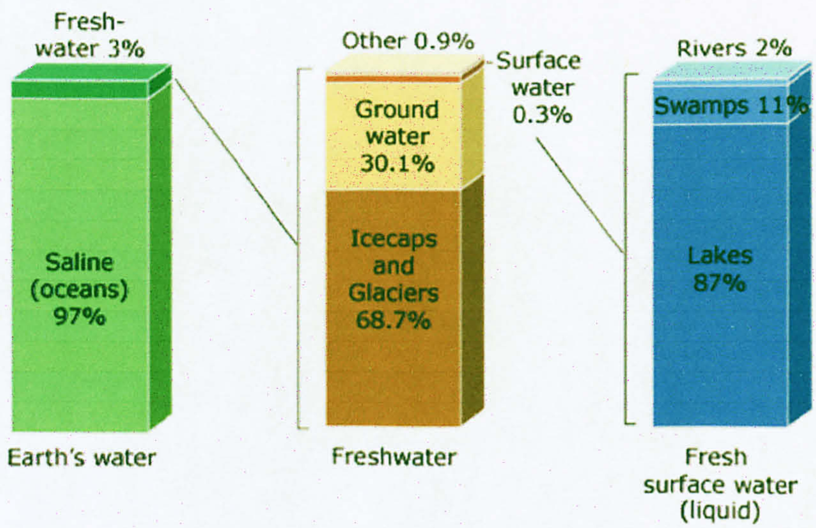

Figure 1 Global water distribution

From the Figure 1, we can see that only 3 percent of earth's water is usable freshwater and out of the 3 percent, only 0.3 percent is fresh surface water in liquid. As a whole, only 0.009 percent of earth's water is usable by humans. The percentage is decreasing due to widely use and waste of freshwater and also pollution of freshwater by human beings.

These are among the major issues in a plant that need to be overcome to gain competitive advantage in this competitive industry and preserve the environment from pollution. Consequently, it is timely to build know how on the potential adoption and implementation of water minimization and water recovery approaches and strategies.

1.2 Motivation

The rapid growth of chemical, oil and gas industry intense the competition between companies or plants. In order to gain competitive advantage, the process must be in optimal condition, where cost and resources usage are minimized and profit is maximized. Plant utility optimization is one of the approaches to achieve the optimal condition to gain competitive advantage. Apart from economical point of view, environmental issue also receives significant attention. Fresh water consumption and wastewater produced of the plant have been the main concern nowadays due to higher costs for freshwater supply and wastewater treatment, increased of environmental awareness, the more stringent regulations on discharges and lastly limited freshwater resources. The concept of water minimization through water reuse, regeneration, and recycle (W3R) has become a worthy alternative to achieve the optimal condition.

1.3 Problem Statement

The problem addressed in this work can be stated as follows.

Problem:

a) heightened demand of water consumption in refinery operations;
b) higher cost of freshwater supply and operating cost of water-using and water-treatment units, and
c) increasingly serious water pollution caused by higher pollutants discharge

Given:

a) set of water using and water treatment units, and
b) supply source of freshwater to satisfy demand in water using processes,

Determine:

The optimal retrofit design of water network for potential reuse, regeneration, and recycle (W3R), with the aim of

a) minimum freshwater usage, treatment capacity and discharge to environment;
b) optimal stream flowrates and contaminant concentrations, and
c) optimal retrofit structure

1.4 Objectives and Scope of Work

1.4.1 Objective

a) To develop a superstructure representation for the retrofit of an existing water network design by incorporating possible options for water reuse, regeneration, and recycle (W3R);

b) To construct an optimization model based on the superstructure representation that includes:

- nonlinear mass balances with bilinear terms arising from variable stream flowrates and compositions;
- specifications of the water content including chemical oxygen demand (COD), total dissolved solids (TSS), and other relevant parameters as stipulated in the Malaysian Environmental Quality Act 1974.

c) To solve the mixed-integer nonlinear program (MINLP) optimization model using the modeling language GAMS for determining the decision variables of flowrates and compositions.

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:

a) development of water balance based on a refinery plant;
b) 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
c) formulation of a mathematical model with 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;
d) 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 Literature Review

From the reviewed literatures, there are a few approaches proposed by different authors to solve optimization for water network. The approaches includes,

a) Pinch approach;

b) State-Task-Network approach;

c) Fixed-Load approach, and

d) Fixed-Flow approach.

Theses approaches have different way of constructing the superstructure and model formulation. In line with the case study, the author only concentrated on Fixed-Load and Fixed-Flow approach. This is due to Fixed-Load and Fixed-Flow approach take into account large number of variables, i.e. flowrate and concentration of contaminants. Table 1 shows the literature reviewed by the author and some description of the approach.

TABLE 1 Literature review and descriptions

Author (year)	General description	Optimization model type	Modeling technique	Solution strategy
Fixed-Load Model Formulation				
Karuppiah and Grossmann (2006)	Integrated water management network	NLP	• Superstructure with all possible interconnections of process units and treatment units using mixers and splitters • Accounts for mass load of contaminants	• Bound strengthening cuts based on overall contaminant flow balances • Logic cuts • Global optimization algorithm
Chang and Li (2005)	Integrated water management network	NLP	• Superstructure incorporates additional design options and a fixed number of repeated treatment units • Inequality constraints on concentrations to account for possible existence of unrecoverable contaminants	• Method to produce a good initial guess to enhance convergence efficiency • Techniques to manipulate structural properties of water networks
Huang et al. (1999)	Integrated water usage and distributed wastewater treatment network	NLP	• Extended version of Takama et al.'s (1980) superstructure by incorporating multiple water sources and sinks, water losses, and repeated water treatment units • Uses the strategy/heuristic/technique of "repeated water treatment units" to	Initial feasible points are generated through water pinch analysis or by solving nonlinear system of equations resulting from fixing several key design variables at

TABLE 1 Literature review and descriptions (continue)

Author (year)	General description	Optimization model type	Modeling technique	Solution strategy
			represent effect of recycling wastewater requiring further treatment (i.e., another "round" of treatment using the same treatment technology)	reasonable levels in the NLP
Fixed-Flowrate Model Formulation				
Meyer & Floudas (2006)	Global optimization of a complex generalized pooling problem	MINLP	Model formulation based on source–interceptor (treatment)–sink representation	Global optimization algorithm of augmented Reformulation–Linearization Technique (RLT)
Gabriel & El-Halwagi (2005)	Rigorous graphical targeting for resource conservation via material recycle/reuse networks	NLP	Source–interceptor–sink superstructure representation	Reformulation into linear program to obtain global optimal solution

2.2 Techniques for Water 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 water water minimization. Figure 1 below showing a simple configuration of which fresh water is used in all operations.

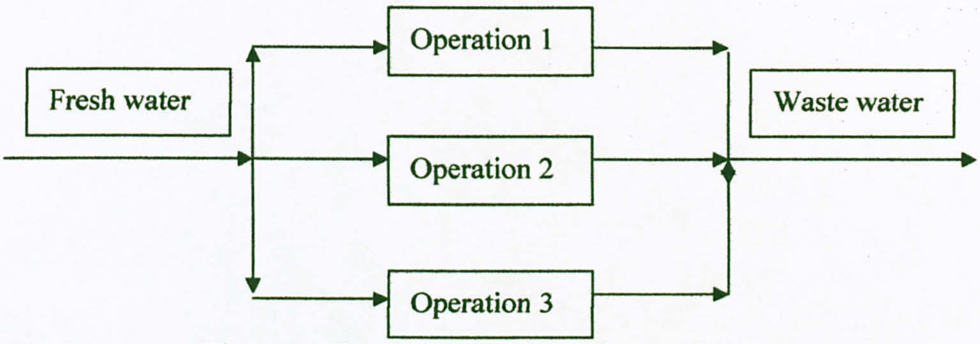

Figure 2 Fresh water used in all operation

2.2.1 Water Reuse

For water reuse, 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 usage of the freshwater and wastewater, as the same water is used twice. For multistage washing operation, low quality water could be used in initial stages, while high-quality water used in the final stages (Smith, 2005). Figure 2 shows the implementation of water reuse in a simple water network.

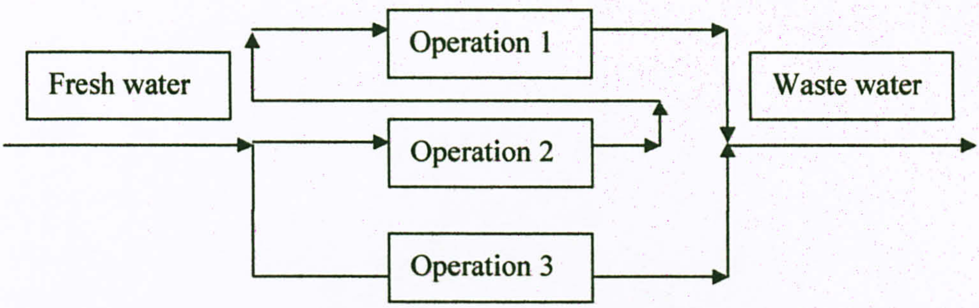

Figure 3 Water Reuse

2.2.2 *Water Regeneration-Recycle*

In this technique, the used water is fed into a treatment unit to regenerate water of which the quality is acceptable for further use. Regeneration also reduces both the usage of the freshwater and wastewater, and also removes part of the effluent load before reuse to prevent contaminants build up. 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.

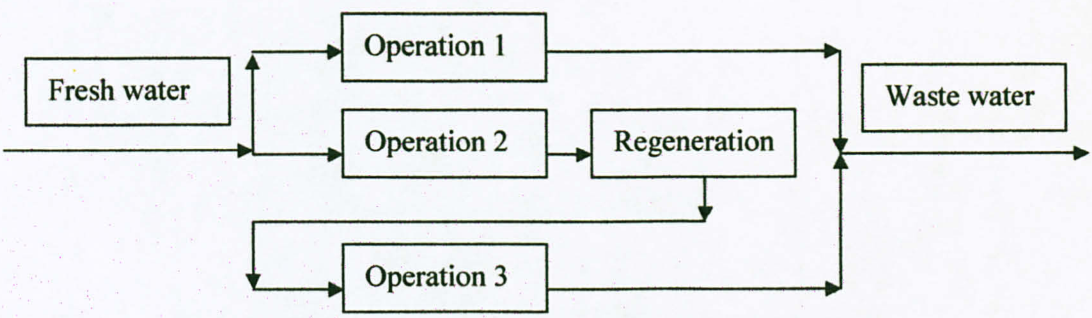

Figure 4 Regeneration-Reuse

2.2.3 Water Recycle-Reuse

For 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. Recycling reduces both the usage of the freshwater and 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).

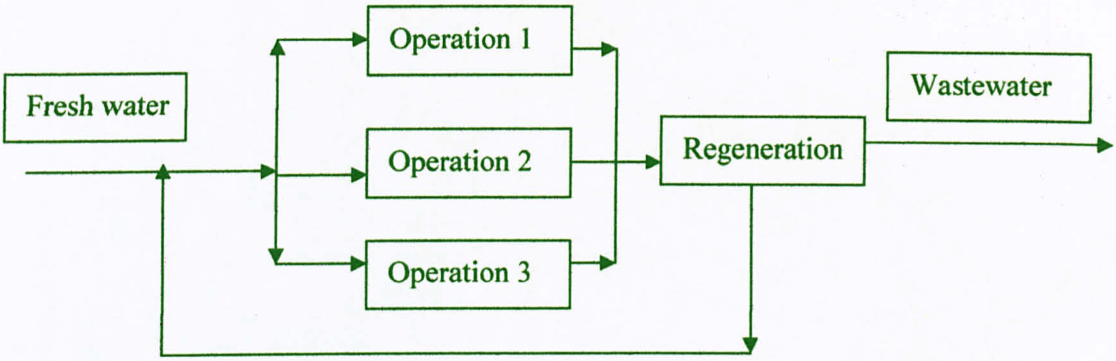

Figure 5 Regeneration Recycle

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).

Table 2 shows the example of treatment units that are considered in the case study.

TABLE 2 List of treatment units with respective removal ratio

Treatment units	Abbreviation	Contaminants Removed or Treated
Mud trap	**MT**	**Oil and Grease**
Corrugated plate interceptor	**CPI**	**Oil and Grease**
Dissolved air flotation	**DAF**	**Oil and Grease**
Effluent treatment system	**ETS**	**Oil and Grease, TSS, COD,**
Sand filtration	**SF**	**TSS, Fe**
Ultrafiltration	**UF**	**TSS, COD**
Reverse osmosis	**RO**	**TSS, COD**
Multimedia filtration	**MMF**	**TSS, Fe**
Carbon filtration	**CF**	**TSS, Fe**
Ion Exchange	**IX**	**Fe**

CHAPTER 3
METHODOLOGY

3.1 General Methodology

In general, the mathematical programming approach to process synthesis and design activities and problems consists of four major steps (Grossmann, 1990; Floudas, 1995;), which are,

1. Development of the superstructure to represent the space of topological alternatives of the water recovery 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.

In line with the case studies, the methodology is slightly modified. The block diagram of the modified method is shown in Figure 6.

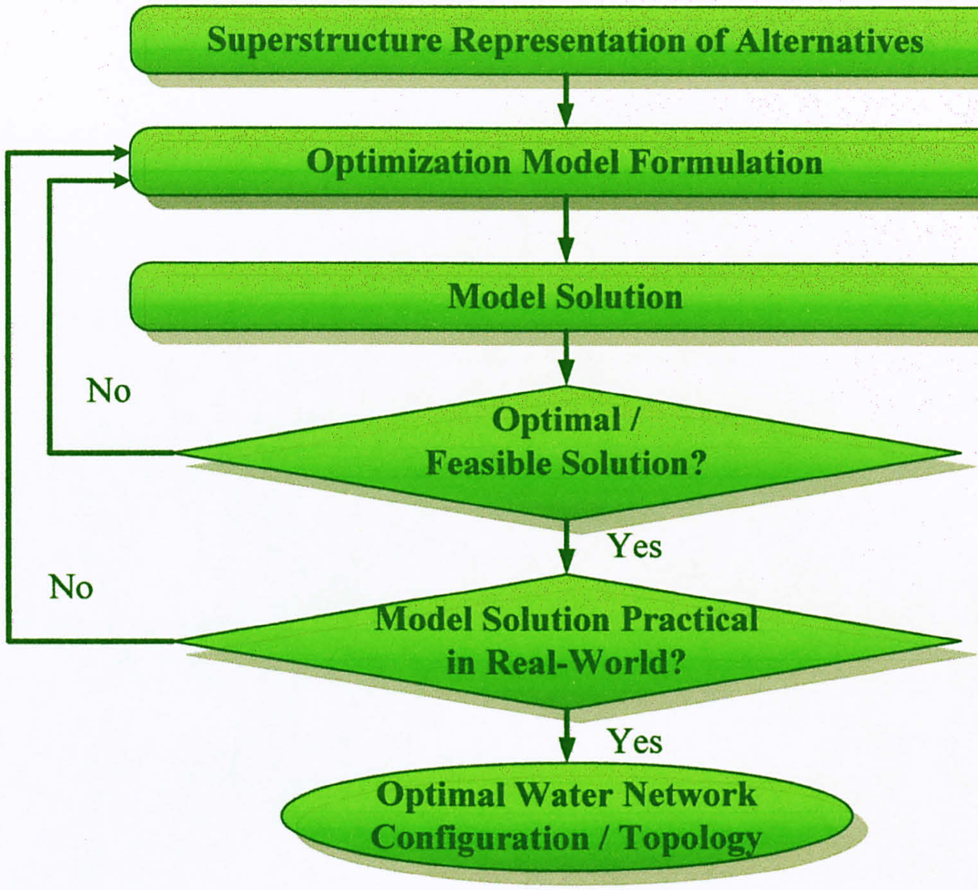

Figure 6 Methodology

CHAPTER 4
RESULT AND DISCUSSION

4.1 Optimization Model Formulation

In this work, we consider the implementation of two leading modeling and computational approaches for water network design problems, namely the fixed-load problem formulation by Karuppiah and Grossmann (2006) and the fixed-flowrate formulation by Meyer and Floudas (2006), as mention in previous chapter. The main contribution of our work, as demonstrated in the next section on Computational Experiments and Numerical Results, is to implement these two methods for the retrofit of the water network structure of a petroleum refinery. It is acknowledged that retrofit problems are more restricted compared to grassroot design problems in terms of the available degrees of freedom, thus making retrofit problems harder to solve.

4.1.1 Model 1: Fixed-Load Problem Formulation of Karuppiah and Grossmann (2006)

4.1.1.1 *Step 1: Superstructure Representation of Alternatives*

Consider a system with two major elements:

- water-using units that are termed generally as process units that consume fixed amounts of water and introduce contaminants into the system, and
- wastewater treatment units.

We construct a superstructure that considers all possible interconnections involving these process units and treatment units by utilizing mixers and splitters.

The superstructure can be divided into eight (8) stages.

1. the first stage: first-level splitter units

   These splitter units diverge the flows of the single water source that in this case is the single source of freshwater at the inlet to the system.

2. the second stage: first-level mixer units

   These mixer units collect streams from the split water source and also streams for water reuse and recycle. The collected streams are then sent to the process units.

3. the third stage: process units

   The process units use fixed amounts of water and introduce contaminants into the system. These contaminants are represented by fixed load of contaminants that we simply refer to as mass load, and they are assumed to be generated in each of the process units.

4. the fourth stage: second-level splitter units

   These splitter units are placed after the process units. They diverge the contaminated streams either to the treatment units, for reuse or recycle or for discharge. The directions of the streams are generally decided based on optimization (except for those that have been pre-specified). The optimization decisions consider a few conditions, such as,

   (a) maximum allowable inlet concentrations for the process units;

   (b) type of treatment units;

   (c) performance of treatment units;

   (d) maximum allowable discharge concentration, and

   (e) objective function.

5. The fifth stage: second-level mixer units

   These mixer units collect streams from the first-level splitter units (after the sources), the second-level splitter units (after the process units), and the third-level splitter units (after the treatment units). The decisions on the actual stream directions are also decided by optimization.

6. The sixth stage: treatment units

   Treatment units reduce the contaminant level in the water before reuse, recycle, or discharge to the environment. Different treatment technologyies remove different amounts of contaminants and also different type of contaminants.

7. The seventh stage: third-level splitter units

   These splitter units diverge flow from the treatment units to the following units:

   (a) first level mixer units for reuse or recycle;

   (b) second-level mixer units for further treatment; or

   (c) third-level mixer units for discharge to the environment.

8. The eighth stage: third-level mixer units

   These mixer units collect streams from any splitter unit for discharge to the environment or to represent water loss, for instance, due to evaporation. For discharge to the environment, the maximum allowable discharge concentration limits must be obeyed. On the other hand, flows due to water loss are normally fixed.

Figure 7 shows the interconnections of the mixer units, splitter units, process units, and treatment units.

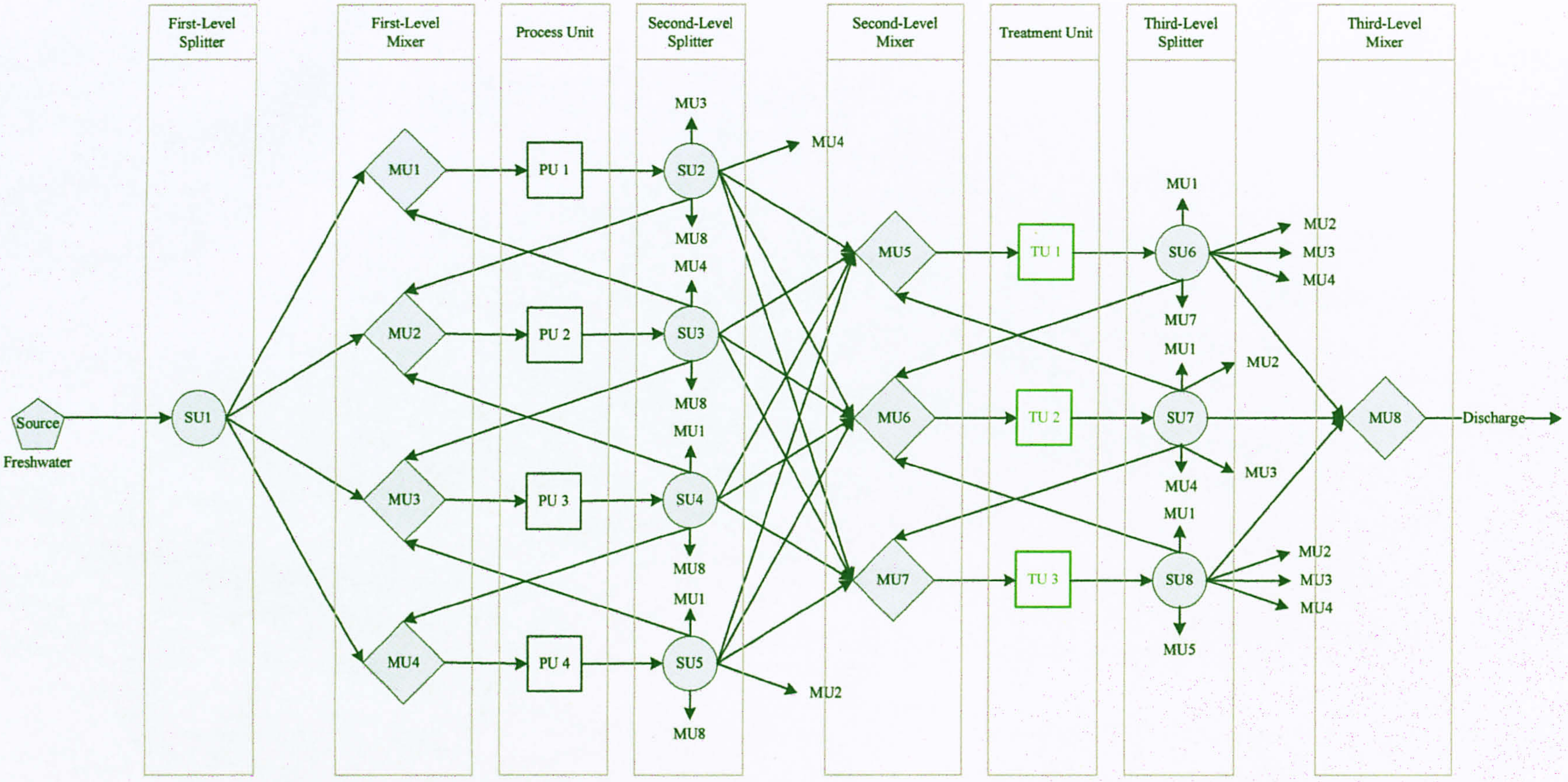

Figure 7 General superstructure representation of alternatives for water network design

4.1.1.2 *Step 2: General Optimization Model Formulation*

The optimization model formulation for fixed-mass load problem can be divided into 4 main parts, which are formulation for mixer units, splitter units, process units and treatment units. For every unit, there will be mass balance for water flow and contaminant flow.

(a) Material Balances for Mixer Units (Convergent-Flow-Path Units)

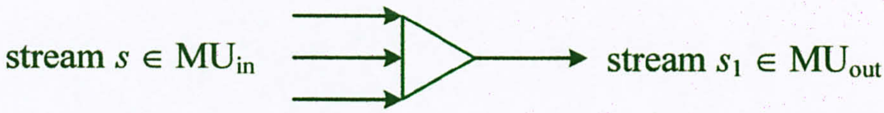

Figure 8 Mixer unit

Mass balance for water flow for mixer unit (MU):

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

The summation of inlet flow is equal to the single outlet flow.

Mass balance for contaminant flow for mixer unit (MU):

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

The left hand side of the equation represents the inlet contaminant flow, while the right hand side represents the contaminant flow single outlet. This is a bilinear constraint that causes difficulty for the optimization model to converge into global optimal solution.

(b) Material Balances for Splitter Units (Divergent-Flow-Path Units)

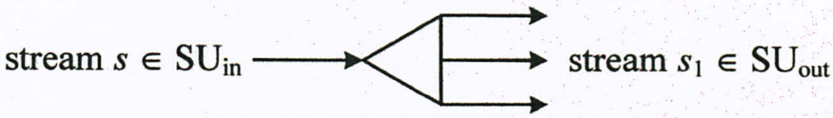

Figure 9 Splitter unit

Mass balance for water flow for splitter unit (SU):

$$F_s = \sum_{s_1 \in \mathrm{SU_{out}}} F_{s_1} \qquad \forall s \in \mathrm{SU_{in}} \tag{3}$$

The single outlet flowrate (left hand side) is equal to the summation of the diverged flows (right hand side).

Mass balance for contaminant flow for splitter unit (SU):

$$F_s C_{j,s} = \sum F_{s_1} C_{j,s_1} \quad \forall j \in J, \forall s \in \mathrm{SU_{in}}, \forall s_1 \in \mathrm{SU_{out}} \tag{4}$$

The outlet concentration is the same for the single inlet concentration.

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

As a result,

$$\begin{aligned} F_s \cancel{C_{j,s}} &= \sum F_{s_1} \cancel{C_{j,s_1}} \\ F_s &= \sum F_{s_1} \end{aligned} \qquad \forall j \in J, \forall s \in \mathrm{SU_{in}}, \forall s_1 \in \mathrm{SU_{out}} \tag{6}$$

After both sides of the concentration is canceled out, the balance left is actually the mass balance for water flow (see equation **(3)**). Thus, the important constraint is equation (5), which specifies that every diverged outlet stream from a splitter has the same concentration as the single inlet stream into the splitter.

(c) Material Balances for Process Unit

Figure 10 Process unit

Mass balance for water flow for process unit (PU):

$$F_k = F_i = P_p \quad \forall p \in \text{PU}, i \in \text{PU}_{\text{in}}, k \in \text{PU}_{\text{out}} \tag{7}$$

Process unit has one single inlet and one single outlet. The outlet flowrate is equal to the outlet flow rate. This flow represents the operating flowrate of water in a process unit or water using unit. Normally this value is a parameter, not a variable to be determined. Besides, it is a crucial parameter that need to be specified in order for the optimization model to yield feasible and practical result.

An assumption in this constraint formulation is that the contaminants introduced from the process unit are negligible.

Mass balance for contaminant flow for process unit (PU):

$$P_p C_{j,i} + L_{j,p} = P_p C_{j,k} \qquad \forall j \in J,\ \forall p \in \text{PU},\ i \in \text{PU}_{\text{in}},\ k \in \text{PU}_{\text{out}} \tag{8}$$

The term $L_{j,p}$ is the mass load term. This represents the amount of contaminant introduced by the process unit (or water using unit) to the system. If the mass load is expressed in the unit ton/hour, then it is not required to multiply it with a conversion factor to ensure that the material balance on contaminant concentration for a process unit is dimensionally correct.

Representation of Mass Load in Process Unit Modeling

We propose a method to convert fixed flowrate operations to fixed contaminant load operations as explained in the following.

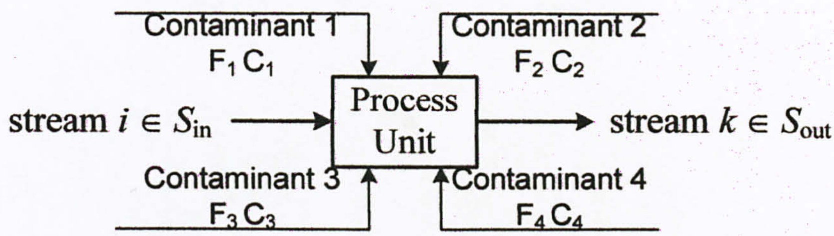

Figure 11 Contaminant is introduced to the system in term of multiplication of flowrates (F) and concentrations (C)

Figure 11 shows the contaminants are introduced to a process unit in fixed-flow form. In this case, the model formulation is different from the conventional model formulation for a process unit. The following explains why the conventional model formulation is not applicable.

The proposed formulation adopts constraint (7) in which there is only a single inlet stream and a single outlet stream. As a result, the inlet flowrate is equal to the outlet flowrate. But for constraint (8), the term $L_{j,p}$ will be replaced by the product of flowrates and concentrations ($F \times C$), which we term as the calculated mass load (because mass load is typically obtained from process data).

Consider the case in Figure 11 in which a contaminant is introduced to a process unit with a significant flowrate. As a result, this fixed-flowrate condition violates constraints (7) and (8), which assume the term P_p representing the equivalence of the single inlet flow and the single outlet flow.

Our proposed approach to adapt such model formulation is detailed as follows.

1. Connect the involved process units to the freshwater source using an imaginary stream, F_{in}, as shown in the figure below.

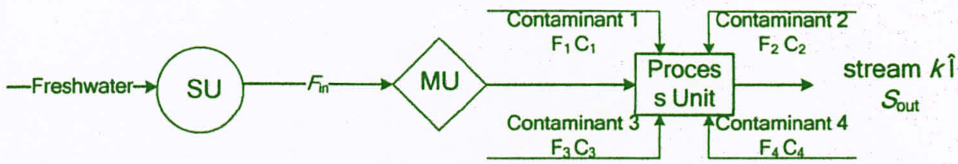

Figure 12 Transformation of model formulation for process units from fixed flowrate operations to fixed contaminant load operations

2. The value of F_{in} is equals to the sum of the flowrates of the contaminants, which in this case are F_1, F_2, F_3 and F_4, as shown in equation (9):

$$F_{in} = \sum F_{\text{fixed-flow}} \tag{9}$$

Steps 1 and 2 turn the multiple inlet contaminant flowrates into a single inlet flow into a process unit.

3. Check the quality of the freshwater so that compensation on the contaminants can be performed in the next step. Normally, freshwater is free from any contaminant, thus compensation is not required in most cases. On the other hand, if there are contaminants in the freshwater source, then compensation is performed by subtracting the concentration of these contaminants from the calculated mass load for a process unit.

4. Substitute the fixed mass-load term, $L_{j,p}$ as the summation of the product of flowrates and concentrations:

$$L_{j,p} = \sum F_{\text{fixed-flow}} C_{\text{fixed-flow}} \tag{10}$$

For Figure 12, this is given by:

$$L_{j,p} = F_1C_1 + F_2C_2 + F_3C_3 + F_4C_4 \tag{11}$$

Steps 3 and 4 convert the fixed flowrate operations to fixed contaminant load operations, in which we now have a process unit with a single inlet flow and a single outlet flow and a calculated mass load value for the term $L_{j,p}$.

Finally, apply the conventional model formulation for process units, as represented by constraints (7) and (8), but again, with the mass load $L_{j,p}$ known.

The advantage of this approach is that a problem might consist of both fixed-flow and fixed-flow problem. This approach enables the model formulation to be pplicable for both fixed flowrate operations to fixed contaminant load operations.

(d) Material Balances on Treatment Units

Figure 13 Treatment unit

Mass balance for water flow for treatment unit (TU):

$$F_s = F_{s_1} \quad \forall s \in \mathrm{TU}_{in}, \forall s_1 \in \mathrm{TU}_{out} \tag{12}$$

Like process unit, treatment unit has only single inlet and outlet. As aresult, the flowrate into the unit is the same with the flowrate coming out from the unit. The **assumption** made for this constraint is the loss contaminant does not affect the total flow balance. The loss contaminant is too small and is negligible.

Mass balance for contaminant flow for treatment unit (TU):

$$C_{j,s_1} = \left(1 - R_{j,t}\right) C_{j,s} \qquad \forall j \in J, \forall s \in \mathrm{TU}_{in}, \forall s_1 \in \mathrm{TU}_{out}, \forall t \in \mathrm{TU} \tag{13}$$

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 leftover contaminant after treatment. The value of $R_{j,t}$ is always between 0 and 1. The $R_{j,t}$ value for high performance treatment unit is near 1 and vice versa. The left hand side of the equation is the contaminant of the outlet flow, while the right hand side of the equation is the outlet of the treatment unit. This shows that the level of contaminant is less (decreased) after the treatment unit. The assumption for this constraint is the removal ratio, $R_{j,t}$ is assumed to be constant, independent on the level of contaminant in the inlet flow.

For a membrane-based type of treatment units, the model formulation is different from a typical non-membrane-based treatment unit. This is due to the fact that this type of treatment unit consists of two outlet flows with different concentrations, namely: (1) a permeate stream or also referred to as a lean stream and (2) a reject stream or also referred to as a rish stream. Examples of membrane-based treatment units include ultrafiltration (UF) and reverse osmosis (RO). Figure 14 graphically depicts the conventional method of modeling a treatment unit (while Figure 16 displays our proposed method to model membrane type of treatment units).

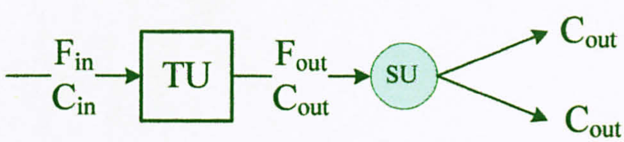

Figure 14 Conventional model for a treatment unit

The conventional model for treatment units consist of one inlet flow into the treatment unit and one outlet flow from the treatment unit. Although the outlet flow can be diverged into multiple streams (using the splitter modeling unit), it is noteworthy that the concentration for each diverged outlet stream is the same as the outlet concentration from the treatment unit. Figure 15 shows the consequences of modeling a membrane-based treatment unit using this conventional model.

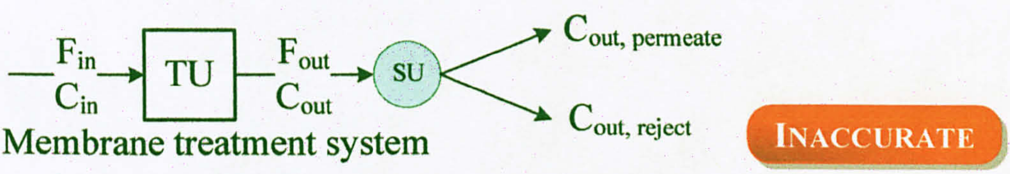

Figure 15 Modeling a membrane-based treatment unit using the conventional model for treatment units

The drawbacks of employing the conventional method for a membrane-based treatment unit are as follows:

1. the outlet concentration of a contaminant in the permeate stream is the same as that in the reject stream;
2. unable to specify the flow split ratio between the permeate stream and the reject stream.

To overcome these shortfalls, we proposed a new approach for modeling a membrane-based treatment unit, as shown in Figure 16.

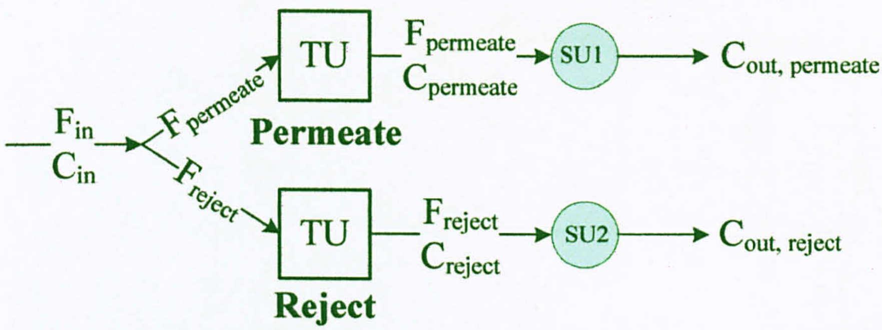

Figure 16 Proposed new approach for modeling a membrane-based treatment unit

An inlet stream to a membrane-based treatment unit is diverged into two streams using a split ratio (whose values lie between 0 and 1) prior to entering two imaginary treatment units, say $TU_{permeate}$ and TU_{reject}. These two units are imaginary because in actuality, the are the same single treatment unit. The typical range of split ratios for a permeate stream is 0.6–0.9, and they are defined according to the following relations:

$$\text{split ratio for permeate stream} = \frac{F_{\text{permeate}}}{\text{Total inlet flow to membrane unit}} \quad \textbf{(14)}$$

$$\text{split ratio for reject stream} = \frac{F_{\text{reject}}}{\text{Total inlet flow to membrane unit}} \quad \textbf{(15)}$$

The removal ratios $R_{j,t}$ for $TU_{permeate}$ ($R_{j,TU_{permeate}}$) and TU_{reject} ($R_{j,TU_{reject}}$) are different. Naturally, $R_{j,t}$ for the $TU_{permeate}$ unit, which represents the lean (or cleaner) permeate stream, is higher than $R_{j,t}$ for the TU_{reject}, which represents the rich (or dirtier) reject stream The relationship between $R_{j,t}$ for $TU_{permeate}$ and $R_{j,t}$ for TU_{reject} is given below:

$$R_{j,TU_{permeate}} + R_{j,TU_{reject}} = 1$$
$$0 \le R_{j,TU_{permeate}} \le 1 \qquad (16)$$
$$0 \le R_{j,TU_{reject}} \le 1$$

Therefore, the advantages of employing our proposed approach of introducing two imaginary units for modeling the permeate and reject streams of a membrane-based treatment unit are as follows:

1. the outlet concentration of a contaminant in the permeate stream is different from that in the reject stream;
2. the two imaginary treatment units can explicitly account for different removal ratios (in which the removal ratio for one is the complement of the other);
3. we are able to specify the flow split ratio between the permeate stream and the reject stream.

It is noted also that our proposed approach for modeling a membrane-based treatment unit applies to both the fixed-load and fixed flowrate model formulations (without the need for modification).

(e) Non-negativity Constraints

All the optimization decision variables are specified to be non-negative as follows:

$$F_i, F_k, C_{j,i}, C_{j,k} \ge 0 \quad \forall i \in S_{\text{in}}, \forall k \in S_{\text{out}} \qquad (17)$$

4.1.1.3 *Step 3: Objective Function*

Objective function is the function that we want to optimize (maximize or minimize) in order to obtain optimize design variables. The design variables in this case are mainly flowrate and concentration of contaminant. The general objective function for W3R problem can be expressed as:

$$\text{minimize } F_{\text{FW}} + \sum_{s_1 \in \text{TU}_{\text{out}}} F_{s_1} + F_{\text{DISCHARGE}} \quad \textbf{(18)}$$

The first term in the objective function is flow of freshwater, F_{FW}. The purpose of minimizing freshwater is to reduce cost of freshwater, reduce waste of freshwater unnecessarily and conserved the limited freshwater. The second term in the objective function represents the flow through treatment unit, F_{S1}. In the objective function showed above, only outlet flowrate of treatment unit is used to represent the flow through treatment unit, because treatment unit only consists of single inlet and single outlet flow. Both flows have the same value of flowrate. Flowrate of treatment unit is included in the objective function as it directly affects both capital and operating cost. A treatment unit with high flowrate means the capacity of the treatment unit is large, which will increase the capital cost of building the treatment unit. Apart from that, cost of treating the water, which is also the operating cost, is directly proportional to the flowrate of water being treated by a treatment unit. Lastly, the last term in the objective function represent the amount of water discharge to the environment, $F_{DISCHARGE}$. The purposes of minimizing this term are reducing the cost of discharge and conserving the environment.

4.1.2 Model 2: Fixed-Flowrate Problem Formulation of Meyer and Floudas (2006)

4.1.2.1 *Step 1: Superstructure Representation of Alternatives*

The superstructure for the fixed-flowrate model formulation, as based on Meyer and Floudas (2006), shows both the existing units and streams, as well as the proposed treatment units and the associated streams. This superstructure is categorized into sources, interceptors (that is, treatment units), and sinks. Sources represent the effluent streams from a set of industrial plants. Each of these streams contains a different load of contaminants. These streams have the potential to be reused or recycled. Interceptors refer to treatment units that maybe used to reduce the contaminant levels in the waste water streams. Each of these plants uses a different treatment technology. Contaminant reduction levels and processing costs therefore vary from plant to plant. Lastly, sinks represent the units or discharge which treated waste flows. Sinks also are units that have potential to accept certain level of contaminant in the water. The proposed treatment units for the retrofit structure are represented in green.

Below are the notations for representation of colour streams

Maroon line: source to sink

Blue line: source to interceptor

Red line: interceptor to interceptor, this considers interconnections from one treatment unit to another treatment unit

Green line: interceptor to sink

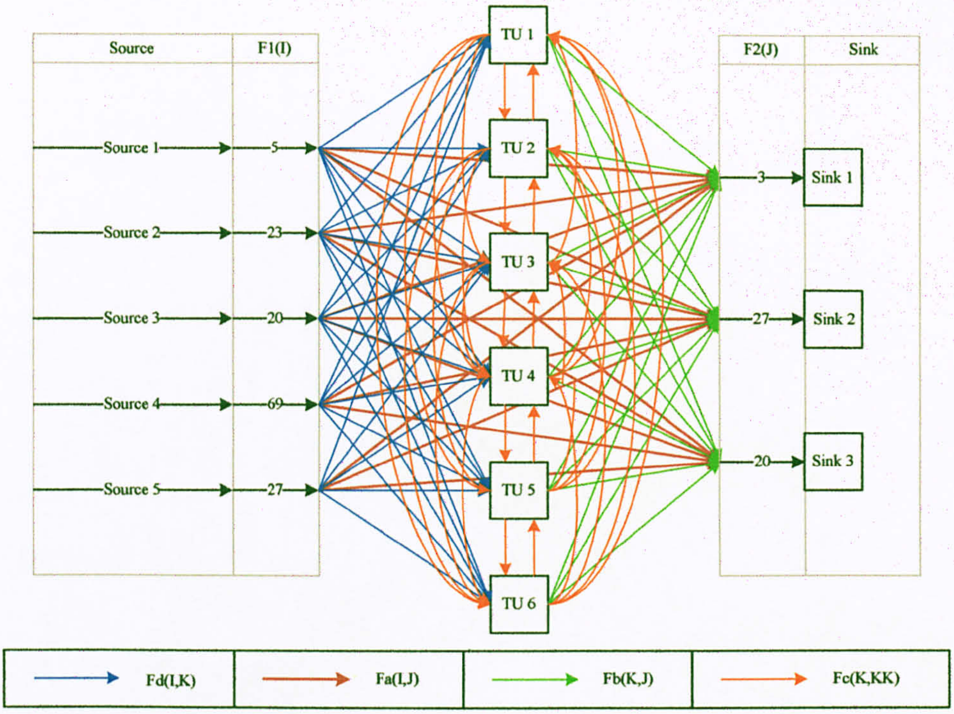

Figure 17 Superstructure representation proposed by Meyer and Floudas (2006) for generalized pooling problem

4.1.2.2 *Step 2: General Optimization Model Formulation*

(a) Material balances for source:

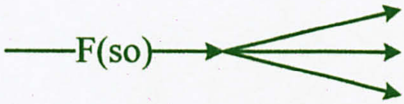

Figure 18 Source

The *source* nodes, in the set *S*, represent the effluent streams that are the outlets of a set of industrial plants. Each of these streams contains a different load of contaminants.

Mass balance for water flow for source (so):

$$F(\text{so}) = \sum_{\text{int}\in\text{INT}} F(\text{so,int}) + \sum_{\text{si}\in\text{SINK}} F(\text{so,si}) \qquad \forall \text{so} \in \text{SOURCE} \qquad \textbf{(19)}$$

Material balances on contaminant concentrations for a source:

For source, the concentration of diverged stream is the same as concentration at F(so).

$$C_{\text{co}}(\text{so}) = C_{\text{co}}(\text{so,int}) = C_{\text{co}}(\text{so,si}) \qquad \forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT} \qquad \textbf{(20)}$$

$$F(\text{so})C_{\text{co}}(\text{so}) = \sum_{\text{int}\in\text{INTERCEPTOR}} F(\text{so,int})C_{\text{co}}(\text{so,int}) + \sum_{\text{si}\in\text{SINK}} F(\text{so,si})C_{\text{co}}(\text{so,int})$$
$$\forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT} \qquad \textbf{(21)}$$

Replacing all concentration to C_{CO}(so) as mention in constraint (20),

$$F(\text{so})C_{\text{co}}(\text{so}) = \sum_{\text{int}\in\text{INTERCEPTOR}} F(\text{so,int})C_{\text{co}}(\text{so}) + \sum_{\text{si}\in\text{SINK}} F(\text{so,si})C_{\text{co}}(\text{so}) \qquad \textbf{(22)}$$
$$\forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT}$$

$$F(\text{so})\cancel{C_{\text{co}}(\text{so})} = \cancel{C_{\text{co}}(\text{so})}\left(\sum_{\text{int}\in\text{INTERCEPTOR}} F(\text{so,int}) + \sum_{\text{si}\in\text{SINK}} F(\text{so,si})\right) \qquad \textbf{(23)}$$
$$\forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT}$$

Since the concentration term C(co,so) can be eliminated from the concentration balance, it simplifies to flow balance.

$$F(\text{so}) = \sum_{\text{int}\in\text{INTERCEPTOR}} F(\text{so,int}) + \sum_{\text{si}\in\text{SINK}} F(\text{so,si}) \Rightarrow \text{flow balance} \qquad \textbf{(24)}$$

Therefore, the constraint for contaminant flow for source need to be specified as,

$$C_{co}(\text{so}) = C_{co}(\text{so,int}) = C_{co}(\text{so,si}) \quad \forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT} \tag{25}$$

(b) Material balance for interceptor:

Figure 19 Interceptor

The node set T represents the set of wastewater treatment plants that maybe used to reduce the contaminant levels and processing costs therefore vary from plant to plant.

Mass balance for water flow for a general interceptor int:

$$\underbrace{\sum_{\text{so}\in\text{SO}} Fd(\text{so,int}) + \sum_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fcc(\text{int}',\text{int})}_{\text{inlet to interceptor}} = \underbrace{\sum_{\text{si}\in\text{SI}} Fb(\text{int,si}) + \sum_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fc(\text{int,int}')}_{\text{outlet of interceptor}}$$

$$\forall \text{int} \in \text{INT} \tag{26}$$

The summation of inlet flowrate into the interceptor equal to the summation of the flowrate out of the interceptor.

Material balances on contaminant concentrations for a general interceptor:

$$\underbrace{(1-\text{RR}(\text{co,int}))\left(\begin{array}{l}\sum_{\text{so}\in\text{SO}} Fd(\text{so,int})C_{co}(\text{so,int}) \\ + \sum_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fcc(\text{int}',\text{int})C_{co}(\text{int}',\text{int})\end{array}\right)}_{\text{inlet to treatment}} = \underbrace{\left(\begin{array}{l}\sum_{\text{si}\in\text{SI}} Fb(\text{int,si})C_{co}(\text{int,sink}) \\ + \sum_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fc(\text{int,int}')C_{co}(\text{int,int}')\end{array}\right)}_{\text{outlet of treatment}}$$

$$\forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO} \tag{27}$$

Outlet of interceptor consist of multiple streams with same concentration.

$$C_{co}(\text{int,si}) = C_{co}(\text{int,int}') = C_{co}(\text{int}) \quad \forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO} \qquad \textbf{(28)}$$

Thus,

$$\left(1-\text{RR}(\text{co,int})\right)\begin{pmatrix} \sum\limits_{\text{so}\in\text{SO}} Fd(\text{so,int})C(\text{co,so}) \\ + \sum\limits_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fcc(\text{int}',\text{int})C(\text{co,int}') \end{pmatrix} = C_{co}(\text{int}) \underbrace{\begin{pmatrix} \sum\limits_{\text{si}\in\text{SI}} Fb(\text{int,si}) \\ + \sum\limits_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fc(\text{int,int}') \end{pmatrix}}_{\text{can be substituted from flow balance}}$$

(29)

$$\left(1-\text{RR}(\text{co,int})\right)\begin{pmatrix} \sum\limits_{\text{so}\in\text{SO}} Fd(\text{so,int})C(\text{co,so}) \\ + \sum\limits_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fcc(\text{int}',\text{int})C(\text{co,int}') \end{pmatrix} = C(\text{co,int}) \begin{pmatrix} \sum\limits_{\text{so}\in\text{SO}} Fd(\text{so,int}) \\ + \sum\limits_{\text{int}'\in\text{INT}\setminus\{\text{int}\}} Fcc(\text{int}',\text{int}) \end{pmatrix}$$

$$\forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO}$$

(30)

Constraints (29) and (30) consist of bilinear variables in both left hand side and right hand side of the equation. This will cause difficulty for the model to converge into optimal solution.

The general interceptor formulation is applicable for non-membrane-type interceptor. For membrane type interceptor, refer part 4.1.1.2 (d) for detail.

(c) Material balance for interceptor:

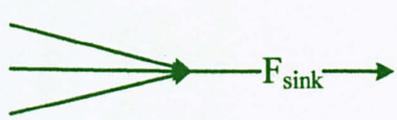

Figure 20 Sink

The *sink* nodes, in the set E, represent rivers into which the treated wastewater flows. Environmental regulations stipulate a maximum level of pollutant concentration for each of these sinks.

Mass balance for water flow for sink (si):

$$\sum_{so \in SO} Fa(so,si) + \sum_{int \in INT} Fb(int,si) = F_2(si) \qquad \forall si \in SI \qquad \textbf{(31)}$$

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.

Material balances on contaminant concentrations for sink:

$$\sum_{so \in SO} Fa(so,si) C_{co}(so,si) + \sum_{int \in INT} Fb(int,si) C_{co}(int,si) = F_2(si) C_{co}(si) \qquad \textbf{(32)}$$
$$\forall si \in SI$$

But 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 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_{co}(si). As long as C_{co}(si) is less than the maximum inlet concentration for a contaminant $C_{co,\max}$(si) for a sink, then the water can be reused or recycled. Hence, the above equality is replaced by the following inequality in the model:

$$\sum_{so \in SO} Fa(so,si) Cso(co,so) + \sum_{int \in INT} Fb(int,si) C_{co}(co,int) \leq F_2(si) C_{co,\max}(si) \qquad \textbf{(32)}$$
$$\forall si \in SI$$

Constraint (32) consists of bilinear variables on the left hand side of the equations that cause difficulty for the model to converge into optimal solution.

(d) Variables' bounds

$$0 \le Fa(so, si) \le Fa(s, e) \quad \textbf{(33)}$$

The purpose of variables' bound is to narrow the solution search. Apart from that, variables' bounds also include non-negativity constraints.

4.1.2.3 *Step 3: Objective Function*

The design variables in this case are mainly flowrate and concentration of contaminant. The objective function used for this model is same as objective function used in model proposed by Karuppiah and Grossmann (2006). This is due to the objective is design to suit the base study.

$$\text{minimize } F_{\text{FW}} + \sum_{s_1 \in \text{TU}_{\text{out}}} F_{s_1} + F_{\text{DISCHARGE}} \quad \textbf{(34)}$$

The detailed explanation for objective function is shown in part 4.1.1.3.

4.2 Computational Results

Case Study: Water Network Retrofit of a Petroleum Refinery for the Case of PETRONAS Penapisan (Melaka) Sdn. Bhd. (PP(M)SB)

4.2.1 Model Data for Case Study

In general, this case study is consist of the following given information.

1. Water using units and tanks

TABLE 3 Water using units and tanks

	Units	Description
1	FIREWATER	firewater purpose
2	OSW_SB	oily surface water storm basin
3	POT	potable water
4	OWS	oily water sewer tank
5	PSR1_CT	cooling tower 1
6	COGEN_CT	cooling tower 2
7	MG3_CT	cooling tower 3
8	PSR2_SW	service water to PSR2
9	PSR1_SW	service water to PSR1
10	CITYWATER	city water tank
11	Demin_Tank	demineralization tank
12	BOILER	Boiler system
13	HPU1	hydrogen production unit 1
14	HPU2	hydrogen production unit 2
15	BDBLu	sump pit of collection of all blowdown streams from cooling towers

2. Nominal throughput flowrate for water-using units and tanks

TABLE 4 Nominal throughput for water using units and tanks

	Process units	Nominal throughput, P(Pu)
1	FIREWATER	30
2	OSW_SB	161
3	POT	40
4	OWS	375.3
5	PSR1_CT	25.6
6	COGEN_CT	54
7	MG3_CT	25
8	CITYWATER	522.9
9	PSR1_SW	2
10	PSR2_SW	67.2
11	Demin_Tank	272
12	BOILER	212
13	HPU1	30
14	HPU2	30
15	BDBLu	56.3333

3. Treatment units

TABLE 5 Type of treatment units

	Treatment Units	Description
1	RO1	reverse osmosis unit 1
2	RO2	reverse osmosis unit 2
3	RO3	reverse osmosis unit 3
4	UF1	ultra-filtration unit 1
5	UF2	ultra-filtration unit 2
6	UF3	ultra-filtration unit 3
7	MB_EDIu	membrane or electrodialysis unit
8	RO_EDI	Reverse osmosis - electrodialysis unit
9	MT_CPI_A	mud trap and corrugated plate inceptor Basin A
10	MT_CPI_B	mud trap and corrugated plate inceptor Basin B
11	MT_CPI_C	mud trap and corrugated plate inceptor Basin C
12	DAFu	dissolved air flotation unit
13	MMF	multimedia filtration unit
14	IX	ion exchange unit
15	CFu	carbon filter unit
16	SFu	sand filter unit
17	ETS	effluent treatment system

4. Removal ratio treatment units

TABLE 6 Treatment units' performance

	Treatment Units	Removal Ratio for a contaminant				
		OnG	TSS	COD	CHLORIDE	SULPHIDE
1	RO1	0	0.975	0.90	0.94	0.97
2	RO2	0	0.975	0.90	0.94	0.97
3	RO3	0	0.975	0.90	0.94	0.97
4	UF1	0	0.8	0.80	0.8	0.8
5	UF2	0	0.8	0.80	0.8	0.8
6	UF3	0	0.8	0.80	0.8	0.8
7	MB_EDIu	0	0	0	0	0
8	RO_EDI	0	0	0	0	0
9	MT_CPI_A	0.99	0	0	0	0
10	MT_CPI_B	0.99	0	0	0	0
11	MT_CPI_C	0.99	0	0	0	0
12	DAFu	0.815	0	0	0	0
13	MMF	0	0	0	0	0
14	IX	0.5	0	0	0	0
15	CFu	0	0	0	0	0
16	SFu	0	0	0	0	0
17	ETS	0.84	0.68	0.88	0	0.99

5. Concentration for certain streams
6. Fixed flowrate for certain streams

4.2.2 Superstructure representation

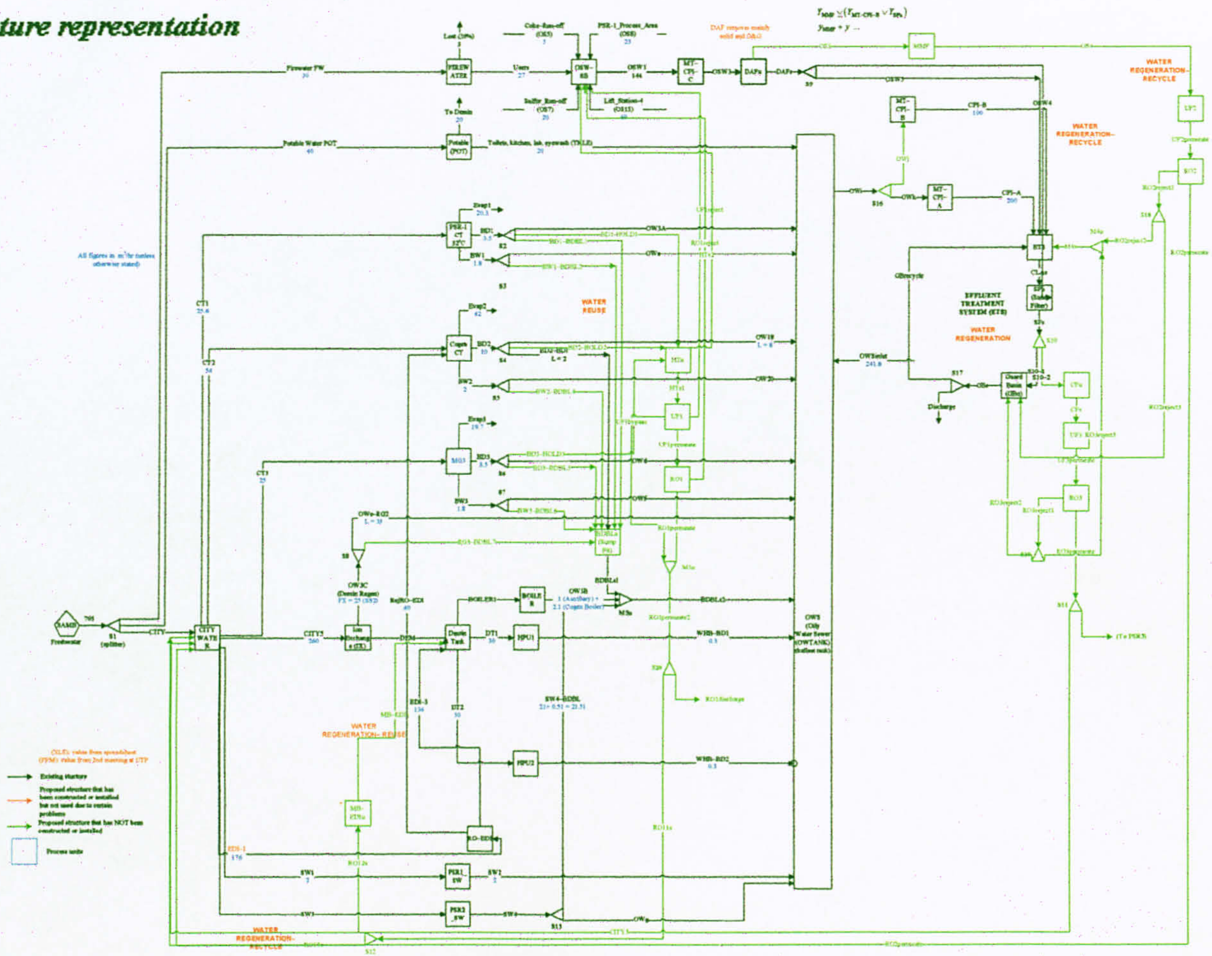

Figure 21 Superstructure representation of water network design of PP(M)SB based on the conventional state–task network (STN) approach

4.2.3 Model 1: Implementation of Computational Approach Based on Karuppiah and Grossmann (2006)

(a) Step 1: Superstructure Representation of Alternatives

We adopt the general superstructure for water network design proposed by Karuppiah and Grossmann (2006) to the problem of retrofitting the existing network of water-using and water-treatment units of PP(M)SB.

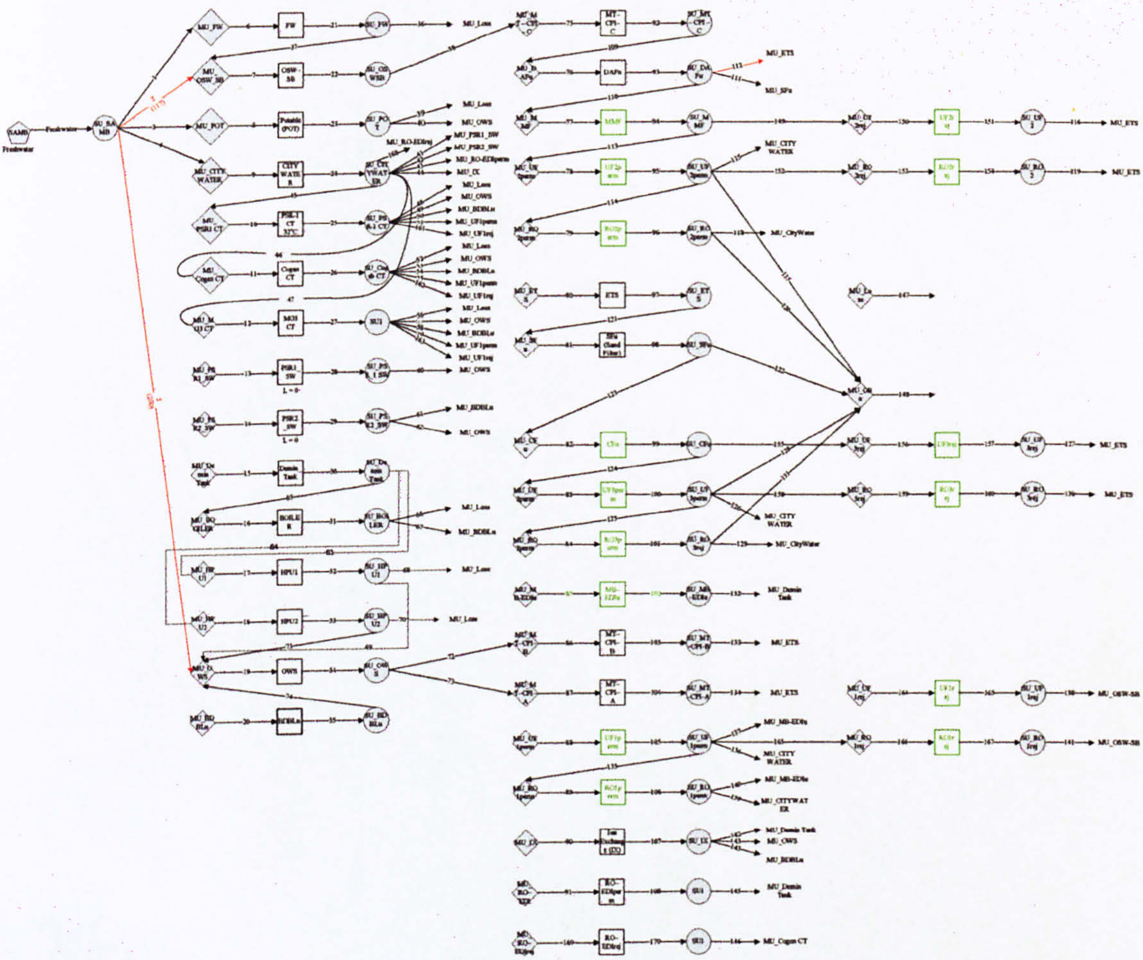

Figure 22 Superstructure representation based on of Karuppiah and Grossmann (2006) for the retrofit of the water network of PP(M)SB

In developing the superstructure representation, the most important issue is to categorize the units into process units and treatment units. Treatment units are not difficult to be differentiated, unlike water using units and tank. Some water using unit and tank can be categorized as mixer as they do not contribute contaminant to the system.

Secondly, the units need to be arranged accordingly as discussed in part 4.1.1.1. This method eases the model formulation for every unit.

(b) Step 2: Optimization Model Formulation

In this case study, the objective function is to minimize freshwater usage and also operating cost. The important data that must be included in the model includes:

1. Mass load, L for process units,
2. Nominal throughput (flow) for process units, P(Pu),
3. Maximum allowable inlet concentration for process units,
4. Removal ratio for treatment units,
5. Freshwater quality,
6. Maximum allowable discharge concentration (standard B).

The data given is transferred into mathematical model as shown in part 4.1.1.2 and solve the optimization model using GAMS.

Due to the enormous size of the optimization model formulated for the case study, we apply the incremental cost solution algorithm as proposed by Wicaksono and Karimi (2006). We refer the interested reader to this excellent paper for more details.

(c) Results

i) Optimal structure:

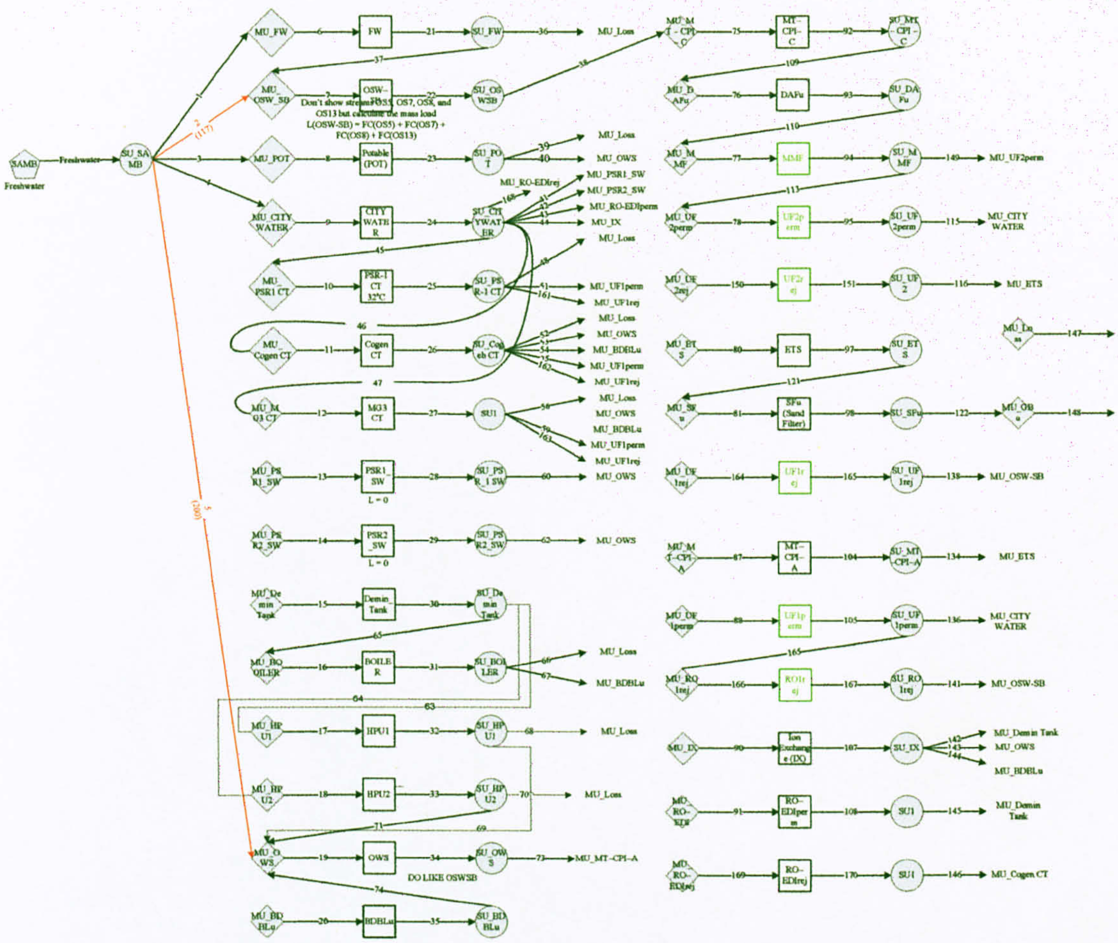

Figure 23 Optimal retrofit structure of the PP(M)SB water network with the optimal flowrates

ii) Numerical results:

TABLE 7 Numerical results and computational statistucs

Paramter	Current Plant Situation	Optimum Value
Freshwater, m^3/h	705	471.9
Discharge, m^3/h	648.6	415.5

COMPUTATIONAL STATISTICS	VALUES
Solver	GAMS / BARON
Total number of continuous variables	1899
Number of constraints	2900
Number of iterations	255
Solution	OPTIMAL
Solving time (seconds)	(negligible)

(d) Discussions on Numerical Results

The proposed optimal retrofit structure of the PP(M)SB water network is able to achieve a reduction in freshwater of 33.06 percent, and 35.94 percent reduction in discharge. The statistics on the model size and computational expense is provided in Table 7. Apart from promising results, the model can also solve the problem in very short time.

4.2.4 Model 2: Implementation of Computational Approach Based on Meyer and Floudas (2006)

(a) Step 1: Superstructure Representation of Alternatives

We adopt the general superstructure for water network design proposed by Meyer and Floudas (2006) to the problem of retrofitting the existing network of water-using and water-treatment units of PP(M)SB. The superstructure representation for this case study is shown at Figure 24, next page.

(b) Step 2: Optimization Model Formulation

In this model, the objective function is to minimize freshwater usage and also operating cost. The important data that must be included in the model includes:

1. Mass load, L for process units,
2. Nominal throughput (flow) for process units, P(Pu),
3. Maximum allowable inlet concentration for process units,
4. Removal ratio for treatment units,
5. Freshwater quality,
6. Maximum allowable discharge concentration (standard B).

The data given is transferred into mathematical model as shown in part 4.1.1.2 and solve the optimization model using GAMS.

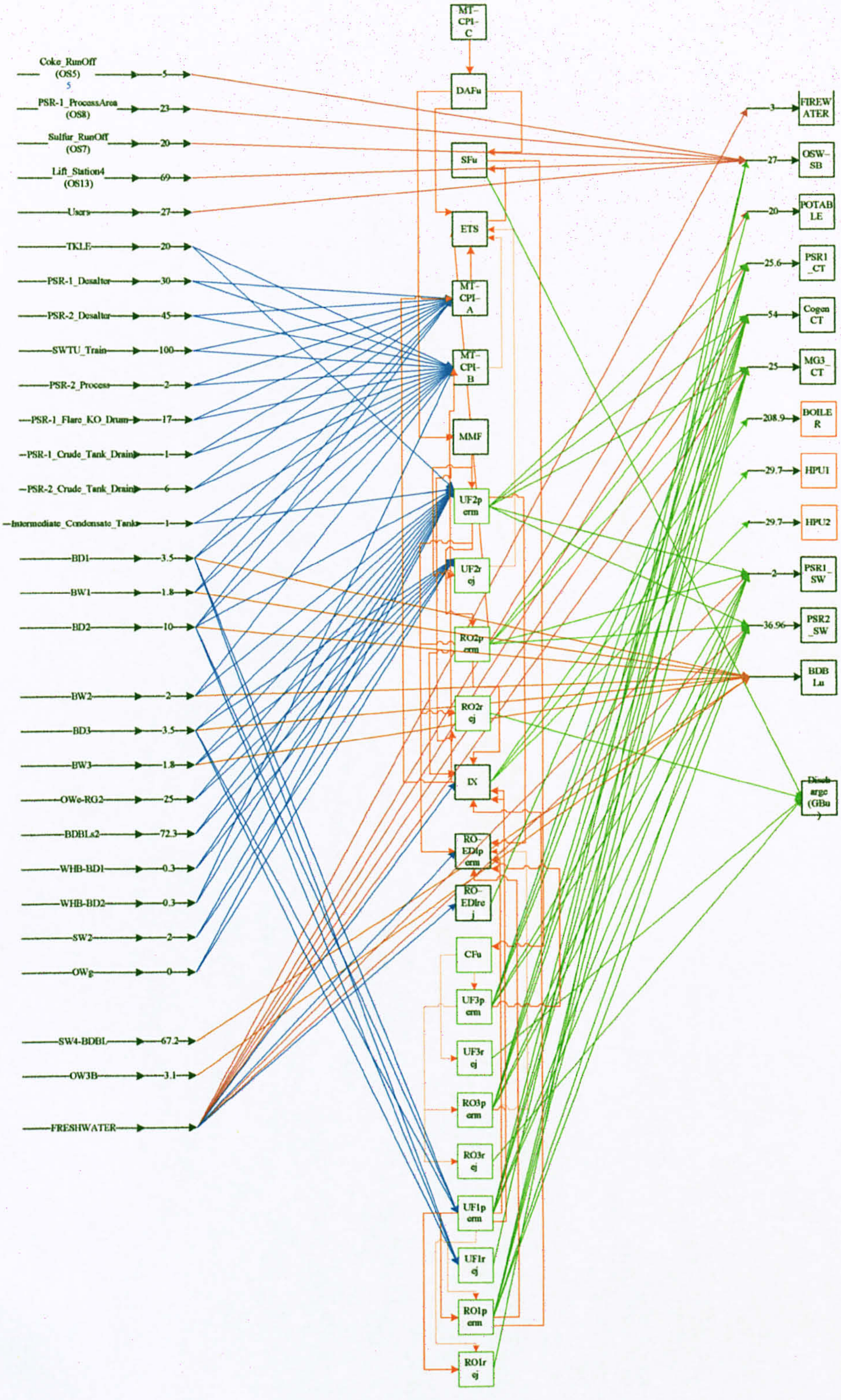

Figure 24 Superstructure representation based on of Meyer and Floudas (2006) for the retrofit of the water network of PP(M)SB

(c) Results

i) Numerical Results

TABLE 8 Numerical results and computational statistics

Paramter	Current Plant Situation	Optimum Value
Freshwater, m^3/h	705	434.86
Discharge, m^3/h	648.6	296.9

COMPUTATIONAL STATISTICS	VALUES
Solver	GAMS / BARON
Total number of continuous variables	254
Number of constraints	97
Number of iterations	32
Solution	OPTIMAL
Solving time (seconds)	(negligible)

(e) Discussion of Results

The proposed optimal retrofit structure of the PP(M)SB water network is able to achieve a reduction in freshwater of 38.32 percent, and 54.22 percent reduction in discharge. The statistics on the model size and computational expense is provided in Table 8. The results showed in Table 8 is only preliminary results, future investigation and modification need to be done to improve the result and overcome some problems (infeasible solution) faced.

4.2.5 Discussion

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.

On the other hand, the modeling tool GAMS is suitable because it allows the user to focus solely on the model formulation of the problem without being concerned about the solution method or algorithm (which is the computation engine that is running in the background of the software GAMS in order to generate the optimal solution). thus, the engineer has full control and understanding in the development of the model for the problem at hand. However, it is fair to caution that at best, the outcome or solution from the model should be relied upon to provide insights on the feasibility of the W3R alternatives being evaluated, and that the computed values should only be trusted to provide a sense of the magnitude to be expected in actual operations.

Proposed Optimal Structure

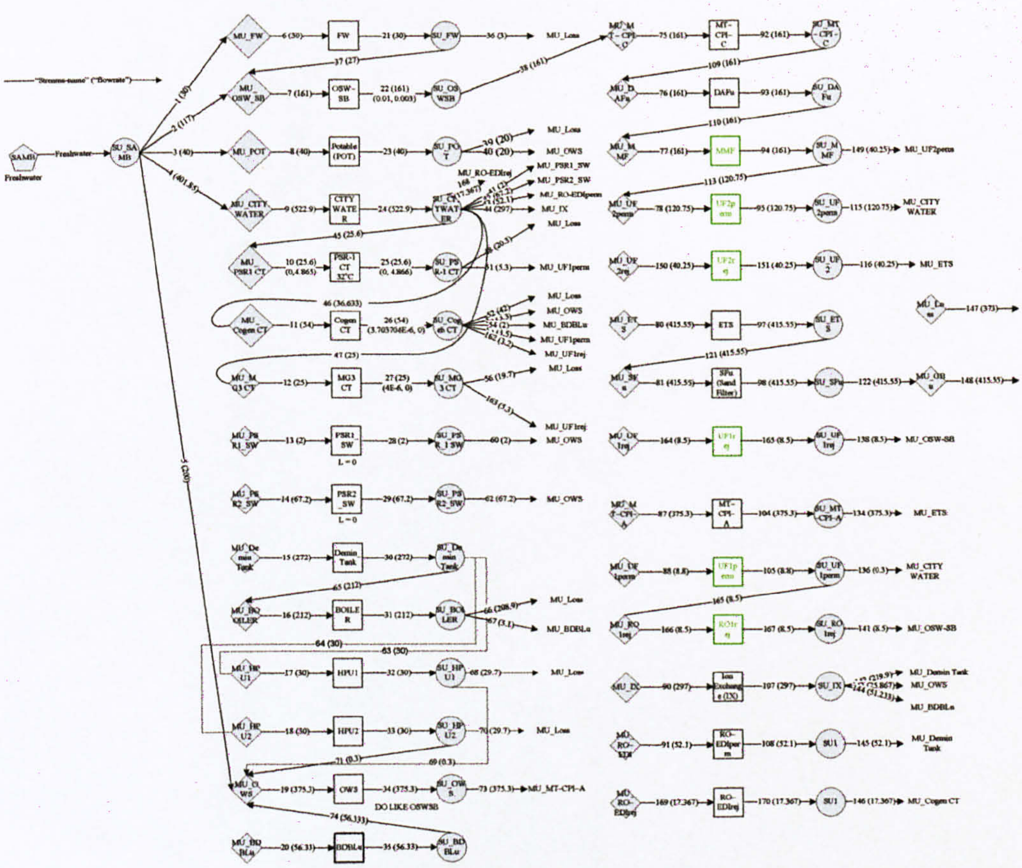

Figure 25 Optimal structure in modified superstructure proposed by Karuppiah and Grossmann

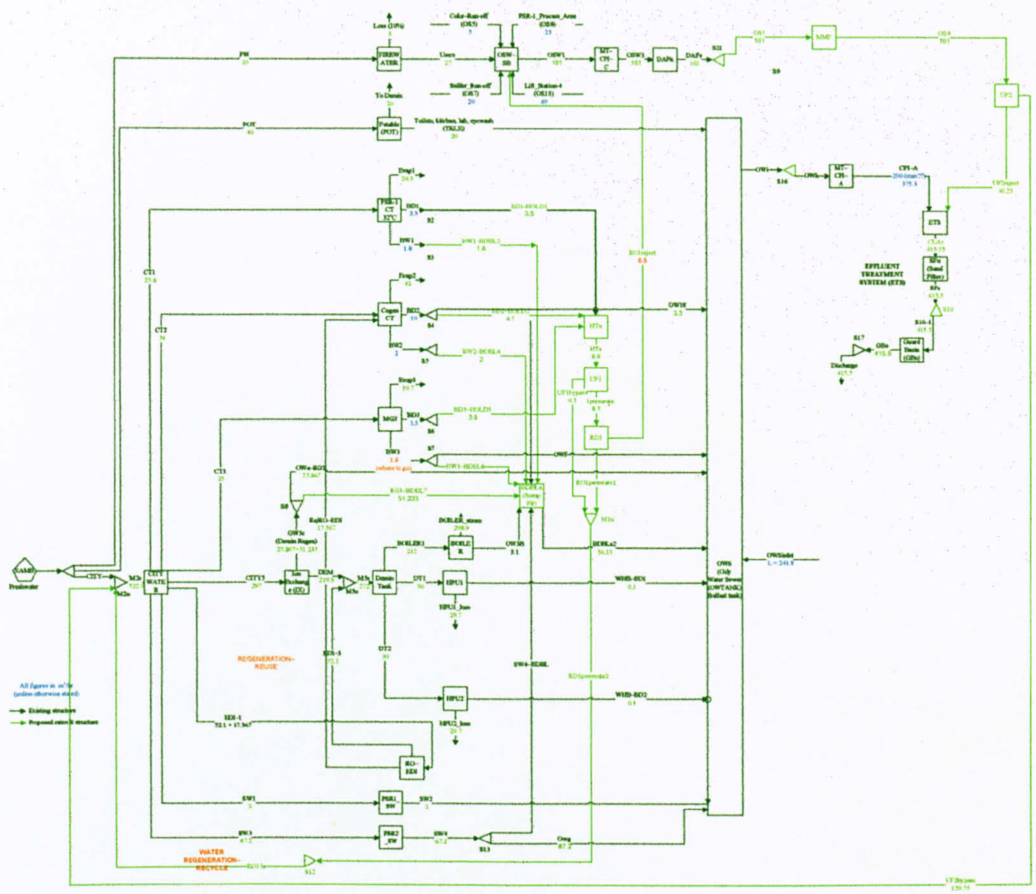

Figure 26 Optimal structure in PFD form

Economic Evaluation

Optimization model is able to aid decision-making in determining optimal retrofit design (and grassroot design) of refinery water network systems. Through the optimization model, minimum freshwater consumption, minimum wastewater discharge and minimum treatment capacity can be achieved. Minimum consumption of freshwater means reducing freshwater cost, where in the case study, the freshwater is bought from Syarikat Air Melaka Berhad (SAMB). Apart from cost, minimum consumption of water also plays the role of conserving the usable freshwater left on earth, so that our next generation can still use the freshwater like we are enjoying today.

Minimum wastewater discharge means minimizing the pollution to the environment. Apart from pollution issue, every volume of water discharge is also incurred cost. As a result, minimizing wastewater discharged is very important as well.

Lastly, minimum throughput of treatment units means minimum capital cost and operating cost. Capital cost is directly involved because a treatment unit with high throughput needs large capacity which is directly proportional to capital cost. On the other hand, treating more wastewater means incurring more operating cost, especially treatment units which use chemical to reduce level of contaminant. The new optimal retrofit should consist of trade off between the three condition discussed.

Apart from determining the optimal retrofit, the optimization model is a versatile tool to be applied to water network retrofit or grassroot design. User can manipulate the data or information to yield new result. An example is manipulating the objective function to put priority to certain variables.

Sustainability Issues

In order to overcome the problems discuss earlier in Chapter 1, optimal use of resources play significant roles. One of the resources that must be taken into account is water. A lot of people have neglected the value of water as the cost to obtain freshwater is low. As a responsible people we need to always remember that although the cost of water is high, but the value is high. Apart from freshwater, discharge of wastewater to the environment is also an issue. This issue can be overcome by designing an optimization model to minimize the discharge of contaminant to environment, or achieve zero discharge if possible. However, to achieve least freshwater consumption and zero discharge, water treatment cost is the trade off. Through the optimization model, a well-balance retrofit can be achieved.

CHAPTER 5
CONCLUSIONS AND FUTURE WORK

5.1 Conclusion

In conclusion, the research project has achieve the following objectives,

1. Developed superstructure representation for retrofit of existing water network
2. Formulated NLP & MINLP optimization model based on superstructure
3. Solved optimization model using GAMS modeling language for determining flowrates and compositions

All three objectives are achieved for this project. However there are still a lot of improvement to be done, especially fix-flow model formulation.

5.2 Recommendations for Future Work

In the process of achieving these objectives, we found that there are still a lot of improvements can be done to produce better optimization model and results. These findings include,

1. Incorporate economics optimization: formulate objective function that explicitly considers capital & operating costs
2. More detailed nonlinear models for wastewater treatment units in stead of just considering fixed removal ratio, rr.
3. Application of proposed techniques to more industrial case studies, including petrochemical plants.
4. Further comparison between fixed-load problem and fixed-flow problem.

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