# DESIGN OF OPTIMAL WATER ALLOCATION NETWORK IN CHLOR-ALKALI PLANT

IZYAN BINTI ISMAIL

BACHELOR OF CHEMICAL ENGINEERING
UNIVERSITI MALAYSIA PAHANG

# OPTIMAL WATER ALLOCATION NETWORK IN CHLOR-ALKALI PLANT

IZYAN BINTI ISMAIL

Thesis submitted in fulfillment of the requirements for the award of the degree of Bachelor of Chemical Engineering in Chemical Engineering

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## SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering in Chemical Engineering.

Signature
Name of Supervisor: MISS ZAINATUL BAHIYAH HANDANI
Position: LECTURER OF FKKSA, UMP
Date:

## STUDENT'S DECLARATION

I hereby declare that the work in this thesis is my own except for quotations and summaries which have been duly acknowledgement. The thesis has not been accepted for any degree and it not concurently submitted for award of other degree.

Signature:
Name : IZYAN BINTI ISMAIL
ID Number: KA08131
Date:

Dedicated to my parents

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# ABSTRACT

Water is the most common raw material in the industries. Due to the increasing water scarcity in certain countries, many industries are exposed to the fresh water risk. In order to overcome this problem, optimal water allocation network is applied in many industrial plants. In this study, a new generic mixed integer non-linear programming (MINLP) involving multiple contaminants, pH, hardness and total dissolved solid (TDS) is present to maximize the fresh water saving in the plant. All options including source of elimination, source of reduction, reuse or recycle, outsourcing and regeneration are considered in water minimization network. Four major steps, limiting water data extraction, superstructure representative, developing mathematical formulation and applying GAMS software are followed in this work. Minimum water target is then design based on the steps used to achieve the maximum freshwater saving and wastewater generation. By the end of this study, the design of water network system give higher percentage reduction of the freshwater consumption and the waste water generation.

# ABSTRAK

Air adalah bahan mentah utama yang paling biasa dalam industri. Oleh kerana kekurangan air yang semakin meningkat di beberapa buah negara-negara, banyak industri yang terdedah kepada risiko air bersih. Dalam usaha mengatasi bagi mengatasi masalah ini, peruntukan rangkaian air optimum di gunakan dalam kawasan industri. Dalam kajian ini, generik pengaturcaraan campuran integer bukan lurus (MINLP) yang melibatkan pelbagai bahan cemar seperti pH, kekerasan, dan jumlah pepejal larut (TDS) yang hadir untuk memaksimumkan jumlah penjimatan air bersih dalam kawasan industri. Semua pilihan termasuk sumber penghapusan, pengurangan, penggunaan semuala atau kitar semula, sumber luar dan penggunaan semula di beri penekanan dalam rangkaian meminimumkan air. Empat langkah utama iaitu pengekstrakan data had air, wakil rangkaian, membentuk formulasi matematik dan penggunaan perisian GAMS digunakan dalam kerja ini. Minimum sasaran air dibentuk berdasarkan langkah-langkah yang di gunakan untuk mencapai penjimatan air bersih dan penggunaan semula sisa air yang maksimum. Pada akhir kajian ini, reka bentuk sistem rangkaian air memberi peratusan pengurangan air bersih dan penggunaan sisa semula yang lebih tinggi.

# TABLE OF CONTENT

## LIST OF TABLES

## LIST OF FIGURES

# LIST OF SYMBOLS

| | |
|---|---|
| $\sigma_{j,\mathrm{re}}$ | Certain percentage of reduction |
| $A_i$ | Adjusted water source flow rate |
| $B_j$ | Adjusted water demand flow rate |
| $Cd_{j,k}$ | Contaminant concentration of water demand |
| $Cos_{os,k}$ | Contaminant concentration of outsource |
| $Cro_{r,k}$ | Contaminant concentration of regenerated water |
| $Cs_{i,k}$ | Contaminant concentration of source demand |
| $Cw_k$ | Contaminant concentration of fresh water |
| $Da_{j,e}$ | Elimination demand flow rate |
| $Da_{j,re}$ | Reduction demand flow rate |
| $F_{i,j}$ | Reuse / recycle flow rate |
| $F_{os,j}$ | Outsource water flow rate |
| $F_{r,j}$ | Regenerated water flow rate |
| $FW_j$ | Freshwater flow rate |
| $S_i$ | Water source flow rate |
| $X_{j,e}$ | Variable for elimination selection |
| $X_{j,o}$ | Variable for original selection |
| $X_{j,re}$ | Variable for reduction selection |
| $WW_i$, | Discharge water flow rate |

# LIST OF ABBREVIATIONS

| | |
|---|---|
| BOD | Biochemical oxygen demand |
| COD | Chemical oxygen demand |
| DCS | Distributed control system |
| HCl | Hydrochloric acid |
| GAMS | General algebraic modeling system |
| LP | Linear programming |
| MATLAB | Matrix laboratory |
| MILP | Mixed integer linear programming |
| MINLP | Mixed integer non-linear programming |
| MTB | Mass transfer-based |
| NaOH | Sodium hydroxide |
| NMTB | Non-mass transfer-based |
| NLP | Non-linear programming |
| PAC | Polyaluminium chlorine |
| RLT | Reformulation-linearization technique |
| TDS | Total dissolved solid |
| WCA | Water cascade analysis |
| WMH | Water management hierarchy |

# CHAPTER 1

# INTRODUCTION

## 1.1 Introduction

This chapter gives an overview on the global water outlook and Malaysia water outlook. In this chapter, it also includes the research background, problem statement, research objective, and the scope of study.

## 1.2 Global Water Outlook

About 70% of the world's surface is covered by water. From this percentage, 97% of the water is salty and only 3% is freshwater. Out of the total freshwater, two–thirds (77%) is locked up as snow, polar ice caps and glaciers while other 22% is stored deep underground as inaccessible groundwater, soil moisture and swamp water. Less than 1% of the world's freshwater resources is accessible for human use (Johannesburg Summit, 2002).

The uses of fresh water divided into three major sectors. There are agriculture, domestic and industry. From the research done by World Water Assessment Programme (WWAP), about 70% of fresh water used in irrigation, 22 % used for industry and the balance for the domestic use. Figure 1.1 shows the pie chart for the percentage of freshwater use for the common sectors.

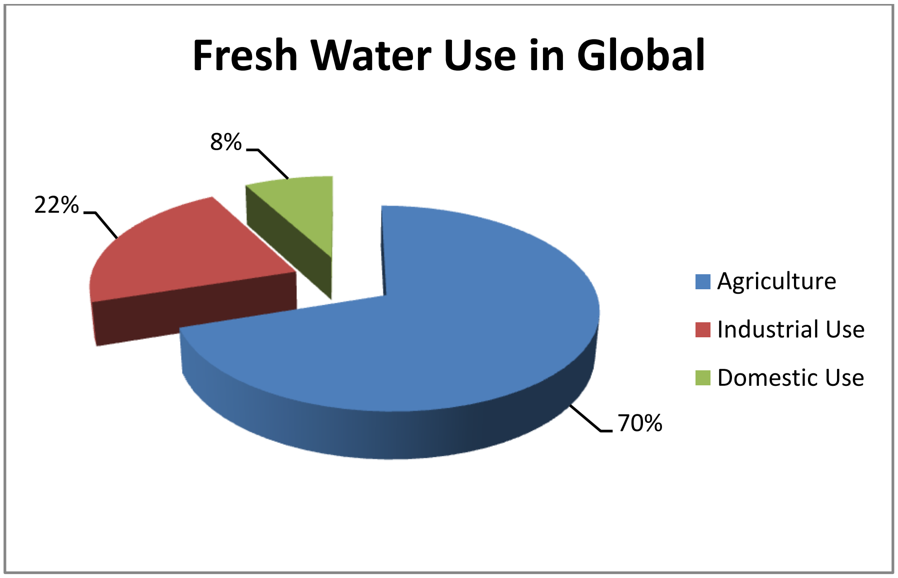



**Figure 1.1**: Percentage fresh water use in three major sectors for global outlook

Source: World Water Assessment Programme, WWAP

Water is increasingly scarce and become more valuable as populations expand and economies grow over years. Instead of that, mismanaging water use also leads to this problem. In the last century, water use has been growing at more than the rate twice of population increase. Due to this rate, about one-third of the world's population lives in countries suffering from moderate-to-high water stress. An area is experiencing water stress when annual water supplies drop below 1 700 $m^3$ per person. When annual water supplies drop below 1 000 $m^3$ per person, the population faces water scarcity (United Nations Environment Programme (UNEP, 2008). By 2025, water withdrawals are predicted to increase 50% due to the population growth (UNEP, 2008). The global water consumption and withdrawal is shown in Figure 1.2.

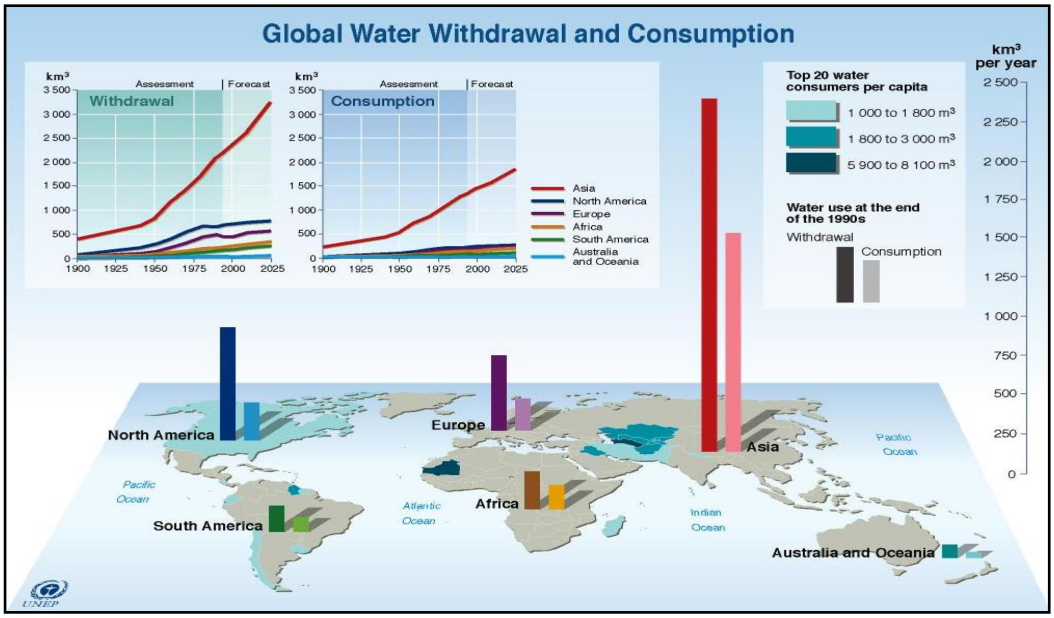



**Figure 1.2:** Global water withdrawal and consumption

Source: UNEP (2008)

## 1.3 Malaysia Water Outlook

Malaysia at present is highly dependent on the more than 189 river systems that contribute 97% of the total national water use, with the remainder 3% being contributed by groundwater (World Wide Fund for Nature, WWF Malaysia). The critical factors having an impact on our freshwater resources include population growth, economic growth and climate change. Due to the population growth, people are demanding more on the water resource to sustain life and to improve the economic activities. Although the earth's water cycle remains, but there still some problems need to be considered such as rainfall.

Similar to global water outlook, Malaysia Water Outlook also divided the uses of fresh water into three major groups which agriculture, domestic and industry. The percentage of the water consumption is slightly different with the global whereby in Malaysia, the percentage of the water use in agriculture is 76%, 13% in industry and 11%

for the domestic use. Although there are some differences in term of values, but Malaysia still expose to the limitation of the water which leads by increasing population (Earth Trend, 2003).

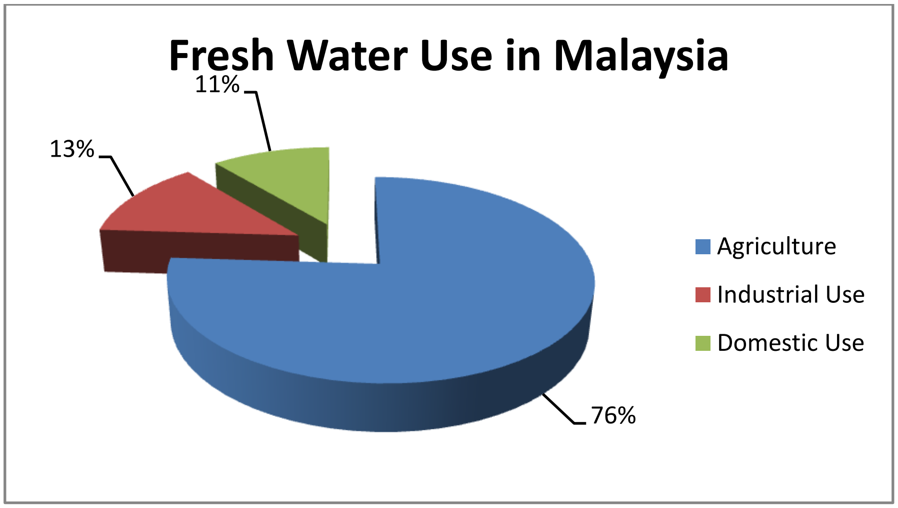



**Figure 1.3**: Percentage fresh water use in three major sectors for Malaysia outlook

Source: Earth Trend (2003)

The water shortage issues are due to the insufficient water quantity and quality at the high water demand location such as urban area, industrial and agricultural areas. As reported by Ujang et al. (2008), the areas found as the abundant fresh water are Kuala Lumpur city, petrochemical complex at Melaka and Kerteh also Muda agricultural area and facing this problem during extended dry weather periods which last up to maximum four months. By 2020, Malaysia will become a fully industrialized nation and this will increase the water demand in Malaysia. With the cost of water usage, sewerage and rising the effluent trade, industry people are conscious on the cost saving.

## 1.4 Problem Statement

Water is probably the most common raw material in the industries. It works as separating agent, cooling and heating medium, cleaning agent and etc. Nowadays, many industries are exposed to the freshwater risks due to growing water stress. If the water stress keeps continuing, it will cause the water scarcity. Water stress is refer to an area experiencing annual water supplies drop to 1700 $m^3$ per person while a country said to experience water scarcity when the annual water drop below 1700 $m^3$ per person (Institute for Global Environmental Strategies, 2003). This problem will be the serious challenge to the investors and companies if they unaware about this matter. In order to reduce the risk, an alternative way, the optimal water allocation network is design to give the minimum fresh water consumption and wastewater generations also minimize the water cost.

Given a set of global water operations of various water sources and water demand containing multiple contaminants, it is desired to design a minimum water network using mathematical programming approach.

## 1.5 Objective of Study

The main objective of this study is to design an optimal water allocation network by using the mathematical programming approach in order to minimize the fresh water consumption for chlor-alkali plant.

## 1.6 Scope of Study

This research is to minimize the fresh water consumption and wastewater generation for system involving multiple contaminants. For multiple contaminants, there are many parameters need to be consider such as biochemical oxygen demand (BOD), chemical oxygen demand (COD), total dissolved solid (TDS), pH and others. In this work, three contaminants are being focusing on which are pH, TDS and hardness. pH is refer to the concentration of hydrogen ions in the solution to determine the alkalinity and acidity of the solution. TDS itself is the amount of all dissolved solid in water which contains either organic or inorganic material while hardness can be defined as the concentration of multivalent metallic cations, magnesium and calcium ions in solution. The mathematical modeling that will be use in this work is Mixed Integer Non-linear Programming and commercial software, General Algebraic Modeling System (GAMS) is employ in this study.

## 1.7 Significance and Rationale

This work will give an alternative way to maximize the fresh water saving as well as minimize the cost of water usage in chemical industry. Other than that, the amount of wastewater discharge as effluent from the operation process can be reduce and this can reduce the treatment cost of the effluent.

# CHAPTER 2

# LITERATURE REVIEW

## 2.1 Introduction

Industrial application usually involved the removal of undesired substances. The most common material used for this purpose is water due to its physical and chemical properties which allow water to pick up substances in any circumstance. Large consumption of water in industry, its increasing cost, as well as strict environmental regulations on the industrial effluents. This has motivated the development of new methods that enable the reduction of effluents to the environment. One way which can minimize the water use and wastewater generation is through reuse or recycles. Two approaches have been used to obtain a good design for the optimal water network through pinch analysis and mathematical programming techniques.

## 2.2 Operation of Water Usage

Operation of water usage in a process can be classified into two categories. There are mass transfer-based (MTB) and non-mass transfer-based (NMTB). A MTB water usage process can be explained as transfer of a species from a rich stream to water as stated in Handani *et al*. (2009) work. This type of operation also known as fixed contaminant load problem and the important assumption for MTB is inlet and outlet flow rates are equal. On the other hand, NMTB water using operation which also known as fixed flow rate problem is defined as function of water besides a mass separating agent. For this operation, water flow rate is more important than the contaminants amount. Hence, the assumption used for the MTB cannot be applied in the NMTB water using operation.

## 2.3 Graphical Method

Wang and Smith (1994) firstly introduced the graphical method to minimize water and wastewater flow rates prior to any network. This method was based on the pinch analysis techniques for heat integration. The water using operation is modelled as MTB for single contaminant. In this work, there are two-step procedures are considered, the composite profile is introduced to locate the minimum fresh water and wastewater flowrates. Later, Dhole et al. (1996) corrected the graphical method introduced by introducing new composite curves. Two composites, water source and demand are plotted together and the potential for water reuse is showed by the overlapping between the two composites. Besides, it also represented the minimum fresh water required and wastewater generation.

The same concept is further improved by Doyle and Smith (1997) for multiple contaminants. Two cases are considered in this paper, mass transfer is modeled based on fixed mass load and fixed outlet concentration. In the first case, it can be solved by non-linear optimization where as for the second case, it can be solved by linear optimization. To overcome non-linear optimization problem, the linear model is used to initialize non-linear optimization problem. This solution is combined with the graphical method that has been introduced by the previous researchers. For multiple contaminants, Wang et al. (2003) proposed water networks with single internal water main. This method reduces the water consumption and approached the minimum target of water consumed.

More recently, a new graphical method for minimum fresh water and wastewater target is presented by Hallale (2002). This is to overcome the source and demand composite curves which the targets obtained may not be the true solution. The approach used is based upon a new representation of water composite curves and the concept of water surplus. Advantage of this method is being able to deal with wide range of water using operation.

The research discussed on the network design, process modifications and water regeneration where the insights obtained from the graphical tools are most valuable.

However, the tedious graphical drawing in locating minimum water target is a problem in water surplus diagram. Apart of that, the diagram is usually based on the assumed of the fresh water value. This leads to the inaccuracy of this graphical method. Lately, Tan et al. (2002) introduced water cascade table to overcome the limitation of water surplice diagram methodology. Manan et al. (2004) presented the water cascade analysis (WCA) as a new technique to establish the minimum water and wastewater targets for continuous water-using processes. This analysis is an alternative to the water surplus diagram. By eliminating the tedious iterative steps of the water surplus diagram, the WCA can yield accurate minimum water targets and pinch point locations. This method only relies on a single water main and it is not guarantee for optimal water solutions. Most previous researches focusing on the pure fresh water but the fresh water might contain contaminants. By realizing this issue, Foo (2007) extended the studies for single and multiple impure fresh water feed. The problems are addressed by numerical targeting tool of water cascade analysis.

On the basis of pinch analysis method that has been presented by Wang and Smith (1994), graphical methods have been applied to analyze the regeneration recycling water system by several authors (Mann and Liu, 1999; Bagajewicz, 2001). The targets for freshwater consumption, regeneration concentration and regenerated water flow rate for regeneration recycling were involved in their research. Basically, regeneration recycling means that the used water from some processes is recycled back to the same processes after regeneration while regeneration reuse means water can be generated by partial treatment to remove the contaminants and then reused by the other processes as stated in Feng et al. (2007).

## 2.4 Water Management Hierarchy

Wan Alwi et al. (2008) introduced water management hierarchy (WMH) to improve in process modification. In WMH, it consists of five levels, source of elimination, source of reduction, direct reuse or outsourcing of external water, regeneration and use of fresh water. Basically, the levels in WMH are arranged according to most preferred option to the least preferred. There also a set of heuristics used as a guide for design. Figure below shows the priority level of the WMH.

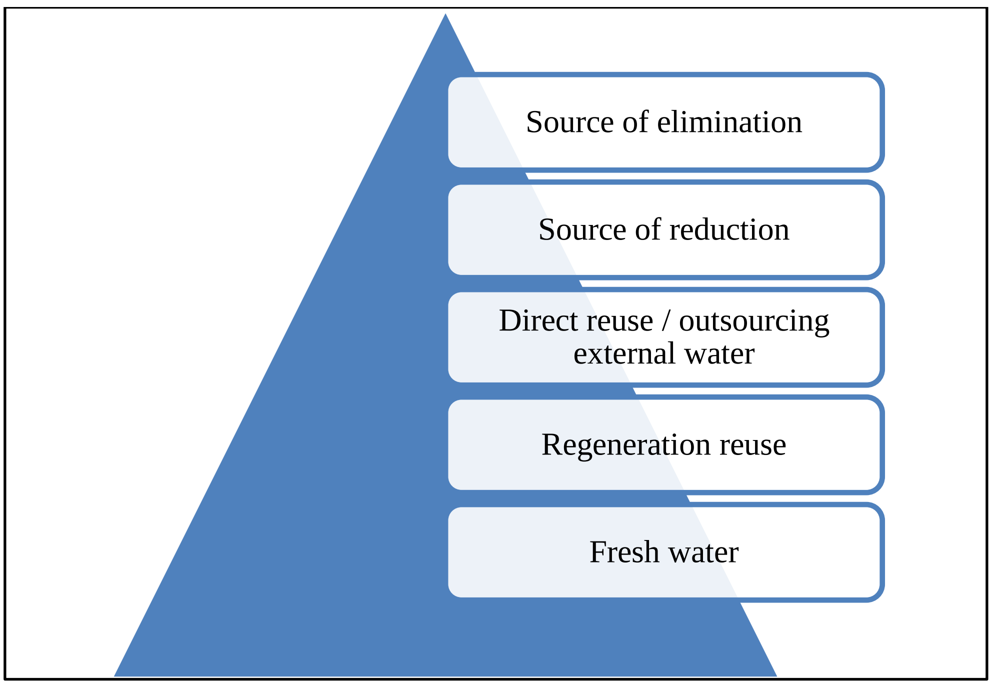



**Figure 2.1:** Levels of water management hierarchy

Source: Wan Alwi et al. (2008)

Source of elimination is placed at the top in the hierarchy and it concerned to complete eliminate the fresh water usage in the process. As stated above where, water is the most crucial element in the industrial process and it make this option is possible to be apply in the water system. An example is by using the air, which is free cost as cooling medium instead of using water.

The next place in WMH is source of reduction. This option is more correspond to be applying in reducing fresh water demand. It is possible to reduce fresh water compared to the first option although it is the ultimate goal in WMH. The water usage can be reduce by using water saving toilet flushing rather than using commercial toilet flushing system.

Direct reuse or outsourcing external water is the third option this hierarchy can be describe as using the spent water within the process plant or using the external water such as rainwater as the water supply. Although this types of water have different quality, but they still acceptable to perform the water demand usage. Rainwater can be channel to the ablution task while the water from wash basin can be used in the toilet flushing system.

Level four is the next option after direct reuse/outsourcing external water. Regeneration is refers to the water treatment to achieve the water quality as the water requirement before it being reuse or recycle. This regeneration can be divided into two types which are regeneration-recycle and regeneration-reuse. The type is involves the reuse of treated water in the same process while the regeneration-recycle indicates the usage of treated water in different process or equipment. When those four options in WMH are not possible to be applied, hence the fresh water can be considered.

## 2.5 Mathematical Programming Technique

Compared to graphical method, mathematical programming is more reliable and more guarantee for optimal water solution. Takama et al. (1980) were the first to address problem of optimal water allocation network in a petroleum refinery. The optimization problem is solved based on both design of water usage and the water treatment networks with non-linear programme (NLP) formulation. A relaxed linear programme (LP) formulation was obtained by Quesada and Grossmann in 1994. The technique used is reformulation-linearization. Bagajewicz and Savelski (2001) have addressed a mathematical modeling using linear programming (LP) formulation to obtain maximum water recovery when single contaminant is present. Both of them improve their research and in 2003, they came out with necessary conditions of optimality proved for single component. The condition is the outlet concentration must be equal to the maximum values for the optimal water network. In their work stated that mathematical modeling can produce global optimal solution.

An automated design of total water systems has been proposed by Gunaratnam et al. (2005) based on the optimization of the superstructure that gives a mixed integer non-linear (MINLP) formulation. The binary variables are taking into consideration. In the first stage, the problem is divided into both MILP and LP problems. This method is used in order to get the initial starting point that then used in the second stage through the solution of the MINLP. Since then, many researchers (Doyle et al., 1997; Gunaratnam et al., 2005; Teles et al., 2008) using two stage optimization methods to solve the optimal water solution. Recently, Alva-Argáez et al. (2006) proposed a systematic methodology that empowers the previous engineering concept by novel decomposition approach which simplifies the optimization problem. This approach used the water pinch insight to define successive projections in the solution. The method focused on the petroleum refineries and explained the saving between freshwater costs, wastewater treatment, piping costs and environmental constraints on the discharge.

Another new approach has been proposed by Teles et al. (2008) which using a standard technique with multiple starting points for the optimal design of water using network including both MTB and NMTB operations. This procedure replacing a non-linear programme (NLP) by a succession of linear programme (LP) that solved during initial procedures. Different with Castro et al. (2007), they used heuristic procedure to obtain good starting points.

Recently, a generic linear programming (LP) model has been developed by Handani et al. *(*2009) based on the water network superstructure to simultaneously generate the maximum water recovery for both MTB and NMTB problems involving single contaminant. To date, the authors extended their research by proposing a new generic mixed integer linear programming (MILP) model to holistically minimize fresh water consumption and wastewater generation for multiple contaminants systems which considered various options for water minimization. The superstructure is constructed based on the water management hierarchy where freshwater concentrations for all contaminants are assumed to be either zero or non-zero. In addition, Reformulation-Linearization technique (RLT) was proposed by Sherali and Tuncbilek, (1992). A linear programming relaxation is derived based on this technique which generates nonlinear implied constraints to be included in the problems and subsequently linearizes the resulting problems by defining a new variable. Then, the construct is used to obtain lower bound in the context of a proposed branch and bound scheme.

Most recently, Matijasevic, Dejanovic and Spoja (2010) proposed a water network optimization using MATLAB. The methodology of mass and energy integration is applied in this study based on relaxation of a non-convex non-linear programming problem into a mixed integer linear programming (MILP). The MILP then was simplified according to the heuristic rules and solved using MATLAB.

# CHAPTER 3

# METHODOLOGY

## 3.1 Introduction

In multiple contaminants system, a mixed-integer nonlinear programming (MINLP) is always being used in maximizing freshwater consumption and waste water in a plant through water reuse and recycle. There are four important steps that need to be taken in order to produce global optimal solutions. Figure 3.1 shows the overall methodology for this study.

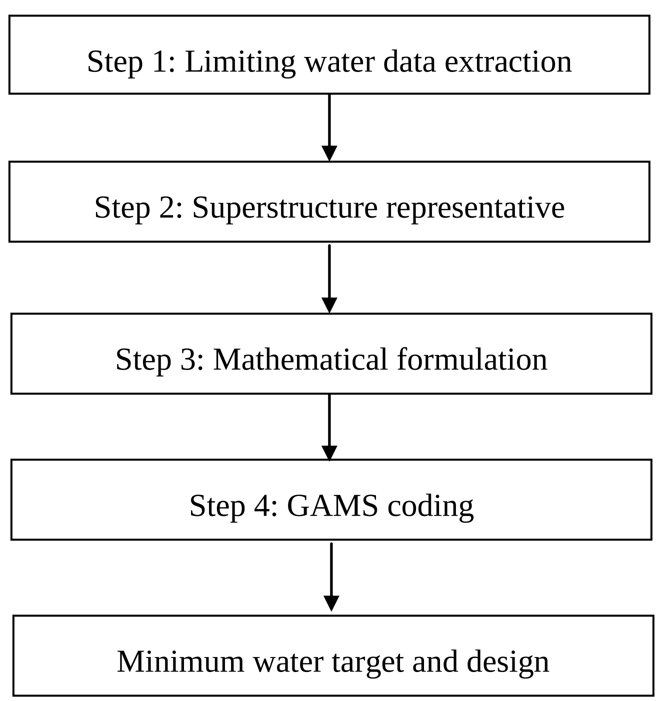


**Figure 3.1:** The steps of minimum water targets through maximum water recovery network

### 3.1.1 Step 1: Limiting Water Data Extraction

The first step is to identify water sources and water demand in the chlor alkali plant. In this step, the limiting water data was taken from Handani et al. (2010) that consist of information regarding water demands and water sources. Those data were listed in terms of flow rate and concentration. The water sources are referred to water possible for recycling or reuse while water demands are the actual requirements for each system.

Figure 3.2 illustrates the operation in the chlor-alkali plant. In this plant, it involved fifthteen water sources and fourteen water demands in the whole operation. The fresh water usage is separated into three major uses which are process uses, non-process uses and domestic uses. From these uses, non-process conquered the water usage where it consists of the most demand and sources required among others.

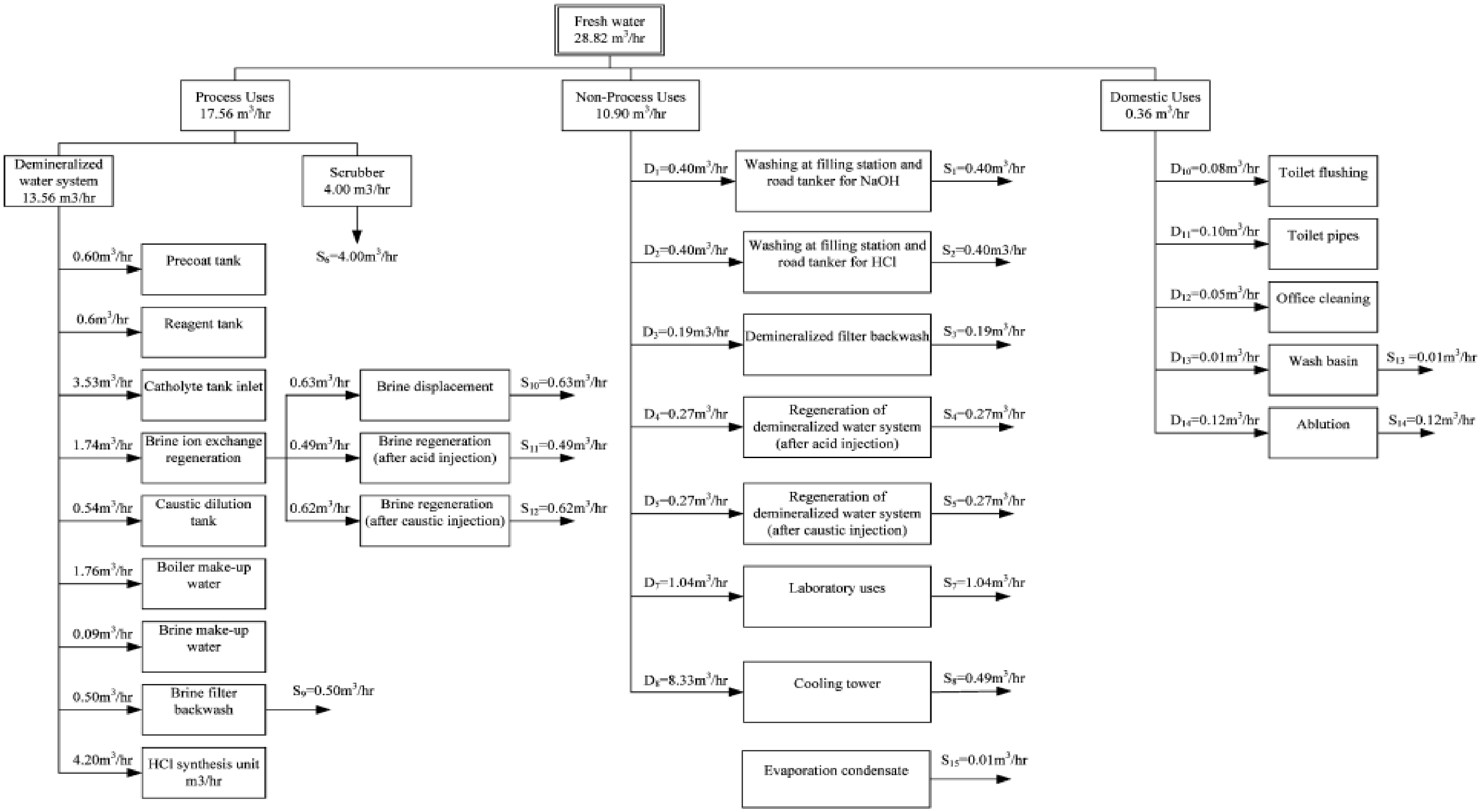
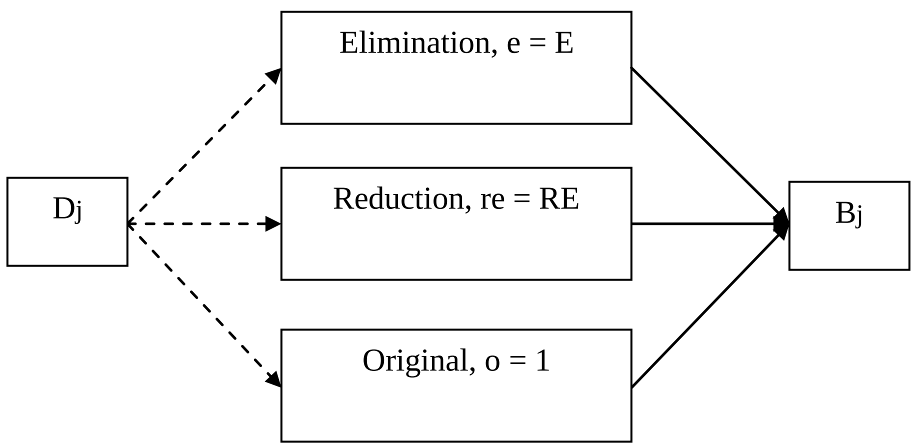



**Figure 3.2:** Water distribution in chlor-alkali plant

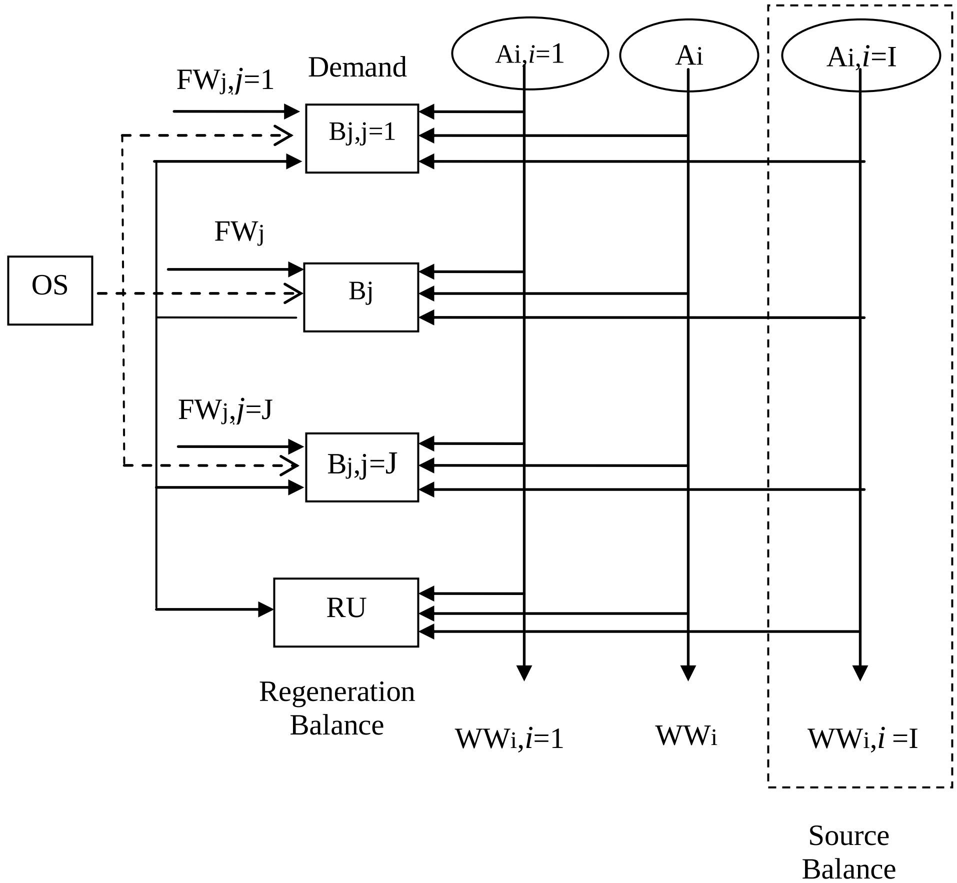
Source: Handani et al. (2010)

### 3.1.2 Step 2: Superstructure Representation

Superstructure representation is used to determine the possible connection between water demands, water sources and wastewater discharge from a plant. Generally, in each operation, there must be an inlet and outlet stream. The inlet stream referred to the water needed in a stream and the water can be either from fresh water or the recycled water from regeneration unit. For the outlet stream, it described the unwanted water in that stream which can be directly discharge from the stream or treated in regeneration unit before it being used by other operation. Figure 3.3 shows the general superstructure for water utilization network based on the WMH that consider both MTB and NMTB operations.




(a)




**(b)**

**Figure 3.3:** General superstructure for a minimum water utilization network with WMH options that consider both MTB and NMTB operations. (a) Water network superstructure to obtain the adjusted demand flow rate, $B_j$, when possible source elimination and reduction are considered (b) Water network superstructure for maximum water recovery that includes outsourcing and regeneration options.

Source: Handani et al. (2010)

In this work, water management hierarchy (WMH) is used to illustrate the minimum water network superstructure. All possible options or methods including elimination, reduction, direct reused or outsourcing, and regeneration are considered to minimize the fresh water consumption. Figure 3.3a shows the superstructure to obtain adjusted water demand flow rate, $B_j$ when three possible options; elimination, reduction and original are considered in water minimization scheme. Only one option can be selected at one time. In this superstructure, the binary variables $X_{j,e}$ represent the source of elimination, $X_{j,re}$ represent source of reduction and $X_{j,o}$ represent the original. If those option s are implement in water minimization scheme, the flow rates are indicate as $Da_{j,e}$, $Da_{j,re}$ and $Da_{j,o}$.

Figure 3.3b illustrates all the possible configuration of water connection in a plant. For the water demand, $B_j$, the water can be supplied from fresh water, $FW_j$, reused or recycle water, outsource water such as rainwater or river, or regenerated water. Meanwhile, the generated water from the water source, $A_i$, can be directly discharge, reused or treated in regeneration unit.

### 3.1.3 Step 3: Mathematical Formulation

Based on the superstructure in Step 2, a mathematical model will be developed. This model is to determine the minimum freshwater consume in the operation and the minimum wastewater discharged. The mathematical models proposed in this work can be used to solve water network design problem to simultaneously generate the minimum water targets and use process changes guided by water management hierarchy.

1 Assumption

a) No changes in water flow rate in the operation
b) The water system is operate continuously
c) The system is isothermal

2 Objective Function: the objective of this work is to minimize fresh water consumption where

$$Min\ \Sigma_j FW_j \tag{1}$$

3 Constraints

a) Demand: The adjusted water demand flow rate, $B_j$ is equal to the demand flow rate after the selection of the three options, elimination, $Da_{j,e}$, reduction, $Da_{j,re}$ and original, $Da_{j,o}$. Binary variables, $X_{j,e}$, and $X_{j,re}$ are introduced to represent the selection of elimination or reduction.

$$\sum_e Da_{j,e}X_{j,e} + \sum_{re} Da_{j,re}X_{j,re} + \sum_o Da_{j,o}X_{j,o} = B_j \tag{2}$$

b) Reduction Option: The flow rate for the reduction demand, $Da_{j,re}$ is reduce to a certain percentage, $\sigma_{j,re}$. Therefore,

$$Da_{j,re} = \sigma_{j,re} D_j \tag{3}$$

By substituting (3) into (2), a new equation was obtained.

$$\sum_e Da_{j,e}X_{j,e} + \sum_{re} D_j\, \sigma_{j,re}\, X_{j,re} + \sum_o Da_{j,o}X_{j,o} = B_j \tag{4}$$

c) Water Balance for Demand: The water supplied for the adjusted water demand, $Bj$ are from freshwater, $FW_j$, reused/recycle water, $F_{i,j}$, outsource water, $F_{os,j}$ and regenerated water from regeneration unit, $F_{r,j}$. The balance can be written as

$$FW_j + \sum_i F_{i,j} + \sum_{os} F_{os,j} + \sum_r F_{r,j} = B_j \tag{5}$$

d) Water Balance for Source: The water generated from each source, $A_i$ can either directly discharge, $WW_i$, directly reuse or recycle from source to demand, $F_{i,j}$ or treated in generation unit, $F_{i,r}$ before used. The balance is given by

$$WW_i, + \sum_i F_{i,j} + \sum_j F_{i,r} = A_i \tag{6}$$

e) Demand Contaminant Load Satisfaction: Contaminant mass load for the adjusted water demand, $B_j Cd_{j,k}$ is supplied from the mixed contaminant mass load from the different sources, fresh water, $FW_j Cw_k$, potential reused/recycle water, $F_{i,j} Cs_{i,k}$, outsources, $F_{os,j} Cos_{os,k}$ and regenerated water from regeneration unit, $F_{r,j} Cro_{r,k}$. The contaminant load is given by

$$FW_j Cw_k + \sum_i F_{i,j} Cs_{i,k} + \sum_{os} F_{os,j} Cos_{os,k} + \sum_r F_{r,j} Cro_{r,k} \leq B_j Cd_{j,k} \quad (7)$$

*f)* Mass Balance on Regeneration Unit: The total inlet flow rate is equal to the total outlet regeneration unit. The amount of wastewater to be regenerated in the regeneration unit, $F_{i,r}$ depends on the demand for regenerated water, $F_{r,j}$.

$$\sum_i F_{i,r} = \sum_j F_{r,j} \quad (8)$$

g) External Water Sources Constraint: The total water outsources flow rate to the demand, $Fos_{os,j}$ must equal or lower than maximum design limit, $Fos_{os}^{max}$

$$\sum_j Fos_{os,j} \leq Fos_{os}^{max} \quad (9)$$

h) Selection of Water Minimization Scheme: The water minimization options which involving elimination, reduction and original operation are introduced by binary variables, $X_{j,e}$, $X_{j,re}$ and $X_{j,o}$. The total of binary variables must equal to 1.

$$\sum_e X_{j,e} + \sum_{re} X_{j,re} + \sum_o X_{j,o} = 1 \quad (10)$$

i) MTB Constraint: The adjusted flow rate of water demand, $B_j$ is equal to the adjusted water source flow rate, $A_i$.

$$B_j = A_i \quad (11)$$

j) NMTB Constraint: The adjusted water source flow rate, $A_i$ is equal to the water source flow rate, $S_i$ before WMH implementation.

$$A_i = S_i \tag{12}$$

k) Concentrations constraint: The concentration of contaminant *k* for each demand and source must be less than maximum concentration of contaminant *k*.

$$Cs_{i,k} \leq Cs_{i,k}^{max} \tag{13}$$
$$Cd_{j,k} \leq Cd_{j,k}^{max} \tag{14}$$

l) Positive Constraints: The flow rate of fresh water supply, $FW_j$, water reuse or recycle, $F_{i,j}$, outsources water, $Fos_{os,j}$, regenerated water, $F_{i,r}$ or $F_{r,j}$, adjusted water demand, $B_j$, adjusted water source, $A_i$, and water reduction option, $Da_{j,re}$ must larger or equal to zero.

$$FW_j , F_{i,j}, Fos_{os,j}, F_{i,r}, F_{r,j}, B_j, A_i, Da_{j,re} \geq 0 \tag{15}$$

### 3.1.4 GAMS Coding

The fourth step is to implement the mathematical models into General Algebraic Modeling System (GAMS) software. This problem is formulated as MINLP and coded in GAMS. GAMS is a language for setting up and solving mathematical programming optimisation models. GAMS is a flexible and powerful optimisation package. Through GAMS software, the optimal water-using network can be found.

# CHAPTER 4

# RESULT AND DISCUSSION

## 4.1 CHLOR-ALKALI PLANT CASE STUDY

### 4.1.1 Water Distribution in Chlor-Alkali Plant

Water supply from SAJ Holding Sdn Bhd is stored in the water reservoirs. Then, the raw water is pumped to the elevated water head tanks before distributed to the water network in the plant by gravity. About 680 $m^3$ of raw water is being used by PGW1 daily. Water plays an important role in chlor-alkali plant where it is act as the fluid servicing the operation demand in the plant. As the main raw material in the plant, large amount of water is being used every day.

The fresh water fed to the plant is divided into three main uses which are process uses, non-process uses and domestic uses. The process uses involved the water usage for the demineralised water and scrubber. The demineralised water is being used in the process such as preparation in precoat and reagent tank, regeneration of ion exchange in the salt solution, caustic dilution, boiler and brine make up water. For the scrubber, water act as medium to trap the acidic fumes to prevent it from release to the air.

In non-process uses, water supply is used as washing purpose, make up water for cooling tower, scrubber, laboratory uses also in filter backwash and regeneration at demineralised water system. Meanwhile, the fresh water for domestic is used in the ablution, toilet and cleaning activities.

### 4.1.2 Water Balance

Figure 4.3 gives the exact illustration regarding the water using process in CCM Chemicals chlor-alkali plant. All water requirements in each stream are shown in water flow rate terms. The inlet stream or the arrow into the box indicates the water consumed by the stream while the outlet stream referred to the water removed from the stream which can be used as the sources for the other process or may be directly discharge as the effluent.

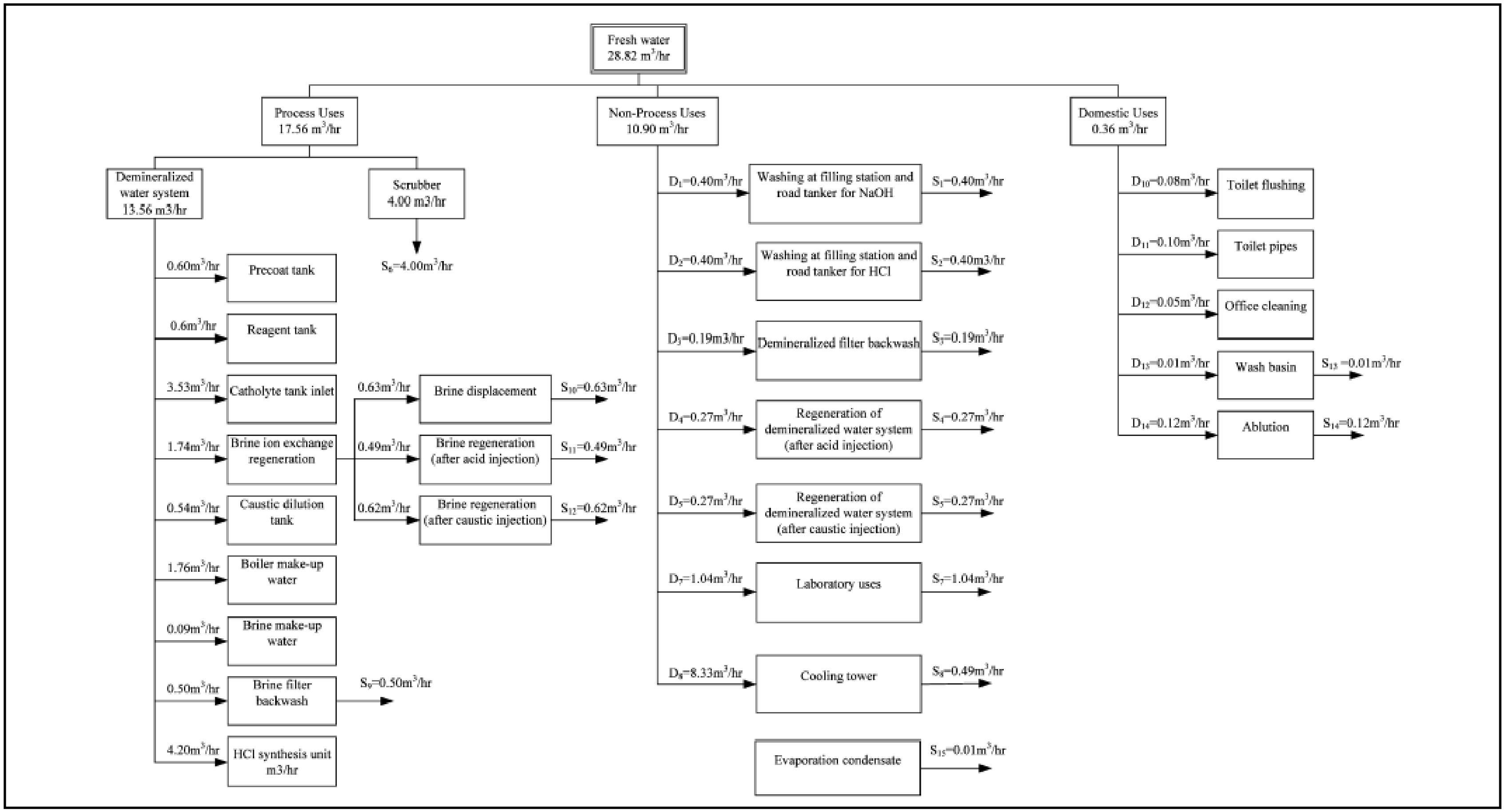



**Figure 4.1:** Water distribution in chlor-alkali plant

Source: Handani et al. (2010)

### 4.1.3 Optimization Model for Water Network

#### *4.1.3.1 Limiting Water Data Extraction*

The purpose of the limiting water data extraction is to identify the water sources and demands and the concentration of contaminants that are needed to perform this work. Overall water network comprising water sources and demands are given in the limiting water data. There are fourteen water demand and fifteen water sources in chlor-alkali process. The water network is including the three main uses of the fresh water which are process, non-process and domestic use.

Instead of flow rate, the contaminant concentrations are taken into account in this water data extraction. Three parameters are taken as the limiting contaminants in this research which are pH, TDS and hardness since they are the dominant parameters related to the water quality in CCM Chemicals chlor-alkali plant. As usual, the pH is measured using the pH meter and TDS is monitored by using conductivity meter. For the hardness, it is differ from the other two dominant contaminants where a simple experiment work is prepared in order to obtain the result.

Water contamination is divided into three general categories which are clean water, grey water and black water. Clean water originates from a source that does not pose harm to human and other living thing. Example of this category may include melting ice or snow, rainwater and broken water supply line.

For grey water, it contains a significant level of contaminants and has potential to cause sickness to human if consumed or exposed to it. Basically this type of water does not contain sewage but only chemicals. It can come from dishwashing and washing machine discharge, shower, overflows from toilet bowl and others. Grey water could be reused for processes that do not involved body contact.

Black water contains pathogenic agents and is grossly sanitary. It is includes sewage and other contaminated water sources entering and not suitable for indoor uses. Examples of black water are office cleaning wastewater, toilet flushing and toilet pipes which are not preferred to be reused.

The limiting water data are listed in Table 4.1 and Table 4.2 for the water sources and demands with the flow rate and contaminants concentration. Meanwhile the concentration of the contaminant for the fresh water sources are fixed and given as $Cw_{pH}$ = 7.5, $Cw_{TDS}$ = 40 ppm and $Cw_{hardness}$ = 14 ppm.

**Table 4.1:** Flow rate and contaminant concentration of the water source, $S_i$ for CCM Chemicals

| $S_i$ | Source | Flow rate (t/hr) | pH | TDS (ppm) | Hardness (ppm) |
|---|---|---|---|---|---|
| $S_1$ | Washing at filling station and road tanker for NaOH | 0.40 | 10.80 | 30360 | 14 |
| $S_2$ | Washing at filling station and road tanker for HCl | 0.40 | 2.50 | 704 | 16 |
| $S_3$ | Demineralised filter backwash | 0.19 | 7.40 | 75 | 20 |
| $S_4$ | Regeneration of demineralised water system (after acid injection) | 0.27 | 1.20 | 3300 | 14 |
| $S_5$ | Regeneration of demineralised water system (after caustic injection) | 0.27 | 9.30 | 60 | 14 |
| $S_6$ | Scrubber | 4.00 | 0.30 | 528 | 40 |
| $S_7$ | Laboratory uses | 1.04 | 8.30 | 400 | 100 |
| $S_8$ | Cooling tower blow down | 0.49 | 6.90 | 3300 | 147 |
| $S_9$ | Brine filter backwash | 0.50 | 10.60 | 6579 | 14 |
| $S_{10}$ | Brine ion exchange regeneration (brine displacement) | 0.63 | 10.20 | 526 | 0 |
| $S_{11}$ | Brine ion exchange regeneration (after acid injection) | 0.49 | 0.02 | 396 | 0 |

| | | | | | |
|---|---|---|---|---|---|
| $S_{12}$ | Brine ion exchange regeneration (after caustic injection) | 0.62 | 13.60 | 1254 | 0 |
| $S_{13}$ | Wash basin | 0.01 | 7.70 | 60 | 20 |
| $S_{14}$ | Ablution | 0.12 | 7.70 | 60 | 20 |
| $S_{15}$ | Evaporation condensate | 0.01 | 11.10 | 76 | 0 |

**Table 4.2:** Flow rate and contaminant concentration of the water source, $D_j$ for CCM Chemicals

| $D_j$ | **Demand** | **Flow rate (t/hr)** | **pH** | **TDS (ppm)** | **Hardness (ppm)** |
|---|---|---|---|---|---|
| $D_1$ | Washing at filling station and road tanker for NaOH | 0.40 | 7.50 | 65 | 17.1 |
| $D_2$ | Washing at filling station and road tanker for HCl | 0.40 | 7.50 | 65 | 17.1 |
| $D_3$ | Demineralised filter backwash | 0.19 | 7.50 | 65 | 17.1 |
| $D_4$ | Regeneration of demineralised water system (after acid injection) | 0.27 | 7.50 | 40 | 17.1 |
| $D_5$ | Regeneration of demineralised water system (after caustic injection) | 0.27 | 7.50 | 40 | 17.1 |
| $D_6$ | Scrubber | 4.00 | 7.50 | 100 | 17.1 |
| $D_7$ | Laboratory uses | 1.04 | 7.50 | 65 | 14.0 |

| | | | | | |
|---|---|---|---|---|---|
| $D_8$ | Cooling tower make-up water | 8.33 | 7.50 | 100 | 14.0 |
| $D_9$ | Carbon filter inlet | 13.56 | 7.50 | 60 | 14.0 |
| $D_{10}$ | Toilet flushing | 0.08 | 7.50 | 100 | 17.1 |
| $D_{11}$ | Toilet pipes | 0.10 | 7.50 | 65 | 17.1 |
| $D_{12}$ | Office cleaning | 0.05 | 7.50 | 65 | 17.1 |
| $D_{13}$ | Wash basin | 0.01 | 7.50 | 65 | 17.1 |
| $D_{14}$ | Ablution | 0.12 | 7.50 | 65 | 17.1 |

Source: Handani et al. (2010)

## 4.2 OPTIMAL DESIGN OF WATER ALLOCATION NETWORK

Using MINLP model and WMH in this study, a new optimal water network design was obtained. The targets of minimizing fresh water consumption in the plant was achieved through maximum water reused or recycled and regenerated from all process. This model considered the multiple contaminants that are the most significance in this water network design. They are pH, TDS and hardness. The process data by Handani et al. (2010) consist of fourteen water demand and fifteen water sources were used. Both linear and non-linear equations were involved to achieve the goal of this study. By applying the formulated model, the total fresh water flow rate in chlor-alkali plant is 18.507 t/h and 0 t/h wastewater discharge from the process plant. Figure 4.3 shows the optimal water network diagram that have been drawn from the results obtained after all the five elements in the water management hierarchy are considered simultaneously. In this figure, it illustrates the connection between fifteen water sources, $S_i$ and fourteen water demands, $D_j$.

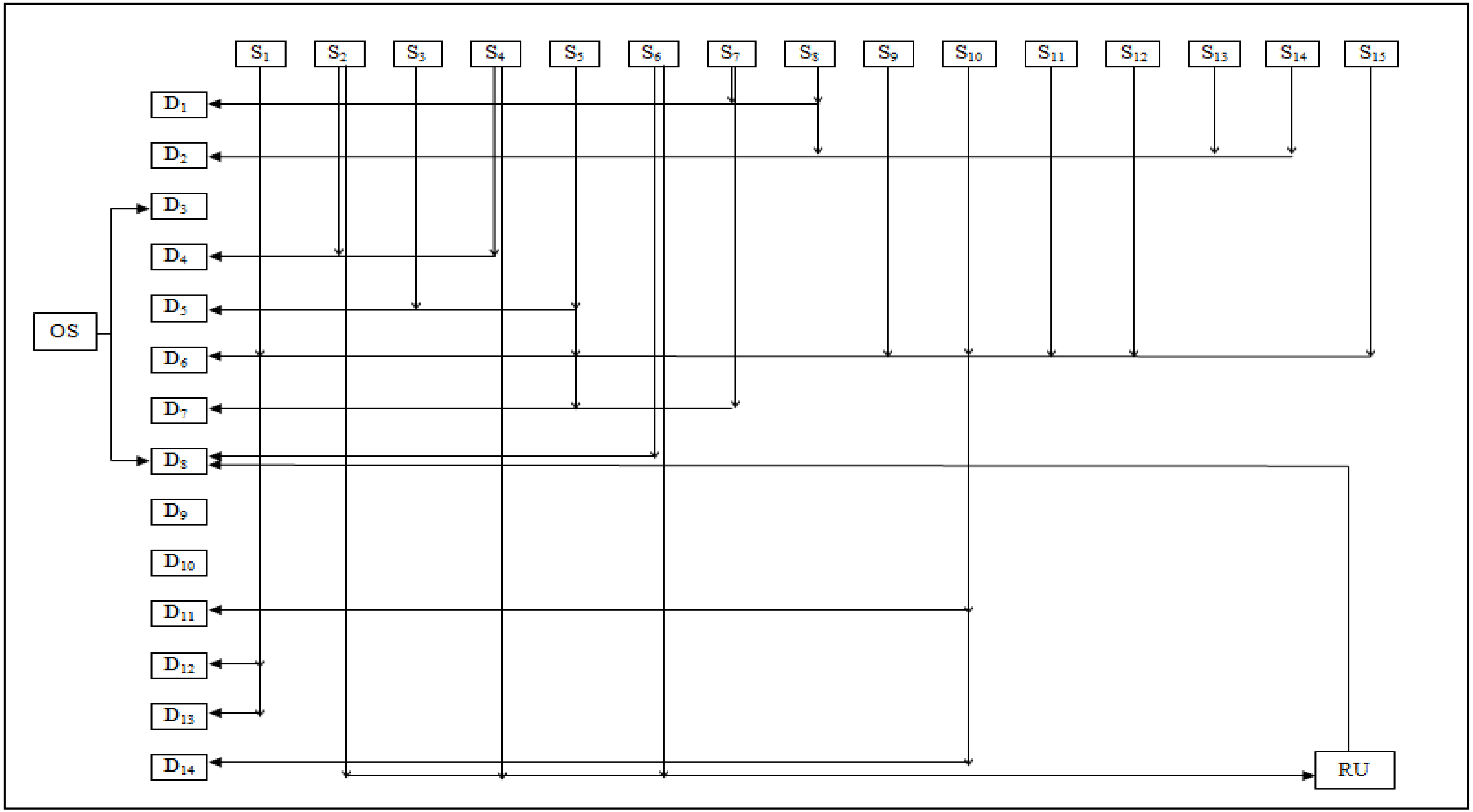



**Figure 4.2:** Optimal water network diagram

As the implementation of WMH options, the new water demands in the process plant were obtained. From the result, it is possible to completely eliminate the fresh water usage at $D_{10}$, water demand at flushing toilet by replacing the flushing toilet to the composting toilet with a new design technology. Composting toilet is known as the dry toilet that using aerobic decomposition process system. Meanwhile, the reduction option occurs at $D_{8}$, the cooling tower make-up. The cooling tower act as removal heat device and the amount of TDS and hardness must be control to ensure the effectiveness of the cooling tower. The chemicals used in this water treatment can be replacing by a new type of polymer chemical which will help to reduce the make-up water demand.

In addition, the average annual rainfall in Johor is about 1778mm and this make the rainwater as suitable outsourcing water in this chlor-alkali plant. Based on the available roof area requirement and rain distribution, about 0.21 $m^3$/h of rainwater is yielded within the process plant with concentration of the contaminants for pH ($Cos_{pH}$), TDS ($Cos_{TDS}$) and hardness ($Cos_{hardness}$) are 5.50, 16 ppm and 5 ppm respectively. The rain water to be use was treated using alkali or acid before it being use as the water demand.in this work, the outsource is supplied to the two demands which are $D_{3}$, demineralised filter backwash and $D_{8}$, cooling tower make-up. The regeneration option, it is divided into two where it can be from source water to the regeneration unit and from regeneration unit to the water demand. The water from source is described as the water to be treated to achieve the standard condition while the water from the regeneration unit is mean by the treated water that attain it level. Three water source are channel to the regeneration unit, ($Fr$); $S_{2}$, source washing at filling station and road tanker for HCl, $S_{4}$, source of regeneration of demineralised water system after acid injection and $S_{6}$, source from scrubber. Treated water from the regeneration unit ($Fro$) is used as the water demand for $D_{8}$, cooling tower make-up. Table 4.4 summarizes the accomplished optimal results from the WMH implementation.

**Table 4.3:** Optimal results from WMH and MINLP model implementation

| WMH option | Location | Optimal results (t/h) |
|---|---|---|
| Elimination | $D_{10}$, flushing toilet | 0 |
| Reduction | $D_8$, cooling tower make-up | 7.75 |
| Outsource water, | $D_3$, demineralised filter backwash<br>$D_8$, cooling tower make-up | 0.21 |
| Regeneration, *Fr* | $S_2$, source washing at filling station and road tanker for HCl<br>$S_4$, source of regeneration of demineralised water system after acid injection<br>$S_6$, source from scrubber | 0.48 |
| Regeneration, *Fro* | $D_8$, cooling tower make-up | 0.48 |
| Freshwater, | $D_3$, demineralised filter backwash<br>$D_6$, scrubber<br>$D_8$, cooling tower make-up<br>$D_9$, carbon filter inlet | 18.51 |
| Wastewater generation | 0 | 0 |

The water sources and demands by Handani et al. (2010) were changed as the WMH and MINLP model were applied through this study. The adjusted water sources, $S_i$ and demands, $D_9$ are tabulated in Table 4.5 and Table 4.6 as below.

**Table 4.4:** Adjusted water sources, $A_i$

| $S_i$ | Source | Flow rate (t/hr) |
|---|---|---|
| $S_1$ | Washing at filling station and road tanker for NaOH | 0.40 |
| $S_2$ | Washing at filling station and road tanker for HCl | 0.40 |
| $S_3$ | Demineralised filter backwash | 0.19 |
| $S_4$ | Regeneration of demineralised water system (after acid injection) | 0.27 |
| $S_5$ | Regeneration of demineralised water system (after caustic injection) | 0.27 |
| $S_6$ | Scrubber | 4.00 |
| $S_7$ | Laboratory uses | 1.04 |
| $S_8$ | Cooling tower blow down | 0.49 |
| $S_9$ | Brine filter backwash | 0.50 |
| $S_{10}$ | Brine ion exchange regeneration (brine displacement) | 0.63 |
| $S_{11}$ | Brine ion exchange regeneration (after acid injection) | 0.49 |
| $S_{12}$ | Brine ion exchange regeneration (after caustic injection) | 0.62 |
| $S_{13}$ | Wash basin | 0.01 |
| $S_{14}$ | Ablution | 0.12 |
| $S_{15}$ | Evaporation condensate | 0.01 |

**Table 4.5:** Adjusted water demand, $B_j$

| $D_j$ | Demand | Flow rate (t/hr) |
|---|---|---|
| $D_1$ | Washing at filling station and road tanker for NaOH | 0.40 |
| $D_2$ | Washing at filling station and road tanker for HCl | 0.40 |
| $D_3$ | Demineralised filter backwash | 0.19 |
| $D_4$ | Regeneration of demineralised water system (after acid injection) | 0.27 |
| $D_5$ | Regeneration of demineralised water system (after caustic injection) | 0.27 |
| $D_6$ | Scrubber | 4.00 |

**Table 4.5:** Continued

| | | |
|---|---|---|
| $D_7$ | Laboratory uses | 1.04 |
| $D_8$ | Cooling tower make-up water | 7.75 |
| $D_9$ | Carbon filter inlet | 13.56 |
| $D_{10}$ | Toilet flushing | 0 |
| $D_{11}$ | Toilet pipes | 0.10 |
| $D_{12}$ | Office cleaning | 0.05 |
| $D_{13}$ | Wash basin | 0.01 |
| $D_{14}$ | Ablution | 0.12 |

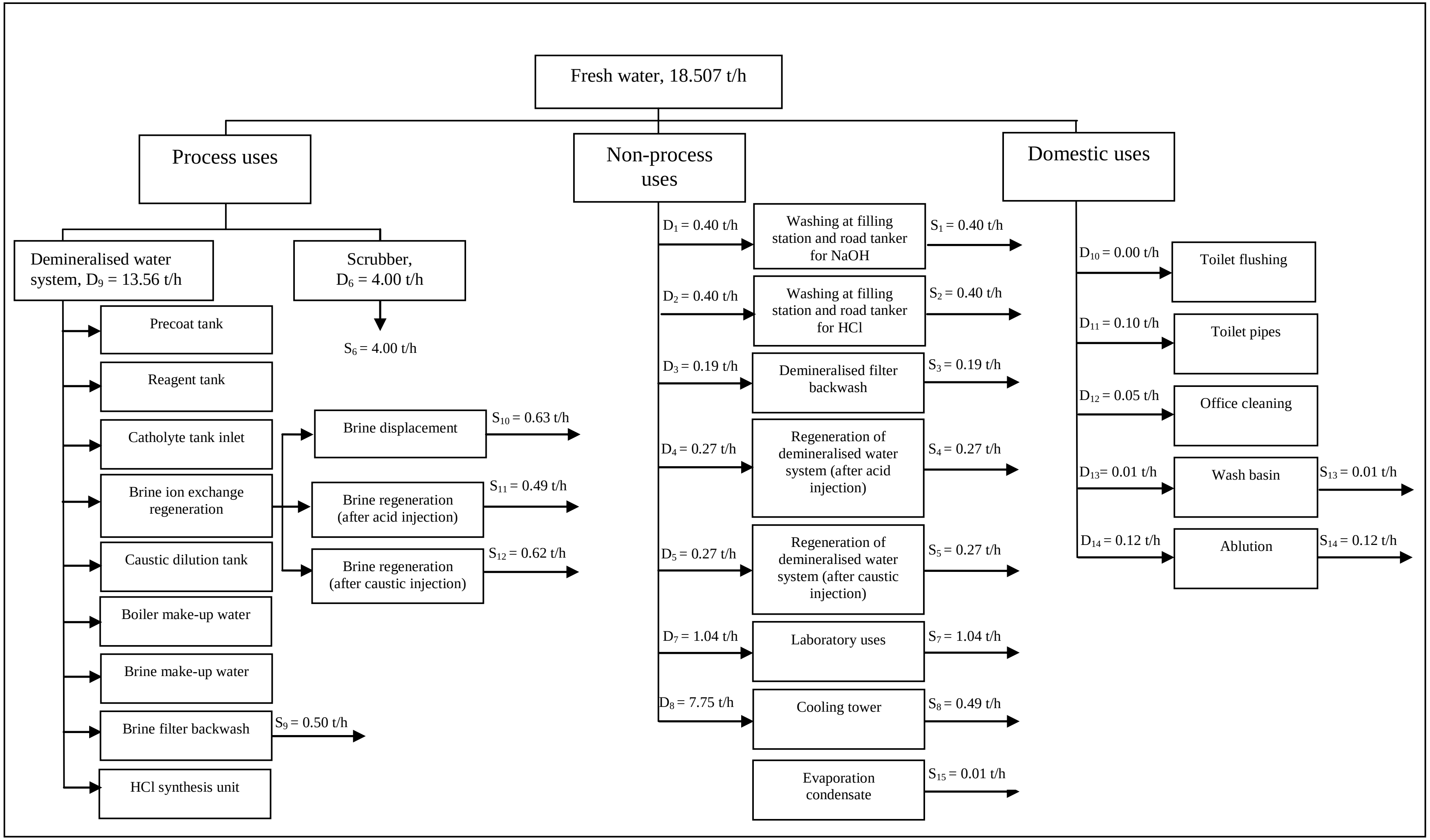



**Figure 4.3:** A new water distribution network by MINLP technique

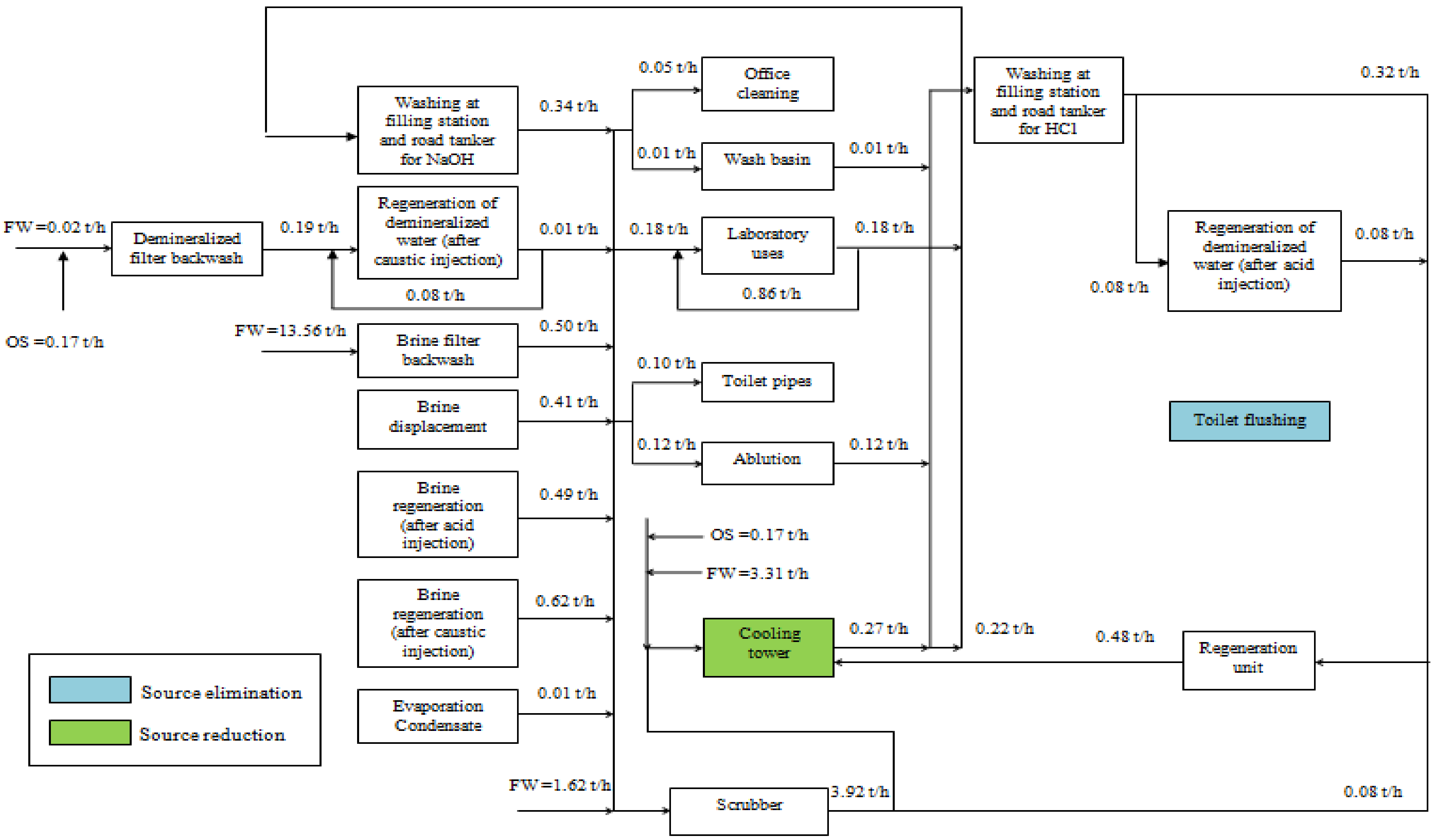



**Figure 4.4:** Optimal water network design in chlor-alkali plant

The mathematical model was formulated in GAMS software with a 2.30 GHz Pentium (R) Dual-Core processor. From the finding through MINLP model using the BARON solver in GAMS, it proved that the minimum water target was achieved at flow rate 18.51 t/h while the wastewater generation is 0 t/h. By this flow rate, the percentage reduction of freshwater consumption and wastewater generation are 35.8% and 100% respectively. The results from MINLP model show the similar results as the previous research, Handani et al. (2010). The differences between both models are the location of selection of the WMH options and this affected the amount of water at the selection points. From both results it can be conclude that the percent of reduction of the freshwater consumption and wastewater generation are achieved the global optimal values which are 35.8% for the freshwater consumption and 100% for the wastewater generation.

**Table 4.6:** Comparison between proposed method and MILP approach for chlor-alkali plant

| | Proposed MINLP model | Handani et al. (2010) |
|---|---|---|
| Technique | MINLP | MILP |
| Fresh water consumption (t/h) | 18.51 | 18.51 |
| Wastewater generation (t/h) | 0.00 | 0.00 |
| Percentage reduction (%) | Fresh water : 35.80<br>Wastewater : 100.00 | Fresh water : 35.80<br>Wastewater : 100.00 |
| Elimination selection | $D_{10}$ | $D_{10}$ |
| Reduction selection | $D_8$ | $D_6$, $D_8$, $D_{10}$, $D_{14}$ |
| Outsource water, | 0.21 | 0.21 |
| Regeneration | 0.48 | 6.57 |
| Reused/recycle | 8.96 | 2.53 |

# CHAPTER 5

# CONCLUSION

## 5.1 Conclusion

An optimal water allocation network was developed in maximizing fresh water saving in chlor-alkali plant by MINLP model. This network was involved multiple contaminants and the contaminants were used to obtained this water network. The given data in the previous research were used as the maximum concentration while the lower concentrations are set in the range not exceeds the maximum concentration. The water management hierarchy consideration was successfully implemented in this work since the minimum water target was achieved through this mathematical model. From this work the total fresh water consumption and wastewater generation are 18.507 t/h and 0 t/h. which are the global optimum amount in chlor-alkali plant. Percentage reduction for both fresh water consumption and wastewater generation are 35.8 % and 100% respectively.

## 5.2 Recommendation

As the recommendation, the future researchers need to work on economic study on the water network instead of apply different method. This will help in obtaining the efficient water network design and results. Besides, other parameters should take into account in order to get a more reliable result and reflects the real water system. Instead of using a centralized regeneration unit, parallel regeneration units should be applied as there are three different contaminants are considered.

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# APPENDIX A1
# GAMS CODING

```
*Chlor-Alkali Plant Case Study
*Minimum fresh water consumption

SETS
 i index for water sources /1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15/
 j index for water demand /1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14/
 k index for contaminant /pH, TDS, hardness/
 r index for regeneration /1/
 o index for original /1/
 e index for elimination /1/
 re index for reduction /1, 2/
 os index for outsource /1/

PARAMETERS
 S(i) flowrate of water sources in tonne per hr
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 0.49, 9 0.50, 10 0.63, 11 0.49,
12 0.62, 13 0.01, 14 0.12, 15 0.01/
 D(j) flowrate of water demand in tonne per hr
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 8.33, 9 13.56, 10 0.08, 11 0.10,
12 0.05, 13 0.01, 14 0.12/
 Fwo(j) initial freshwater consumption
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 8.33, 9 13.56, 10 0.08, 11 0.10,
12 0.05, 13 0.01, 14 0.12/
 Wwo(i) initial wastewater generation
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 0.49, 9 0.50, 10 0.63, 11 0.49,
12 0.62, 13 0.01, 14 0.12, 15 0.01/
*Beta(j)adjusted flowrate of water demand
*/6 1, 8 1, 10 8, 14 7/
 Fosmax(os)   maximum outsource flowrate (ton per hr)
  /1  0.21/
```

Cw(k) freshwater concentration ;

Cw('pH')=3.16E-8;

Cw('TDS')=40;

Cw('hardness')=14;

Table Cos(os,k) outsource concentration

| | pH | TDS | hardness | |
|---|---|---|---|---|
| 1 | 3.16E-8 | 16 | 5 | ; |

Table Cro(r,k) regenerated water concentration

| | pH | TDS | hardness | |
|---|---|---|---|---|
| 1 | 3.16E-8 | 30 | 2 | ; |

Table Cs(i,k) concentration limit of contaminants k in water source i

| | pH | TDS | hardness | |
|---|---|---|---|---|
| 1 | 1.58E-11 | 30360 | 14 | |
| 2 | 3.16E-3 | 704 | 16 | |
| 3 | 3.98E-8 | 75 | 20 | |
| 4 | 6.31E-2 | 3300 | 14 | |
| 5 | 5.01E-10 | 60 | 14 | |
| 6 | 5.01E-1 | 528 | 40 | |
| 7 | 5.01E-9 | 400 | 100 | |
| 8 | 1.26E-7 | 3300 | 147 | |
| 9 | 2.51E-11 | 6579 | 14 | |
| 10 | 6.31E-1 | 526 | 0 | |
| 11 | 9.55E-1 | 396 | 0 | |
| 12 | 2.51E14 | 1254 | 0 | |
| 13 | 2.00E-8 | 60 | 20 | |
| 14 | 2.00E-8 | 60 | 20 | |
| 15 | 7.40E-12 | 76 | 0 | ; |

Table Cd(j,k) concentration limit of kontaminants k in water demand j

| | pH | TDS | hardness |
|---|---|---|---|

```
1    3.16E-8    65     17.1
2    3.16E-8    65     17.1
3    3.16E-8    65     17.1
4    3.16E-8    40     17.1
5    3.16E-8    40     17.1
6    3.16E-8    100    17.1
7    3.16E-8    65     14.0
8    3.16E-8    100    14.0
9    3.16E-8    60     14.0
10   3.16E-8    100    17.1
11   3.16E-8    65     17.1
12   3.16E-8    65     17.1
13   3.16E-8    65     17.1
14   3.16E-8    65     17.1    ;

Table Da1(j,e) elimination flowrate
     1
1    0    ;

Table Alpha(j,re) portion of water reduction for demand
     1      2
6    0.93   0
8    0.93   0
10   0.03   0.5
14   0.5    0    ;

FREE VARIABLE
Ftot       Total freshwater flowrate    ;

VARIABLES
A(i)       Source flowrate
B(j)       Demand flowrate
FW(j)      Freshwater flowrate from supply to demnad
```

```
 F(i,j)        Flowrate from source to demand
 Fos(os,j)    Outsource flowrate
 Fr(i,r)       Regenerated water flowrate from source
 Fro(r,j)      Regenerated water flowrate from regeneration unit to demand
 WW(i)        Unused portion of water source
* Da1(e,j)
  Da2(j,re)
  Da3(j,o)
  Csa(i,k)
  Cda(j,k)    ;

BINARY VARIABLES
  X1(j,e), X2(j,re), X3(j,o)      ;

POSITIVE VARIABLES
 A(i), B(j), FW(j), F(i,j), Fos(os,j), Fr(i,r), Fro(r,j), WW(i), Da2(j,re), Da3(j,o), Csa(i,k),
Cda(j,k)    ;

EQUATIONS
SUPPLY                  Define Objective Function
 MASSSOURCE(i)   Mass balance for each source
 MASSDEMAND(j)  Mass balance for each demand
 MASSLOAD(j,k)      Massload for every internal demand
 REGEN(r)                Balance for regeneration
OUTSOURCE(os)    Balance for outsource
 SCHEME(j)              Water minimization scheme
 DEMAND(j)
 SELWATERSCHEME1(j)
 SELWATERSCHEME2(j)
 SELWATERSCHEME3(j)
 SELWATERSCHEME4(j)
 SELWATERSCHEME5(j)
 SELWATERSCHEME6(j)
```

```
SELWATERSCHEME7(j)
SELWATERSCHEME8(j)
SELWATERSCHEME9(j)
SELWATERSCHEME10(j)
SELWATERSCHEME11(j)
SELWATERSCHEME12(j)
SELWATERSCHEME13(j)
SELWATERSCHEME14(j)
SELDS1
SELDS2
SELDS3
SELDS4
SELDS5
SELDS6
SELDS7
SELDS13
SELDS14
SOURCE8(i)
SOURCE9(i)
SOURCE10(i)
SOURCE11(i)
SOURCE12(i)
SOURCE15(i)
CON1(i,k)
CON12(i,k)

SUPPLY..
Ftot =e= sum(j,FW(j));

MASSSOURCE(i)..
WW(i) + sum(j,F(i,j)) + sum(r,Fr(i,r)) =e= A(i);

MASSDEMAND(j)..
```

```
 FW(j) + sum(i,F(i,j)) + sum(os,Fos(os,j)) + sum(r,Fro(r,j)) =e= B(j);

 MASSLOAD(j,k)..
 FW(j)*Cw(k) + sum(i,F(i,j)*Csa(i,k)) + sum(os,Fos(os,j)*Cos(os,k)) +
sum(r,Fro(r,j)*Cro(r,k)) =l= B(j)*Cda(j,k);

 REGEN(r)..
 sum(i,Fr(i,r)) =e= sum(j,Fro(r,j));

 OUTSOURCE(os)..
 sum(j,Fos(os,j))=l= Fosmax(os);

 SCHEME(j)..
 sum(e,Da1(j,e)*X1(j,e)) + sum(re,D(j)*Alpha(j,re)*X2(j,re)) + sum(o,D(j)*X3(j,o))=e=
B(j);

*SEL(j)..
*sum(e,X1(j,e)) + sum(re,X2(j,re)) + sum(o,X3(j,o)) =e= 1;

  SELWATERSCHEME1('1')..
  X3('1','1') =e= 1;

  SELWATERSCHEME2('2')..
  X3('2','1') =e= 1 ;

  SELWATERSCHEME3('3')..
  X3('3','1') =e= 1 ;

  SELWATERSCHEME4('4')..
  X3('4','1') =e= 1 ;

  SELWATERSCHEME5('5')..
  X3('5','1') =e= 1 ;
```

```
SELWATERSCHEME6('6')..
X2('6','1')+X3('6','1') =e= 1 ;

SELWATERSCHEME7('7')..
X3('7','1') =e= 1 ;

SELWATERSCHEME8('8')..
X2('8','1')+ X3('8','1') =e= 1 ;

SELWATERSCHEME9('9')..
X3('9','1') =e= 1 ;

SELWATERSCHEME10('10')..
X1('10','1')+X2('10','1')+X2('10','2')+X3('10','1') =e= 1 ;

SELWATERSCHEME11('11')..
X3('11','1') =e= 1 ;

SELWATERSCHEME12('12')..
X3('12','1') =e= 1 ;

SELWATERSCHEME13('13')..
X3('13','1') =e= 1 ;

SELWATERSCHEME14('14')..
X2('14','1')+X3('14','1') =e= 1 ;

DEMAND(j)..
B(j) =l= D(j);

*for MTB in water system
SELDS1..
B('1') =e= A('1');
```

```
SELDS2..
B('2') =e= A('2');
SELDS3..
B('3') =e= A('3');
SELDS4..
B('4') =e= A('4');
SELDS5..
B('5') =e= A('5');
SELDS6..
B('6') =e= A('6');
SELDS7..
B('7') =e= A('7');
SELDS13..
B('13') =e= A('13');
SELDS14..
B('14') =e= A('14');

*if source stream exist for NMTB operations
SOURCE8('8')..
S('8') =e= A('8');

SOURCE9('9')..
S('9') =e= A('9');

SOURCE10('10')..
S('10') =e= A('10');

SOURCE11('11')..
S('11') =e= A('11');

SOURCE12('12')..
S('12') =e= A('12');
```

```
 SOURCE15('15')..
 S('15') =e= A('15');

CON1(i,k)..
 Csa(i,k) =l= Cs(i,k);

 CON2(j,k)..
 Cda(j,k) =l= Cd(j,k);

MODEL MWN /ALL/;
SOLVE MWN USING MINLP MINIMIZING Ftot ;
DISPLAY WW.L, FW.L, F.L, Fos.L, Fr.L, Fro.L, A.L, B.L, X1.L, X2.L,
X3.L,Ftot.L,Csa.L, Cda.L  ;
```

# APPENDIX A2

# RESULTS OBTAINED FROM GAMS

GAMS Rev 237 WIN-VS8 23.7.3 x86/MS Windows 01/12/12 01:24:31 Page 1

G e n e r a l A l g e b r a i c M o d e l i n g S y s t e m

C o m p i l a t i o n

```
*Chlor-Alkali Plant Case Study
*Minimum fresh water consumption

SETS
 i index for water sources /1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14,
15/
 j index for water demand /1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14/
 k index for contaminant /pH, TDS, hardness/
 r index for regeneration /1/
 o index for original /1/
 e index for elimination /1/
 re index for reduction /1, 2/
 os index for outsource /1/

PARAMETERS
 S(i) flowrate of water sources in tonne per hr
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 0.49, 9 0.50,
10 0.63, 11 0.49, 12 0.62, 13 0.01, 14 0.12, 15 0.01/
 D(j) flowrate of water demand in tonne per hr
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 8.33, 9 13.56,
10 0.08, 11 0.10, 12 0.05, 13 0.01, 14 0.12/
 Fwo(j) initial freshwater consumption
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 8.33, 9 13.56,
10 0.08, 11 0.10, 12 0.05, 13 0.01, 14 0.12/
 Wwo(i) initial wastewater generation
 /1 0.40, 2 0.40, 3 0.19, 4 0.27, 5 0.27, 6 4.00, 7 1.04, 8 0.49, 9 0.50,
```

```
    10 0.63, 11 0.49, 12 0.62, 13 0.01, 14 0.12, 15 0.01/
 Fosmax(os)   maximum outsource flowrate (ton per hr)
  /1  0.21/
 Cw(k) freshwater concentration ;
 Cw('pH')=3.16E-8;
 Cw('TDS')=40;
 Cw('hardness')=14;

Table Cos(os,k) outsource concentration
              pH         TDS     hardness
 1        3.16E-8       16        5          ;

Table Cro(r,k) regenerated water concentration
              pH         TDS     hardness
 1        3.16E-8       30        2          ;

Table Cs(i,k) concentration limit of contaminants k in water source i
              pH         TDS                 hardness
 1       1.58E-11      30360         14
 2       3.16E-3       704           16
 3       3.98E-8       75            20
 4       6.31E-2       3300          14
 5       5.01E-10       60           14
 6       5.01E-1       528            40
 7       5.01E-9       400           100
 8       1.26E-7       3300          147
 9       2.51E-11       6579         14
 10      6.31E-1       526            0
 11      9.55E-1       396           0
 12      2.51E14       1254          0
 13      2.00E-8       60            20
 14      2.00E-8       60            20
 15      7.40E-12      76            0          ;
```

```

Table Cd(j,k) concentration limit of kontaminants k in water demand j
             pH          TDS      hardness
 1       3.16E-8       65        17.1
 2       3.16E-8       65        17.1
 3       3.16E-8       65        17.1
 4       3.16E-8       40        17.1
 5       3 .16E-8      40        17.1
 6       3.16E-8       100       17.1
 7       3.16E-8       65        14.0
 8       3.16E-8       100       14.0
 9       3.16E-8       60        14.0
 10      3.16E-8       100       17.1
 11      3.16E-8       65        17.1
 12      3.16E-8       65        17.1
 13      3.16E-8       65        17.1
 14      3.16E-8       65        17.1        ;

Table Da1(j,e) elimination flowrate
          1
 1        0      ;

Table Alpha(j,re) portion of water reduction for demand
          1       2
 6       0.93    0
 8       0.93    0
 10      0.03    0.5
 14      0.5     0      ;

FREE VARIABLE
 Ftot          Total freshwater flowrate       ;

```

```
VARIABLES
 A(i)          Source flowrate
 B(j)          Demand flowrate
 FW(j)         Freshwater flowrate from supply to demnad
 F(i,j)        Flowrate from source to demand
 Fos(os,j)     Outsource flowrate
 Fr(i,r)       Regenerated water flowrate from source
 Fro(r,j)      Regenerated water flowrate from regeneration unit to
                demand
 WW(i)         Unused portion of water source
* Da1(e,j)
  Da2(j,re)
  Da3(j,o)
  Csa(i,k)
  Cda(j,k)    ;

BINARY VARIABLES
  X1(j,e), X2(j,re), X3(j,o)      ;

POSITIVE VARIABLES
 A(i), B(j), FW(j), F(i,j), Fos(os,j), Fr(i,r), Fro(r,j), WW(i), Da2(j,re),
Da3(j,o), Csa(i,k), Cda(j,k)    ;

EQUATIONS
 SUPPLY                   Define Objective Function
 MASSSOURCE(i)            Mass balance for each source
 MASSDEMAND(j)            Mass balance for each demand
 MASSLOAD(j,k)            Massload for every internal demand
 REGEN(r)                  Balance for regeneration
 OUTSOURCE(os)            Balance for outsource
 SCHEME(j)                Water minimization scheme
DEMAND(j)
SELWATERSCHEME1(j)
```

```
SELWATERSCHEME2(j)
SELWATERSCHEME3(j)
SELWATERSCHEME4(j)
SELWATERSCHEME5(j)
SELWATERSCHEME6(j)
SELWATERSCHEME7(j)
SELWATERSCHEME8(j)
SELWATERSCHEME9(j)
SELWATERSCHEME10(j)
SELWATERSCHEME11(j)
SELWATERSCHEME12(j)
SELWATERSCHEME13(j)
SELWATERSCHEME14(j)
SELDS1
SELDS2
SELDS3
SELDS4
SELDS5
SELDS6
SELDS7
SELDS13
SELDS14
SOURCE8(i)
SOURCE9(i)
SOURCE10(i)
SOURCE11(i)
SOURCE12(i)
SOURCE15(i)
CON1(i,k)
CON2(j,k);

SUPPLY..
Ftot =e= sum(j,FW(j));
```

```
MASSSOURCE(i)..
WW(i) + sum(j,F(i,j)) + sum(r,Fr(i,r)) =e= A(i);

MASSDEMAND(j)..
FW(j) + sum(i,F(i,j)) + sum(os,Fos(os,j)) + sum(r,Fro(r,j)) =e= B(j);

MASSLOAD(j,k)..
FW(j)*Cw(k) + sum(i,F(i,j)*Csa(i,k)) + sum(os,Fos(os,j)*Cos(os,k)) +
sum(r,Fro(r,j)*Cro(r,k)) =l= B(j)*Cda(j,k);

REGEN(r)..
sum(i,Fr(i,r)) =e= sum(j,Fro(r,j));

*FWREGEN..
*sum(j,FW(j) =g= sum(i,Fr(i,'1'));

OUTSOURCE(os)..
sum(j,Fos(os,j))=l= Fosmax(os);

SCHEME(j)..
sum(e,Da1(j,e)*X1(j,e)) + sum(re,D(j)*Alpha(j,re)*X2(j,re)) +
sum(o,D(j)*X3(j,o))=e= B(j);

*SEL(j)..
*sum(e,X1(j,e)) + sum(re,X2(j,re)) + sum(o,X3(j,o)) =e= 1;

 SELWATERSCHEME1('1')..
 X3('1','1') =e= 1;

 SELWATERSCHEME2('2')..
 X3('2','1') =e= 1 ;
```

```
SELWATERSCHEME3('3')..
X3('3','1') =e= 1 ;

SELWATERSCHEME4('4')..
X3('4','1') =e= 1 ;

SELWATERSCHEME5('5')..
X3('5','1') =e= 1 ;

SELWATERSCHEME6('6')..
X2('6','1')+X3('6','1') =e= 1 ;

SELWATERSCHEME7('7')..
X3('7','1') =e= 1 ;

SELWATERSCHEME8('8')..
X2('8','1')+ X3('8','1') =e= 1 ;

SELWATERSCHEME9('9')..
X3('9','1') =e= 1 ;

SELWATERSCHEME10('10')..
X1('10','1')+X2('10','1')+X2('10','2')+X3('10','1') =e= 1 ;

SELWATERSCHEME11('11')..
X3('11','1') =e= 1 ;

SELWATERSCHEME12('12')..
X3('12','1') =e= 1 ;

SELWATERSCHEME13('13')..
X3('13','1') =e= 1 ;
```

```
 SELWATERSCHEME14('14')..
 X2('14','1')+X3('14','1') =e= 1 ;

DEMAND(j)..
B(j) =l= D(j);

*for MTB in water system

SELDS1..
B('1') =e= A('1');
SELDS2..
B('2') =e= A('2');
SELDS3..
B('3') =e= A('3');
SELDS4..
B('4') =e= A('4');
SELDS5..
B('5') =e= A('5');
SELDS6..
B('6') =e= A('6');
SELDS7..
B('7') =e= A('7');
SELDS13..
B('13') =e= A('13');
SELDS14..
B('14') =e= A('14');

*if source stream exist for NMTB operations

SOURCE8('8')..
S('8') =e= A('8');

SOURCE9('9')..
```

```
S('9') =e= A('9');
SOURCE10('10')..
S('10') =e= A('10');
SOURCE11('11')..
S('11') =e= A('11');
SOURCE12('12')..
S('12') =e= A('12');
SOURCE15('15')..
S('15') =e= A('15');
CON1(i,k)..
Csa(i,k) =l= Cs(i,k);
CON2(j,k)..
Cda(j,k) =l= Cd(j,k);
MODEL MWN /ALL/;
SOLVE MWN USING MINLP MINIMIZING Ftot ;
DISPLAY WW.L, FW.L, F.L, Fos.L, Fr.L, Fro.L, A.L, B.L, X1.L, X2.L,
X3.L,Ftot.L,Csa.L, Cda.L  ;
```

COMPILATION TIME     =        0.000 SECONDS      3 Mb  WIN237-237 Aug 23, 2011

GAMS Rev 237  WIN-VS8 23.7.3 x86/MS Windows           01/12/12 01:24:31 Page 2

S O L V E     S U M M A R Y

```
MODEL   MWN              OBJECTIVE  Ftot
TYPE    MINLP            DIRECTION  MINIMIZE
```

SOLVER BARON FROM LINE 296

**** SOLVER STATUS 1 Normal Completion

**** MODEL STATUS 1 Optimal

**** OBJECTIVE VALUE 18.5069

RESOURCE USAGE, LIMIT 0.230 1000.000

ITERATION COUNT, LIMIT 0 2000000000

EVALUATION ERRORS 0 0

Total no. of BaR iterations: -1

Best solution found at node: -1

Max. no. of nodes in memory: 0

GAMS Rev 237 WIN-VS8 23.7.3 x86/MS Windows 01/12/12 01:24:31 Page 6

G e n e r a l A l g e b r a i c M o d e l i n g S y s t e m

E x e c u t i o n

---- 297 VARIABLE WW.L Unused portion of water source

( ALL 0.000 )

---- 297 VARIABLE FW.L Freshwater flowrate from supply to demnad

3 0.016, 6 1.620, 8 3.311, 9 13.560

---- 297 VARIABLE F.L Flowrate from source to demand

| | 1 | 2 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|
| 1 | | | | | 0.340 | |
| 2 | | | 0.077 | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 3 | | | | 0.190 | | |
| 4 | | | 0.193 | | | |
| 5 | | | | 0.080 | 0.010 | 0.180 |
| 7 | 0.180 | | | | | 0.860 |
| 8 | 0.220 | 0.270 | | | | |
| 9 | | | | | 0.500 | |
| 10 | | | | | 0.410 | |
| 11 | | | | | 0.490 | |
| 12 | | | | | 0.620 | |
| 13 | | 0.010 | | | | |
| 14 | | 0.120 | | | | |
| 15 | | | | | 0.010 | |

| + | 8 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|
| 1 | | | 0.050 | 0.010 | |
| 6 | 3.916 | | | | |
| 10 | | 0.100 | | | 0.120 |

---- 297 VARIABLE Fos.L Outsource flowrate

| | 3 | 8 |
|---|---|---|
| 1 | 0.174 | 0.036 |

---- 297 VARIABLE Fr.L Regenerated water flowrate from source

| | 1 |
|---|---|
| 2 | 0.323 |
| 4 | 0.077 |
| 6 | 0.084 |

---- 297 VARIABLE Fro.L Regenerated water flowrate from regeneration unit to demand

8

1 0.484

---- 297 VARIABLE A.L Source flowrate

1 0.400, 2 0.400, 3 0.190, 4 0.270, 5 0.270, 6 4.000
7 1.040, 8 0.490, 9 0.500, 10 0.630, 11 0.490, 12 0.620
13 0.010, 14 0.120, 15 0.010

---- 297 VARIABLE B.L Demand flowrate

1 0.400, 2 0.400, 3 0.190, 4 0.270, 5 0.270, 6 4.000
7 1.040, 8 7.747, 9 13.560, 11 0.100, 12 0.050, 13 0.010
14 0.120

---- 297 VARIABLE X1.L

1

10 1.000

---- 297 VARIABLE X2.L

1

8 1.000

---- 297 VARIABLE X3.L

| | 1 |
| --- | --- |
| 1 | 1.000 |
| 2 | 1.000 |
| 3 | 1.000 |
| 4 | 1.000 |
| 5 | 1.000 |
| 6 | 1.000 |
| 7 | 1.000 |
| 9 | 1.000 |
| 11 | 1.000 |
| 12 | 1.000 |
| 13 | 1.000 |
| 14 | 1.000 |

---- 297 VARIABLE Ftot.L = 18.507 Total freshwater flow rate

EXECUTION TIME = 0.016 SECONDS 3 Mb WIN237-237 Aug 23, 2011

USER: Zainatul Bahiyah Handani G111101:1719AP-WIN

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Output C:\Users\win\Documents\gamsdir\projdir\Untitled_1.lst