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BORANG PENGESAHAN
LAPORAN AKHIR PENYELIDIKAN

TAJUK PROJEK : FORMULATION OF MATHEMATICAL MODELLING FOR THE DESIGN OF MAXIMUM WATER RECOVERY

Saya DR HASLENDA BT HASHIM

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FORMULATION OF MATHEMATICAL MODELLING FOR THE DESIGN OF MAXIMUM WATER RECOVERY

(FORMULASI PEMODELAN MATEMATIK UNTUK MEREKABENTUK PEMULIHAN AIR MAKSIMA)

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ABSTRACT

FORMULATION OF MATHEMATICAL MODELLING FOR THE DESIGN OF MAXIMUM WATER RECOVERY

(Keyword: Optimisation, minimum water network, water management hierarchy, water minimisation, cost)

Mathematical programming technique has become an essential tool for design of optimal water networks due to the limitations of conceptual approaches in dealing with complex industrial water systems involving multiple contaminants. This report presents the development of a *Model for Optimal Design of Water Networks (MODWN)* applicable for water operations involving multiple contaminants and multiple utilities. The approach is based on the optimisation of a superstructure which represents a set of all possible water flow configurations in a process system. MODWN can be analysed in two stages, i.e. *fresh water savings mode (FWS-mode)* and *economic mode (E-mode).* The first stage consists of mixed integer linear program (MILP) formulation that is solved to provide some initial values for the second stage. In the second stage, the model is formulated as a mixed integer nonlinear program (MINLP) that is used to optimise an existing design of water systems.

The model considers all levels of water management hierarchy (i.e. elimination, reduction, reuse, outsourcing and regeneration) and cost constraints simultaneously to select the best water minimisation schemes that can achieve the maximum net annual savings at a desired payback period. In addition, MODWN can also be used to solve water network design simultaneously. This work also includes cases where fresh water concentrations for all contaminants are assumed to be either zero or non-zero.

The approach has been successfully implemented in case studies involving an urban building (Sultan Ismail Mosque, UTM) for retrofit scenario. The results show that the potential maximum reductions of fresh water of 95.3% and wastewater of 64.7% for Sultan Ismail Mosque, giving an investment payback period of within 5 years. By considering more constraints, the MODWN has successfully yielded more accurate results as compared to the heuristics and graphical approaches, and will be very beneficial for the design and retrofit of real-life urban and industrial water networks.

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ABSTRAK

FORMULASI PEMODELAN MATEMATIK UNTUK MEREKABENTUK PEMULIHAN AIR MAKSIMA

(Katakunci: Pengoptimuman, rangkaian air minima, hirarki pengurusan air, pengurangan air, kos)

Teknik pengaturcaraan matematik telah menjadi alat yang penting untuk merekabentuk rangkaian air yang optimum kerana keterbatasan pendekatan heuristik dalam menangani sistem air industri yang kompleks dan melibatkan pelbagai bahan cemar. Laporan ini membentangkan pembangunan *Model for Optimal Design of Water Networks (MODWN)* bagi merekabentuk rangkaian pengendalian air melibatkan pelbagai bahan cemar serta utiliti. Pendekatan ini berdasarkan kepada pengoptimuman superstruktur yang mewakili semua kemungkinan aliran air dalam sistem proses. MODWN boleh dianalisa dalam dua peringkat, iaitu mod penjimatan air bersih *(FWS-mode)* dan mod ekonomi *(E-mode).* Peringkat pertama terdiri daripada formulasi *mixed integer linear program (MILP)* yang diselesaikan untuk menyediakan nilai-nilai awal bagi peringkat kedua. Pada peringkat kedua, model ini diformulasikan sebagai *mixed integer nonlinear program (MINLP)* yang digunakan untuk mengoptimumkan rekabentuk sistem air yang sedia ada.

Model tersebut mengambil kira semua peringkat hierarki pengurusan air (iaitu penghapusan, pengurangan, perolehan semula, penggunaan sumber luar dan penjanaan semula) dan kos secara serentak dan memilih skim peminimuman air yang terbaik bagi mencapai penjimatan tahunan bersih yang maksima dalam jangka masa bayar balik yang diingini. Selain itu, MODWN juga boleh digunakan secara serentak untuk menyelesaikan rekabentuk rangkaian air. Kerja ini juga meliputi kes-kes di mana kepekatan air bersih untuk pelbagai bahan cemar dianggapkan sifar atau bukan sifar.

Pendekatan ini telah berjaya dilaksanakan dalam kajian kes yang melibatkan sebuah bangunan bandaran (Masjid Sultan Ismail, UTM). Keputusan kajian menunjukkan bahawa potensi penurunan maksima air bersih dan air sisa buangan adalah 95,3% dan 64,7% untuk Masjid Sultan Ismail dalam 5 tahun jangka masa pulangan pelaburan. Dengan mengambil kira lebih banyak halangan, MODWN berjaya menghasilkan keputusan yang lebih tepat berbanding pendekatan secara heuristik dan grafik, dan akan memberi manfaat yang besar dalam merekabentuk dan mengubahsuai rangkaian air untuk sektor bandaran dan industri.

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A_i	-	Adjusted flow rate of water source i
AOT	-	Annual operating time
B_j	-	Adjusted flow rate of water demand j
$Cd_{j,k}^{max}$	-	Maximum concentration limit of contaminant k in demand j
$Cos_{os,k}$	-	Outsource concentration of contaminant k
$CostOsU_{os}^{A}$	-	Cost of outsourcing unit os with given water flow rate A
$CostRegU_{r}^{A}$	-	Cost of regeneration unit r with given water flow rate A
$CostChemReg$	-	Cost of chemicals needed for regeneration
$CostElect$	-	Cost of electricity
$CostFW$	-	Cost of fresh water supply
$CostPipe$	-	Cost of piping
$CostPump$	-	Cost of pump
$CostUE_{j,e}$	-	Cost of elimination unit e for demand j
$CostURe_{j,re}$	-	Cost of reduction unit re for demand j
$COsU$	-	Total cost of outsourcing unit
$CostWW$	-	Cost of wastewater generation
$CRegU$	-	Total cost of regeneration unit
$CReuse$	-	Total cost for reuse unit
$Cri_{r,k}$	-	Inlet concentration of contaminant k to regeneration unit r
$Cro_{r,k}$	-	Outlet concentration of contaminant k from regeneration unit r
$Cs_{i,k}^{max}$	-	Maximum concentration limit of contaminant k from water source i
Cw_k	-	Fresh water concentration of contaminant k
$Da_{j,e}$	-	Flow rate of elimination option e for demand j

$Da_{j,o}$ - Original flow rate o for demand j

$Da_{j,re}$ - Flow rate of reduction option e for demand j

D_j - Flow rate of water demand j

$F_{i,j}$ - Water flow rate from source i to demand j

$F_{i,j}^{initial}$ - Initial water flow rate from source i to demand j

$F_{i,r}$ - Water flow rate from source i to regeneration unit r

$F_{i,r}^{initial}$ - Initial water flow rate from source i to regeneration unit r

$Fos_{os,j}^{initial}$ - Initial outsource flow rate os to demand j

$Fos_{os,j}$ - Outsource flow rate os to demand j

Fos_{os}^{max} - Maximum flow rate of outsource os

Fos_{os}^{A} - Flow rate of A for outsource os

$F_{r,j}$ - Water flow rate from regeneration unit r to demand j

$F_{r,j}^{initial}$ - Initial water flow rate from regeneration unit r to demand j

$FReg^{A}$ - Flow rate of A for regeneration

Fw_j - Fresh water supplied to demand j

$Fw_j^{initial}$ - Initial fresh water flow rate to demand j

HCl - Hydrochloric acid

Max - Maximum

Min - Minimum

$NaOH$ - Natrium hydroxide

P - Percentage of equipment cost installation

$POPump$ - Power of pump

S_i - Flow rate of water source i

TPP - Total payback period

TPP_{AS} - Total payback period after SHARPS

TPP_{BS} - Total payback period before SHARPS

TPP_{set} - Desired payback period specified by designer

WW_i - Unused portion of water source i (waste)

$WW_i^{initial}$ - Initial wastewater flow rate from source i

$x1_{j,e}$ - Selection of e^{th} elimination options for j^{th} demand

$x2_{j,re}$ - Selection of re^{th} reduction options for j^{th} demand

$x3_{j,o}$ - Selection of original flow rate o for j^{th} demand

$\sigma_{j,re}$ - Water reduction percentage
β - Sixth-tenth rule
ε_j - Number of equipment j
γ - Payback period limit

Greek Letters

$\sum$ - Summation
$\forall$ - All belongs to

Subscripts

i - Index for water source
j - Index for water demand
k - Index for water contaminant
r - Index for regeneration unit
e - Index for water elimination option
re - Index for water reduction option
o - Index for original water demand
os - Index for outsourcing

Acronym

BOD - Biological oxygen demand
CEMWN - Cost-effective minimum water network
COD - Chemical oxygen demand
D - Demand
EDI - Electrodialysis-ion exchange
FW - Fresh water
GAMS - Generalized Algebraic Modeling System
IAS - Net capital investment versus net annual savings plot
LID - Load interval diagram
LP - Linear programming

LPD	-	Litre per capita per day
LPT	-	Load problem table
MILP	-	Mixed integer linear program
MINLP	-	Mixed integer nonlinear program
MODWN	-	Model for optimal design of water networks
MTB	-	Mass transfer-based
MWN	-	Minimum water network
MWR	-	Maximum water recovery
NAS	-	Net annual savings
NCI	-	Net capital investment
NLP	-	Nonlinear programming
NMTB	-	Non-mass transfer-based
NPV	-	Net present value
ppm	-	Part per million
ROI	-	Rate of investment
RW	-	Rainwater
RU	-	Regeneration unit
S	-	Source
SDCC	-	Source and demand composite curve
SHARPS	-	Systematically Hierarchical Approach for Resilient Process Screening
TDS	-	Total dissolved solid
TSS	-	Total suspended solid
TPP	-	Total payback period
WCA	-	Water cascade analysis
WMH	-	Water management hierarchy
WPA	-	Water pinch analysis
WW	-	Wastewater

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Introduction

This chapter provides an overview of the current local and global water issues. The problem background and problem statement are described next. This is followed by research objectives and scope of the study which involves the development of a new systematic technique for designing an optimal water utilisation network involving multiple contaminants based on mathematical programming. This chapter also addresses five main contributions of this work.

1.2 Global Water Outlook

Water is a precious and scarce resource. Nowadays water has become a very valuable resource for use in agriculture, industry and domestic sectors. The major water usages come from agricultural sector which comprises of up to 70% of world water consumption, followed by 22% industry and 8% domestic (Figure 1.1).

Virtually all of these sectors require fresh water. 97.5% of water on the earth is salt water, and 68.9% of fresh water is locked in glaciers and polar ice caps, leaving only one thirds of fresh water available for human use from lakes, river and groundwater (Figure 1.2).

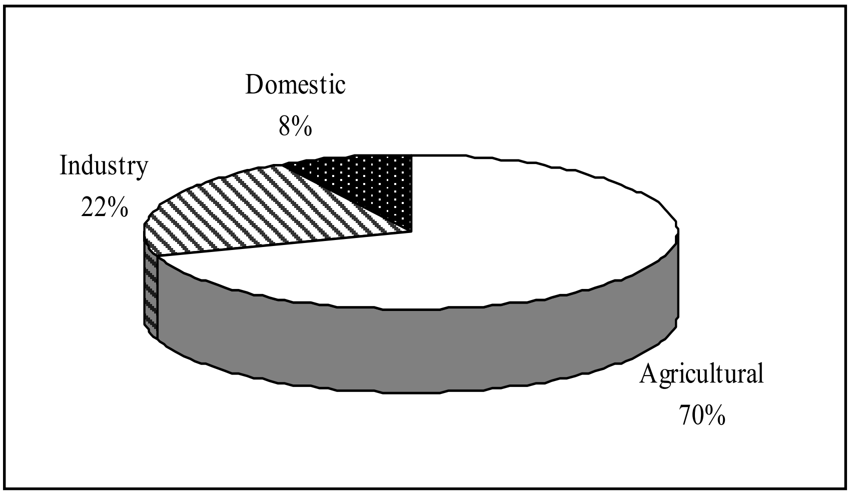


Figure 1.1: Global water use (BBC News Website, 2007).

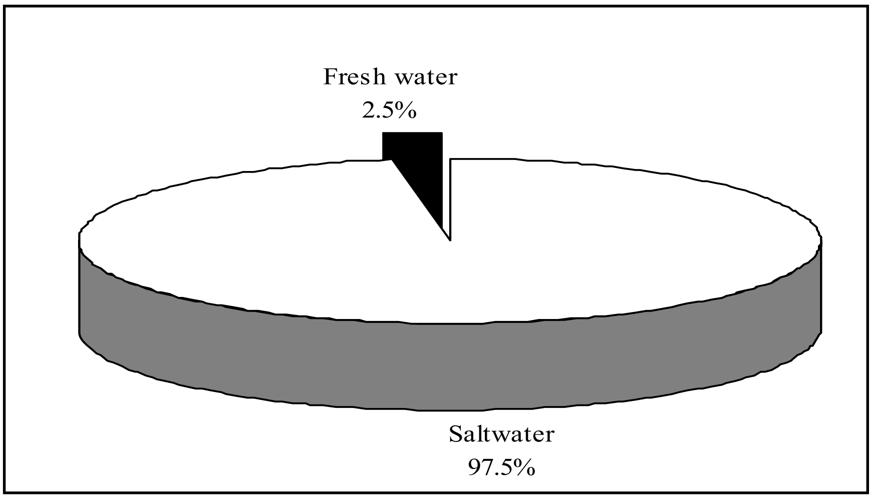


Figure 1.2: The world's water resources (BBC News Website, 2007).

BBC News reported that water demand already exceeds supply in many parts of the world, and as world population continues to rise at an unprecedented rate, many more areas are expected to experience this imbalance in the near future (BBC

News Website, 2007). The increase in water demand doubles every two decades, but the increase in supply is much less (Chan, 2009). As a result, while in the 1950, the council estimated that only 12 countries with 20 million people faced water shortages, this figure has increased more than two folds to afflict 26 countries in 1990 with the affected population increasing to more than 15 folds at 300 million (Chan, 2009). The Council has projected that by 2050, 65 countries will be hit by water supply problems with a total of seven billion people or 60 % of the world's population affected (Chan, 2009).

Most countries in the Middle East and North Africa can be classified as experiencing absolute water scarcity today. By 2025, Pakistan, South Africa, and large parts of India and China will join these countries. Many African countries, with a population of nearly 200 million people, are facing serious water shortages. By the year 2050, the United Nation estimates that there will be an additional 3 billion people, with most of the growth in developing countries that will suffer water stress (United Nation Website, 2007).

In the Middle Eastern countries, water has become the oil-rich region's primary concern over recent years, due to fears of a water shortage. One in every five people live in countries with inadequate fresh water and in 25 years, the ratio is estimated to be one in every three people (Indiana University Website, 2007). In many countries, water either has to be obtained from sources outside their borders (from neighbouring countries) or via desalination. On top of that, many countries that share the same river basin are already now fighting over the resource. It is therefore critical that available water resources be conserved, managed and shared equally to ensure sustainable and high quality supply, as well as to maintain regional co-operation.

1.3 .Water Situation in Malaysia

Malaysia is rich in water resources, receiving an abundant amount of rain every year**.** This country receives heavy annual rainfall with the average annual rainfall of 2,400 mm for the Peninsular Malaysia, 2,360 mm for the state of Sabah and 3,830 mm for the state of Sarawak (The Malaysian Water Association, 2001). Lately, the water supply situation for the country has changed from one of relative abundance to one of scarcity. Population growth and urbanisation, industrialisation and the expansion of irrigated agriculture are imposing rapidly increasing demands and pressure on water resources, besides contributing to the rising water pollution. The way forward to a prosperous and sustainable future is to keep development to a level that is within the carrying capacity of the river basins while protecting and restoring the environment.

Another factor that contributes to water shortages in many parts of the world is the changing in rainfall patterns as an effect of global warming. In Malaysia, the annual rainfall is estimated at about 990 billion m^3 by taking into consideration of the surface area 330,000 km^2 (Subramaniam, 2007). 566 billion m^3 of the annual rainfall becomes surface runoff, 630 billion m^3 evaporated and another 64 billion m^3 infiltrate (absorbed by the ground) the ground to be groundwater (Subramaniam, 2007). It is estimated that water consumption in this country is about 15 to 18 billion m^3 of treated water (Subramaniam, 2007). This means that Malaysia is wasting a lot of rainwater and has not implemented significant measures to recover it. Other major issues must be addressed to ensure sustainability of water resources is water pollution. Water pollution is a serious problem in Malaysia and gives negative impacts on the sustainability of water resources. It reduces total water availability and increases the cost of treating polluted waters.

Another major water issue in Malaysia that needs to be urgently addressed is the high domestic water usage per capita. In Malaysia, the average water usage is about 300 liters of water per capita per day (LPD). This amount however has increased over the years. It is reported that in the 1970s, Malaysians used only about less than 200 LPD. This number then increased to about 250 LPD in the 1980s and more than 300 LPD for now. In urban sector, it has been estimated that the average person uses is about 500 LPD (Renganathan, 2000). United Nations recommended the international standard for water use is 200 LPD. However, Malaysians used 100 LPD more than the amount suggested by the United Nations. This clearly shows that Malaysians do not practice sustainable water consumption.

In addition, Malaysia also faces some water-related problems which have raised concerns among water engineers and the public. In some river basins, there is already the problem of water shortage especially during periods of prolong droughts, and conversely, the problem of excessive water and floods during the wet season. These problems have disrupted the quality of life and economic growth in the country and can result in severe damage and loss of properties, and occasionally loss of human lives. This can be seen in the recent December 2006 and January 2007 floods in Johor as well as the 1998 prolong water rationing widespread in the Klang Valley area. Despite the abundance of rain, Malaysia has experienced the worst water shortage in 1998. The water shortage happened in the most populated and industrialised state such as Selangor, Penang and Malacca. However due to the fact that the water sources is under the authority of the respective states, it is hard to transfer water from one state to another legally (The Malaysian Water Association, 2001).

1.4 Problem Background

Over the past two decades, the primary concern has always focused on end-of-pipe wastewater treatment. End-of-pipe solutions have been seen as the sole remedy to meet the imposed discharge limits. Scarcity of water, stricter environment regulations on industrial effluents and the rising costs of fresh water and effluent treatment underline the growing emphasis on fresh water minimisation in industry, which also influences wastewater minimisation. Water system integration becomes the research focus, being an efficient technology for saving fresh water and reducing wastewater as it can assist organisations to maximise water saving. Therefore, at present, the research on fresh water and wastewater minimization mainly focuses on water system integration.

In the recent years, several researches have been done on the synthesis of process water systems using mathematical programming approach. Mathematical programming technique is a more suitable approach compared to heuristics based-approach for optimum water-using networks, for both grassroots and retrofit application. This technique has emerged primarily to overcome the limitations encountered by the graphical approaches particularly for large-scale and complex problems involving multiple contaminants. They serve as a good synthesis tool in handling complex systems with different complex constraint.

Recently, the idea of water minimisation is dominated by pinch analysis technique. The idea of cost-effective minimum water network (CEMWN) design with consideration of process changes guided by water management hierarchy is first attempted by Wan Alwi (2007). Although the technique provides an interactive, quick and efficient guide to screen design options involving process changes prior to conducting detailed water network but the tedious graphical steps and manually heuristics procedure has limitation when handling large scale and complex problems involving multiple contaminants. Furthermore, the technique is only applicable for single contaminant system. Hence, the development of a new systematic approach to design an optimal water networks by using mathematical programming technique involving multiple contaminants is proposed in this work to overcome the limitations of previous works.

In this study, the optimisation problem is formulated as a mixed integer nonlinear program (MINLP) and is implemented in GAMS. The model known as

Model for Optimal Design of Water Networks (MODWN) is capable of predicting which water source should be eliminated or reduced or how much external source is needed, which wastewater source should be reused/recycled, regenerated or discharged and what is the minimum water network configuration for maximising the net annual savings at a desired payback period. The MODWN is applicable for retrofit design. Note that, this model also can be applied to a wide range of building in urban sector.

1.5 Problem Statement

Given a set of global water operations with multiple contaminants concentrations, it is desired to design an optimal and holistic minimum water network with maximum net annual savings that considers all water management hierarchy options to achieve desired payback period for retrofit design using mathematical programming approach.

1.6 Objective of the Study

The main objective of this research is to develop a new systematic approach for designing an optimal water utilisation network involving multiple contaminants using mathematical programming approach.

1.7 Scope of the Study

To achieve the objective, five key tasks have been identified in this research. The scope of this research includes:

1. Analysing the state-of-art techniques on Water Pinch Analysis (WPA) and mathematical programming approach related to water minimisation.

2. Establishing a new water targeting procedure for maximum water recovery using mathematical programming approach.

3. Performing a new optimisation model on water system that considers water management hierarchy options to obtain the minimum water utilisation network that yield maximum net annual saving within the desired payback period for retrofit scenario.

4. Applying the optimisation models on urban case study to illustrate the effectiveness of the approach.

5. Comparing the optimisation model with CEMWN approach.

1.8 Research Contributions

The key specific contributions of this work are summarised as follows:

1) A new systematic technique to target the minimum fresh water consumption and wastewater generation to achieve maximum water recovery for systems involving single and multiple contaminants.

  - A generic linear programming (LP) model has been developed based on water network superstructure to simultaneously set the targets and design the maximum water recovery network, for both mass transfer-based and non-mass transfer-based problems (i.e., global water operations).

2) A new optimisation model for synthesis of minimum water network (MWN) for multiple contaminants problem.
   - A generic optimisation model has been developed to obtain minimum water utilisation network that considers all process changes options in WMH i.e. elimination, reduction, reuse/outsourcing and regeneration simultaneously.

3) A new optimisation model that ensure cost effective water network for multiple contaminants system for retrofit design.
   - A new generic optimisation model known as Model for Optimal Design of Water Network (MODWN) is able to solve complex water systems involving multiple contaminants that include all levels of water management hierarchy (i.e. elimination, reduction, reuse, outsourcing and regeneration), multiple utilities, and cost constraints simultaneously. The optimisation model is also capable to suggest which process changes from WMH options should be selected in order to achieve desired payback period while maximising net annual savings for retrofit design.

4) The optimisation model can be employed to the cases involving pure and impure fresh water for multiple contaminants.

5) The optimisation model can be applied to a wide range of building in urban and industrial sectors.

Table 1.1 lists all the publications and output of this work and the associated key contributions of this project towards global knowledge on water minimisation.

Table 1.1: Refereed national and international journals; conference papers submitted; patent applied towards contribution of knowledge from this work.

No.	Paper title	Publication type	Status	Contribution towards knowledge
1.	**Handani, Z. B.,** Wan Alwi, S. R., Hashim H., Manan, Z. A. and Sayid Abdullah, S. H. Y. Optimal Design of Water Networks Involving Multiple Contaminants. CHERD-D-09-00015, *Chemical Engineering Research and Design*	International Journal	In review	Contribution (1), (4), (5)
2.	**Handani, Z. B.,** Hashim H., Wan Alwi, S. R., Manan, Z. A. A generic optimisation model for optimal design of water networks. *Computers and Chemical Engineering.*	International Journal	In writing	Contribution (3), (4), (5)
3.	**Handani, Z. B.,** Hashim H., Wan Alwi, S. R., Manan, Z. A., A Review on Optimal Design of Water Networks. *The Scientific World Journal.*	International Journal	In writing	Contribution (3), (4), (5)
4.	**Handani, Z. B.,** Wan Alwi, S. R., Hashim, H. and Manan, Z. A., Optimal Design of Water Networks Involving Single Contaminant, *Jurnal Teknologi, Series E.*	National Journal	In press	Contribution (1), (4), (5)
5.	**Handani, Z. B.**, Wan Alwi, S. R., Hashim, H. and Manan, Z. A. (2008). Simultaneous Targeting and Design of Minimum Water Networks involving Multiple Contaminants. *RSCE-SOMCHE Proceedings 2008.*	International Conference	Published	Contribution (1), (4), (5)
6.	**Handani, Z. B.,** Wan Alwi, S. R., Hashim, H. and Manan, Z. A. (2008). Optimal Design of Water Network Involving Single Contaminant. *International Conference on Environment 2008 (ICENV)* (15-16 December 2008)	International Conference	Published	Contribution (1), (4), (5)
7.	**Z. B. Handani,** S. R. Wan Alwi, H. Hashim and Z. A. Manan (2009). A Generic Approach for Synthesis of Minimum Water Utilisation Networks. *International Conference on Chemical Engineering and Bioprocess. SOMCHE-ICCBPE Proceedings*, 12-14 August 2009.	International Conference	Published	Contribution (1), (4), (5)
8.	Wan Alwi, S. R., **Handani, Z. B**., Hashim, H., and Manan, Z. A. PI 2009 3813. A system for obtaining water network involving multiple contaminants for global water operations and method thereof. UTM Patent.	UTM patent	Filed	Contribution (1), (4), (5)
9.	**Handani, Z. B**., Hashim, H., Wan Alwi, S. R., and Manan, Z. A. A generic optimisation model to obtain cost-effective minimum water utilization network involving multiple contaminants. UTM patent	UTM patent	Submitted	Contribution (3), (4), (5)

1.9 Summary of this Thesis

This thesis consists of six chapters. Chapter 1 gives an overview of the local and global water issues, research background, problem statement, objective and scope of the study which aims to develop new systematic approach for designing an optimal water utilization network involving multiple contaminants using mathematical programming approach. Chapter 2 provides a review of the relevant literatures of this thesis. The development of research in water targeting and network design techniques using pinch analysis and mathematical programming are reviewed. Cost-effective minimum water network is also covered in this chapter. Chapter 3 of this thesis describes the fundamental theory related to water and wastewater minimisation. Chapter 4 shows a detailed methodology of this research to achieve the targeted objectives. It consists of optimal design of water networks methodology for retrofit case for global water operations to achieve maximum net annual savings. Chapter 5 presents and discuss the results on the implementation of the developed methodology on an urban case study to demonstrate the applicability and benefits of using the new mathematical model. Lastly, Chapter 6 summaries the main points and contributions of the thesis and explores the possible potential areas for future works. Figure 1.3 shows the outline of this thesis.

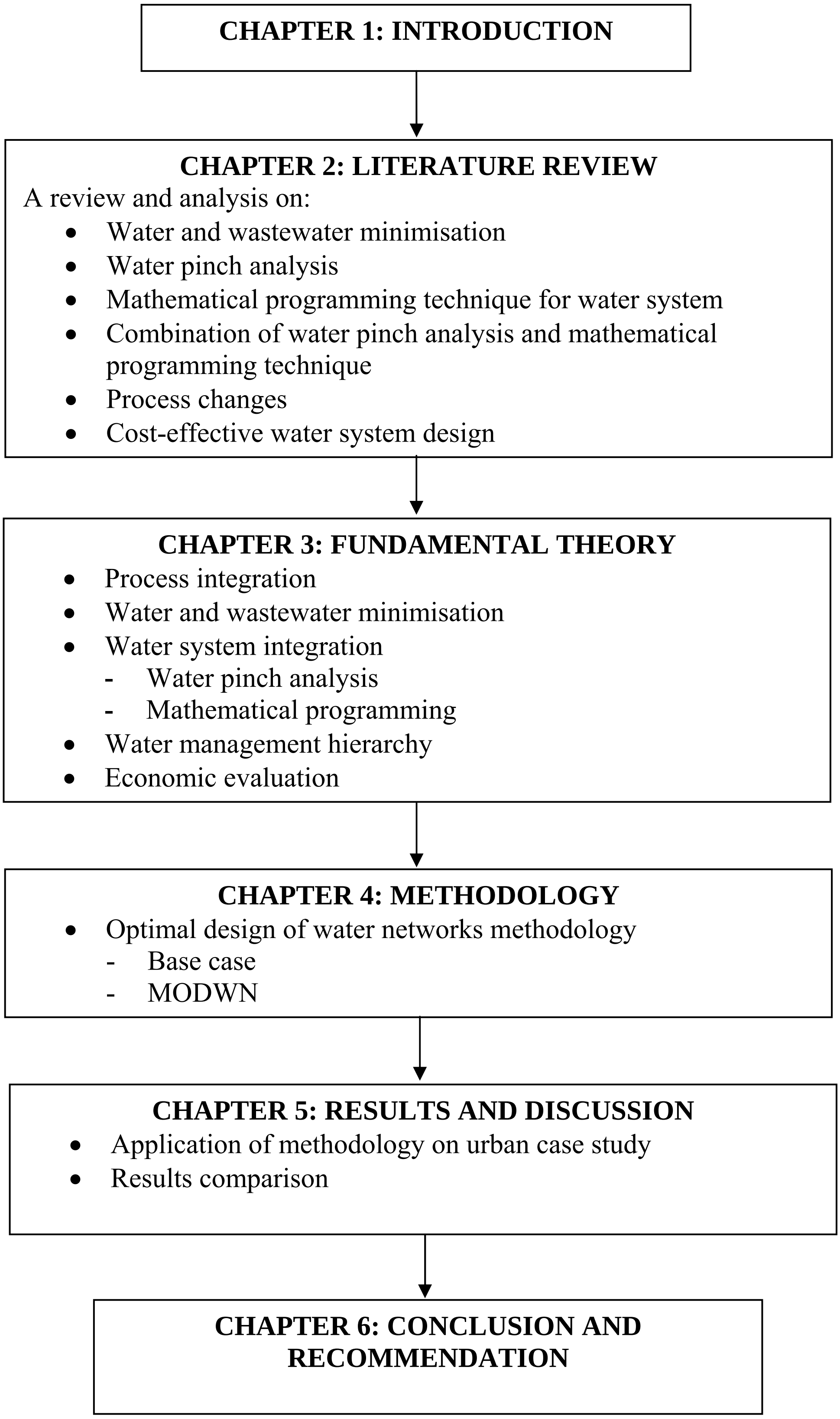


Figure 1.3: A flow diagram illustrating the conceptual link between the chapters.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter summarises prior works related to optimal design of minimum water utilisation network. Section 2.2 reviews on current water and wastewater minimisation techniques. The state-of-the-art of water pinch analysis and mathematical programming for water network synthesis is reviewed in Section 2.3 and Section 2.4 respectively. In these sections, the advantages and disadvantages of water pinch analysis and mathematical programming are evaluated. Section 2.5 reviews the combination of water pinch analysis and mathematical programming technique in solving water network design problems. Implementation of process changes on water minimisation is discussed Section 2.6. In Section 2.7, the current optimal design of water network costing technique is reviewed in the point of view of total cost and profitability as objective function. This chapter also highlights the specific research gap for each review.

2.2 A Review on Water and Wastewater Minimisation

Over the past two decades, the primary concern has always been more focused on end-of-pipe wastewater treatment. End-of-pipe solutions have been seen as the sole remedy to meet the imposed discharge limits. Later, the main concern shifted towards solutions that maximise water reuse from conventional water treatment to more sustainable water minimisation activities. In the early eighties, water reuse started to become one of the active areas for water minimisation activities as a means of reducing the total water requirements. This not only saves upstream treatment of raw water but also reduces wastewater treatment costs. Additionally, zero water discharge cycles became a desired goal for grassroots and retrofit designs.

Takama *et al.* (1980) concluded that it was possible to reduce the large quantities of fresh water intake and wastewater produced by industrial processes by considering the entire water network as a total water system. The authors developed a mathematical formulation and transformed it into a series of problems without inequality constraints by employing a penalty function. In other work, the basic concept underlying the methodology is Mass Exchange Network (MEN) technology, which was first pioneered by El-Halwagi and Manousiouthakis (1989). They introduced the notion of MEN for the preferential transfer of a key contaminant from rich streams into lean streams.

Afterwards, Wang and Smith (1994) considered the water minimisation problem by maximising the water reuse potential using graphical approach for targeting and manual approach to design. The authors also discovered options of regenerating wastewater even when concentration of pollutants has not reach end-of-pipe limits. Besides, they introduced the important concept of ‘water pinch’ and presented a conceptually based approach on wastewater minimisation, by which the minimum fresh water utilisation of a water using system can be obtained in a direct way.

Notably however, the use of graphical approach for targeting the minimum fresh water demand for a system has been shown to be somewhat limited in terms of the number of contaminants and the types of water-using operations that can be considered. As a result, the use of mathematical programming approach has become the preferred method for designing minimum water network. Moreover, this method allows the incorporation of more complicated constraints such as forbidden connections in the network structure. Thus, its use for these purposes was presented by Takama *et al.* (1980) over a decade before Wang's Pinch Analysis (Wang and Smith, 1994) based approach application.

2.3 A Review on Water Pinch Analysis (WPA)

Water pinch analysis approach comprises two distinct stages, targeting followed by design. This approach involves the identification of the minimum fresh water and wastewater targets for the system ahead of design of the network which achieves these targets.

2.3.1 Previous Works on Water Targeting Approach

A method of targeting for maximum water reuse was first introduced by Wang and Smith (1994). This method was based on the concept of limiting water profile which defines the most contaminated water which can be fed to an operation in terms of a maximum inlet concentration and a maximum outlet concentration. They make use of the limiting water profile to pinch point the pinch location and generate the exact minimum water targets prior to network design. Various options for water reuse, regeneration reuse and regeneration recycling are explored. The limiting water profile describes a major stride in establishing the baseline water requirement and wastewater generation for a process in the system. However, its applicability is only limited to mass-transfer based operations. Therefore, the method fails to achieve the true maximum water recovery targets and design as claimed.

Dhole *et al.* (1996) proposed the water source and demand composite curves to overcome the limitation of Wang and Smith (1994) work. They also suggested process changes such as mixing and bypassing to further reduce the fresh water consumption. On the other hand, Polley and Polley (2000) later demonstrated that unless the correct stream mixing system was identified, the apparent targets generated by Dhole's technique (Dhole *et al.,* 1996) could be substantially higher than the true minimum fresh water and wastewater targets.

Additionally, Sorin and Bédard (1999) established *the evolutionary table* to numerically determine the fresh water and wastewater targets. The authors pointed out that the targeting approach introduced by Dhole *et al.* (1996) could result in a number of "local" pinch points, which might not necessary be the actual or the "global" pinch points. However, the method fails to locate pinch point correctly when multiple pinch points exist in water using processes, as mentioned by Hallale (2002).

Hallale (2002) suggested a graphical procedure based on water surplus diagram to find the absolute targets. The idea of surplus diagram was adapted from hydrogen pinch analysis by Alves and Towler (2002). This approach had similar representation to the water source and demand composite curves introduced by Dhole *et al.* (1996). Nevertheless, this approach is more superior where it is capable to handle both mass transfer-based (MTB) and non-mass transfer-based (NMTB) operations. This new work represented by Hallale (2002) has the ability to handle all mixing possibilities and yet still result the true pinch point and water reuse target.

Nonetheless, Hallale (2002) works were improved by Manan *et al.* (2004) by numerical technique development that could give the same effect as the graphical water targeting method proposed by Wang and Smith (1994) and Hallale (2002). They proposed the water cascade analysis (WCA) technique to establish the minimum water and wastewater targets for single contaminant problem in a maximum water recovery (MWR) network. The technique is equivalent to the water surplus diagram (Hallale, 2002), with the elimination of tedious and iterative calculation steps. It is also applicable for global water-using operations.

Aly *et al.* (2005) introduced the load problem table (LPT) which is another numerical technique to establish the minimum water requirement for maximum water recovery and minimum wastewater generated. This technique was adapted from load interval diagram (LID) by El-Halwagi and Almutlaq (2004) for material reuse and recycling. Nevertheless, the LPT is almost similar with the Problem Table Algorithm (PTA) used in heat integration. This table is able to insight on network design and can be applied for MTB and NMTB operations.

A source composite curve-based approach for simultaneous targeting distributed effluent treatment system and minimum fresh water demand is introduced by Bandyopadhyay *et al.* (2006). Similar with previous study, (Hallale, 2002; Manan *et al.,* 2004; Aly *et al.*, 2005) this approach also can caters problem involving MTB and NMTB operations.

2.3.2 Previous Works on Water Network Design

Apart of the targeting stage, various techniques have also been suggested to design the network which achieves the flow rate targets. The first water network design based on composite curves was reported by Wang and Smith (1994). The authors introduced a grid diagram to carry out the design of water network that achieve the water targets. The approach will maximize the driving force in the resulting design.

In other work, Polley and Polley (2000) introduced the concept of source and demand mapping and employed a set of heuristics to successively match the demand with the concentration lowest with source that has lowest concentration in ascending order to satisfy the quantity (flow rate) and quality (load) of the demand. This method however failed when dealing with multiple pinch problems.

Prakash and Shenoy (2005a) proposed a principle of nearest neighbours to synthesise single contaminant water networks. The nearest neighbours algorithm (NNA) based on the principle that the sources to be chosen to satisfy a particular demand must be the nearest available neighbours in terms of contaminant concentration. This principle generated a single network that meets the minimum fresh water target. The NNA principle also has been used by Bandyopadhyay (2006) to satisfy minimum wastewater target for water management. Prakash and Shenoy (2005b) later improved their work by introducing the concept of source shifts to design many different water networks that are applicable to single contaminant water network.

Aly *et al.* (2005) introduced the first numerical technique on simultaneous targeting and network design for maximum water recovery. The authors employed the LPT for identifying the minimum fresh water requirement for maximum water recovery and minimum wastewater generation. They also introduced systematic procedure for water network design to obtain the targets by observing the pinch divisions and following some guidelines (Hallale, 2002; Prakash and Shenoy, 2005).

El-Halwagi *et al.* (2003) as well as Prakash as Shenoy (2005a) introduced the source and demand composite curves (SDCC). The SDCC is a plot of cumulative mass load versus cumulative flow rate. This method can be used to establish the minimum water flow rates targets for both mass transfer-based and non-mass transfer-based operations. In addition, they applied the SDCC for matching and allocation of mass load and flow rates of each source and demand. El-Halwagi *et al.* (2003) employed the source and demand allocation rule known as "cleanest to cleanest" for network design which is also used by Polley and Polley (2000). Kazantzi and El-Halwagi (2005) extended the use of sources and demand allocation for impure fresh water.

Recently, Wan Alwi and Manan (2008) proposed a new technique and a set of heuristics to design water utilisation network based on source and demand allocation composite curves (SDAC) for simultaneous targeting and design of water networks. The authors also introduced Network Allocation Design (NAD) as a useful visualisation tool for designing water networks. The approach can be applied for global water-using operations and generate targets for the cases with mass load as well as flow rate deficits. It can also simultaneously solve complex design problems involving multiple pinches.

2.3.3 Research Gap on Water Pinch Analysis

All the above mentioned water pinch analysis methods have mainly focused on single contaminant cases. Remarkably however, the use of water pinch analysis approach for targeting the minimum fresh water requirement for a system has been shown to be somewhat limited in terms of the number of contaminants. Other major drawbacks of water pinch analysis technique in handling water systems are that the approach is not effective in optimising large-scale system consisting of a large number of water-using operations and complex water distribution systems. Even though water pinch analysis can be applied to multiple contaminants system, the targeting and design step have proved to be too cumbersome and unreliable. As a result, the use of mathematical programming approach has become the preferred method for designing water-reuse networks. A review on mathematical programming approach for water system will be explained in the next section.

2.4 A Review on Mathematical Programming Technique for Water System

Mathematical programming technique has emerged primarily to overcome the limitations encountered by the graphical approaches particularly for large-scale and complex problems involving multiple contaminants. In recent years, several researches have been done to synthesise optimal water networks using mathematical programming approach as described next.

2.4.1 Previous Works on Targeting and Design for Multiple Contaminants System

Since the conceptual approach shows limitations where complex systems are involved particularly in the area of systems involving multiple contaminants, mathematical programming has become the method of choice for water-system design (Bagajewicz, 2000). Typically, a set of candidate network designs is formulated as a superstructure comprising fresh water sources, wastewater sinks, unit operations, mixers and splitters. Similar to any other optimisation study in process synthesis, it is necessary to build a superstructure in which all possible flow configurations are embedded.

The implementation of mathematical programming approach in solving water or wastewater minimisation problems has been reported in the literature since 1980s. Early work was on solving a problem to reduce fresh water consumption in a petroleum refinery involving multiple contaminants system using superstructure coupled with mathematical programming by removing irrelevant and uneconomic connection (Takama *et al.,* 1980). The authors made an important contribution by addressing the management problem as a combination of water and wastewater allocation among processes and wastewater distribution. The problem was solved by using a complex method by employing a penalty function after transforming the nonlinearities into a sequence of linear functions without inequality constraints.

Doyle and Smith (1997) proposed an iterative procedure to solve bilinear constrained problem to overcome the difficulties of the conceptual design approach by presenting a combination of linear and nonlinear formulations for MTB operations. The authors developed the formulation by assuming that all contaminants have reached their maximum outlet concentrations for all operations and solved the problem by linear program (LP) to achieve optimal network design that corresponds to minimum fresh water consumption. Then, with the obtained water network, they reformulate the problem back into nonlinear program (NLP) and optimise it to get the exact value. This method addressed new design problems, in which all possible piping connections can be formulated to get optimum solution of total fresh water consumption. However, the obtained solution may not be a practical solution due to its complexity towards having the optimum solution and other practical constraints.

Alva-Algáez *et al.* (1998) suggested a decomposition of the mixed integer nonlinear program (MINLP) problem into a sequence of relaxed mixed integer linear program (MILP) problems to approximate the optimal solution. They fixed all outlet concentrations to their maximum limits for water-using operations and zero for treatment operations. Later, Alva-Algáez *et al.* (1999) developed multiple contaminant transhipment models at a conceptual stage for mass exchanger network and wastewater minimisation problems using MILP formulation.

Apart from that, Huang *et al.* (1999) presented a mathematical programming solution for the combined problem of water usage and treatment network (WUTN). The authors suggested a superstructure approach that considers the water-using and water-treating subsystems simultaneously. The superstructure included all interactions and possible connections between the water-using and water-treating subsystems, as well as those between the process operations, fresh water sources and wastewater discharges. In this work, the integrated network was optimised using NLP model. However, as stated by the authors, this approach does not guarantee global optimality.

Bagajewicz *et al.* (2000) introduced a tree searching algorithm with efficient branch cutting criteria to solve globally the multiple contaminants for water allocation problem featuring minimum total cost. The approach is also capable in providing alternative sub-optimal solutions for grassroots and retrofit design. Subsequently, Savelski and Bagajewics (2003) presented the necessary conditions of optimality for water utilisation system with multiple contaminants. The authors set up a multiple contaminants necessary conditions for water-using processes when at least one contaminant reaches its maximum possible outlet concentration. Monotonicity conditions have also been derived known as key contaminant and the problem is solved with developed algorithmic procedures that guarantee global optimum.

Dunn *et al.* (2001) reported the results for the only NMTB problem found thus far, which uses an NLP model to target minimum wastewater generation by maximizing wastewater recovery. Even though the approach was said to have managed to reduce wastewater generation, it failed to consider fresh water usage as source. No methodology for solving the problem was presented.

Later, Wang *et al.* (2003) described the application of the water networks with single internal water main for multiple contaminants. Water networks with just one internal water main determined by the presented method can obviously reduce water consumption, approaching the minimum water consumption target. The authors tried to solve the problem by presenting a related design methodology for water network that is easy to design, operate and control. Although the authors used single water main to reduce fresh water consumption, it cannot guarantee global solution. Zheng *et al.* (2006), in their paper, proposed an optimal design procedure for water networks with multiple internal water mains. The methodology permitted experimentation with the number of internal water mains and the number of outlet streams from each process unit.

More recently, Teles *et al.* (2008) proposed two initialisation procedures that provide multiple starting points to design optimal water network for MTB and NMTB operations by reducing NLP to LP during initialisation procedures using global optimisation methods (Quesada and Grossmann, 1995). However, the method also has its drawback since it requires highly computational effort due to the large number of problems that needs to be solved which may lead to an unreasonable computation time for problem involving more than six operations.

Most of the mathematical programming approaches based on NLP or MINLP involving multiple contaminants are focused on mass transfer-based operations. NLP and MINLP are very dependent on starting point and do not guarantee global optimum. Therefore, many authors then solved it using a two-stage optimisation to approximate the optimal solution (Doyle and Smith, 1997; Alva-Algáez, 1999; Gunaratnam *et al.*, 2005; Putra and Amminudin, 2008; Teles *et al.,* 2008). In contrast, Castro *et al.* (2007) claimed that their heuristic procedure was able to generate good starting point and find global optimal solutions up to three orders magnitude faster than when using the global optimisation BARON to solve NLP problem.

2.4.2 Research Gap on Mathematical Programming Technique for Water System

Mathematical programming technique has emerged primarily to overcome the limitations encountered by the graphical approaches particularly for large-scale and complex problems involving multiple contaminants. In recent years, several researches have been done to synthesise optimal water networks using mathematical programming approach. Most of the mathematical programming approaches based on NLP or MINLP involving multiple contaminants are focused on MTB (Takama *et al.,* 1980; Doyle and Smith, 1997; Alva-Argáez *et al.,* 1998; Alva-Argáez *et al.,* 1999; Huang *et al.,* 1999; Bagajewicz and Savelski, 2000) and NMTB operations (Dunn *et al*., 2001; Wang *et al.,* 2003).

The application of water minimisation strategies involving multiple contaminants for both MTB and NMTB operations was first discovered by Teles *et al.* (2008). However, due to the NLP model, it is difficult to converge to the global optimum. The method requires highly computational performance which increases with problem size and may lead to an unreasonable computation time. Furthermore, NLP and MINLP are very dependent on starting point and always lead to sub-optimal local solutions. Therefore, there is a clear need to solve the problem to guarantee global optimum solution is achieved.

2.5 A Review on Combination of Water Pinch Analysis and Mathematical Programming Technique

Although mathematical programming approach offers the advantages in handling complex water systems involving multiple contaminants, it is less popular among engineering practitioners. This is due to the difficulty to master the technique and little insights on water networks design. On the contrary, water pinch analysis helps in getting a physical insight of the problem through its graphical representations and simplified tableau-based calculation procedures. The two approaches are complementary where the visualization ability improves engineering understanding and the mathematical model allows the handling of complex problems.

Alva-Algáez *et al.* (1998 and 1999) developed the integrated approach combining the insights of both water pinch and mathematical programming in handling mass transfer-based problems. Alva-Algáez *et al.* (1999) showed that conceptual model takes the form of a multiple contaminant transhipment model and is formulated as a MILP problem. In other work, Jacob *et al.* (2002) reported that water network of pulp and paper processes is analysed using combination of pinch analysis and LP for the fixed flow rate problems. On top of that, Ulmer *et al.* (2005) proposed a strategy and software system for the synthesis of process water systems that combined the advantages of heuristic rules and mathematical method to generate a promising design.

An automated design of total water systems was suggested by Gunaratnam *et al.* (2005), where the optimal distribution of water to satisfy process demands and treatments of effluent streams are considered simultaneously. It combined engineering insights with mathematical programming tools based on a superstructure model that results in a MINLP problem initially. The design problem is decomposed into two stages. The first stage consists of a relaxed MILP and LP formulation that is solved in an iterative manner to provide an initial starting point. The solution available from the first stage is refined in the second stage to a final solution in a general MINLP. The approach is claimed to overcome the disadvantages of the previous method proposed by Alva-Algáez (1999). This approach offers a reduced number of variables and iterations for convergence. Nonetheless, similar to Alva-Algáez's method (Alva-Algáez, 1999), the method does not show in a greater detail of the variety of water networks as finding one optimum solution is the target of the work.

Pillai and Bandyopadhyay (2007) later proposed a mathematically rigorous methodology to minimise the requirement of a natural resource in chemical industry. It provided a rigorous mathematical proof to the source composite curve graphical approach of pinch analysis proposed by El-Halwagi *et al.* (2003). The authors have successfully tested and proven their mathematical models on various case studies involving resource conservation. The algebraic approach also can handle cases where the resource quality is not the purest.

In recent study by Liao *et al.* (2007), mathematical programming combined with pinch insight has been used in designing flexible multiple plant water networks to obtain the minimum fresh water usage and cross plant interconnection (CPI) without considering the detailed network design. The approach is applicable for both mass transfer-based and non-mass transfer-based operations involving single contaminant problem.

2.6 A Review on Water Minimisation through Process Changes

In the past, many researchers focused on maximum water recovery concept which is related to maximum water reuse, recycle and regeneration. Nevertheless, it does not lead to the minimum water targets as widely claimed by researchers over the years. Moreover, regenerating wastewater without considering the possibility of elimination and reduction may lead to unnecessary treatment units. Process changes implementation is discussed fairly and extensive work on water targeting approaches with the presence of regeneration process on water pinch analysis and mathematical programming approach.

Takama *et al.* (1980) first addressed the problem of optimal water allocation in a petroleum refinery by generating a superstructure of all possible reuse and regeneration opportunities. The problem was solved by removing irrelevant and uneconomic features of the design. Later, Wang and Smith (1994) found that if regeneration is correctly integrated into a water system, water regeneration unit could decrease the water and wastewater flow rates. The authors also illustrated how minimum water targets can be achieved using the composite curve when a source are treated to a new concentration.

Later Mann and Liu (1999) further developed the concept of water pinch technologies for water regeneration by providing guidelines to analysis, synthesis and retrofit of water networks. They also investigated three regeneration techniques and discussed how to determine the optimal contaminant levels and minimum water targets for these regenerations. Castro *et al.* (1999) developed a regeneration reuse algorithm capable to target and design minimum fresh water and regenerated water consumption.

Bagajewicz and Savelski (2001) presented a LP model for optimising regeneration recycling water system at certain outlet concentration in the regeneration unit by applying the necessary conditions of optimality they have proposed earlier (Savelski and Bagajewicz, 2000). Nonetheless, this work is restricted to problems with single contaminant.

A handy graphical method for constructing the optimal water supply line for regeneration recycling water system involving single contaminant was proposed by Feng *et al.* (2007). They adopted sequential optimisation method and summarised three general formulas to achieve the targets for fresh water, regenerated water and regeneration concentration. Nevertheless, this work showed that the optimal regeneration concentration is not correlated with the pinch concentration of the system but dependent on distinctive limiting composite curves.

Bai *et al.* (2007) implemented the sequential optimisation procedure and extended the graphical technique to regeneration reuse systems. The authors presented three categories of water-using systems that have different characteristics. In addition, they also introduced two general formulas for calculating corresponding targets for total regeneration reuse systems based on concept of limiting points.

In contrast, Feng *et al.* (2007) employed sequential optimisation and optimised regeneration recycling water networks at grassroots design stage using NLP and MINLP models. The mathematical models are solved step by step to obtain minimum fresh water consumption, minimum regenerated water flow rate and minimum contaminant regeneration load. Moreover, this method can be applied for both single and multiple contaminants regeneration recycling water networks.

Tan *et al.* (2009) developed a new superstructure-based model for synthesis of water networks with centralised partitioning regenerators. The wastewater from different sources are purified and partially treated in the regeneration system which then discharge to lean and reject streams before further reused/recycled in other operation in the process system. The regenerators can be modelled as a fixed outlet concentration or fixed removal ratio of the total contaminant in the system. This work however is limited to single contaminant system since the performance of common partitioning regenerator is measured in terms of single contaminant.

As stated before, implementations of regeneration reuse/recycle can reduce fresh water demand and wastewater generation, but it does not lead to the minimum water targets. Minimum water targets only can be achieved when all conceivable methods are implemented. Earlier work on the use of water minimisation strategy beyond recycling had been done by El-Halwagi (1997), who proposed targeting technique involving water elimination, segregation, recycle, interception and source/sink manipulation. Hallale (2002) gave clear guidelines for process modifications and regenerations through pinch approach and how water surplus diagram can offers this insight to the designers.

Bandyopadhyay (2006), in his work reported that appropriate process changes or process modification can further reduce the waste regeneration. The author presented a methodology for waste reduction through process modifications by changing quality and/or demands and sources flow rate. They also discussed issues related to process modification and their effect on waste generation.

More recently, Wan Alwi and Manan (2006) and Wan Alwi *et al.* (2008) introduced a water management hierarchy (WMH) to give new insight in process modification. The minimum water network (MWN) design not only considers reuse and recycling but all conceivable methods to holistically reduce fresh water consumption through elimination, reduction, reuse/outsourcing and regeneration based on the WMH. All this process changes are systematically implemented in terms of priority through a clear guidance.

2.7 A Review on Cost-Effective Water System Design

2.7.1 Previous Works on Cost-Effective Water Network Design

Previously, most of researchers have focused on minimising fresh water consumption with assumption that fresh water cost is the dominant portion of the cost function. Even though the aforementioned tendency is focused on fresh water minimisation, there are several works done on minimising cost objective for water system design.

Optimal wastewater reuse designs using process integration tools frequently suggest designs which ignored constraints as well as expensive pipes needed. Olesen and Polley (1996) discussed the influence of piping costs in their work. The authors also had incorporated some geographical constraints when setting water targets using composite curves developed by Wang and Smith (1994). They were able to set water targets for the various zone and considered intrazonal and interzonal water transfer by decomposing site water networks into zones. This approach tends to simplify network modifications and help ensure a feasible and cost effective network design. However, they did not present any cost analysis for further understanding. In other work, 'minimum composition difference' was introduced by Hallale and Fraser (1998) as a basis to determine the minimum number of units and ultimately the capital cost targets for mass exchanger networks which utilise water as a solvent.

Koppol *et al.* (2003) suggested zero or partial liquid discharge solution. The cost optimisation on the zero or partial liquid discharge networks is presented by varying the regeneration cost, fresh water cost as well as the treatment outlet concentration. Feng and Chu (2004) later established the optimum regeneration and treatment outlet concentrations can lead to the minimum total cost of a water system. The cost-optimisation models for water network in this work involved placement of the regeneration unit. Tan and Manan (2006) later adapted the finding for optimisation of existing regeneration units and presented a systematic approach for the retrofit of water networks involving single contaminant problem. They found various retrofit profiles were generated by varying regeneration flow rate and regeneration outlet concentration. After that, retrofit targets were determined from savings versus investment diagram at a certain limits on payback period or capital expenditure.

Earlier work on implementation of total cost as objective function had been done by Alva-Argáez *et al.* (1998). Later, Alva-Argáez *(*1999) employed the insights of water system design problem given by Kuo (1996) and formulated the problem with MINLP model. They then decomposed the model to MILP and NLP to solve the mathematical problems. This approach is intended to seek for minimum total annual investment and operating cost of water-using operations network by applying water reuse scheme. Their method is meant to get an optimum solution by incorporating practical constraints in the beginning of the mathematical formulations.

However, the method does not show in a greater detail of the development of the water network, especially when it is applied in retrofit scenarios. The proposed model included all possibilities for water reuse, regeneration-reuse and regeneration recycling.

Bagajewicz *et al.* (2000) presented a combination of mathematical programming and necessary conditions of optimality to automatically generate the optimal solution featuring minimum capital and operating costs. This approach was presented for the grassroots and retrofit design of water utilisation systems with multiple contaminants.

Jödicke *et al.* (2001) presented a MILP model which described the reusability constraints with connectivity matrix. The model attempts to minimise the operating cost (fresh water, wastewater treatment and pumping) and investment costs (piping and holding tanks). The approach is proposed as a screening tool to design wastewater network with minimal total cost for a given optimisation horizon.

Gunaratnam *et al.* (2005) later solved the total water system problem by considering complex trades-off involving the capital and operating costs as well as other practical constraints such as piping and sewer costs. They also included minimum or maximum allowable flow rates, compulsory and forbidden connections as well as geographical, control and safety considerations. In addition, the approach is capable to design water-using systems and effluent treatment systems simultaneously.

Even though the implementation of total cost as objective function have been successfully presented by previous works and gave minimum total cost, the idea however may not be attractive for most plant or building owners. This is due to the difficulty in applying the concept of minimum water network to the plants without being certain of its profitability. Therefore, economic evaluation using profitability as objective function becomes of more concern.

Wan Alwi and Manan (2006) and Wan Alwi *et al.* (2008) investigated a cost-effective minimum water network design for grassroots and retrofit cases involving single contaminant problem. The authors suggested a hierarchical procedure where each level of water management hierarchy is explored to obtain minimum water targets. They introduced a cost screening technique known as *Systematic Hierarchical Approach for Resilient Process Screening Approach (*SHARPS) to attain cost effective minimum water network for urban and industrial sectors. The SHARPS technique provides clearly quantitative insights to screen various water management options. By applying this methodology in accordance with the water management hierarchy, it is possible to identify which schemes should be partially applied or eliminated in order to satisfy a desired payback period, thereby allowing the designer to estimate maximum potential annual savings prior to design. Some processes can be replaced if the total payback period does not agree with the desired payback period set by a plant owner.

Lim *et al.* (2007) developed a mathematical model to maximise the profitability of water network system by maximising its net present value (NPV) using NLP model. They studied the profitability of the optimised network having the conventional water network as a baseline and applying incremental costs and benefits to rearrange the given network to more economically friendly water network system. The principal contributors to incremental costs including piping, maintenance and repairs (M&R), pipe decommissioning and fresh water consumption were formulated to calculate incremental costs and benefits required for the NPV evaluation. However, this work is only considered maximum water reuse and recycling.

Faria and Bagajewicz (2009) performed a grassroots design and retrofit cases for water systems with single and multiple contaminants using mathematical optimisation and profitability insights. In both cases, they considered regeneration process. The proposed methodology is used to maximise NPV and/or return of investment (ROI), instead of minimising fresh water consumption. Although the authors incorporated regeneration processes into the water system design, it does not yield minimum water targets as claimed by the authors. Furthermore, this work is only applicable for MTB operations.

2.7.2 Research Gap on Cost-Effective Minimum Water System Design

Previously, a lot of work had been done to achieve cost-effective minimum water utilisation networks. Although total cost as objective function has been successfully presented by previous works, the idea however may be unattractive to plant or building owners. The economic evaluation based on profitability with consideration of process changes becomes more attractive because it may lead to optimal design of minimum water utilisation network. As proposed by Wan Alwi and Manan (2006) and Wan Alwi *et al.* (2008) in their work, the sequence of priority water management steps is conducted in order to obtain cost-effective pre-design water network. Nonetheless, the graphical method and heuristics steps are quite cumbersome and tedious and only can be applied for single contaminant problem. Therefore, there is a clear need to develop a cost-effective of water networks using mathematical programming technique involving multiple contaminants that considers all water minimisation options to holistically reduce fresh water usage through elimination, reduction, reuse/outsourcing and regeneration. Furthermore, in mathematical programming technique, the WMH options are consider simultaneously.

2.8 The State-of-the-art on Optimal Design of Water Networks – Addressing the Research Gap

From the studies associated with the optimal design of water networks using mathematical programming approach previously mentioned, there are four issues that remain unsolved. These issues will be overcome with the new design procedure proposed in this study.

1. Water and wastewater minimisation problems involving multiple contaminants system are successfully solved using mathematical programming approach. Nevertheless, previous studies mainly focused on MTB operation for multiple contaminants problem. However, in real system there is also NMTB operation in industrial and urban sectors. In this study, the models are developed to simultaneously generate the minimum water targets and design minimum water network for global water-using operations involving multiple contaminant systems.

2. The concept of MWN design introduced by Wan Alwi *et al.* (2008) considered all conceivable methods to reduce water usage through elimination, reduction, reuse/recycle, outsourcing and regeneration. Hence, to guarantee that the MWN benchmark is obtained, process changes at each of WMH level must be prioritised based on heuristic procedures. These rules are applied based on technical experience and offer the possibility to consider those details. This method is however very tedious. In this work, the process changes will be modelled using mathematical programming to overcome the tedious step of the heuristic procedure. In mathematical programming technique, the WMH options are consider simultaneously. The consideration of process changes will lead to optimal design of minimum water utilisation network.

3. Most previous studies assumed pure fresh water feed. It is important to note that fresh water source may contain dilute concentration of contaminant. Foo (2007) extended the algebraic water cascade analysis (WCA) technique to problems involving impure fresh water feed. Nevertheless, the technique is only limited to a single contaminant system. Therefore, there is clear need to include cases involving pure and impure fresh water for multiple contaminants.

4. Although there is a simple cost screening technique (SHARPS) for plant design preliminary cost estimation with consideration of process changes using graphical method and heuristics, the steps is quite tedious. In addition, the main feature of this work is the development of a methodology for simultaneous analysis of water network with consideration of options for process changes using WMH through a MINLP with the overall objective of maximising net annual savings. The nonlinear term is due to the presence of power term that represents the capital cost functions that exist in the capital investment and payback period constraints.

Figure 2.1 provides the research gaps in mathematical programming technique on water and wastewater minimisation.

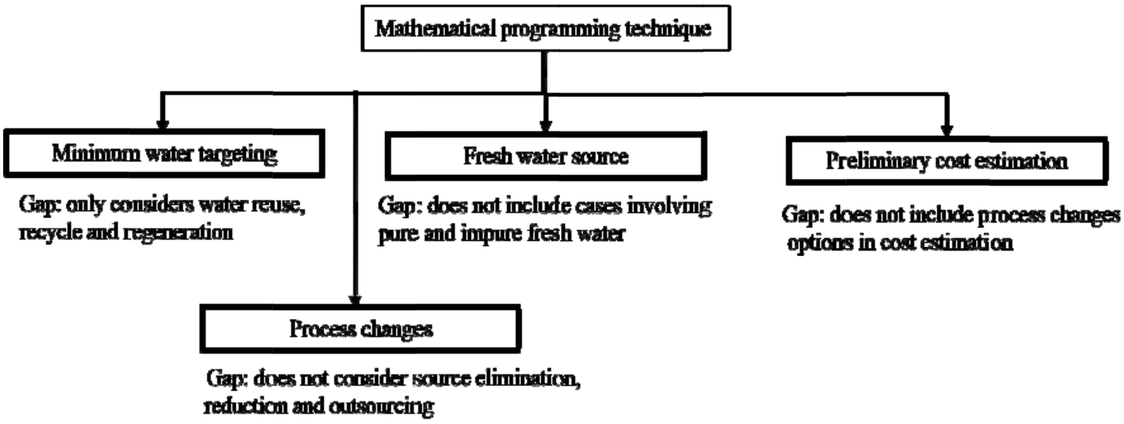


Figure 2.1: Research gaps associated with mathematical programming technique.

CHAPTER 3

FUNDAMENTAL THEORY

3.1 Introduction

In this chapter, the basic concepts of process integration are described first. This is followed by the description of the application of conventional method and process integration for water and wastewater minimisation. Understanding of the concepts is important in order to apply mathematical programming technique to water system. The final part of the chapter explains the fundamental concept related to water pinch analysis and mathematical programming techniques.

3.2 Process Integration

El-Halwagi (1997) defines process integration as *a holistic approach to process design which considers the interactions between different unit operations from the outset, rather than optimising them separately*. In the late 1970’s, process integration emerged as an important branch of process engineering. It refers to the system-oriented, thermodynamics-based, integrated approaches to the analysis, synthesis and retrofit of process plants. Process integration provides a unique framework for fundamentally understanding the global insights of a process, methodically determining the achievable performance targets and systematically making decision leading to the realisation of these targets (El-Halwagi, 1997).

Process integration design tools have been developed over the past three decades to achieve process improvement, productivity enhancement, conservation in mass and energy resources, and reductions in the operating and capital costs of chemical processes. The major applications of these integrated tools have focused on resource conservation, pollution prevention and energy management. Process integration methodology involves three important key components; synthesis, analysis and optimisation (El-Halwagi, 1997).

3.2.1 Process Synthesis

Westerberg (1987) defined process synthesis as *"the discrete decision-making activities of conjecturing which of the many available component parts one should use and how they should be interconnected to structure the optimal solution to a given design problem"*. Thus, process synthesis field is involved with the activities in which the various process elements are integrated and the flow sheet of the system is generated to meet certain objectives. Normally, a designer synthesises a few process alternatives based on experience and corporate preference without a systematic approach for process synthesis. They will select the alternative and most promising economic potential and used it as the optimum solution. However, by doing this, the designer may easily miss the true optimum solution of the problem.

There are two main approaches that can be implemented to determine the optimum solution, namely the structure independent and structure based approaches (El-Halwagi, 1997). The structure independent (also known as targeting) approach is based on tackling the synthesis task through a sequence of stages. A design target can be identified within each stage and applied in subsequent stages. The second approach is structure based. The structural technique involves in development of a framework that embeds all potential configurations of interest. The frameworks examples include process graphs, state-space representation and superstructures (Bagajewicz and Manousiouthakis, 1992).

Two important process synthesis models are the hierarchical approach and the "onion model" (Figure 3.1). The onion model is an alternative way to represent the hierarchical approach for process design (Smith, 1995). Process design begins at the centre of the onion, with the reactor and proceeds outward. The reactor designs influences the separation and recycle structures (the second layer of the onion) which are designed next. The reactor, separator and recycle structures dictate the overall heat recovery requirements, so the heat recovery network design comes next. Finally, the process utility system is designed to provide additional heating and cooling requirements that cannot be satisfied through heat recovery (Smith, 1995). The onion model is complemented with an arrow crossing the layers to emphasise the need for interactions between the different layers while applying optimisation techniques and simplification efforts to generate ideas to achieve the optimum process design. The model emphasise on the sequential and hierarchical nature of process flow sheet synthesis.

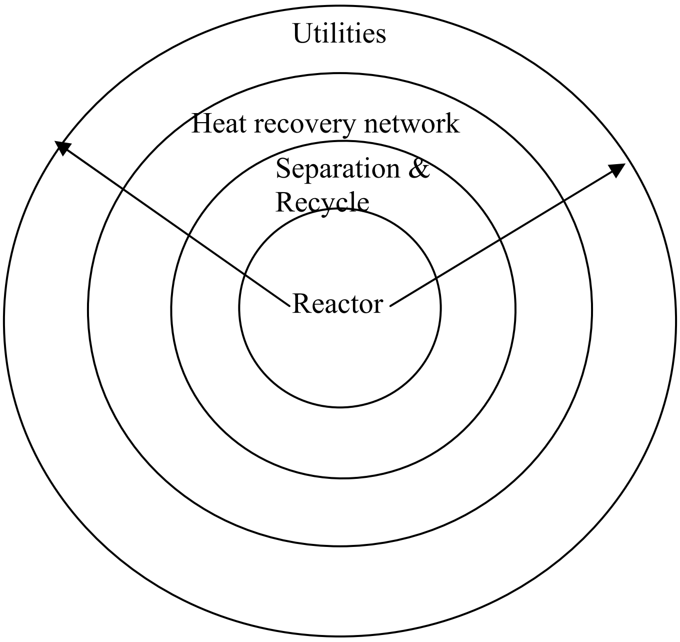


Figure 3.1: The onion model of process design (Smith, 1995).

3.2.2 Process Analysis

Process analysis involves the decomposition of a whole process into its constituent elements for each individual study performance. Therefore, once a process has been synthesised its detailed characteristics are predicted using analysis approaches. The approaches include mathematical models, empirical correlations and computer-aided simulation tools. Besides, process analysis may involve anticipating and validating performance through lab and pilot plant scale experiments and though studies conducted on an existing plant facility (El-Halwagi, 1997).

3.2.3 Process Optimisation

Process optimisation is the use of specific techniques that involves the selection of the best solution from among a set of candidate solutions. The degree of goodness of a solution is quantified using an *objective function* which is to be minimised or maximised. Examples of objective function include cost, profit and generated waste. The search process is undertaken subject to the system model and restrictions which are termed as *constraint.* These constraints can be in the form of equality or inequality. Examples of the equality constraints include material and energy balances, process modelling equations and thermodynamic requirements. On the other hand, the nature of inequality constraints may include environmental policies and regulations, technical specifications and thermodynamic limitations (El-Halwagi, 1997).

The optimisation component of process integration drives the iterations between synthesis and analysis towards optimal closure. In many cases, optimisation is also used within the synthesis activities. For example, in the targeting approach for synthesis, the various objectives are reconciled using optimisation.

3.3 Water and Wastewater Minimisation

Until now, many efforts have been done to minimise fresh water use, which corresponds to wastewater minimisation. Reduction of fresh water consumption and wastewater discharge has become one of the main targets of design and optimisation of process design. Reducing wastewater affects both effluent treatment and fresh water costs. In general, there are a least four approaches to water minimisation (Figure 3.2) (Wang and Smith, 1994):

a) Process changes

Process changes can reduce the inherent demand for water. For example, wet cooling towers can be changed to air coolers, or washing operations can have the number of stages increased.

b) Reuse

Wastewater is reused directly in other operations subject to the level of contamination to operations within the process system.

c) Regeneration reuse

Wastewater is purified and partially treated to remove contaminant before reused in other operation in the process system.

d) Regeneration recycling

Contaminants from wastewater are partially eliminated and the wastewater is returned to the same process afterwards or operations in which it has previously been used.

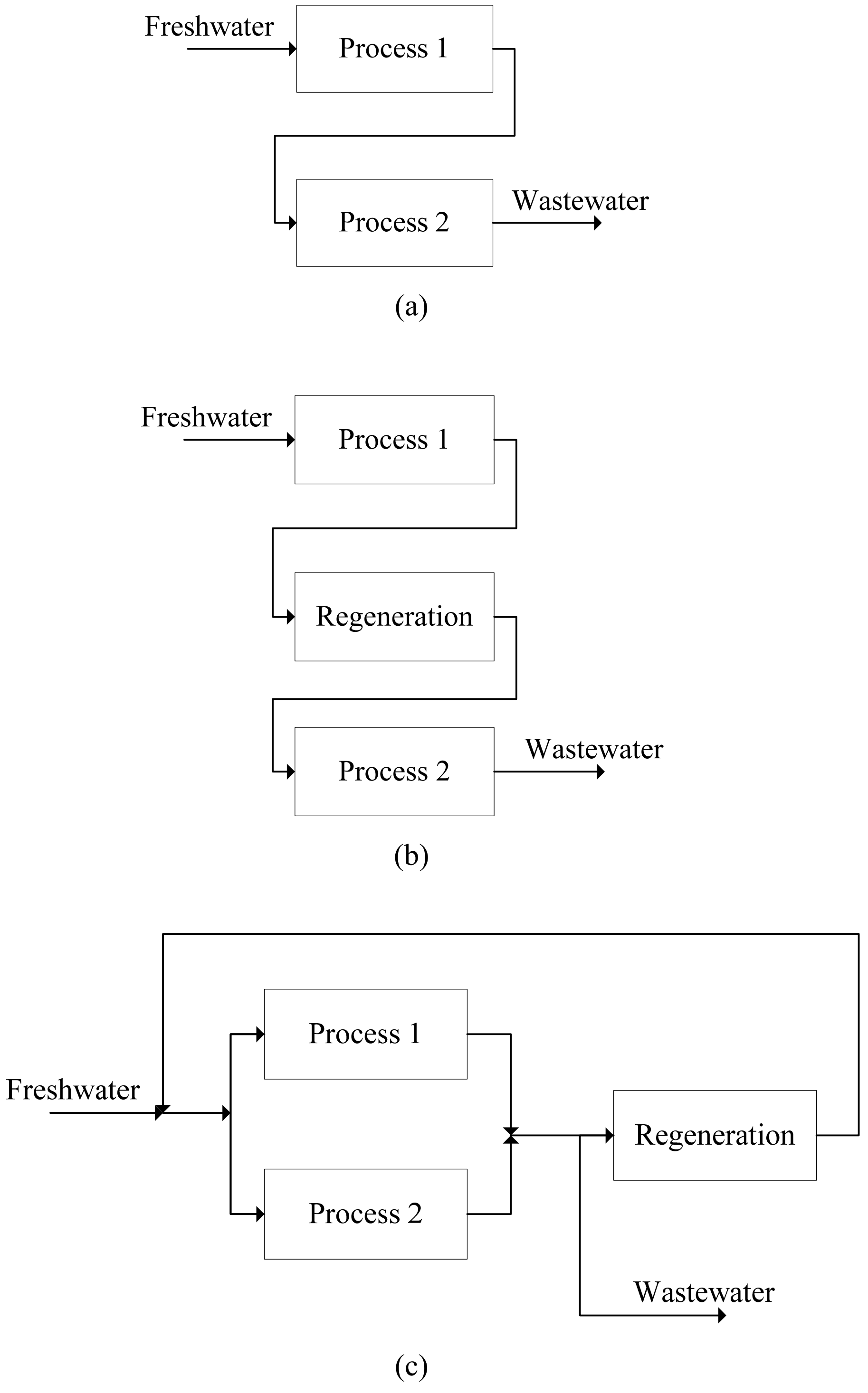


Figure 3.2: Water minimisation through (a) reuse, (b) regeneration reuse (c) regeneration recycling (Wang and Smith, 1994).

3.3.1 Conventional Approach for Water and Wastewater Minimisation

Systematic efforts have been done to increase the reuse of water on a plant-wide scale and such projects have been implemented to industry for past years using conventional water reuse strategies. Conventional water reuse is often grouped according to three strategies for fresh water savings and wastewater minimisation (Rossain, 1993):

i) Cascade reuse

Cascade reuse involves the direct water reuse with little treatment. The example of cascade reuse is storm water runoff can often be used as makeup water for cooling towers, with partial treatment.

ii) Waste minimisation

Waste minimisation can be obtained by reducing fresh water requirements in a process, such as by using mechanical cleaning rather than water to avoid wastewater generation.

iii) Source reduction

Source reduction is concerned with reduction of inherent need for water by a process. Counter current- rinsing stages can greatly reduce the fresh water demand for rinsing operations

The conventional approach in order to meet the goals for water reuse involves four key steps (Byers *et al.,* 1995):

a) Establish the scope or boundary limits for the project.

The limits of a water reuse study must be broad enough to include all key potential water reuses. A preliminary evaluation will often include the entire site.

b) Identify water sources and sinks.

This step involves identification of water-using operations that can be considered as sources of water for reuse, including water currently going to wastewater treatment, and identification of water-using operations that can potentially accept reused water in place of fresh water. Establishing a water-balance diagram for an existing plant requires looking at the piping and instrumentation diagrams (P&IDs), field-verifying piping connections and identifying the process uses, utility uses and other uses (e.g., housekeeping) of water sources including instances of undocumented water use (Rossain, 1993).

c) Identify and evaluate the factors that limit water reuse.

Identify and evaluate the specific contaminants present in each water source, together with the physical, chemical and biological water-quality factors that influence water reuse in each water sink. This step involves a complete inventory of water flow rates and qualities for each water source and sink. The physical location of each water source within the plant and the corresponding piping requirement to reuse the water source must be recognised to meet the need of a water sink.

d) Prepare an engineering and economic evaluation of a water utilisation network.

Evaluate water reuse based on typical water-reuse opportunities from experiences. In conventional case, the most obvious options for water reuse are investigated. These typically include replacing any once-through operations with a closed loop system featuring makeup and blowdown to regulate contaminant build-up.

3.3.2 Process Integration for Water and Wastewater Minimisation

Process integration methodologies are broadly classified into two categories; methodologies based on mathematical optimisation techniques and methodologies based on the conceptual approaches of pinch analysis (Figure 3.3). For a given water minimisation problem, a different solution technique maybe required to solve the problem. Figure 3.4 illustrates the tools of process integration.

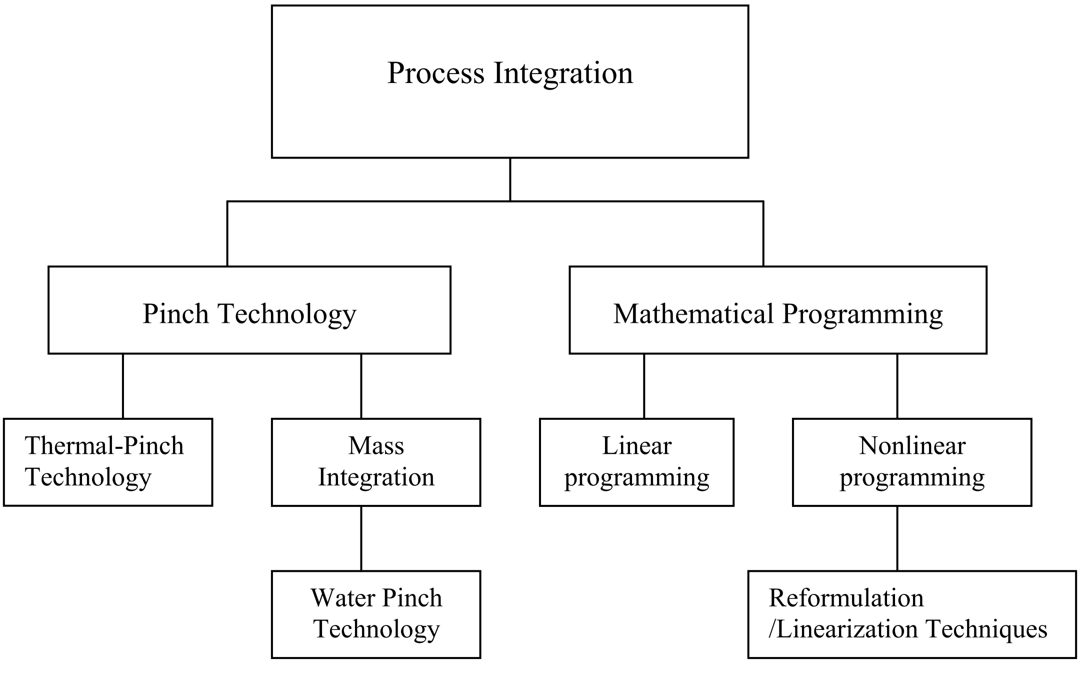


Figure 3.3: The tools of process integration (Mann, 1999).

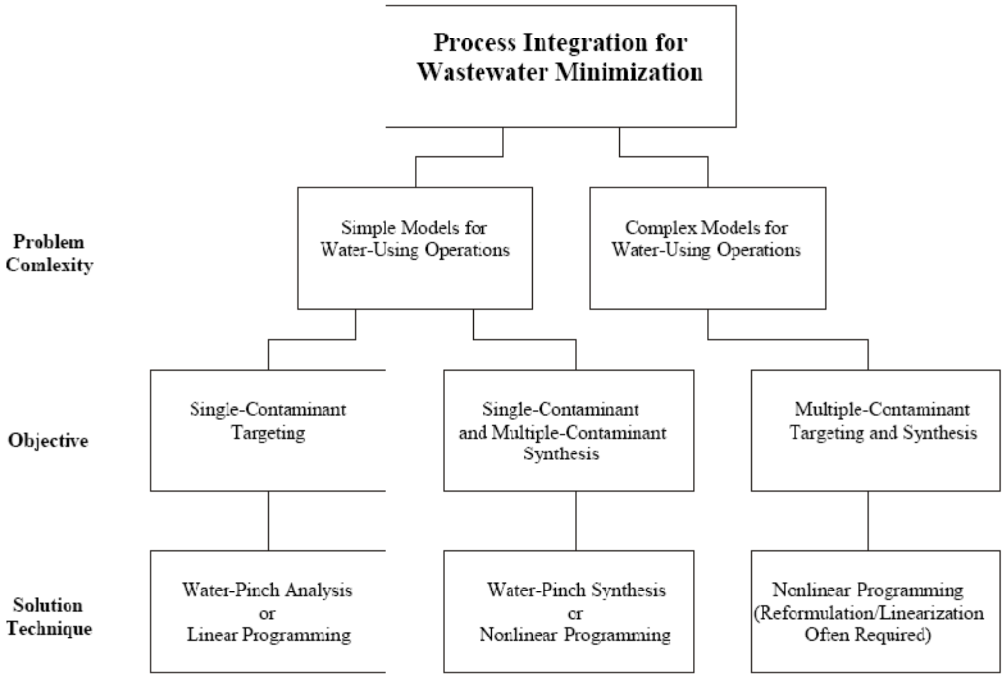


Figure 3.4: Solution techniques for water and wastewater minimisation (Mann, 1999).

3.4 Water Pinch Analysis

Water pinch analysis (WPA) evolved out of broader concept of process integration of materials and energy and the minimisation of emissions and wastes. WPA can be defined as a systematic approach of implementing water minimisation strategy through integration of processes for maximum water efficiency. WPA is a combination of new graphical and mathematical techniques for water and wastewater minimisation (Dhole *et al*., 1996). WPA does not replace conventional water reuse principles. Instead, it provides a means to first identify a goal for water reuse and then to pinpoint the key water reuse opportunities. The WPA uses five main key steps:

i) Analysis of water network

The first step in WPA is to analyse the existing or the base case of water network through plant auditing.

ii) Data extraction

The second step is data extraction where the water sources and water demands having potential for reuse recycling are identified.

iii) Targeting of minimum utility

The third step is to establish the minimum possible quantity of fresh water requirement and wastewater generation. This is also known as minimum water targets.

iv) Water network design

The fourth step is to design a water network to achieve minimum water targets.

v) Economic analysis

The last step is to evaluate and analysis the economics of the new water network design

3.5 Mathematical Programming Technique for Water Minimisation

Mathematical programming is gaining effectiveness in optimizing of large-scale systems, with many streams, multiple contaminants and cost optimality. They serve as a good synthesis tool in handling complex systems with different complex constraint. This technique is more suitable approach for optimum water-using networks, for both grassroots and retrofit application. Mathematical programming sees the targeting and design stages as being performed simultaneously, so the problem under consideration can be of a more complex nature.

This technique can be used as an effective method for the analysis, synthesis, and retrofit of water-using networks for industrial water reuse and wastewater minimisation and distributed effluent treatment systems for minimising the wastewater treatment flow rate. Fresh water and wastewater minimisation can be achieved using mathematical optimisation. Mathematical programming is effective tool for minimising or maximising an objective function (e.g., total cost, fresh water consumption and wastewater generation) subject to constraint relationships among the independent variables. It is typically done by simultaneously considering all factors contributing to overall network cost effectiveness and operability.

Linear programming (LP) is a powerful tool capable of finding the minimum value of a linear objective function subject to all linear constraints. The solution methods available for LP problems are guaranteed to find the global optimal solution. On the other hand, nonlinear *programming* (NLP) is useful for minimising a nonlinear objective function subject to nonlinear constraints. The solution approaches for NLP problem however are lead to local optima solution which may or may not coincide with the global optimum. An optimisation formulation that contains continuous variables (e.g., pressure, temperature or flow rate) as well as integer variables (e.g., 0, 1, 2,…) is called *mixed integer program* (MIP). This is depending on the linearity or nonlinearity of MIPs, they are applied as *mixed-integer linear program* (MILP) and *mixed-integer nonlinear program* (MINLP). Recently, several software packages are now commercially available such as LINGO and GAMS. In this work, the optimisation problem will be solved using GAMS software.

Mann and Liu (1999) introduced the method of superstructure to formulate a water network as LP and NLP for single and multiple contaminants systems, respectively. The solution of those models is the optimal allocation of species and streams throughout the process with minimum fresh water flow rate target. Mathematical programming has an advantage when the choice of a model for each water operation must be flexible, such as connection cost, operating cost, piping and pumping costs.

One fundamental difference between mathematical programming and water pinch analysis is that the distinction between the targeting and design phases no longer exists with these being carried out simultaneously. Besides, the so-called pinch point may not arise due to some other constraints.

3.5.1 Analysis of Water Network

The determination of water streams in plant is the most important steps. Water streams can be defined as stream that used or consumed or produced water in the plant. A water mass balance is conducted for all water streams. All the water streams in the plant are divided into two main categories; water demands and water sources. Water demands are the streams that consume water while water sources are the streams that produce or generate water. The mass balance data can be obtained from existing plant records, on-line monitoring, manual measurements and personal communication with plant's expertise.

3.5.1.1 Types of Water-Using Operations

Water is one of most valuable resources to mankind and become life support for us. Water is used for different activities in our daily life such as cleaning, heating, cooling and toilet flushing. In general, water-using operations can be classified into two broad categories i.e. mass transfer-based (MTB) and non-mass transfer-based (NMTB).

(i) Mass Transfer-based Water-Using Operation

A MTB water-using operation is characterized by the preferential transfer of a species from a rich stream to water, which is being utilized as a lean stream or a mass separating agent (MSA) (Manan *et al.,* 2004). Washing, scrubbing and extraction process are included in this category. Figure 3.5 shows water being fed into the absorptions column (as demand) and the wastewater generated (as source). Note that, the water losses from MTB water-using operation are typically assumed to be negligible and input and output flow rates assumed to be the same. This type operation is also known as *fixed contaminant load problem*.

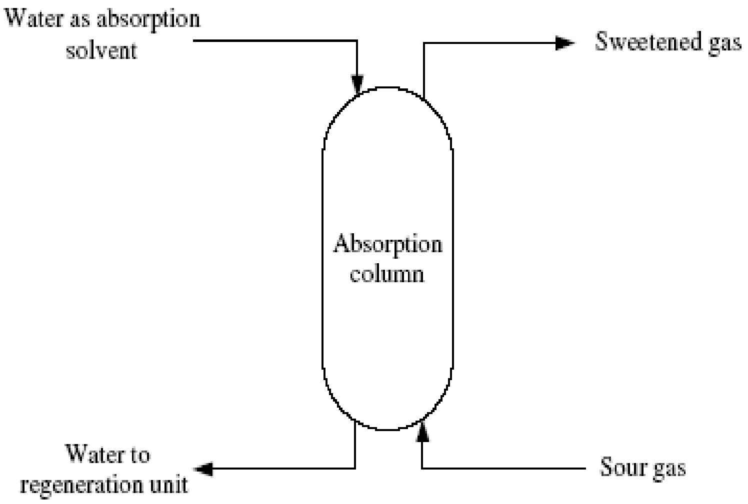


Figure 3.5: Mass-transfer-based water-using operations: Sour gas absorption where water demand and water source exist.

(ii) Non-Mass Transfer-based Water-Using Operation

In contrast, a NMTB water-using operation covers function of water other than as a mass separating agent (Manan *et al.,* 2004). In real system, not all water-using operations can represent using MTB operations. Certain processes may have different input and output flow rates and can not be modelled as MTB. A common example includes water being fed as raw water or being withdrawn as a product or byproduct in chemical reaction (Figure 3.6). The operation in this category also covers water-using operation such as cooling towers, boilers and reactors where water being utilised as heating or cooling media as shown in Figure 3.7, for such operations, water may exist as sources and/or demands. Therefore, the inlet and outlet flow rate for NMTB operation can have different flow rate. Note that, for the NMTB operations, water flow rate is more important than the amount of contaminants accumulated. This operation also widely known as *fixed flow rate problem*.

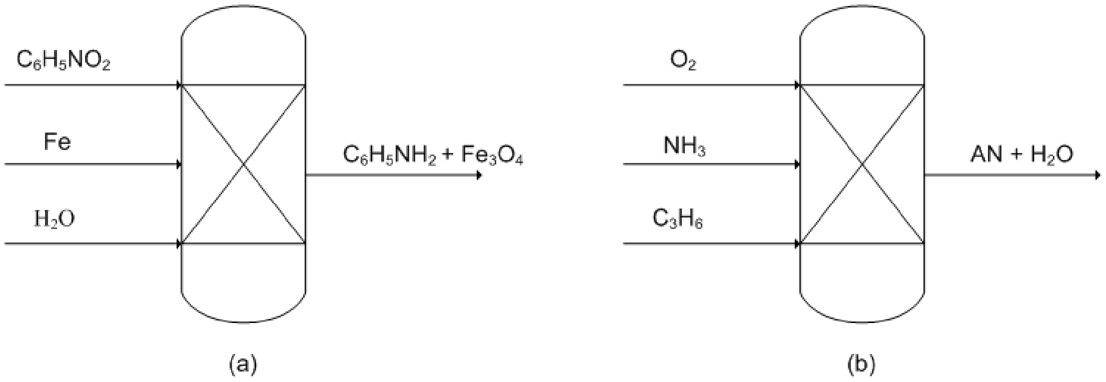


Figure 3.6: Non-mass transfer-based water-using operations (a) a reactor that consumes water in aniline production (b) a reactor that produces water a byproduct in acylonitrile production.

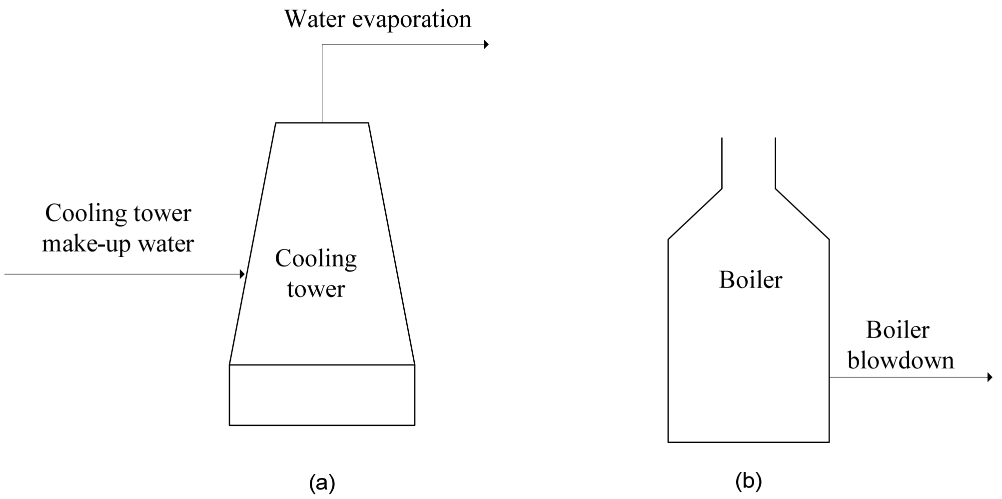


Figure 3.7: Two other common types of non-mass transfer-based water-using operations (a) cooling tower make-up water (b) boiler blowdown.

3.5.1.2 Characteristic of Contaminants

Contaminants are a species removed by a process or limiting water reuse within a system, for example biological oxygen demand (BOD), chemical oxygen demand (COD), total organic carbon (TOC), total solids, chloride or heavy metal concentration. In petroleum refinery process, the principal contaminants that existed in a water network are hydrogen sulfide, ammonia, phenols and mercaptans (Zheng *et al.*, 2005).

Several measures exist to assess the quality of water for discharge. For example, TOC, BOD and COD measurements indicate the organic matter content. Oil and grease (O&G) and total petroleum hydrocarbon (TPH) give a measure of the presence of oil, grease and other hydrocarbons. The physical characteristics of wastewater are also adjusted before disposal. These characteristics include the total suspended solids (TSS), pH, temperature, colour and odour (Bagajewicz, 2000).

If all the contaminants are considered, which usually involve many kinds of contaminants, solving the network will become complicated. As a result, Zheng *et al.* (2005) had proposed some rules to determine contaminants in the water system as stated below:

- Consider contaminants that have obvious or major effects on the processes. The other contaminants will be considered as constraints after the initial network has been obtained.
- Combine the contaminants that have similar effects to reduce the number of contaminants so as to simplify solving for mathematical model. For example, if the effect of Ca and Mg is the hardness of water, total hardness can be used as a contaminant instead of Ca and Mg individually.

The quantity of contaminants should be controlled so that the wastewater generated obeys the rules and regulation stated by the government so that it does not pollute the environment in any ways.

3.5.2 Water System Superstructure

In the application of mathematical programming techniques to design and synthesis problems it is always necessary to postulate a superstructure of alternatives. The superstructure model generates every possible connection between water-using operations and wastewater treatment systems as well as those between the process operations, water sources and wastewater discharges. According to Gianadda (2002), in formulating the superstructure for the model, it remains desirable that the model framework be of a sufficiently general nature such that all process operations can be integrated efficiently and easily. Thus, the superstructure should be formulated in such a way that it represents the set of all flows from any and all sources (supplies) within the process system to any and all sinks (demands) within the process system as well as fresh water supply and wastewater discharges. In addition, water reuse and recycle options and the related generation options are also incorporated. Figure 3.8 shows a general water network superstructure of every possible configuration for a water-using network involving water.

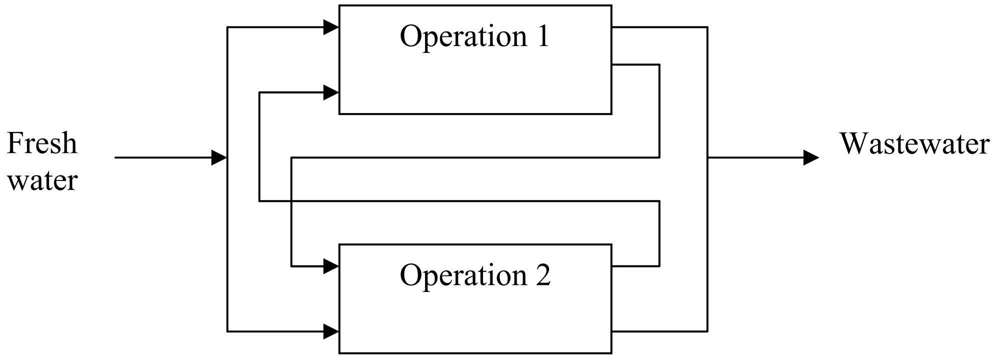


Figure 3.8: General water network superstructure (Mann and Liu, 1999).

3.5.3 GAMS Coding

From the 1950s, there has been a rapid development of algorithms and computer codes to analyse and solve large mathematical programming problems. One important part of this growth was the development in the early 1980's of modelling systems, one of the earlier of which was the Generalized Algebraic Modelling System (GAMS). GAMS is a language for setting up and solving mathematical programming optimisation models. GAMS is a flexible and powerful optimisation package. The model will involve discrete and continuous variables as well as uncertainties. The all in one package of GAMS is designed to (McCarl GAMS User Guide, 2007):

i) Provide an algebraically based high-level language for the compact representation of large and complex models.

ii) Allow changes to be made in model specifications simply and safely.

iii) Allow unambiguous statements of algebraic relationships.

iv) Provide an environment where model development is facilitated by subscript based expandability allowing the modeller to begin with a small data set, then after verifying correctness expand to a much broader context.

v) Be inherently self documenting allowing use of longer variable, equation and index names as well as comments, data definitions etc. GAMS is designed so that model structure, assumptions, and any calculation procedures used in the report writing are documented as a byproduct of the modelling exercise in a self-contained file.

vi) Be an open system facilitating interface to the newest and best solvers while being solver independent allowing different solvers to be used on any given problem.

The GAMS software uses four main key steps. The each step of GAMS software is illustrated in Figure 3.9.

1) Variable specifications - GAMS requires variables in each problem to be identified.

2) Equation specifications
   a) Declaration
      GAMS requires the modeller name each equation, which is active in the model. In the example, the equations are named after the keyword EQUATIONS.
   b) Algebraic structure specification

After naming equations, the exact algebraic structure of equations must be specified by using **“..”** notation. This algebraic form involves use of a special syntax to tell the exact form of the equation that may actually be an inequality.

=E= indicates an equality constraint
=L= indicates a less than or equal to constraint
=G= indicates a greater than or equal to constraint

3) Model statement - model statement is used to identify models that will be solved. It involves 2 steps:
Step 1: give name of the model (e.g. Example1)
Step 2: specify equations that will be included in the model in slashes “/ /”

MODEL Example1 /ALL/ ;
MODEL Example1 /Equation1, Equation2/;

4) Solve statement – solve specification causes GAMS to apply a solver to the model named in the solve statement (Example1) using the data defined just before the solve statement.

SOLVE Example1 USING LP MAXIMISING Z ; LP MIN

SOLVE Example1 USING LP MINIMISING Z ; LP MAX

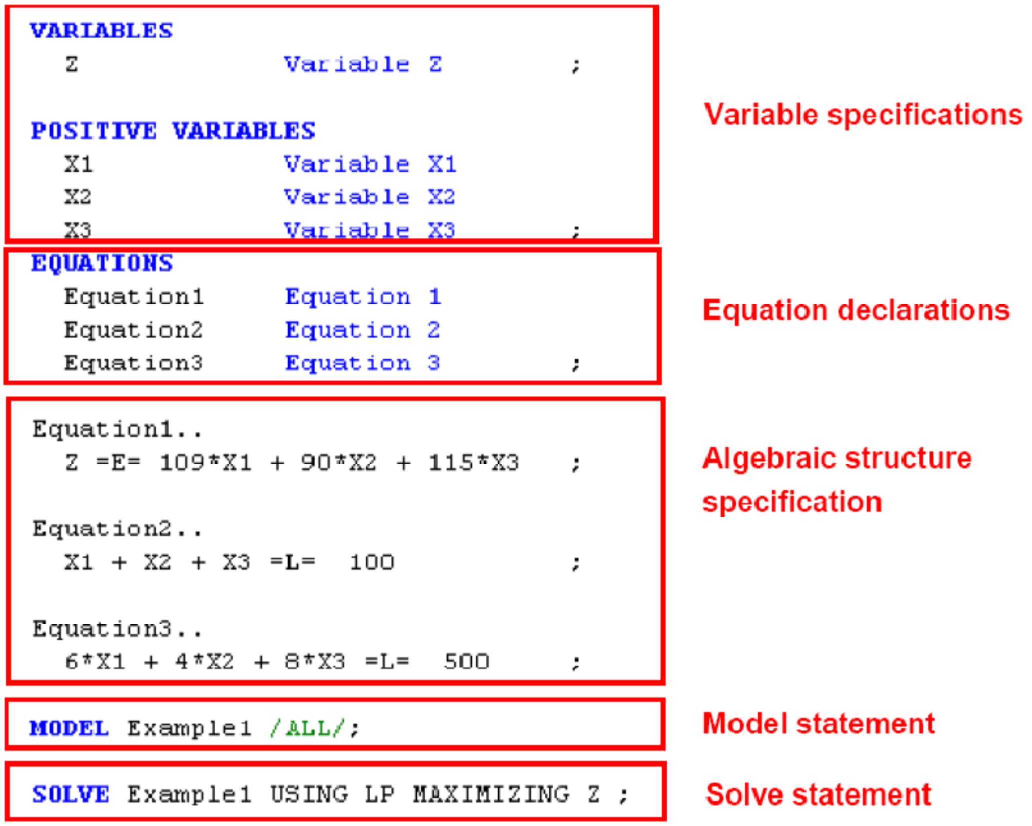
SOLVE Example1 USING MIP MAXIMISING Z ; Mixed Integer Program

SOLVE Example1 USING NLP MAXIMISING Z ; Nonlinear Program

For further understanding, an example of GAMS steps are illustrate as below:

Example 1:

$$
\begin{array}{llcl}
\text{Maximise} & 109X_1 + 90X_2 + 115X_3 & & \\
\text{Subject to:} & X_1 + X_2 + X_3 & \leq & 100 \\
 & 6X_1 + 4X_2 + 8X_3 & \leq & 500 \\
 & X_1 + X_2 + X_3 & \geq & 0 \text{ (non negative)}
\end{array}
$$



```
VARIABLES
   Z               Variable Z          ;

POSITIVE VARIABLES
   X1              Variable X1
   X2              Variable X2
   X3              Variable X3         ;
EQUATIONS
   Equation1       Equation 1
   Equation2       Equation 2
   Equation3       Equation 3          ;

Equation1..
   Z =E= 109*X1 + 90*X2 + 115*X3       ;

Equation2..
   X1 + X2 + X3 =L=   100              ;

Equation3..
   6*X1 + 4*X2 + 8*X3 =L=   500        ;

MODEL Example1 /ALL/;

SOLVE Example1 USING LP MAXIMIZING Z ;
```

Figure 3.9: The application of each step of GAMS software (McCarl GAMS User Guide, 2007).

3.6 The Water Management Hierarchy (WMH)

Based on previous works, most researchers mainly focused on maximum water recovery network and claimed that their methods will lead to minimum water targets. Minimum water targets can only be achieved when all water minimisation options have been completely implemented. On the other hand, minimum water network (MWN) design is the optimum network design that considers not only reuse and recycling, but all conceivable methods to holistically reduce fresh water usage through elimination, reduction, reuse/outsourcing and regeneration according to the Water Management Hierarchy (WMH). The WMH consists of five levels and each levels are arranged in order of preference, from the most preferred option at the top of the hierarchy (level 1) to the least preferred at the bottom (level 5) as in Figure 3.10 (Wan Alwi and Manan, 2006; Wan Alwi *et al.*, 2008). Water minimization is more concern from the first level to fourth level of the hierarchy.

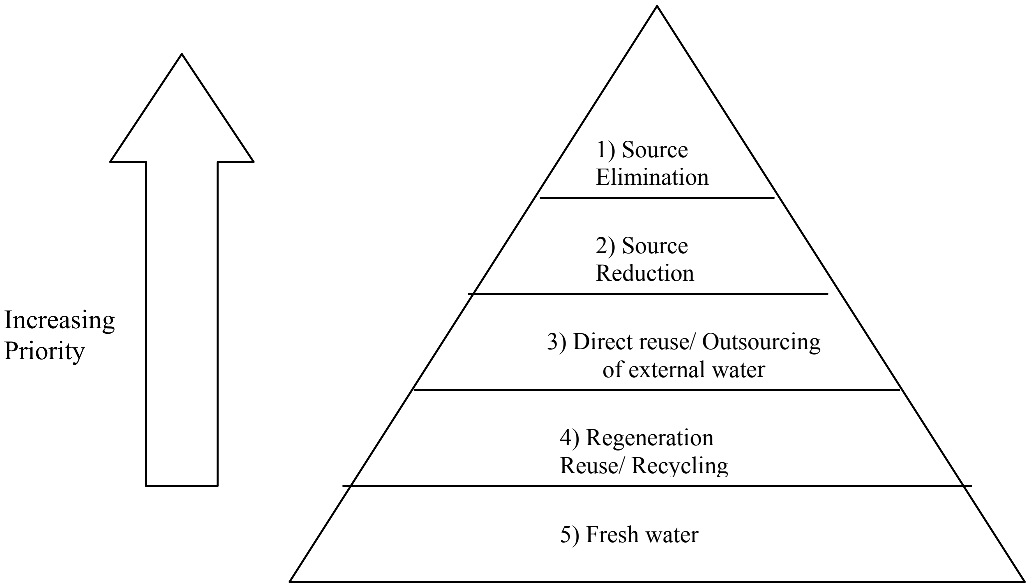


Figure 3.10: The water management hierarchy (Wan Alwi and Manan, 2006).

The top of the hierarchy is s*ource elimination*. It concerns with the complete avoidance of fresh water usage. In different situation, sometimes it is possible to eliminate water rather than to reduce, reuse or recycle water. For example, wet cooling towers can be changed to air coolers. When it is not possible to eliminate fresh water at source, *source reduction* should be considered (level 2). Water saving toilet flushing system and automatic tap are the examples of source reduction equipment.

If it is not possible to eliminate or reduce fresh water at source, wastewater recycling should be considered. *Direct reuse/outsourcing of external* and *regeneration reuse* (level 4) in WMH are two different modes of water recycling. *Direct reuse or outsourcing of external* (level 3) may involve using spent water within the building or using available external water (i.e., rainwater, river water and snow). For instance, water passes automatically through the hand wash basin on its way to the toilet bowl. Besides, rainwater may be used for equipments or processes which need higher quality water such as for ablution. Basically, external water sources are water or wastewater which is not initially considered for integration due to special investment needed on top of the existing building infrastructure and the standard storage and pumping requirements for integration within the building.

The next level for water minimisation is regeneration (level 4). Regeneration refers to treatment of wastewater or even external water source to match the quality of water required for further use. Regeneration can be used to remove contaminants on an intermediate basis, by processes such as gravity settling, microfiltration and membranes. The choice and placement of regenerators are crucial importance. There are two possible cases of regeneration. Regeneration-recycling involves reuse of regenerated water in the same equipment or process after treatment. Contaminants from wastewater are partially eliminated and the wastewater is returned to the same process afterwards. Regeneration-reuse includes reuse of regenerated water in other equipment or process after treatment. Wastewater is purified and partially treated to remove contaminant before reused in other operation in the process.

Fresh water consumption (level 5) should only be considered when all above options cannot be applied. Fresh water usage can be used when wastewater cannot be recycled or when wastewater needs to be diluted to achieve desired purity. Through MWH, the use of fresh water may not eliminate, but it will become more economical.

3.7 Economic Evaluation

Economic evaluation is important in designing water network system to assess the feasibility of the proposed network solution. In order to design water systems, the tendency has been to minimise fresh water requirement, with assumption that fresh water costs is the dominant portion of cost function. For preliminary economical calculations, simple payback period is widely used as a criterion to evaluate the feasibility of a water network design. The payback period is calculated using Equation (3.1)

$$Payback \quad period \quad (yrs) = \frac{Net \quad Capital \quad Investment \quad (\$)}{Net \quad Annual \quad Savings \quad (\$/yrs)} \tag{3.1}$$

The equipment, piping and pumping costs built in equation (3.2) are the three main cost components considered for a building or a plant water recovery system (Takama *et al.*, 1980; Olesen and Polley, 1996; Hallale and Fraser, 1998; Alva-Argáez, 1998; Jödicke *et al.,* 2001; Bagawicz and Savelski, 2001; Koppol *et al.*, 2003; Feng and Chu, 2004; Gunaratnam *et al.,* 2005; Wan Alwi *et al.*, 2008).

$$\sum CC = C_{PE} + C_{PEI} + C_{piping} + C_{IC} \tag{3.2}$$

where, C_{PE} = Total capital cost for the equipment

C_{PEI} = equipment installation cost

C_{piping} = water reuse piping cost investment

C_{IC} = instrumentation and controls cost investment

Economic analysis for the water management options for retrofit and design case can be evaluated by calculating the net capital investment (NCI) for the minimum water network using equations (3.3) and the net annual savings (NAS) using equations (3.4) and (3.5) (Wan Alwi, 2007).

$$Net\ Capital\ Investment,\ \$\ (retrofit) = \Sigma CC_{new\ system} \tag{3.3}$$

where, $CC_{new\ system}$ = capital cost associated with new equipment.

The net annual savings (NAS) is the difference between the base case water operating costs from the water operating costs after employing water management options as in equation (3.4).

$$NAS = OC_{base\ case} - OC_{new} \tag{3.4}$$

where, $OC_{base\ case}$ = base case expenses savings ($/yr)

OC_{new} = new expenses on water ($/yr)

The total operating cost of a water system consists of fresh water cost, effluent disposal charges, energy cost for water processing and the chemical costs as given by equation (3.5).

$$OC = C_{FW} + C_{WW} + C_{OEC} + C_{C} \tag{3.5}$$

Where, OC = total water operating cost

C_{FW} = costs per unit time for fresh water

C_{WW} = costs per unit time for energy for water processing

C_{C} = costs per unit time for chemicals used by water system.

3.7.1 The Systematic Hierarchical Approach for Resilient Process Screening (SHARP) Strategy

Systematic Hierarchical Approach for Resilient Process Screening or SHARPS is a network cost screening technique was introduced by Wan Alwi and Manan (2006) and Wan Alwi *et al.* (2008). SHARPS screening technique involves cost estimation associated with water management hierarchy to detailed design. Since SHARPS is a cost screening tool, standard plant design preliminary cost estimation technique were used to evaluate the capital and operating cost of a proposed water system. SHARPS strategy was used to ensure that the savings achieved was cost-effective and affordable.

Step 1: Set the desired payback period (TPP). The desired payback period is setting by the plant owner as an investment payback limit e.g., two years.

Step 2: Plot an investment versus annual savings for each level of WMH. Figure 8 shows the sample of the IAS plot. The gradient of the plot gives the payback period for each process changes begins with top of the hierarchy. The steepest gradient, m_4 gives the highest capital investment per annual savings indicate the most costly scheme. The new process modification scheme needs lower investment as compared to the grassroots equipment is described by negative gradient, m_3.

Step 3: Draw a straight line from the origin (starting point) to end point of the investment and annual savings plot (Figure 3.11). The slope of this line is a preliminary cost estimate of the total payback period implementing all process changes guided by WMH.

Step 4: The total payback period should match with the maximum desired payback period set by the plant owner.

If $TPP_{BS} \leq TPP_{set}$, network design may be proceed.
If $TPP_{BS} > TPP_{set}$, two strategies may be implemented.

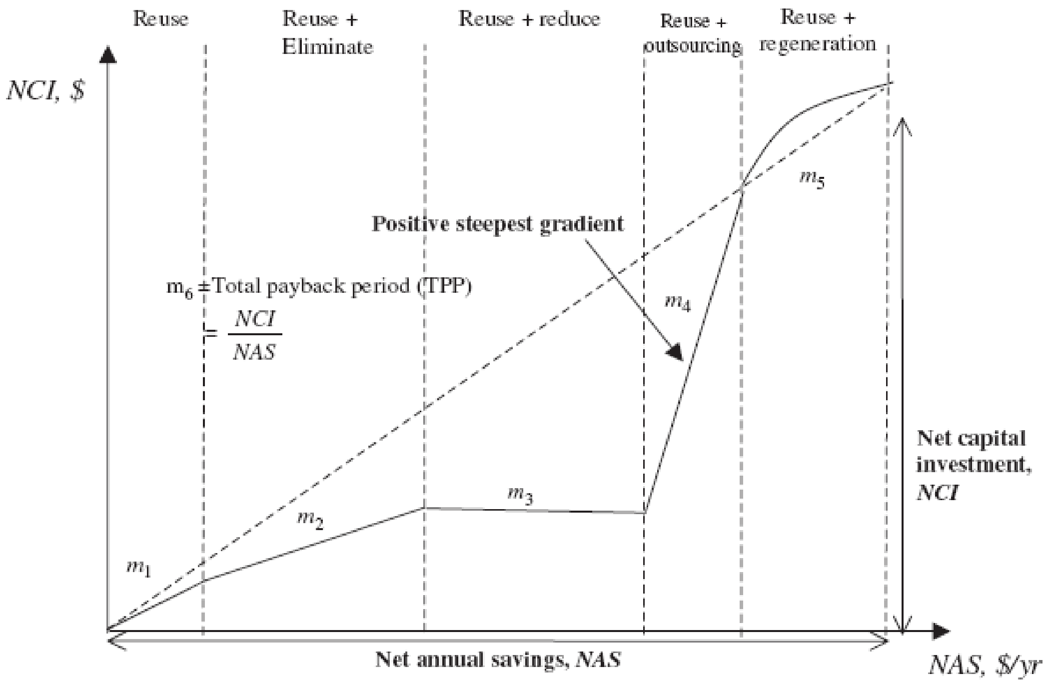


Figure 3.11: IAS plot for each level of WMH, m_4 is the steepest gradient and TPP is the total payback period for a water network system (Wan Alwi and Manan, 2006).

i) Strategy 1: Substitution

The strategy consisted of replacing the equipment /process that resulted in the steepest positive slope with an equipment or process that give a less steep slope (Figure 3.12). This strategy not applicable to reuse line since there was no equipment to replace. Hence, the first strategy is to reduce the length of the steepest positive gradient until TPP_{AS} is equal to TPP_{set}. The process change option gives the highest total annual savings with lesser total investment was selected to substitute the initial process option and trim the steepest gradient.

ii) Strategy 2: Intensification

The intensification strategy applied in reducing the length of the steepest positive gradient until TPP_{AS} was equal to TPP_{set} **(**Figure 3.13**).** The second strategy also not applicable to reuse line since there was no equipment to replace. This strategy involves instead of completely applying each process change, only considers eliminating or partially applying the process change that gives the steepest positive gradient, and hence, a small annual savings compared to investment amount. If TPP_{AS} still exceeds the TPP_{set} after the steepest gradient was adjusted, the length for the next steepest gradient was reduced until TPP was equal to $\text{TPP}_{\text{set.}}$

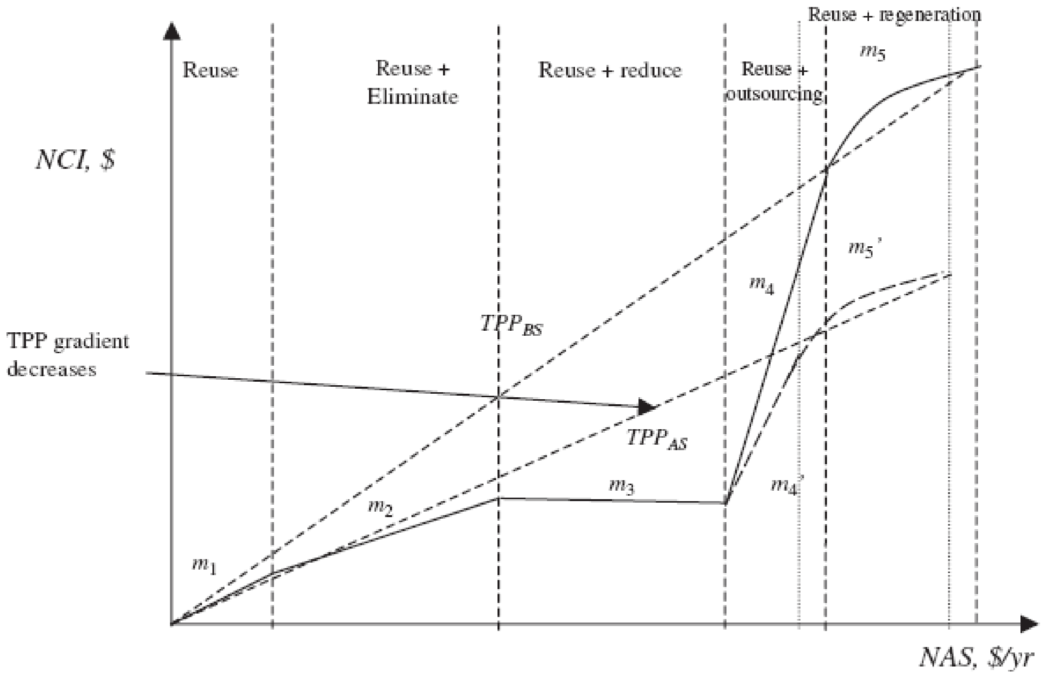


Figure 3.12: IAS plot showing the revised total payback period when the magnitude of the steepest gradient is reduced using SHARPS substitution strategy (Manan and Wan Alwi, 2006).

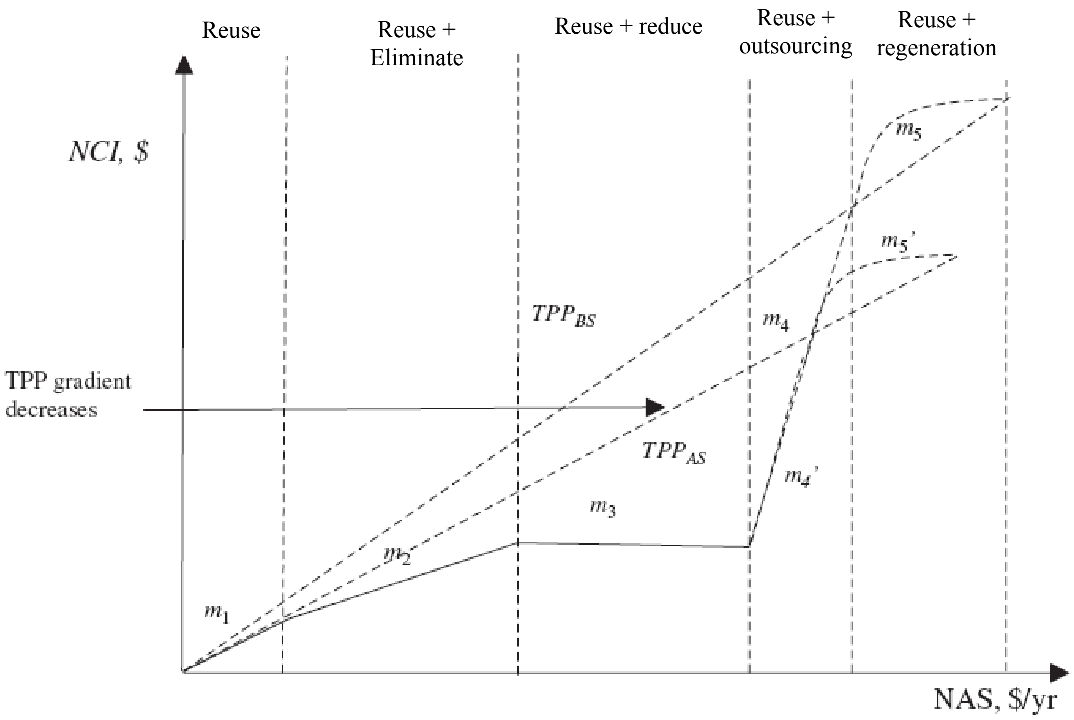


Figure 3.13: IAS plot showing the revised total payback period with a shorter steepest gradient curve (Manan and Wan Alwi, 2006).

The best savings can be achieved when both strategies 1 and 2 is tested and applied together. The overall SHARPS procedure is summarised in Figure 3.14**.**

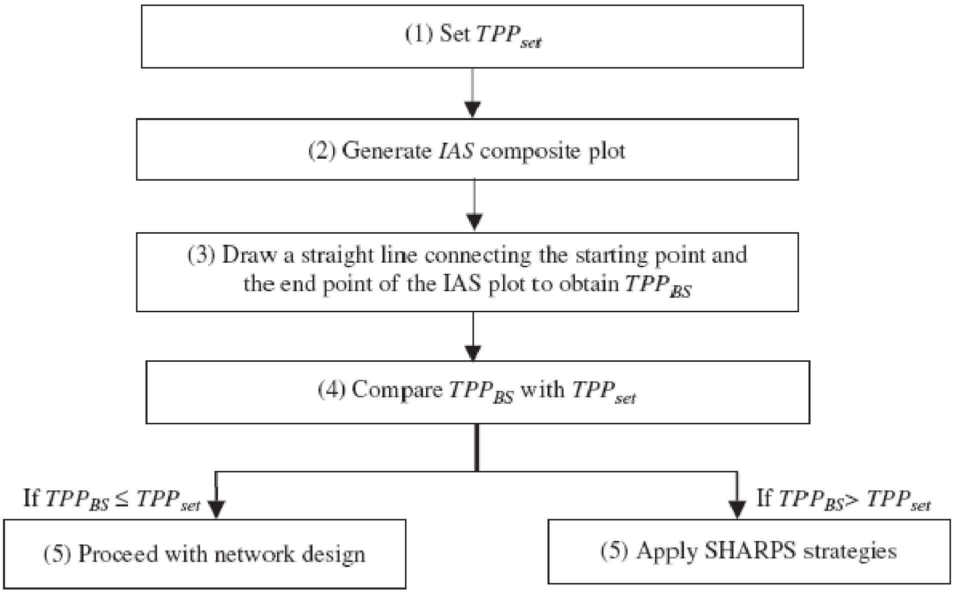


Figure 3.14: The overall SHARPS procedure (Manan and Wan Alwi, 2006).

CHAPTER 4

METHODOLOGY

4.1 Introduction

This chapter presents a detailed procedure for the optimal design of water networks which comprises of five main steps. Step 1 involves extraction of limiting water flow rate and contaminant data retrieved from case studies. Step 2 presents the superstructure framework that features a number of feasible configurations of water networks. Mathematical models for the development of the Model for Optimal Design of Water Networks (MODWN) are performed in Step 3. The MODWN is coded into a commercial mathematical optimisation software package GAMS (Generalized Algebraic Modeling System) in Step 4. Finally, sensitivity analysis is performed in Step 5. Figure 4.1 shows the methodology for this study. Each step is explained next.

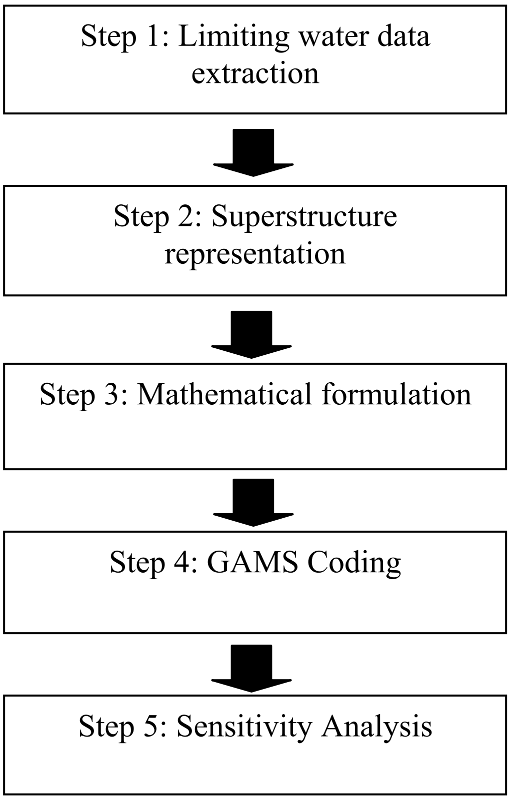


Figure 4.1: Methodology of the research.

4.2 Introduction to a New Systematic Approach for Optimal Design of Water Networks

A new systematic approach for water minimisation applicable to a wide range of urban and industrial sectors is presented in detail. There are two key features adapted from Wan Alwi and Manan (2006) and Wan Alwi *et al.* (2008) work which are the water management hierarchy options as a guide to select appropriate process changes and the Systematic Hierarchical Approach for Resilient Process Screening (SHARPS) as a cost screening technique. These features will be translated into mathematical programming technique to cater for cases involving multiple contaminants.

4.2.1 Step 1: Limiting Water Data Extraction

The first step is to extract the *limiting water data* from a given water-using operations. In minimum water targeting, the main data specification are limiting contaminant data and flow rate for all available water sources (outlet streams with potential to be reused/recycled) and demands (inlet streams representing process water requirements) available in the system. The concepts of water sources and demands are important especially in representing water-using operations. In addition, with the implementation of this concept, the required quality (flow rate) and quantity (contaminant) of water demands can be satisfied by mixing of water sources.

The water sources data are obtained by identifying the maximum concentration limit and the minimum flow rate limit of the wastewater source for each process. Selection of the limiting water sources and demands data are based on the limiting contaminant concentration of water. Contaminant concentration may include total suspended (TSS), total dissolved solids (TDS), biological oxygen demand (BOD), chemical oxygen demand (COD), hardness or may be a specific contaminant (perhaps the concentration of a heavy metal such as iron) to meet a discharge constraint. Assume that for all contaminants concentrations of each demand and source is fixed to their maximum values.

Based on study by Brouckaert and Buckley (2002), once the significant processes and their inter-process connectivity have been established, the water mass flow rates must be determined. There are several sources of flow data:

1) Existing plant records

   This is the most obvious source. Sophisticated facilities may have computerised monitoring of process flows throughout the plant.

2) Design data

Where available and still reasonably relevant, the original design figures can be used to estimate the missing data. However, of all the aspects of a process, the water systems are perhaps the most likely to be altered as circumstances change.

3) Control data

There are several types of control settings that may be of interest, two are mentioned here:

a) *Ratio control*: Flows of inter-process streams dependent on others will have a corresponding control valve setting. For example, the mass flow of dilution water required for dilution of reactor feed may be dependent on the flow rate of raw materials.

b) *Composition*: Valve settings that respond to changes in stream composition or density.

For example, the mass flow of steam to an evaporator may be dependent on the density of the inflow.

4) Unit operation data

Plant operations can offer a various types of flow rate data and relationships:

a) *Through flow*: The typical flow rate that the operation is designed to handle may be used.

b) *Flow relationships*: Design relationships between outlet and inlet flow rates may be useful, such as splitting fractions of inlet streams.

c) *Flow losses*: Some losses are inherent to the process and must be taken into account such as leaks, evaporation rates, overflows, etc.

5) Manual measurements

Many smaller streams or non-process streams may not be monitored. Sometimes these streams cannot be inferred from mass balance calculations. Although not as accurate as plant records, manually measuring streams where data are not available can provide an indication of typical stream flows if several measurements are taken over a representative time interval. Manual measuring techniques range from the simple bucket-and-timer methods (or timing tank levels) to more sophisticated portable magnetic flow meters.

6) Personal communication

Plant personnel experienced with plant operating conditions can provide estimates of relevant flows, when other data are not available. This is the least reliable form of data, but can provide a quick insight into relative flow rates.

4.2.2 Step 2: Superstructure Representation

The second step is to generate a superstructure. Similar to any other optimisation study in process synthesis, it is necessary to build a superstructure in which all possible flow configurations are embedded. The superstructure is applicable for mass transfer-based (MTB) and non-mass transfer-based (NMTB) water-using operations (global water operations). As one can imagine, a superstructure representing all possible alternatives will be very complex.

4.2.2.1 Superstructure for Maximum Water Recovery Network (Base-Case)

The superstructure represents all possible connections among water sources, water demands and wastewater discharges. The following notation is adopted throughout this work: S_i, D_j, *FW* and *WW* which represents water flow rate of source *i*, demand *j*, fresh water and wastewater respectively. The superstructure framework features a number of feasible networks developed based on given limiting water data. Figure 4.2 shows the general water network superstructure.

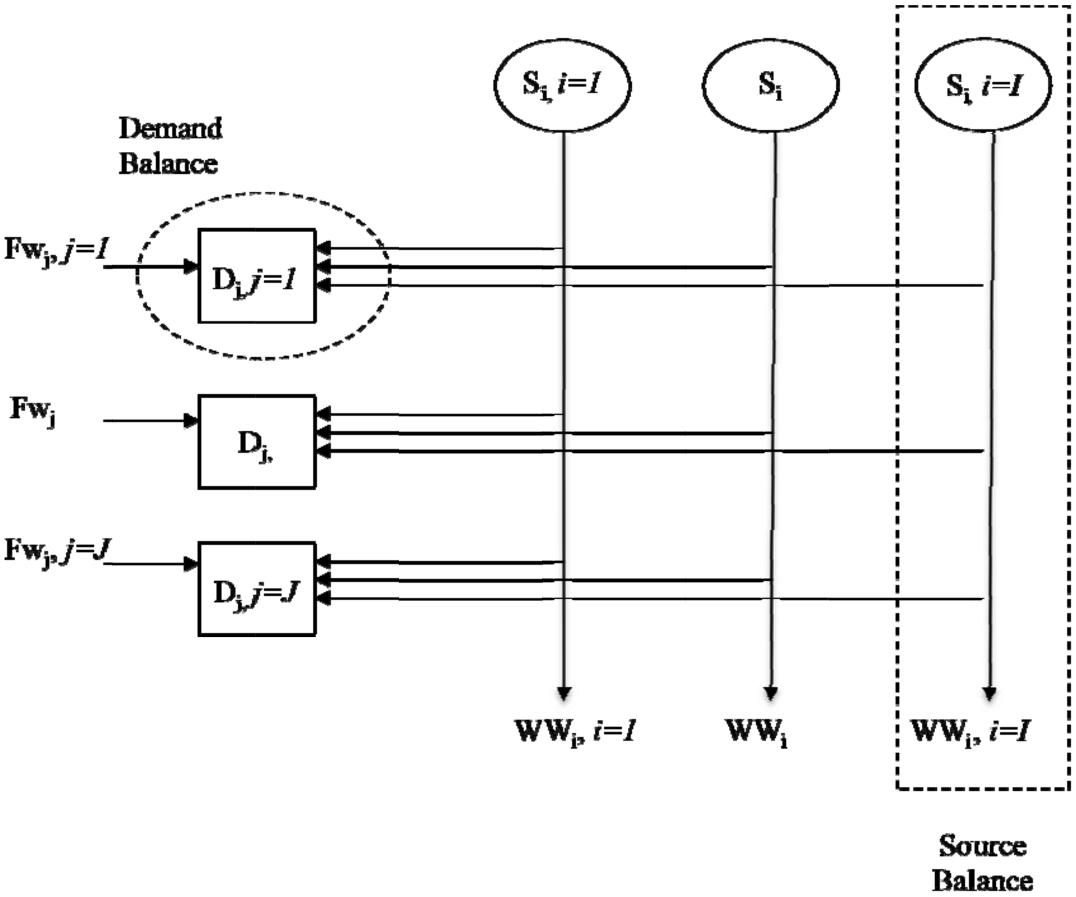
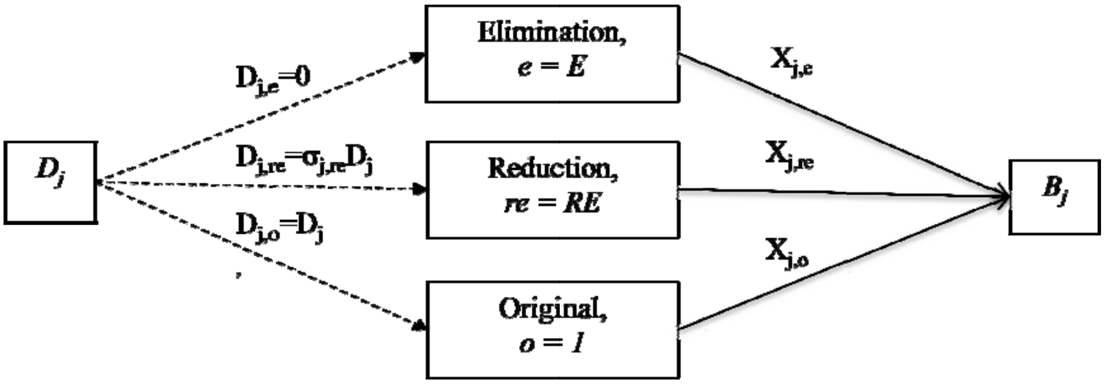


Figure 4.2: General water network superstructure for maximum water recovery that considers both MTB and NMTB operations (base-case scenario).

4.2.2.2 Superstructure for Minimum Water Utilisation Networks (MWN)

The representative superstructure is based on the water management hierarchy (WMH) options. The minimum water network (MWN) considers all conceivable methods to holistically reduce fresh water usage through elimination, reduction, reuse/outsourcing and regeneration in the WMH. Figure 4.3a shows the superstructure on how to obtain the adjusted demand flow rate, B_j when source elimination and reduction are considered. $Da_{j,e}$, $Da_{j,re}$ and $Da_{j,o}$ denotes the flow rate for elimination, reduction or original water demand.

Figure 4.3b represents a superstructure which is an extension of Figure 4.2 but with inclusion of outsourcing and regeneration options. For each water-using operation, the water demand, B_j can be supplied by fresh water, FW_j, outsourced resources, OS (e.g rainwater, river and melted snow), reused/recycled water, or regenerated water from regeneration unit, RU. While at the water source, A_i, the generated wastewater may be directly discharged to the end-of-pipe treatment, WW_i, or reused in the same or different processes or partially treated in the regeneration unit, RU before being reused/recycled. In this case, superstructure of every possible configuration of a water-using network is allowed. The combination of Figure 4.3a and Figure 4.3b gives the general superstructure for the minimum water utilisation network considering all WMH options.



(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.

Figure 4.3: General superstructure for a minimum water utilisation network with WMH options that considers both MTB and NMTB operations.

4.2.3 Step 3: Mathematical Formulation

The third step is to develop a mathematical model that represents the superstructure in Step 2. In order to formulate the model, assumptions are first made, followed by identification of sets, variables, and parameters, objective function and constraints.

4.2.3.1 Assumptions and Limitations

a) All contaminants concentrations for each demand and source are fixed to their maximum values.
b) There are no flow rate losses or gains in the water operations. In other words, the water flow rate does not change for the water operations.
c) No contaminant concentration constraints have been introduced for the discharge of effluent.
d) The water system is assumed to be operating continuously.
e) The system operates isothermally.

4.2.3.2 Sets

There are six sets used in this mathematical model, which is shown in Table 4.1.

Table 4.1: Sets used in the mathematical modelling.

Set	Description
I	Index for water source
J	Index for water demand
K	Index for water contaminant
R	Index for regeneration unit
E	Index for water elimination option
Re	Index for water reduction option
O	Index for original water demand
Os	Index for external water sources

4.2.3.3 Parameters

Table 4.2 lists all the parameters applied in mathematical modelling.

Table 4.2: List of parameters.

Notation	Unit	Description
$Cs_{i,k}^{max}$	ppm	Maximum concentration limit of contaminant *k* from water source *i*
$Cd_{j,k}^{max}$	ppm	Maximum concentration limit of contaminant *k* in demand *j*
Cw_k	ppm	Fresh water concentration of contaminant *k*
$Cos_{os,k}$	ppm	Outsource concentration of contaminant *k*
$Cro_{r,k}$	ppm	Outlet concentration of contaminant k from regeneration unit *r*
S_i	t/hr	Flow rate of water source *i*
D_j	t/hr	Flow rate of water demand *j*
Fos_{os}^{max}	t/hr	Maximum flow rate of outsource *os*
$Fw_j^{initial}$	t/hr	Initial fresh water flow rate to demand *j*

$WW_i^{initial}$	t/hr	Initial wastewater flow rate from source *i*
$F_{i,j}^{initial}$	t/hr	Initial water flow rate from source *i* to demand *j*
$F_{i,r}^{initial}$	t/hr	Initial water flow rate from source *i* to regeneration unit *r*
$Fos_{os,j}^{initial}$	t/hr	Initial outsource flow rate *os* to demand *j*
$F_{r,j}^{initial}$	t/hr	Initial water flow rate from regeneration unit *r* to demand *j*
Fos_{os}^{A}	t/hr	Flow rate of *A* for outsource *os*
$FReg^{A}$		Flow rate of *A* for regeneration
$Da_{j,e}$	t/hr	Flow rate of elimination option *e* for demand *j*
$\sigma_{j,re}$	-	Water reduction percentage
$CostElect$	USD$/kW	Cost of electricity
$CostPipe$	USD$/system	Cost of piping
$CostPump$	USD$/system	Cost of pump
$CRegU$	USD$/unit	Total cost of regeneration unit
$COsU$	USD$/system	Total cost of outsourcing unit
$CReuse$	USD$/system	Total cost for reuse unit
$CostUE_{j,e}$	USD$/unit	Cost of elimination unit *e* for demand *j*
$CostURe_{j,re}$	USD$/unit	Cost of elimination unit r*e* for demand *j*
$CostFW$	USD$/t	Cost of fresh water supply
$CostWW$	USD$/t	Cost of wastewater generation
$CostOsU_{os}^{A}$	USD$/unit	Cost of outsourcing unit *os* with given water flow rate *A*
$CostRegU_{r}^{A}$	USD$/unit	Cost of regeneration unit *r* with given water flow rate *A*
$CostChemReg$	USD$/t	Cost of chemicals needed for regeneration
ε_j	-	Number of equipment for demand *j*
AOT	hr/yr	Annual operating time
$POPump$	kW	Power of pump
γ	-	Payback period limit
β	-	Sixth-tenth rule
P	-	Percentage of equipment cost installation

4.2.3.4 Variables

Table 4.3 and Table 4.4 list all the variables used in mathematical modelling.

Table 4.3: List of continuous variables.

Term	Unit	Description
Fw_j	ton/hr	Fresh water supplied to demand *j*
$F_{i,j}$	ton/hr	Water flow rate from source *i* to demand *j*
WW_i	ton/hr	Unused portion of water source *i* (waste)
$Fos_{os,j}$	ton/hr	Outsource flow rate *os* to demand *j*
$F_{i,r}$	ton/hr	Water flow rate from source *i* to regeneration unit *r*
$F_{r,j}$	ton/hr	Water flow rate from regeneration unit *r* to demand *j*
A_i	ton/hr	Adjusted flow rate of water source *i*
B_j	ton/hr	Adjusted flow rate of water demand *j*
$Da_{j,re}$	ton/hr	Flow rate of reduction option *e* for demand *j*
$Da_{j,o}$	ton/hr	Original flow rate *o* for demand *j*
$Cri_{r,k}$	ppm	Inlet concentration of contaminant k to regeneration unit *r*

Table 4.4: List of binary variables.

Term	Variable selection	Description
$x1_{j,e}$	1 if *e*th elimination options is selected 0 otherwise	Selection of *e*th elimination options for *j*th demand
$x2_{j,re}$	1 if *re*th reduction options is selected 0 otherwise	Selection of *re*th reduction options for *j*th demand
$x3_{j,o}$	1 if original flow rate is selected 0 otherwise	Selection of original flow rate *o* for *j*th demand

4.2.3.5 Objective Function and Constraints

4.2.3.5.1 Base-Case Scenario

The objective of this LP model is to determine the minimum fresh water target which leads to the minimum wastewater generation and maximum total water reused/recycled in the system. S_i and D_j are the water flow rate of source i and demand j with a given maximum concentration of contaminant k, $Cs_{i,k}$ and $Cd_{j,k}$ respectively. Let $F_{i,j}$ denotes the flow transferred from source i to demand j. Similarly, FW_j represents the flow transferred from fresh water to demand j, with a concentration Cw_k (concentration of *kth* contaminant in fresh water). WW_i refers the flow transferred from source i to waste without any maximum concentration limit. For a better understanding of the network superstructure, refer to Figure 4.4.

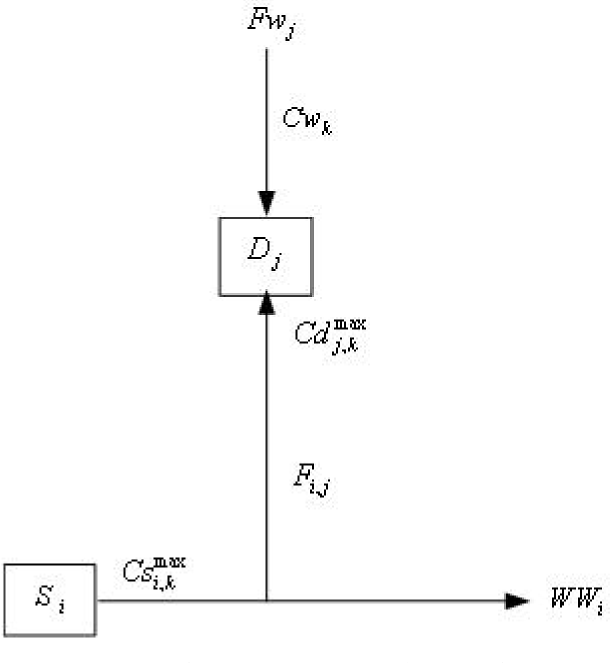


Figure 4.4: A water network superstructure for maximum water recovery.

Objective function:

The objective function is to minimise the total amount of fresh water demand, FW_j.

$$Min\sum_j FW_j \tag{4.1}$$

The minimisation of the objective function represented by equation (4.1) is subjected to the following constraints:

Constraints:

1) Water balance for source

For each source i, the generated wastewater, WW_i and reused/recycled water from source i to demand j, $F_{i,j}$ must be equal to available water source, S_i. The water balance for each source i is given by:

$$WW_i + \sum_j F_{i,j} = S_i \qquad \forall i \in I \tag{4.2}$$

2) Water balance for demand

For each demand j, the water supply from fresh water, FW_j or/and potential reused/recycle water, $F_{i,j}$ must be equal to the desired water demand, D_j. The water balance for each demand j is given by:

$$FW_j + \sum_i F_{i,j} = D_j \qquad \forall j \in J \tag{4.3}$$

3) Demand contaminant load satisfaction

Contaminant mass load for demand j is supplied from a mixed of contaminant mass load from different sources (e.g fresh water, FW_jCw_k or/and potential reused/recycle water, $F_{i,j}Cs_{i,k}$). Thus, the contaminant load from all sources must satisfy the contaminant load for demand j.

$$FW_jCw + \sum_i F_{i,j}Cs_{i,k}^{\max} \leq D_jCd_{j,k}^{\max} \qquad \forall j \in J \tag{4.4}$$

4) Non-negativity constraints

The fresh water supply, wastewater generation and reused/recycled water flow rate must be greater than zero, therefore the fresh water supply, wastewater generation and reuse/recycle water flow rate is defined as positive/non-negativity variables.

$$FW_j, \quad WW_i, \quad F_{i,j} \geq 0 \qquad \forall i \in I, \quad \forall j \in J \qquad (4.5)$$

4.2.3.5.2 Model for Optimal Design of Water Networks (MODWN)

This model, called MODWN, is formulated as a mixed integer nonlinear program (MINLP). However, the MINLP problems are the most complex optimisation problems. The first stage consists of a MILP formulation that is solved to provide initial values. The solution available from the first stage is refined in the second stage to a final solution in a general MINLP.

Stage 1: Fresh Water Savings Mode (FWS-mode)

In the Fresh Water Savings Mode (FWS-mode), the objective is to minimise fresh water target which leads to minimum wastewater generation without considering any economic constraints. Changes can be made to the flow rates and concentrations of water sources and water demands to reduce the MWR targets and ultimately achieve MWN benchmark. Minimum water targets can be obtained through WMH options. It is vital to note that the implementation of process changes options will yield new water targets. In this approach, all the WMH options are considered simultaneously in order to obtain minimum water targets. The water networks obtained in this stage are used as initial values for the optimisation of second stage.

Objective function:

The objective function can be written as:

$$Min\sum_{j} FW_j \tag{4.6}$$

The minimisation of the objective functions in equation (4.6) is subject to the following constraints.

Constraints:

1) Demand constraint

Adjusted demand flow rate, B_j is equal to the given demand flow rate after selections of elimination, $Da_{j,e},$ reduction, $Da_{j,re}$ and original demand flow rate, D_j. Binary variables, $X_{j,e}$ and $X_{j,re}$ are introduced to represent the selection of several possible measures in elimination and reduction levels.

$$\sum_{e} Da_{j,e} X_{j,e} + \sum_{re} Da_{j,re} X_{j,re} + \sum_{o} D_j X_{j,o} = B_j \qquad \forall j \in J \tag{4.7}$$

2) Reduction option constraint

If reduction option is selected, the flow rate for j^{th} demand, $Da_{j,re}$ is reduced by certain percentage, $\sigma_{j,re}.$

$$Da_{j,re} = \sigma_{j,re} D_j \qquad \forall j \in J \tag{4.8}$$

Substituting $Da_{j,re}$ in equation (4.8) into eq (4.7) will result to linear constraint (4.7’). and can be written as below,

$$\sum_{e} Da_{j,e} X_{j,e} + \sum_{re} \sigma_{j,re} D_j X_{j,re} + \sum_{o} D_j X_{j,o} = B_j \qquad \forall j \in J \tag{4.7'}$$

3) Water balance for each demand

The water supplied for each adjusted demand flow rate, B_j is a combination of fresh water, FW_j, potential reused/recycle water, $F_{i,j}$, other resources, $Fos_{os,j}$ (e.g rainwater, river and snow), and regenerated water from regeneration unit, $F_{i,r}$. The water balance for each demand, B_j is given by:

$$FW_j + \sum_i F_{i,j} + \sum_{os} Fos_{os,j} + \sum_r F_{r,j} = B_j \qquad \forall j \in J \qquad (4.9)$$

4) Water balance for each source

The water generated from each source i, A_i is either discharged directly as effluent, WW_i, direct reuse/recycle water from source i to demand j, $F_{i,j}$ or partially treated in regeneration unit. The water balance for each source i is given by:

$$WW_i + \sum_j F_{i,j} + \sum_r F_{i,r} = A_i \qquad \forall i \in I \qquad (4.10)$$

5) Demand contaminant load satisfaction

Contaminant mass load for adjusted demand j, $B_jCd_{j,k}$ is supplied from a mixed of contaminant mass load from different sources (e.g fresh water, FW_jCw_k, potential reused/recycle water, $F_{i,j}Cs_{i,k}$, outsources, $Fos_{os,j}Cos_{os,k}$ or/and regenerated water, $F_{r,j}Cro_{r,k}$). Thus, the contaminant load from all sources must satisfy the contaminant load for demand j.

$$FW_jCw_k + \sum_i F_{i,j}Cs_{i,k}^{\max} + \sum_{os} Fos_{os,j}Cos_{os,k} + \sum_r F_{r,j}Cro_{r,k} \le B_jCd_{j,k}^{\max}$$

$$\forall j \in J \qquad (4.11a)$$

Note that, the regeneration units employed here using centralised wastewater treatment concept and the performance of regeneration units are measured with fixed outlet concentration for all contaminants, $Cro_{r,k}$ or contaminant removal ratio, $RR_{r,k}$.

$$FW_jCw_k + \sum_i F_{i,j}Cs_{i,k}^{\max} + \sum_{os} Fos_{os,j}Cos_{os,k} + \sum_r F_{r,j}((1-RR_{r,k})Cri_{r,k}) \le B_jCd_{j,k}^{\max}$$

$$\forall j \in J \qquad (4.11b)$$

6) Mass balance on regeneration unit

The amount of wastewater needs to be regenerated in regeneration unit, $F_{i,r}$, depends on the needs of water demand to be supplied with the regenerated water, $F_{r,j}$. The total inlet flow rate is equal to the total outlet flow rate for regeneration unit. Water consumption for cleaning of the regeneration unit is assumed to be negligible since the cleaning process only performs once in a while.

$$\sum_{i} F_{i,r} = \sum_{j} F_{r,j} \qquad \forall r \in R \qquad (4.12)$$

7) External water sources constraint

The total external water sources flow rate distributed to demand, Fos_j must be equal to or lower than maximum design limit, Fos^{max}

$$\sum_{j} Fos_{os,j} \leq Fos_{os}^{\max} \qquad \forall os \in OS \qquad (4.13)$$

8) Selection of Water management

This constraint is developed to emphasis that, only one water management options is chosen at one time. Binary variables, $X_{j,e}$, $X_{j,re}$ and $X_{j,o}$ are introduced to represents the selection of water management options involving elimination, reduction or original operation respectively.

$$\sum_{e} X_{j,e} + \sum_{re} X_{j,re} + \sum_{o} X_{j,o} = 1 \qquad \forall j \in J \qquad (4.14)$$

9) MTB constraint

For MTB operations, the adjusted flow rate of water demand, B_j is equal to the adjusted water source flow rate, A_i.

$$B_j = A_i \qquad \forall j \in J \qquad (4.15)$$

10) NMTB constraint

If source streams exist for NMTB operations, the adjusted flow rate of water source, A_i, is equal to water source flow rate before implementation of WMH options, S_i.

$$A_i = S_i \qquad \forall i \in I \qquad (4.16)$$

11) Non-negativity constraints

The fresh water supply, wastewater generation and reused/recycled water flow rate, must be greater than zero, therefore the fresh water supply, wastewater generation and reuse/recycle water flow rate is defined as positive/non-negativity variables.

$$FW_j,\ \ WW_i,\ \ F_{i,j},\ \ F_{i,r},\ \ F_{j,r},\ \ A_i,\ \ B_j,\ Da_{j,re} \geq 0 \qquad (4.17)$$

Stage 2: Economic Mode (E-mode)

In the second mode, the optimiser determines the maximum net annual savings of water networks while satisfying the minimum possible fresh water and wastewater targets and achieving the desired payback period for retrofit design. The objective function includes the operating cost savings of fresh water demand, wastewater generation, chemicals used by water system and electricity required for pumping activities. The water networks obtained in the first stage are used as initial points for the optimisation in this stage.

Objective function:

The objective function is given by:

$$\text{Max NAS} = \begin{bmatrix} \sum_j \left(FW_j^{initial} - FW_j\right) CostFW + \sum_i \left(WW_i^{initial} - WW_i\right) CostWW \\ + \sum_i \sum_r \left(F_{i,r}^{initial} - F_{i,r}\right) CostChemReg \\ + \sum_i \left(WW_i^{initial} - WW_i\right) CostElecPOPump \\ + \sum_j \left(FW_j^{initial} - FW_j\right) CostElecPOPump \\ + \sum_i \sum_j \left(F_{i,j}^{initial} - F_{i,j}\right) CostElecPOPump \\ + \sum_j \left(Fos_{os,j}^{initial} - Fos_{os,j}\right) CostElecPOPump \\ + \sum_i \sum_r \left(F_{i,r}^{initial} - F_{i,r}\right) CostElecPOPump \\ + \sum_r \sum_j \left(F_{r,j}^{initial} - F_{r,j}\right) CostElecPOPump \end{bmatrix} * AOT \tag{4.18}$$

The first part of the equation represents the savings attained from fresh water and wastewater reductions. In this expression, FW_j and WW_i are the flow rate of fresh water and wastewater while $CostFw_j$ and $CostWW_i$ are cost of fresh water and wastewater respectively. This followed by chemical savings that may be used for regeneration system in the second term. *CostChemReg* is devoted as cost of chemicals for regeneration processes. The next terms represent the savings on pumping costs. The costs are proportional to the total flow of fresh water, FW_j, wastewater, WW_i, external water sources, $Fos_{os,j}$, wastewater to regeneration unit, $F_{i,r}$ and regenerated water from regeneration unit, $F_{r,j}$, respectively. *CostElect* and *POPump* are electrical cost and power of pump used for each pumping system.

Constraints:

The maximisation of the objective functions in equations (4.18) is subject to equation (4.7) - (4.17) and (4.19) - (4.24).

12) Capital investment for external water sources unit

The capital investment for outsourcing unit is a function of the maximum flow rate of external water sources Fos_{os}^{max} including pipes and pumps costs are given as below:

$$COsU = \sum_{os} [CostOsU_{os} (Fos_{os}^{\max} / Fos_{os}^{A})^{\beta}] P + CostPipe + CostPump \qquad (4.19)$$

13) Capital investment for regeneration unit

The capital investment for regeneration unit is a function of the total wastewater flow rate entering the regeneration unit, $F_{i,r}$, including pipes and pumps cost are given as below:

$$CRegU = CostRegU_{r}^{A} (\sum_{i} \sum_{r} F_{i,r} / Freg^{A})^{\beta} P + CostPipe + CostPump \qquad (4.20)$$

14) Capital investment for reuse system

The capital investment for reused and recycled water only considers cost of pipes and pumps.

$$CReuse = CostPipe + CostPump \qquad (4.21)$$

Note that, cost estimation for equipment purchased for external water sources, regeneration unit as well as reuse unit are calculated using sixth-tenth factor, β as attached in Appendix A.

15) Total capital investment for elimination unit

The total capital investment for elimination unit is given as below:

$$\sum_{j} \sum_{e} X1_{j,e} CostUE_{j,e} \varepsilon_{j} \qquad (4.22)$$

where $CostUE_{j,e}$ is cost of elimination unit e for demand j; ε_j is number of equipment for demand j; $X1_{j,e}$ is binary variable that indicates the selection of e^{th} elimination options for j^{th} demand.

16) Total capital investment for reduction unit

The total capital investment for reduction unit is given as below:

$$\sum_{j}\sum_{re} X2_{j,re}\, CostURe_{j,re}\, \varepsilon_{j} \tag{4.23}$$

where $CostURe_{j,re}$ is cost of reduction unit e for demand j; ε_j is number of equipment for demand j; $X2_{j,re}$ is binary variable that indicates the selection of re^{th} reduction options for j^{th} demand.

17) Payback period constraint

The total payback period must be set less than or equal to investment payback limit set by a plant owner. The payback period is calculated using equation (3.1).

$$\frac{\text{Net Capital Investment (NCI)}}{\text{Net Annual Savings (NAS)}} \le \gamma$$

$$\frac{\begin{array}{c}\underbrace{CRegU}_{\text{Regeneration unit cost}} + \underbrace{COsU}_{\text{External water sources unit cost}} + \underbrace{CReuse}_{\text{Reuse system cost}} + \\ \underbrace{\sum_{j}\sum_{e} X1_{j,e}\, CostUE_{j,e}\, \varepsilon_{j}}_{\substack{\text{capital cost for}\\ \text{elimination unit}}} + \underbrace{\sum_{j}\sum_{re} X2_{j,re}\, CostURe_{j,re}\, \varepsilon_{j}}_{\substack{\text{capital cost for}\\ \text{reduction unit}}}\end{array}}{\left[\begin{array}{l}\sum_{j}\left(Fw_{j}^{initial} - Fw_{j}\right)CostFW + \sum_{i}\left(WW_{i}^{initial} - WW_{i}\right)CostWW \\ + \sum_{i}\sum_{r}\left(F_{i,r}^{initial} - F_{i,r}\right)CostChemReg \\ + \sum_{i}\left(WW_{i}^{initial} - WW_{i}\right)CostElecPOPump \\ + \sum_{j}\left(Fw_{j}^{initial} - Fw_{j}\right)CostElecPOPump \\ + \sum_{i}\sum_{j}\left(F_{i,j}^{initial} - F_{i,j}\right)CostElecPOPump \\ + \sum_{j}\left(Fos_{os,j}^{initial} - Fos_{os,j}\right)CostElecPOPump \\ + \sum_{i}\sum_{r}\left(F_{i,r}^{initial} - F_{i,r}\right)CostElecPOPump \\ + \sum_{r}\sum_{j}\left(F_{r,j}^{initial} - F_{r,j}\right)CostElecPOPump \end{array}\right] * AOT} \le \gamma \tag{4.24}$$

where γ is investment payback limit set by a plant owner, e.g. two years. This constraint is only applicable if the obtained payback period is more than payback period set by the plant owner.

4.3.4 Step 4: GAMS Coding

The problem is formulated as MINLP and coded into General Algebraic Modeling System (GAMS). Through the commercial mathematical optimisation software package GAMS, the optimal water network can be found. GAMS is a language for setting up and solving mathematical programming optimisation models. GAMS is a flexible and powerful optimisation package. This software also is a high-level modelling system that offers a flexible framework for formulating and solving linear, nonlinear, mixed integer linear and nonlinear optimisation problems. Its syntax allows for declaring associations among equations (objective function, equality constraints and inequality constraints), variables, parameters and scalar. GAMS provides a wide range of solvers to optimise a variety of problem formulation, consist of linear programs (LP), nonlinear programs (NLP), mixed integer linear programs (MIP), and mixed integer nonlinear programs (MINLP). The user can modify the formulation quickly and easily from one solver to another. Refer Section 3.5.3 for details explanation on application of GAMS software.

4.3.5 Step 5: Sensitivity Analysis

A sensitivity analysis studies the variation in model parameters by estimating the change in the optimal solution. Sensitivity analysis is a tool that may be used to study the behaviour of a model and to ascertain how much the outputs of a given model depend on each or some of the input parameters. The information obtained from sensitivity analysis can be utilized to investigate the influence of errors or uncertainty in model parameters to the optimal solution. In design and operation of any process, there are usually several parameters that have a degree of uncertainty and variability associated with them. It is necessary to assess the sensitivity of the optimum flow sheet to model parameters that may be subject to variation and uncertainty. In this work, the impact of fresh water price is discussed.

The possible cost required for the water network systems was estimated throughout incremental of costs. A different scaling factor was used to analyse the sensitivity of the water network due to variation of the component. Results of the sensitivity analysis identified the adequacy of process models and the key areas that affect the process performance. A sensitivity analysis study was carried out in order to investigate the effect of parameter uncertainties. The model sensitivity has been analysed by using deterministic method (Grossmann and Sargent, 1978), in which the uncertainty is provided either by a specific bound or via a finite number of fixed parameter values. From the sensitivity analysis, we can distinguish among the parameters that are critical to the model predictions from those that have negligible effects.

CHAPTER 5

RESULTS AND DISCUSSION

5.1 Introduction

This chapter describes and discusses thoroughly the results of applying each step of the methodology. The MODWN models are applied on an urban case study involving a mosque for a retrofit design.

5.2 Urban Case Study – Sultan Ismail Mosque, UTM

5.2.1 Sultan Ismail Mosque Background

Sultan Ismail Mosque (SIM) which is situated in Universiti Teknologi Malaysia (UTM), Skudai, Johor was chosen as the case study for this work. This mosque is mainly used by the Muslim students and staff of UTM for prayer and educational activities.

5.2.2 Process Description

In the mosque, water is being used for various activities including ablution, irrigation, shower, kitchen and toilet services as well as mosque cleaning (Wan Alwi, 2007). Fresh water is supplied by SAJ and stored in four interconnected distribution tank. The estimated fresh water usage for SIM is 11, 550 m^3/yr (Ujang and Larsen, 2000). 79.5% of this value is used for ablution and the rest is for irrigation, mosque cleaning, toilet flushing, wash basin and toilet pipes (Ujang and Larsen, 2000). The total amount of water consumed fluctuates throughout the year between academic semesters and holidays. During academic semesters, the amount of water used for ablution is 60 m^3/day on Friday and 25 m^3/day on other days. In order to estimate a reasonable typical water savings for the mosque, daily water usage calculations will be based on academic semester days (Ujang and Larsen, 2000). Water distribution network for SIM is shown in Figure 5.1.

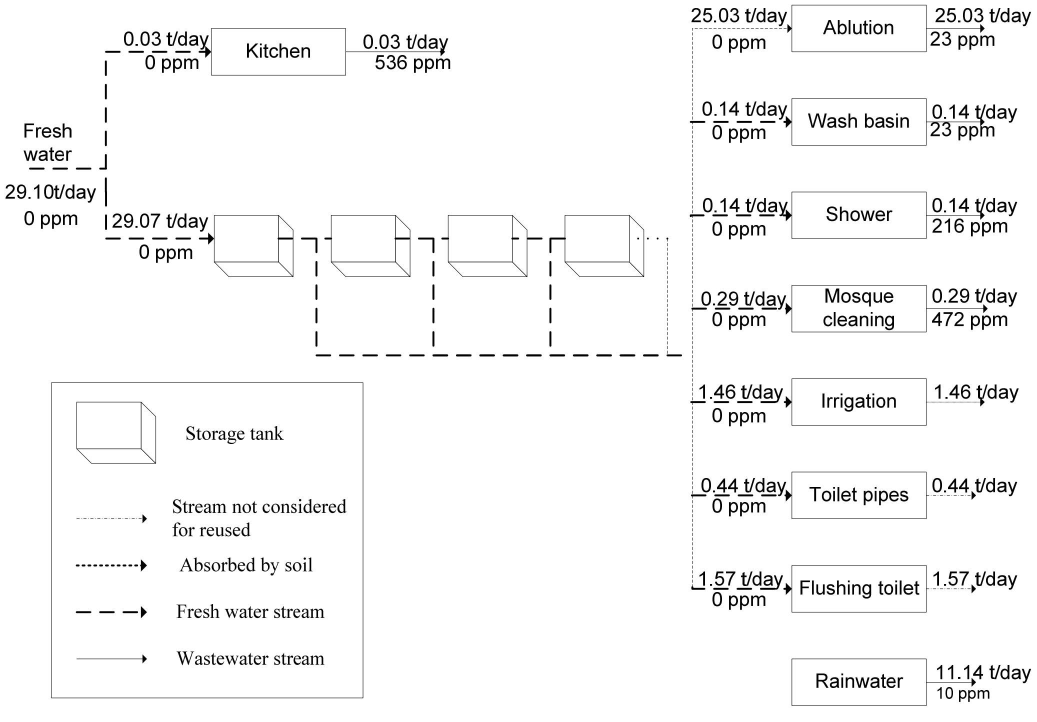


Figure 5.1: Water distribution network for Sultan Ismail Mosque (Wan Alwi, 2007).

5.2.3 Optimal Design of Water Networks

5.2.3.1 Limiting Water Data extraction

The SIM limiting water data taken from Wan Alwi (2007) is modified by adding another contaminant data. Contaminants concerned for this water minimisation study are biological oxygen demand (BOD) and turbidity. The limiting water flow rate data for each operation is sorted to source and demand as presented in Table 5.1. Tables 5.2 and 5.3 show the contaminant concentrations for water demands and sources. The data for water demands was adapted from USEPA water quality standards for water reuse (Al-Jayyousi, 2003) (Table 5.5). The fresh water source available is free of all contaminants ($Cw_{BOD} = 0$ ppm, $Cw_{turbidity} = 0$ NTU). In this case, there are eight water demands and five water sources. Wastewater derived from toilet flushing and toilet pipes is referred to as black water and will not considered to be reused since it is highly faecally contaminated. Water from irrigation is assumed to be completed absorbed by the soil.

Table 5.1: Demands, D_j and sources, S_i water data for Sultan Ismail Mosque.

D_j	Demand	Flow rate (t/day)	S_i	Source	Flow rate (t/day)
D_1	Ablution	25.03	S_1	Ablution	25.03
D_2	Wash basin	0.14	S_2	Wash basin	0.14
D_3	Showering	0.14	S_3	Showering	0.14
D_4	Mosque cleaning	0.29	S_4	Mosque cleaning	0.29
D_5	Kitchen	0.03	S_5	Kitchen	0.03
D_6	Irrigation	1.46			
D_7	Toilet pipes	0.44			
D_8	Flushing toilet	1.57			

Table 5.2: Contaminant concentrations data for water demands, $Cd_{j,k}^{max}$.

D_j	**Demand**	**BOD (ppm)**	**Turbidity (NTU)**
D_1	Ablution	10	2
D_2	Wash basin	10	2
D_3	Showering	10	2
D_4	Mosque cleaning	10	2
D_5	Kitchen	0	0
D_6	Irrigation	10	2
D_7	Toilet pipes	10	2
D_8	Flushing toilet	10	2

Table 5.3: Contaminant concentrations data for water sources, $Cs_{i,k}^{max}$.

S_i	**Source**	**BOD (ppm)**	**Turbidity (NTU)**
S_1	Ablution	23	43
S_2	Wash basin	23	49
S_3	Showering	216	375
S_4	Mosque cleaning	472	444
S_5	Kitchen	536	132

Table 5.4: Summary of water quality and criteria suitable for domestic water recycling (Al-Jayyousi, 2003).

	Total coliform count/100 ml	**Faecal coliforms**	**BOD_5 (mg/l)**	**Turbidity (NTU)**	**Cl_2 residual (mg/L)**	**pH**
Bathing water Standards[a]	10,000(m) 500(g)	2,000(m) 100(g)	-	-	-	6-9
USA, NSF	-	<240	45	90	-	-
USA, EPA	Non-detectable	-	10	2	1	6-9
Australia	<1	<4	20	2	-	-
UK (BSIRA)	Non-detectable	-	-	-	-	-
Japan	<10	<10	10	5	-	6-9
WHO	1,000(m) 500(g)	-	-	-	-	-
Germany	100	500	20	1-2	-	6-9

5.2.3.2 Base-Case Scenario – Maximum Water Recovery

For base case scenario, the LP model is applied to existing SIM water system to establish the minimum water targets through maximum reuse and recycling of available water sources. After the LP model is coded into GAMS, the results give the minimum fresh water requirement and wastewater generation targets of 27.75 t/day and 24.28 t/day respectively for this water system. This gives a reduction of 4.8% for fresh water consumption and 5.2% for wastewater generation as compared to the base case scenario. Table 5.5 shows the freshwater and wastewater cost comparison before and after implementation of maximum water recovery while the corresponding water network design is given in Figure 5.2. The GAMS input and report files for MWR are shown in Appendix C.1.

Table 5.5: Comparison of fresh water consumption and wastewater generation before and after water integration.

	Before MWR	**After MWR**
Total fresh water consumption (t/day)	29.10	27.75
Total wastewater generation (t/day)	25.63	24.28
Savings of fresh water (USD/yr)	0	276
Fresh water reduction (%)	0	4.8
Wastewater reduction (%)	0	5.3

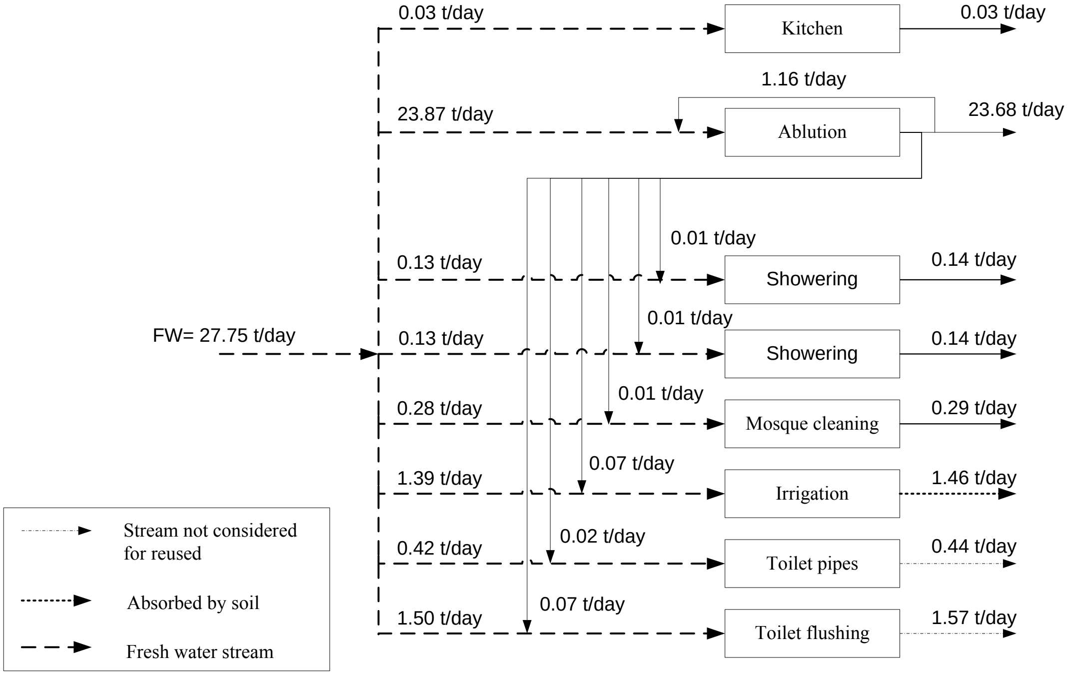


Figure 5.2: Maximum water recovery network design for Sultan Ismail Mosque.

5.2.3.3 The Water Management Hierarchy Implementation

After calculating the base-case MWR targets, all potential process changes to improve SIM water system were implemented according to WMH options. The various water minimisation schemes were listed in Table 5.6. The WMH options SIM water system is described next:

Table 5.6: Various water minimisation schemes for SIM.

WMH	Strategy
Elimination	D_8: Change 12 litre flushing toilet to composting toilet
Reduction	D_1: Change normal ablution tap to laminar flow tap D_8: Option 1: Change 12 litre flushing toilet to dual flush toilet Option 2: Change 12 litre flushing toilet to vacuum toilet
Reuse	Total water reuse
External water sources	Rainwater harvesting
Regeneration	Wastewater regeneration

i. Source elimination

Source elimination is concerned with the complete avoidance of fresh water usage. In order to maximise fresh water savings, all possible means for process changes or to change existing equipment to new equipment in order to eliminate water demands were considered. In this case, it was possible to eliminate D_8 (toilet flushing) by changing all 12 litre flushing toilet to composting toilet.

ii. Source reduction

When it was not possible to eliminate water demands, water reduction should be considered. It was possible to reduce water demand at D_1 (ablution) by changing normal water tabs to laminar taps. This also reduced source S_1. Another possibility to reduce fresh water demand at D_8 is by changing the 12 litre flushing to dual flush toilet. Next, fresh water usage can also be reduced by changing the 12 litre flushing toilet to vacuum toilet. The vacuum toilet only requires 0.4 litre water per flushing.

iii. External water sources

Rainwater harvesting is one of possible water sources to be used at SIM water system. In Johor, the average annual rainfall is approximately 1778mm (Wikipedia, 2008). Based on SIM available roof area and rain distribution, it was possible to harvest 11.14 t/day (maximum design limit, Fos_{os}^{max}) of rainwater at concentration of BOD, Cos_{BOD} =10 ppm (Janikowski, 2000) and turbidity, $Cos_{turbidity}$ = 1.5 NTU (Kim *et al.*, 2006).

iv. Regeneration reuse/recycle

The next level for water minimisation is regeneration. Regeneration refers to treatment of wastewater or even external water source to match the quality of water required for further reuse. Regeneration can be used to remove contaminants on an intermediate basis. In this case, the regeneration process consists of three main steps. First of all, grey water is filtered for particles. After that, it is passed through an activated carbon to remove unpleasant odour and turbidity. Finally, UV system is used to disinfect the grey water for storage purposes. Regeneration of wastewater using a microfiltration, activated carbon and UV system yielded 4.2 ppm of BOD concentration (Cro_{BOD}) and 1 NTU of turbidity ($Cro_{turbidity}$) (Ahn *et al.,* 1999).

5.2.3.4 Application of MODWN

The applicability and advantages of the proposed approach for designing optimal water network is demonstrated. In order to obtained optimal solution for *FWS-mode*, GAMS/CPLEX solver was employed for MILP problem. The first stage consists of an MILP formulation that is solved to provide the initial points. The solution available from the first stage is used as the initial points for the second stage, *E-mode* to obtain optimal solution in a general MINLP. The models were encoded and solved using GAMS/BARON. The case study was carried out using a notebook with 2.00 GHz Intel Core Duo Processor. The economic data for SIM case study are listed in Appendix B while the GAMS input and report files for MODWN are presented in Appendix C.2 and C.3.

5.2.3.4.1 Stage 1: Fresh Water Savings Mode (FWS-Mode)

In the FWS-mode, the objective is to minimise fresh water target which leads to minimum wastewater generation. Process changes can be made to the flow rates and concentrations of water sources and water demands to reduce the MWR targets and ultimately achieve MWN benchmark. Minimum water targets can be obtained by screening process changes using WMH options. Solving equation (4.6) with constraint of equations (4.7)-(4.17) yielded an optimal solution and can be used as initial points to solve MINLP problem in the second stage. From the developed model, the minimum fresh water and wastewater flow rate targets were at 0.03 t/day and 0.14 t/day respectively.

5.2.3.4.2 Stage 2: Economic Mode (E-Mode)

The optimal results attained from the first stage were used as initial points to determine the maximum net annual savings for retrofit scenario for SIM. Table 5.7 presents optimal results for SIM with and without setting payback period limit. In the beginning, the total payback period for retrofit design was 9.98 years for SIM and gave the minimum water targets at 0.03 t/day fresh water and 9.27 t/day wastewater. In order to obtain the maximum annual savings for water system, the optimiser favoured to eliminate water demand at D_8 (toilet flushing) by changing all 12 litre flushing toilet to a composting toilet. In addition, changing normal water taps to laminar taps at demand D_1 also led to reductions of fresh water consumption.

Nonetheless, the maximum limit for payback period for retrofit scenario was set at 5 years by plant owner (Wan Alwi, 2007). From the developed model, the maximum net annual savings was USD 5366 per year and minimum fresh water and wastewater flow rate targets were at 1.37 t/day and 9.04 t/day respectively. The minimum water network targeted 95.3% fresh water and 64.7% wastewater savings after implementing WMH options. Because of the payback period constraint, the optimiser chose to reduce water flow rate at D_1 since much less capital investment was needed as compared to eliminating or reducing fresh water usage at demand D_8.

Table 5.7: Optimal results for SIM with and without setting payback period limit.

	Without setting payback period limit	**Payback period limit to 5 yrs**
Water elimination (t/day)	$D_8=0$	-
Water reduction (t/day)	$\alpha_{1,1}D_1 = 12.52$	$\alpha_{1,1}D_1 = 12.52$
Total fresh water consumption (t/day)	0.03	1.37
Total wastewater generation (t/day)	9.27	9.04
Total reused/recycled water (t/day)	0.23	0.29
Total regenerated water (t/day)	3.62	3.78
Total external water sources (t/day)	11.14	11.14
Net annual savings (USD/yr)	5646	5366
Net capital investment (USD)	56341	26830
Total payback period (yr)	9.98	5

The external water source was added at the maximum limit of rain water harvesting for both scenarios. As mentioned before, rain water source becomes favourable to be used because of its high water quality compared to reuse and recycling. On the contrary, the total regenerated water flow rate and reused/recycled water flow rate were slightly increased when payback period limit was set to 5 years in order to fulfil flow rate and mass load of water demand. The increase in regenerated and reused/recycled water flow rates also resulted in decreased wastewater generation.

5.2.3.5 Sensitivity Analysis

Similar to the previous case study, the impact of fresh water price is discussed. It was assumed that the price of fresh water was increased by 10%, 20%, 40%, 80% and 100% from the base line price of USD 0.56/t.

5.2.3.5.1 Effects of Fresh Water Prices on Total Water Demand and Source Flow Rates

Figures 5.3 and 5.4 show the effects of fresh water prices on total water demand flow rate and total water source flow rate respectively. The figures also demonstrate the selection of water minimisation schemes for each increment of fresh water price. It was clearly shown that the total water demand flow rate was maintained at 16.58 t/day even though the price of fresh water increased to 20% higher than base line. This is due the selection of water minimisation schemes involving elimination and reduction. The optimiser recommended reducing fresh water usage at D_1 in order to fulfil the desired payback period. However, as fresh water price increased to 40% and 60% higher than the base line, the optimiser favoured to reduce fresh water consumption at D_1 and D_8 by changing the 12 litre flush toilet to dual-flush toilet in order to achieve the payback period constraint. Consequently, the total water demand was slightly reduced to 15.80 t/day.

While the price of fresh water was increased to 80% higher than the base line price, the total water demand flow rate was further decreased since the optimiser proposed to change the base case toilet to vacuum toilet at demand D_8. Nonetheless, when fresh water price was doubled, elimination of demand D_8 by changing from a 12 litre toilet to a composting toilet became more attractive. Reduction of fresh water usage at D_1 was still favourable. Elimination of fresh water usage at D_8 did not give significant reduction of total water demand, but affected the net capital investment as well as the payback period, as will be discussed in the next section.

In contrast, there were no changes in the total water source flow rate even though the price of fresh water increased to 100% higher than the base line. This was because the elimination of water demand D_8 only affected the total water demand.

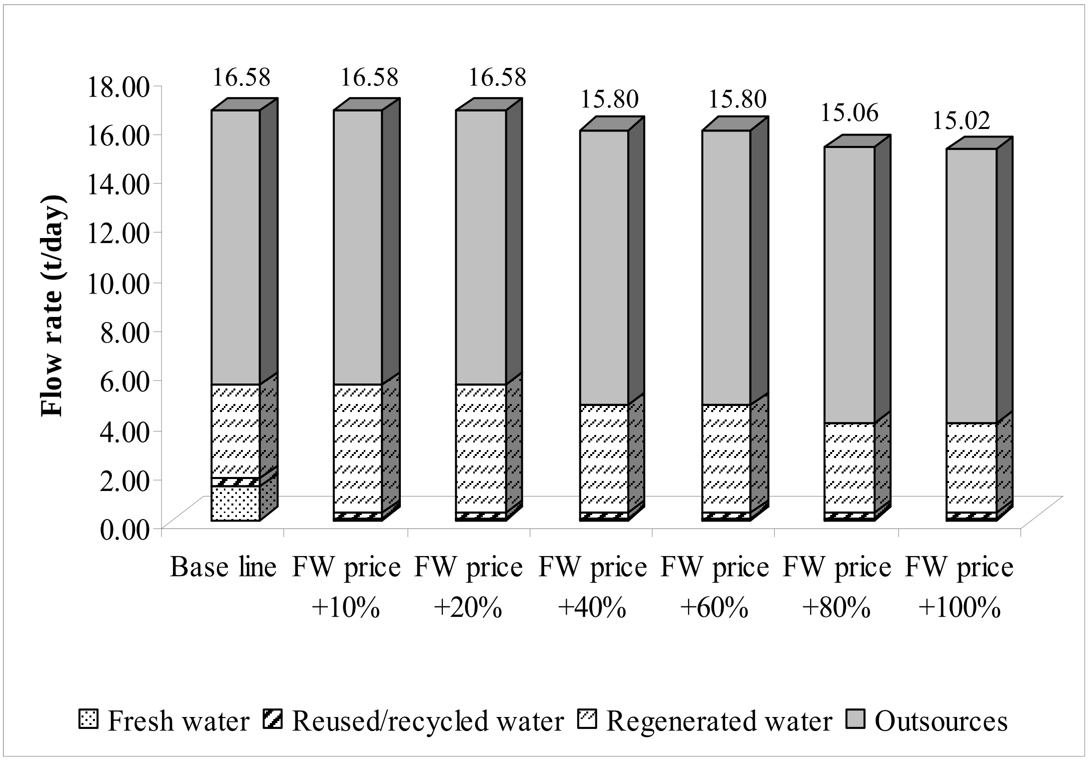


Figure 5.3: Effects of fresh water prices on the total water demand flow rate.

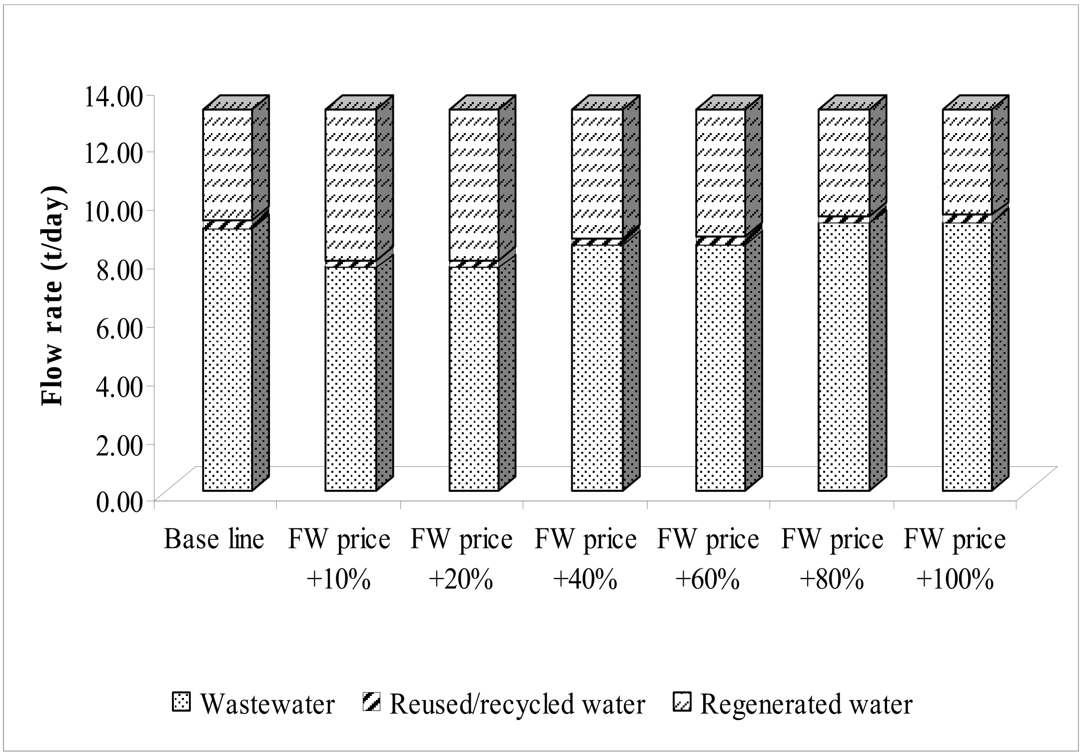


Figure 5.4: Effects of fresh water prices on the total water source flow rate.

5.2.3.5.2 Effects of Fresh Water Prices on Selection of Water Minimisation Schemes

Fluctuating fresh water price has a strong influence on the selection of water minimisation schemes as shown in Figure 5.3. The fresh water consumption was decreased when fresh water price increased to 10% higher than the base line price. The fresh water flow rate dropped from 1.37 t/day to 0.03 t/day. The fresh water flow rate remained the same even though the price of fresh water increased from 10% to 100%. This was because the minimum limit of fresh water requirement had already been achieved with the increment of fresh water price. Due to fresh water reduction, more wastewater needed to be regenerated in order to fulfil the water demand flow rate and massload. However, wastewater regeneration decreased as fresh water price increased from 10% to 100% higher than base line, in order to satisfy desired payback period. Hence, more wastewater was discharged to the environment within this price increment. Meanwhile, direct reused/recycled water was still favourable. In addition, the external water source with maximum flow rate became the biggest contributor in order to satisfy water demand.

5.2.3.5.3 Effects of Fresh Water Prices on Net Annual Savings, Net Capital Investment and Payback Period

Figure 5.5 shows the effects of fresh water prices on net annual savings, net capital investment as well as payback period. As mentioned before, capital investment for most of water minimisation schemes was a function of the water flow rate. Therefore, the changes in the water flow rate will affect to the net capital investment while the changes of fresh water flow rate gave the impact to net annual savings. From the figure, it was clearly shown that when the price of fresh water increased, the net annual savings also increased. However, the net capital investment was slightly increased when fresh water price increased to 10% higher than base line, and was maintained as the price of fresh water increased to 20% higher than base line. This was because more water needed to be regenerated in order to fulfil water demand. A similar scenario occurred when the fresh water price was increased by up to 60% from 40% higher than base line. Nevertheless, the net capital investment was increased as the price of fresh water increased to 80% and 100% due to the different selection of water minimisation schemes involving demand D_8. The pattern of payback period was not stable due to it was really depending on net annual savings and net capital investment. Table 5.8 presents the results obtained for sensitivity analysis on fresh water price.

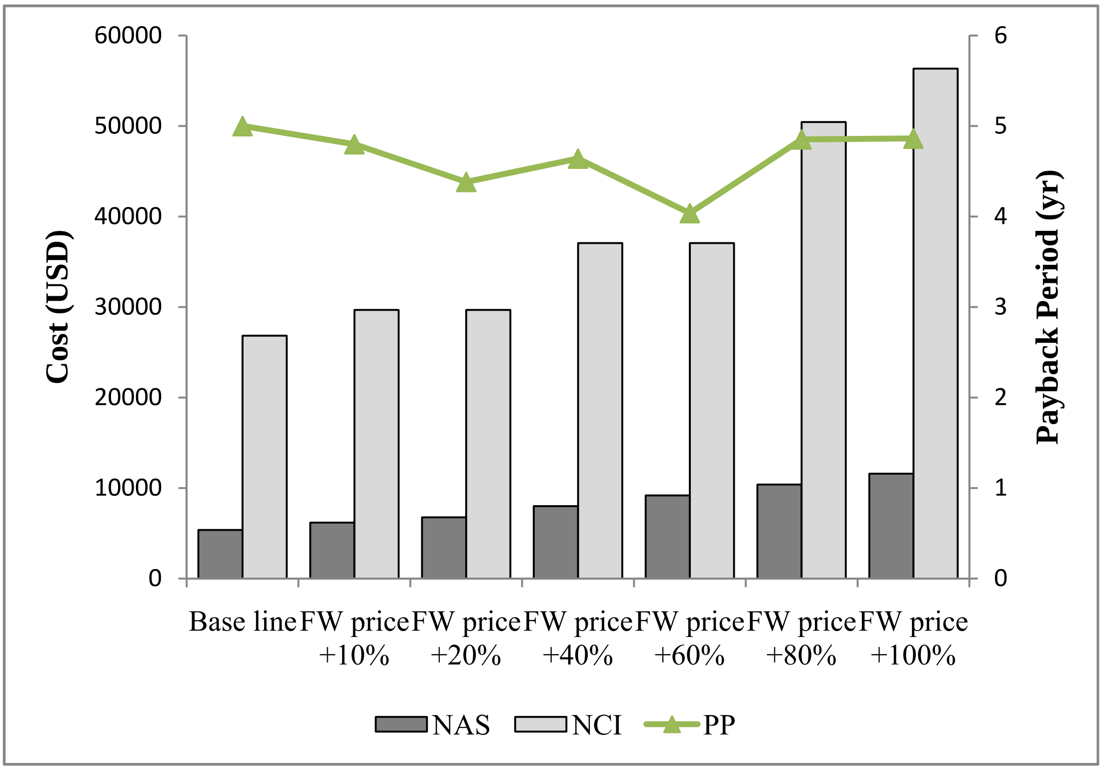


Figure 5.5: Effects of increasing fresh water prices on net annual savings, net capital investment and total payback period.

Table 5.8: Effects of increasing fresh water price on optimal design of water networks.

	Set payback period limit at 5 years (Base line)	**Fresh water price +10%**	**Fresh water price +20%**	**Fresh water price +40%**	**Fresh water price +60%**	**Fresh water price +80%**	**Fresh water price +100%**
Water elimination (t/day)	-	-	-	-	-	-	$D_8 = 0$
Water reduction (t/day)	$\alpha_{1,1}D_6 = 12.52$	$\alpha_{1,1}D_1 = 12.52$	$\alpha_{1,1}D_1 = 12.52$	$\alpha_{1,1}D_1 = 12.52$ $\alpha_{8,1}D_8 = 0.79$	$\alpha_{1,1}D_1 = 12.52$ $\alpha_{8,1}D_8 = 0.79$	$\alpha_{1,1}D_1 = 12.52$ $\alpha_{8,2}D_8 = 0.05$	$\alpha_{1,1}D_1 = 12.52$
Total reused/recycled water (t/day)	0.29	0.26	0.26	0.24	0.24	0.23	0.22
Total external water sources (t/day)	11.14	11.14	11.14	11.14	11.14	11.14	11.14
Total regenerated water (t/day)	3.78	5.16	5.16	4.39	4.39	3.67	3.62
Total fresh water consumption (t/day)	1.37	0.03	0.03	0.03	0.03	0.03	0.03
Total wastewater generation (t/day)	9.04	7.70	7.70	8.49	8.49	9.22	9.27
Net annual savings (USD/yr)	5,366	6,184	6,773	7,998	9,181	10,398	11,587
Net capital investment (USD)	26830	29,678	29,678	37,067	37,067	50,449	56,341
Total payback period (yr)	5	4.80	4.38	4.64	4.64	4.85	4.86

5.2.3.6 Optimal Water Network Design

The minimum water targets and the optimal water network design were generated simultaneously similar to the previous case study. The optimal water network design for SIM case study is shown in Figure 5.6.

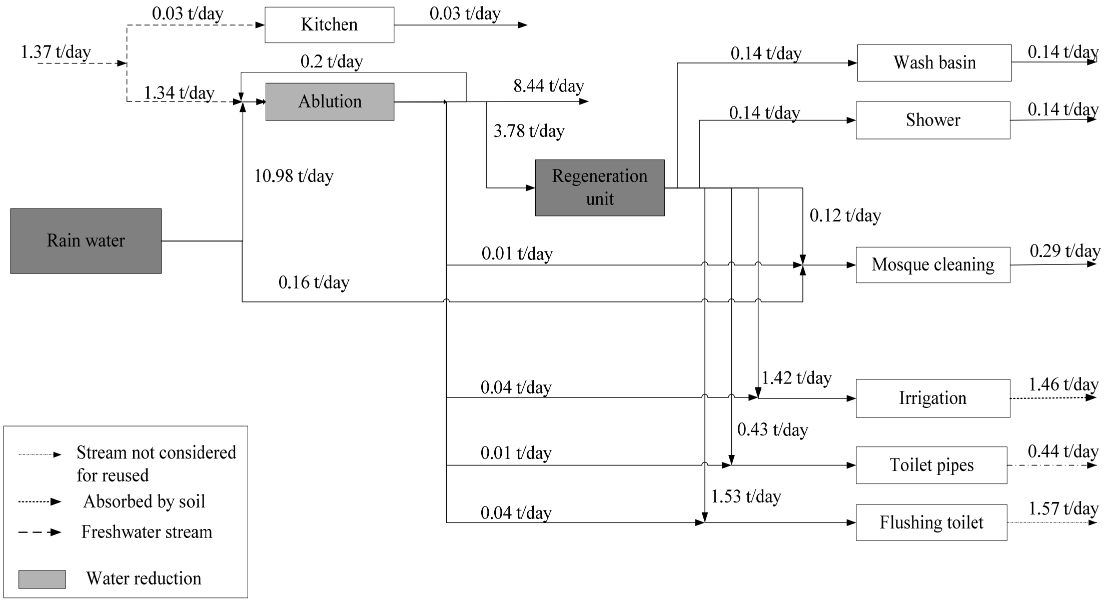


Figure 5.6: Optimal water network design for SIM case study.

5.3.4 Comparison of MODWN and CEMWN

Table 5.9 compares the results between MODWN and CEMWN approach proposed by Wan Alwi (2007). The results obtained from MODWN are better than that for CEMWN in terms of net annual savings and payback period. It is also expected that the minimum fresh water target attained by MODWN is higher than that for CEMWN due to consideration of multiple contaminants in the water system. In real water system, there are various contaminants. These contaminants present additional constraints and prevent wastewater reuse or recycle.

Table 5.9: Comparison of MODWN and CEMWN for Sultan Ismail Mosque Case Study.

	MODWN	**CEMWN**
Contaminant	Multiple contaminant	Single contaminant
Approach	Mathematical programming	Water pinch Analysis (Graphical)
Total fresh water consumption (t/day)	1.37	0.73
Total wastewater generation (t/day)	9.04	8.4
Total reused/recycled water (t/day)	0.29	1.83
Total regenerated water (t/day)	3.78	2.89
Total external water sources (t/day)	11.14	11.14
Net annual savings (USD/yr)	5366	5343
Net capital investment (USD)	26830	26757
Total payback period (yr)	5	5.01
Selection of elimination option	-	-
Selection of reduction option	D_1	D_1

5.3 Advantages and Disadvantages of MODWN and CEMWN

In this section, the advantages and disadvantages of Model for Optimal Design of Water Networks (MODWN) and Cost-Effective Minimum Water Network

(CEMWN) were discussed. The idea of CEMWN design with consideration of process changes guided by water management hierarchy was first accomplished by Wan Alwi (2007). The technique provides an interactive, quick and insightful guide to screen design options involving process changes prior to conducting detailed water network. Besides that, this technique offers an advantage in providing physical insight of the problem through graphical procedures.

However, the graphical steps are tedious and the technique is only applicable for single contaminant system and suitable for simple systems with simple constraints. As mentioned before, in actuality, water systems typically involve various contaminants. Hence, the development of a new systematic approach to design an optimal water networks by using mathematical programming technique involving multiple contaminants known as MODWN is proposed in this work to overcome the limitations of CEMWN.

The MODWN can solve complex water systems involving multiple contaminants that include all levels of water management hierarchy (i.e. elimination, reduction, reuse, outsourcing and regeneration), multiple utilities and cost constraints simultaneously. Furthermore, the optimisation models is able to predict which water source should be eliminated or reduced or needed external source, which wastewater source should be reused/recycled, regenerated or discharged and what is the minimum water network while maximising net annual savings at a desired payback period. In addition, the MODWN can also be used to solve water network design problem to simultaneously generate the minimum water targets and design the minimum water network for global water-using operations.

Although a few additional features can be solved simultaneously, the MODWN is however disadvantaged in terms of providing good insights to designers during network synthesis. In addition, the MINLP is very dependent on good starting points and do not always guarantee a global optimum solution. The advantages and disadvantages for both MODWN and CEMWN approaches are summarised in Table 5.10**.**

Table 5.10: Advantages and disadvantages of MODWN and CEMWN.

MODWN		**CEMWN**	
Advantages	**Disadvantages**	**Advantages**	**Disadvantages**
Can handle multiple contaminants problem	Not providing good insight to designer during network synthesis	Provides an interactive, quick and efficient guide to screen design options involving process changes	Only applicable for single contaminant system
Considers simultaneously all factors that contributes to overall network cost effectiveness	Very dependent on good starting points and do not always guarantee global optimum	Help in getting physical insight of the problem through graphical procedures	Tedious graphical step and manual heuristic procedures
Able to predict which water management schemes should be implemented			Only suitable for simple systems with simple constraints
Minimum water targets and design an optimal water network is generated simultaneously			

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

The work in this thesis offers some major contributions in the area of water minimisation for industrial and urban facilities using mathematical programming technique as mentioned in Section 1.8. The main aim of this study is to develop a new systematic approach for designing an optimal and holistic water utilisation network involving multiple contaminants using mathematical programming.

The model known as *Model for Optimal Design of Water Networks (MODWN)* is capable of predicting which water source should be eliminated or reduced or and how much external water source is needed, which wastewater source should be reused/recycled, regenerated or discharged and what is the minimum water network configuration for maximising the net annual savings at a desired payback period. The optimisation models can be applied to wide range of buildings for both MTB and NMTB water operations involving multiple contaminants. This model also can be employed to the cases involving pure and impure fresh water with multiple contaminants.

The method has been successfully implemented in an urban (Sultan Ismail Mosque at UTM) case study for retrofit scenario. For the mosque case study, the fresh water concentrations for all contaminants were assumed to be zero. The results show that the maximum potential freshwater and wastewater reductions are 95.3% and 64.7% respectively, within 5 years desired payback period specified by the building owner of Sultan Ismail Mosque. This corresponds to an annual savings of USD 5366 per year. Due to the payback period constraint, the optimiser favoured to reduce fresh water flow rate at D_1. Moreover, the maximum net annual savings can be obtained by adding the external water source as well as regenerated and reused/recycled water. The water savings was slightly lower than water savings obtained by Wan Alwi (2007) due to the existence of multiple contaminants.

In addition, sensitivity analysis on fresh water price was performed for both case studies. From the sensitivity analysis, it can be concluded that different water minimisation schemes will be selected as the price of fresh water increased. Furthermore, the sensitivity analysis can also be used to predict future water minimisation scenario.

6.2 Recommendations

i. Simultaneous mass and energy reduction by considering multiple contaminants

The models developed in this work are based on the assumption that the system is operated isothermally. However, certain water-using operations involve energy consumption. Therefore, it is possible to minimise heat and water simultaneously. For example, integrating cold streams with hot streams could result in chilled water reduction. A reduction in chilled water usage could reduce cooling tower make up water and also save energy.

ii. Batch process system

Batch processes are commonly encountered in the production of food, beverages and pharmaceutical. In batch processes, the water streams cannot be characterised only by their flow rate and concentration, the timing of each operation also needs to be taken into account. Thus, the existing methodologies for continuous processes cannot be applied directly to time-dependent processes.

iii. Total water system

Total water system is an overall framework that considers simultaneous the combination of water-using operations and wastewater treatment system. The water system consists of water reuse/recycle and water regeneration, as well as effluent treatment. Before wastewater is discharged to the environment, wastewater will be treated to meet the environmental regulations. Hence, it is possible to reduce a large quantity of freshwater and wastewater by considering an entire water network.

iv. Optimal design of resource network

The optimisation program can be used as a tool for conservation of other resources including mass, heat and gas with slight changes in the model.

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APPENDIX A: PRE-DESIGN CAPITAL COST ESTIMATION

Basically, an equipment capital cost is calculated based on a function of the equipment capacity or flow rate. The calculation for capital cost estimation is presented as below:

(i) Estimation of equipment purchased cost and installation cost (C_{PE} and C_{PEI})

As stated by Peters *et al.* (2003), the capital cost of an equipment of a given size can be predicted using the power relationship known as *sixth-tenth factor rule*. According to this rule, if the cost of an equipment *b* at given capacity is known, the cost of *a* similar equipment *a* at *X* times the capacity of b is $X^{0.6}$ times the cost of equipment *b* as given by equation (A.1) (Peters *et al.,* 2003). The application of 0.6 rule of thumb is only used when the actual cost component is unknown. The typical exponents for equipment cost as a function of capacity can be obtained from most literatures on plant economics. For example the exponential value of a flat-head, carbon steel tank is 0.57 (Peters *et al.,* 2003).

$$\text{Cost of equipment } a = (\text{cost of equipment } b)\, X^{0.6} \tag{A.1}$$

The capital cost is a function of the flow rate. For example, the total flow rate, FTU entering a treatment unit (steam-stripping column) is given by (Gunaratnam *et al.,* 2005). Equation (A.2) is a capital cost correlation for steam-stripping column (Gunaratnam *et al.,* 2005). Hence, the capital cost of a 20 t/hr wastewater treatment unit is USD 136, 782.

$$CC_{TU} = Cost_{TU} (\$) = 16800F_{TU} (t/hr)^{0.7} \quad (A.2)$$

Cost data are often old with different ages. Such data can be updated by putting a common basis using costs indexes. In this study, the plant cost index (PCI) was obtained from Chemical Engineering (CE) Plant Cost Index, which published in Chemical Engineering Magazine to estimate the purchased cost. The PCI is based on 2007 value, which is 525.4.

ii) Instrumentation and control, C_{IC}

To enable water reuse, pumps and control systems must also be installed. This should include instrumentation cost, installation labor cost and the operating cost for auxiliary equipment such as pumps and motors. For preliminary design, the costs of instrumentation and control may range between 8 to 50% of the total delivered equipment cost depending on the extent of control required (Peters *et al.*, 2003).

APPENDIX B: ECONOMIC EVALUATION FOR SULTAN ISMAIL MOSQUE

B.1: Operating Cost Calculations

The economic data used for operating cost calculation is given in **Table B.1**.

Table B.1: Economic data for SIM operating cost (Wan Alwi, 2007)

Types	**Unit**
Fresh water cost, *CostFW*	USD 0.56/t
UV lamp	USD 0.03/t
Pumping	USD 0.014/t
Annual Operating Time, *AOT*	365 day/yr

B.2: Capital Cost Calculations

Table B.2: Capital cost for individual equipment (Wan Alwi, 2007).

Process	New equipment	No. of unit	Cost formula (USD)	Unit
Ablution	Laminar flow with installation. ($\alpha_{i,re} = 0.5$)	126	25	USD/unit
Toilet flushing	Option 1: Composing toilet with installations	30	1000	USD/unit
	Option 2: Vacuum toilet with installations ($\alpha_{j,re} = 0.97$)	30	800	USD/unit
	Option 3: Dual flush toilet with installations. ($\alpha_{i,re} = 0.5$)	30	300	USD/unit
Reuse	Reuse system and pumps with installations	-	$[(499*(\Sigma F_{i,j}/22.71)^{0.6})+(30*\Sigma F_{i,j}) + 8,000*(\Sigma F_{i,j}/29.1)^{0.6}]*150\%$	USD/system
Regeneration	Treat WW by using microfiltration, activated carbon and UV system with installation and control	-	$[10,000*(\Sigma F_{i,r}/7.27)^{0.6})*150\%]+[499*(\Sigma F_{i,r}/22.71)^{0.6}+(30*\Sigma F_{i,r})+8,000*(\Sigma F_{i,r}/29.1)^{0.6}]*150\%$	USD/system
Rainwater harvesting	Rainwater system and pumps with installation	-	$[499*(Fos^{max}/22.71)^{0.6}+(30*Fos^{max})+8,000*(Fos^{max}/29.1)^{0.6}]*170\%$	USD/system

APPENDIX C: GAMS INPUT AND REPORT FILES FOR SULTAN ISMAIL MOSQUE

C.1 (a): GAMS Input File for MWR

```
SETS
  i   index for water source /1, 2, 3, 4, 5/
  j   index for water demand /1, 2, 3, 4, 5, 6, 7, 8/
  k  index for contaminant /BOD, Turb/    ;

PARAMETERS

  S(i) flow rate of water source (ton per day)
  /1 25.03, 2 0.14, 3 0.14, 4 0.29, 5 0.03/

  D(j) flow rate of water demand (ton per day)
  /1 25.03, 2 0.14, 3 0.14, 4 0.29, 5 0.03, 6 1.46, 7 0.44, 8 1.57/;

Table Cd(j,k) concentration limit of contaminant k in water stream for demand j (ppm)
       BOD    Turb
   1    10        2
   2    10        2
   3    10        2
   4    10        2
   5     0        0
   6    10        2
   7    10        2
   8    10        2   ;

Table Cout(i,k) concentration limit of contaminant k in water source i (ppm)
       BOD     Turb
   1    23        43
   2    23        49
   3    216      375
   4    472      444
   5    536      132;
```

```
PARAMETER Cw(k) fresh water concentration (ppm) ;
  Cw('BOD')=0;
  Cw('Turb')=0;

FREE VARIABLE    Ftot    total fresh water flow rate (ton per day);

VARIABLES
  Fw(j)   flow rate of fresh water supply to demand j(ton per day)
  W(i)  unused portion of water source i (ton per day)
  F(i,j)  flow rate from source i to demand j (ton per day);

POSITIVE VARIABLES Fw(j), W(i), F(i,j);

EQUATIONS
SUPPLY         define objective function
MASSSOURCE(i)  mass balance for each source
MASSDEMAND(j)  mass balance for each demand
MASSLOAD(j,k)    massload every internal demand for contaminant k;

SUPPLY..Ftot =E= sum (j,Fw(j));
MASSSOURCE(i)..W(i)+ sum (j,F(i,j)) =e= S(i);
MASSDEMAND(j)..Fw(j)+ sum (i,F(i,j)) =e= D(j);
MASSLOAD(j,k)..sum (i, F(i,j)*Cout(i,k))+ Fw(j)*Cw(k)=l= D(j)*Cd(j,k);

MODEL MWR /ALL/;
SOLVE MWR USING LP MINIMIZING Ftot  ;
DISPLAY W.L, Fw.L, F.L, Ftot.L ;
```

C.1 (b): GAMS Report File for MWR

```
MODEL STATISTICS

BLOCKS OF EQUATIONS         5    SINGLE EQUATIONS        30
BLOCKS OF VARIABLES         4    SINGLE VARIABLES        54
NON ZERO ELEMENTS         182


GENERATION TIME    =      0.203 SECONDS     4 Mb  WIN230-230 Feb 12, 2009

EXECUTION TIME     =      0.203 SECONDS     4 Mb  WIN230-230 Feb 12, 2009


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

   MODEL   MWRMC             OBJECTIVE  Ftot
   TYPE    LP                DIRECTION  MINIMIZE
   SOLVER  CPLEX             FROM LINE  70

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      1 OPTIMAL
**** OBJECTIVE VALUE             27.7479

 RESOURCE USAGE, LIMIT          0.000      1000.000
 ITERATION COUNT, LIMIT        10          10000


----   VARIABLE W.L  unused portion of water source i (waste)

1    23.678,   2     0.140,   3    0.140,   4    0.290,   5    0.030


----   VARIABLE Fw.L  flow rate of fresh water supply to demand j

1   23.866,   2    0.133,   3   0.133,   4  0.277,   5  0.030,   6  1.392
7    0.420,   8   1.497


----     71 VARIABLE F.L  flow rate from source i to demand j

          1           2             3           4            6           7

1      1.164      0.007      0.007      0.013      0.068      0.020

+          8

1      0.073


----     71 VARIABLE Ftot.L              =       27.748  total fresh water flow
```

C.2 (a): GAMS Input File for MODWN (STAGE 1)

```
SETS
  i    index for water source /1, 2, 3, 4, 5/
  j    index for water demand /1, 2, 3, 4, 5, 6, 7, 8/
  r    index for regeneration unit /1/
  k    index for contaminant /BOD, turb/
  e    index for elimination /1/
  re   index for reduction /1, 2/
  o    index for original /1/
  os  index for outsource /1/;

PARAMETERS

  S(i) flow rate of water source (ton per day)
  /1 25.03, 2 0.14, 3 0.14, 4 0.29, 5 0.03/

  D(j) flow rate of water demand (ton per day)
  /1 25.03, 2 0.14, 3 0.14, 4 0.29, 5 0.03, 6 1.46, 7 0.44, 8 1.57/

  Fosmax(os)   max outsource flow rate (ton per hr)
  /1  11.14/;;

PARAMETER Cw(k) fresh water concentration (ppm) ;
  Cw('BOD')=0;
  Cw('Turb')=0;

Table  Cos(os,k) outsource concentration (ppm)
        BOD     Turb
  1      10       1.5           ;

Table Cro(r,k)  regenerated water concentration (ppm)
       BOD    Turb
  1     4.2       1    ;

Table Cd(j,k) concentration limit of contaminant k in water stream for demand j (ppm)
       BOD    Turb
  1     10       2
  2     10       2
  3     10       2
  4     10       2
  5      0       0
  6     10       2
  7     10       2
  8     10       2   ;

Table Cs(i,k) concentration limit of contaminant k in water source i (ppm)
      BOD     Turb
  1    23       43
  2    23       49
  3   216       375
  4   472       444
  5   536       132  ;

Table Da1(j,e) elimination flow rate (ton per day)
      1
 8    0  ;
```

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

FREE VARIABLE    Ftot     Total fresh water consumption (ton per day)

VARIABLES
  Fw(j)          flow rate of fresh water supply to demand j (ton per day)
  W(i)           unused portion of water source i (ton per day)
  F(i,j)         flow rate from source i to demand j (ton per day)
  Fos(os,j)    outsource flow rate (ton per day)
  Fr(i,r)        regenerated water flow rate from source i (ton per day)
  Fro(r,j)       regenerated water flow rate from regeneration unit r to demand j (ton per day)
  A(i)           variable for source flow rate (ton per day)
  B(j)           variable for demand flow rate  (ton per day);

BINARY VARIABLES
  X1(j,e)     elimination option
  X2(j,re)    reduction option
  X3(j,o)     original  ;


POSITIVE VARIABLES Fw(j), W(i), F(i,j), Fos(os,j), Fr(i,r), Fro(r,j), A(i), B(j);

EQUATIONS
  SUPPLY                          total fresh water supply
  SCHEMES1(j)                    water minimisation scheme
  MASSDEMAND(j)                  mass balance for each demand
  MASSLOAD(j,k)                   massload every internal demand
  MASSSOURCE(i)                  mass balance for each source
  REGEN(r)                       regeneration balance
  OUTSOURCE(os)                  outsource balance
  SELWATERSCHEME1(j)      water minimisation scheme selection for D1
  SELWATERSCHEME2(j)      water minimisation scheme selection for D2
  SELWATERSCHEME3(j)      water minimisation scheme selection for D3
  SELWATERSCHEME4(j)      water minimisation scheme selection for D4
  SELWATERSCHEME5(j)      water minimisation scheme selection for D5
  SELWATERSCHEME6(j)      water minimisation scheme selection for D6
  SELWATERSCHEME7(j)      water minimisation scheme selection for D7
  SELWATERSCHEME8(j)      water minimisation scheme selection for D8
  DEMAND(j)                      demand relationship
  SELDS1                         source demand relationship for mtb 1
  SELDS2                         source demand relationship for mtb 2
  SELDS3                         source demand relationship for mtb 3
  SELDS4                         source demand relationship for mtb 4
  SELDS5                         source demand relationship for mtb 5    ;


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

  SCHEMES1(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)) =l= B(j);

  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)..
 sum (i, F(i,j)*CS(i,k))+ Fw(j)*Cw(k)+ sum (os, Fos(os,j)*Cos(os,k))+ sum (r, Fro(r,j)*Cro(r,k)) =l=
B(j)*Cd(j,k);

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

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

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

 SELWATERSCHEME1('1')..
 X2('1','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')..
 X3('6','1') =e= 1 ;

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

 SELWATERSCHEME8('8')..
 X1('8','1')+ sum (re, X2('8',re))+ X3('8','1') =e= 1 ;

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

 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');


MODEL MWN /ALL/;
SOLVE MWN USING MIP MINIMIZING Ftot;
DISPLAY W.L, Fw.L, F.L, Fos.L, Fr.L, Fro.L, A.L, B.L,Ftot.L, X1.L,X2.L,X3.L;
```

C.2 (b): GAMS Report File for MODWN (STAGE 1)

```
MODEL STATISTICS

BLOCKS OF EQUATIONS        22        SINGLE EQUATIONS        61
BLOCKS OF VARIABLES        12        SINGLE VARIABLES       100
NON ZERO ELEMENTS          332       DISCRETE VARIABLES       12


GENERATION TIME     =      0.266 SECONDS     4 Mb  WIN230-230 Feb 12, 2009

EXECUTION TIME      =      0.266 SECONDS     4 Mb  WIN230-230 Feb 12,


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

   MODEL   MWN              OBJECTIVE  Ftot
   TYPE    MIP              DIRECTION  MINIMIZE
   SOLVER  CPLEX            FROM LINE  333

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      1 OPTIMAL
**** OBJECTIVE VALUE               0.0300

 RESOURCE USAGE, LIMIT         0.109      1000.000
 ITERATION COUNT, LIMIT         25        100000


----   VARIABLE W.L  unused portion of water source i (waste)

2    0.140


----   VARIABLE Fw.L  flow rate of freshwater supply to demand j

5    0.030


----   VARIABLE F.L  flow rate from source i to demand j

          1           4           6           7

1      0.274       0.007       0.035       0.010


----   VARIABLE Fos.L  outsource flow rate

          1

1      2.010
```

```
----   VARIABLE Fr.L  regenerated water flow rate from source i

          1

1      12.182
3       0.140
4       0.290
5       0.030


----   VARIABLE Fro.L  regenerated water flow rate from regeneration unit r to demand j

            1            2            3            4            6            7

1      10.231       0.137       0.137       0.283       1.425       0.430


----   VARIABLE A.L  variable for source flow rate

1    12.515,    2  0.140,    3  0.140,    4  0.290,    5  0.030


----   VARIABLE B.L  variable for demand flow rate

1    12.515,    2  0.140,    3  0.140,    4  0.290,    5  0.030,    6  1.460
7    0.440


----    334 VARIABLE Ftot.L               =       0.030


----    334 VARIABLE X1.L  elimination option

          1

8       1.000


----    334 VARIABLE X2.L  reduction option

          1

1       1.000


----    334 VARIABLE X3.L  original

          1

2       1.000
3       1.000
4       1.000
5       1.000
6       1.000
7       1.000
```

C.3 (a): GAMS Input File for MODWN (STAGE 2)

```
SETS
  i   index for water source /1, 2, 3, 4, 5/
  j   index for water demand /1, 2, 3, 4, 5, 6, 7, 8/
  r   index for regeneration unit /1/
  k   index for contaminant /BOD, turb/
  e   index for elimination /1/
  re  index for reduction /1, 2/
  o   index for original /1/
  os  index for outsource /1/;

PARAMETERS
  S(i) flow rate of water source (ton per day)
  /1   25.03, 2   0.14, 3   0.14, 4   0.29, 5   0.03/

  D(j) flow rate of water demand (ton per day)
  /1   25.03, 2   0.14, 3   0.14, 4   0.29, 5   0.03, 6   1.46, 7   0.44, 8   1.57/

  Fwo(j) existing system fresh water consumption (ton per day)
  /1   25.03, 2   0.14, 3   0.14, 4   0.29, 5   0.03, 6   1.46, 7   0.44,   8 1.57/

  Wo(i) existing system wastewater generation (ton per day)
  /1    25.03, 2   0.14, 3   0.14, 4   0.29, 5   0.03/

  epsil(j)
  /1   126, 8   30/

  Fosmax(os)   max outsource flow rate (ton per day)
  /1    11.14/;

PARAMETER Cw(k) fresh water concentration (ppm);
  Cw('BOD')=0;
  Cw('Turb')=0;

Table  Cos(os,k)  outsource concentration (ppm)
       BOD     Turb
   1    10       1.5            ;

Table Cro(r,k)  regenerated water concentration (ppm)
       BOD     Turb
   1    4.2       1    ;

Table Cd(j,k) concentration limit of contaminant k in water stream for demand j (ppm)
       BOD     Turb
   1    10        2
   2    10        2
   3    10        2
   4    10        2
   5     0        0
   6    10        2
   7    10        2
   8    10        2   ;
```

```
Table Cs(i,k) concentration limit of contaminant k in water source i (ppm)
       BOD     Turb
  1    23       43
  2    23       49
  3    216     375
  4    472     444
  5    536     132  ;

Table Da1(j,e) elimination flow rate (ton per day)
     1
 8   0   ;

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

Table Fo(i,j) existing flow rate for reuse or recycle water (ton per day)
      1    2     3    4    5    6   7   8
1   0     0     0    0    0    0   0   0
2   0     0     0    0    0    0   0   0
3   0     0     0    0    0    0   0   0
4   0     0     0    0    0    0   0   0
5   0     0     0    0    0    0   0   0  ;

Table Foso(os,j) existing flow rate for outsource(ton per day)
     1    2    3    4    5    6   7   8
1   0    0    0    0    0    0   0   0 ;

Table Frold(i,r) existing flow rate for inlet regeneration (ton per day)
    1
1   0
2   0
3   0
4   0
5   0    ;

Table Froold(r,j) existing regenerated flow rate regeneration (ton per day)
     1    2    3    4    5    6   7   8
1   0    0    0    0    0    0   0   0  ;

Table CostUE(j,e) cost unit for elimination (ton per day)
     1
8   1000    ;

Table CostURE(j,re) cost unit for reduction (ton per day)
       1      2
1      25     0
8    300    800;


SCALAR AOT            annual operating time (day per year) /365/;
SCALAR FWCost        price of fresh water for domestic (USD per ton)/ 0.56/;
SCALAR ElectCost    average electricity tariff (USD per kW.h) /0.014/;
SCALAR CostPump   cost of pump (USD) /499/;
SCALAR RegUCost   regeneration unit cost for equipment a (USD) /10000/;
SCALAR CostPipe    cost of piping (USD)  /8000/;
SCALAR P1              cost component percentage /1.5/;
SCALAR P2              cost component percentage /1.7/;
SCALAR Beta           cost exponential / 0.6/;
```

```
FREE VARIABLE
NAS        Net annual savings (USD per year)
Ftot       Total fresh water consumption (ton per day)
NCI        Net capital investment (USD)
PP         Payback period (year)
CRegU      Total regeneration unit cost (USD)
COsU       Total outsourcing unit cost (USD)
CReuse     Reuse cost (USD);

VARIABLES
  Fw(j)      flow rate of fresh water supply to demand j (ton per day)
  W(i)       unused portion of water source i (ton per day)
  F(i,j)     flow rate from source i to demand j (ton per day)
  Fos(os,j)  outsource flow rate (ton per day)
  Fr(i,r)    regenerated water flow rate from source i (ton per day)
  Fro(r,j)   regenerated water flow rate from regeneration unit r to demand j (ton per day)
  A(i)       variable for source flow rate (ton per day)
  B(j)       variable for demand flow rate (ton per day) ;

BINARY VARIABLES
  X1(j,e)    selection of elimination option
  X2(j,re)   selection of reduction option
  X3(j,o)    selection of original flow rate ;

POSITIVE VARIABLES Fw(j), W(i), F(i,j), Fos(os,j), Fr(i,r), Fro(r,j), A(i), B(j) ;

EQUATIONS
  OF                       objective function
  PPERIOD                  payback period
  NETCAPINV                net capital investment
  costreg                  total regeneration unit cost
  costos                   total outsource unit cost
  costreuse                total reuse cost
  SUPPLY                   total fresh water supply
  SCHEMES1(j)              water minimisation scheme
  MASSDEMAND(j)            mass balance for each demand
  MASSLOAD(j,k)            massload every internal demand
  MASSSOURCE(i)            mass balance for each source
  REGEN(r)                 regeneration balance
  OUTSOURCE(os)            outsource balance
  SELWATERSCHEME1(j)       water minimisation scheme selection for D1
  SELWATERSCHEME2(j)       water minimisation scheme selection for D2
  SELWATERSCHEME3(j)       water minimisation scheme selection for D3
  SELWATERSCHEME4(j)       water minimisation scheme selection for D4
  SELWATERSCHEME5(j)       water minimisation scheme selection for D5
  SELWATERSCHEME6(j)       water minimisation scheme selection for D6
  SELWATERSCHEME7(j)       water minimisation scheme selection for D7
  SELWATERSCHEME8(j)       water minimisation scheme selection for D8
  DEMAND(j)                demand relationship
  SELDS1                   source demand relationship for mtb 1
  SELDS2                   source demand relationship for mtb 2
  SELDS3                   source demand relationship for mtb 3
  SELDS4                   source demand relationship for mtb 4
  SELDS5                   source demand relationship for mtb 5   ;

  OF..  NAS =e= (FWCost*AOT*sum(j, Fwo(j)-Fw(j))+
                 0.03*sum((i,r), Frold(i,r)-Fr(i,r))*AOT+0.03*sum((i,j),F(i,j)-F(i,j))*AOT+
                 0.03*sum((os,j), Foso(os,j)-Fos(os,j))*AOT+
                 ElectCost*AOT*sum((i,j),Fo(i,j)-F(i,j))+
                 ElectCost*AOT*sum((os,j), Foso(os,j)-Fos(os,j))+
```

```
                      ElectCost*AOT*sum((i,r), Frold(i,r)-Fr(i,r))+
                     ElectCost*AOT*sum((r,j), Froold(r,j)-Fro(r,j))) ;

 PPERIOD.. NCI / NAS =l= 5 ;

 NETCAPINV..
 NCI =e= (CRegU+ COsU+ CReuse+
      sum((j,e),X1(j,e)*CostUE(j,e)*epsil(j))+sum((j,re),X2(j,re)*CostURE(j,re)*epsil(j)));

 costreg..
 CRegU =e= ((sum((i,r), Fr(i,r))/7.27)**Beta*RegUCost)*P1+ sum((i,r), Fr(i,r))*30*P1+
        (sum((i,r), Fr(i,r))/22.71)**Beta*CostPump*P1+ (sum((i,r), Fr(i,r))/29.1)**Beta*CostPipe*P1
;

 costos..
 COsU =e= sum (os, ((Fosmax(os)/22.71)**Beta*CostPump)*P2)+sum(os,
((Fosmax(os)/29.1)**Beta*CostPipe*P2))+ sum(os, (Fosmax(os)*30*P2));

 costreuse..
 CReuse =e= ((sum((i,j), F(i,j))/22.71)**Beta*CostPump)*P1+(sum((i,j),
F(i,j))/29.1)**Beta*CostPipe*P1+ sum((i,j), F(i,j))*30*P1;


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

 SCHEMES1(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);

 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)..
 sum (i, F(i,j)*CS(i,k))+ Fw(j)*Cw(k)+ sum (os, Fos(os,j)*Cos(os,k))+ sum (r, Fro(r,j)*Cro(r,k)) =l=
B(j)*Cd(j,k);

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

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

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


 SELWATERSCHEME1('1')..
 X2('1','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')..
 X3('6','1') =e= 1 ;

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

 SELWATERSCHEME8('8')..
 X1('8','1')+ sum (re, X2('8',re))+ X3('8','1') =e= 1 ;

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

 SELDS1..
 B('1') =e= A('1') ;

* for mtb in the water system

 SELDS2..
 B('2') =e= A('2');

 SELDS3..
 B('3') =e= A('3');

 SELDS4..
 B('4') =e= A('4');

 SELDS5..
 B('5') =e= A('5');

 NAS.l = 1  ;
 F.l(i,j) = 0.001;
 Fos.l('1','2') = 0.14 ;
 Fos.l('1','3') = 0.14 ;
 Fos.l('1','4') = 0.29 ;
 Fos.l('1','2') = 1.3 ;
 Fr.l('1',r) = 12.515   ;
 Fr.l('2',r) = 0.14   ;
 Fr.l('3',r) = 0.14   ;
 Fr.l('4',r) = 0.29   ;
 Fr.l('5',r) = 0.03  ;
 Fro.l(r,'1') = 12.515;
 Fro.l(r,'6') = 0.16 ;
 Fro.l(r,'7') = 0.44 ;
 W.l(i) = 0;
 F.lo(i,j) = 0;
 F.up(i,j) = 25.63  ;

 Fos.lo(os,j) = 0  ;
 Fos.up(os,j) = Fosmax(os) ;

 Fw.lo(j) = 0;
 Fw.up(j) = D(j);

 W.lo(i) = 0;
 W.up(i) = 25.63;

 Fr.lo(i,r) = 0;
 Fr.up(i,r) = 25.63;
```

```
  Fro.lo(r,j) = 0;
  Fro.up(r,j) = 25.63;

MODEL MODWN /ALL/;

option LIMROW = 0;
option LIMCOL = 0;
Options iterlim  = 100000 ;
Option optcr=0.1;

SOLVE MODWN USING MINLP MAXIMIZING NAS;
DISPLAY W.L, Fw.L, F.L, Fos.L, Fr.L, Fro.L, A.L, B.L, NAS.L, PPERIOD.L, Ftot.L, NCI.L, X1.L,
X2.L, X3.L;
```

C.3 (b): GAMS Report File for MODWN (STAGE 2)

```
MODEL STATISTICS

BLOCKS OF EQUATIONS        28     SINGLE EQUATIONS        67
BLOCKS OF VARIABLES        17     SINGLE VARIABLES       105
NON ZERO ELEMENTS         460     NON LINEAR N-Z          47
DERIVATIVE POOL            86     CONSTANT POOL           25
CODE LENGTH             1,035     DISCRETE VARIABLES     12


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

   MODEL   MWN               OBJECTIVE  NAS
   TYPE    MINLP             DIRECTION  MAXIMIZE
   SOLVER  BARON             FROM LINE  329

**** SOLVER STATUS     1 NORMAL COMPLETION
**** MODEL STATUS      8 INTEGER SOLUTION
**** OBJECTIVE VALUE            5366.0392

 RESOURCE USAGE, LIMIT          0.270      1000.000
 ITERATION COUNT, LIMIT           0        100000
 EVALUATION ERRORS                0            0


----  VARIABLE W.L  unused portion of water source i (waste)

1   8.441,   2    0.140,   3   0.140,   4     0.290,   5   0.030


----  VARIABLE Fw.L  flow rate of freshwater supply to demand j

1   1.341,   5   0.030


----  VARIABLE F.L  flow rate from source i to demand j

          1          4          6          7

1      0.199      0.005      0.035      0.010

+         8

1      0.037


----  VARIABLE Fos.L  outsource flow rate

          1          4

1     10.975      0.165
```

```
----  VARIABLE Fr.L  regenerated water flow rate from source i

         1

1      3.781

----   VARIABLE Fro.L  regenerated water flow rate from regeneration unit r to demand j

          2           3            4            6            7            8

1      0.137      0.137      0.120      1.425      0.430      1.533


----   VARIABLE A.L  variable for source flow rate

1    12.515,    2    0.140,    3    0.140,    4    0.290,    5    0.030


----   VARIABLE B.L  variable for demand flow rate

1 12.515,    2  0.140,    3  0.140,    4  0.290,    5  0.030,    6  1.460
7  0.440,    8  1.570


----      VARIABLE NAS.L                  =       5366.039  net annual savings
           EQUATION PPERIOD.L           =        5.000  payback period
           VARIABLE Ftot.L                 =        1.371
           VARIABLE NCI.L                   =       26830.196


----   VARIABLE X1.L  elimination option

                   ( ALL       0.000 )


----   VARIABLE X2.L  reduction option

         1

1      1.000


----   VARIABLE X3.L  original

         1

2      1.000
3      1.000
4      1.000
5      1.000
6      1.000
7      1.000
8      1.000
```