Optimization of Water Network Design for a Petroleum Refinery

by

Ilmiah Binti Moksin

Dissertation submitted in partial fulfillment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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Approved by,

C. S. KHOR

(Khor Cheng Seong)

UNIVERSITI TEKNOLOGI PETRONAS

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JULY 2010

CERTIFICATION OF ORIGINALITY

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

Ilmiah.

ILMIAH BINTI MOKSIN

ABSTRACT

This work discusses about the basic understanding and research done on the final year project entitled Optimization of Water Network Design for a Petroleum Refinery. A few sets of parameter were identified by a set of water-producing streams process sources with known flowrate and contaminant concentration, a set of water-using operations of process sinks with known inlet flowrate and maximum allowable contaminant concentration, a set of water-treatment technologies interception units and a set of freshwater sources. The objectives are to determine minimum freshwater used and wastewater discharged, optimum allocation of sources to sinks and optimum selection of interception devices or regeneration technologies with a fast computational time. Formulation of mixed-integer nonlinear programming (MINLP) optimization model involved a source-interceptor-sink superstructure representation with the application of water reuse, regeneration and recycle (W3R). Bilinear variables and big-M logical constraints are considered as a major problem in the optimization model which necessitates a solution strategy of using piecewise linear relaxation and tight specification of lower and upper bounds to ensure a global optimal solution is achieved within a reasonable time. A preliminary optimal solution will be obtained by implementing the model into GAMS modeling language.

ACKNOWLEDGEMENT

This project would not be successful if there were no guidance, assistance and support from certain individuals and organizations whose have the substantial contribution to the completion of this project.

Firstly, I would like to personally express my utmost appreciation and gratitude to the project supervisor, Mr. Khor Cheng Seong for his valuable ideas and guidance throughout the progress of the project until its completion. His advice, support and assistance have helped me greatly which enable this project to meet its specified objectives and completed within the particular time frame.

A special gratitude is extended to the Chemical Engineering Department of Universiti Teknologi PETRONAS (UTP) for providing this opportunity of undertaking the remarkable Final Year Project. All the knowledge obtained from the lecturers since five years of study have been placed into this project implementation.

Last but not least, I would like to thank Miss Norafidah binti Ismail, Miss Foo Ngai Yoong and all parties that were involved directly or indirectly in making this project a success. All the concerns and compassion while completing the project are deeply appreciated.

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ABBREVIATIONS

General

FYP II	Final Year Project II
GAMS	General Algebraic Modeling System
HFRO	Hollow Fiber Reverse Osmosis
MINLP	Mixed-integer nonlinear programming
PLR	Piecewise Linear Relaxation
PP(M)SB	PETRONAS Penapisan (Melaka) Sdn. Bhd.
RO	Reverse osmosis
RON	Reverse osmosis network
W3R	Water reuse, regeneration and recycle

Sets and Indices

co	contaminant
int	interceptor
perm	permeate stream
rej	reject stream
si	sink
so	source

Parameters

AOT	annual operating time
μ	viscosity of water
A	water permeability coefficient
C_{max} (si,co)	maximum allowable contaminant concentration *co* in sink *si*
C_{so} (so,co)	contaminant concentration *co* in source stream *so*
$C_{chemicals}$	cost of pretreatment chemicals
$C_{discharge}$	unit cost for discharge (effluent treatment)
$C_{electricity}$	cost of electricity
C_{module}	cost per module of HFRO membrane
C_{pump}	cost coefficient for pump
$C_{turbine}$	cost coefficient for turbine
C_{water}	unit cost for freshwater
D	Manhattan distance
$D_{2M}/K\delta$	solute (contaminant) flux constant
K_C	solute (contaminant) permeability coefficient
L	HFRO fiber length
L_s	HFRO seal length
m	fractional interest rate per year
M_a (so,si)	big-M parameter for interconnection between source stream *so* to sink unit operation *si*
$M_{b,perm}$ (int,si)	big-M parameter for interconnection between interceptor *int* permeate *perm* to sink unit operation *si*
$M_{b,rej}$ (int,si)	big-M parameter for interconnection between interceptor *int* reject *rej* to sink unit operation *si*
M_d (so,int)	big-M parameter for interconnection between source stream *so* to interceptor *int*
n	number of years
p	parameter for piping cost based on CE plant index
q	parameter for piping cost based on CE plant index
P_p	permeate pressure from interceptor
ΔP_{shell}	shell side pressure drop per HFRO membrane module
Q_1 (so)	flowrate of source stream *so*

Q_2 (si)	flowrate of sink unit operation *si*
r_i	inside radius of HFRO fiber
r_o	outside radius of HFRO fiber
RR	removal ratio (fraction of the interceptor inlet mass load that exits in the reject stream)
α	liquid phase recovery (fixed fraction of the interceptor inlet flowrate that exits in the permeate stream)
S_m	HFRO membrane area per module
η_{pump}	pump efficiency
$\eta_{turbine}$	turbine efficiency
OS	osmotic pressure coefficient at HFRO
π_F	osmotic pressure at HFRO feed side

Continuous Variables

C_F (int,co)	contaminant concentration in feed *F* of interceptor
C_{perm} (int,co)	contaminant concentration in interceptor permeate
C_{rej} (int,co)	contaminant concentration in interceptor reject
Q_a (so,si)	flowrate of source stream to sink unit operation
$Q_{b,perm}$ (int,si)	flowrate of interceptor permeate to sink unit operation
$Q_{b,rej}$ (int,si)	flowrate of interceptor reject to sink unit operation
Q_d (so,int)	flowrate of source stream to interceptor
Q_F (int)	total feed flowrate into interceptor
C_S	average contaminant concentration in shell side of HFRO
N_{solute}	solute flux through the HFRO membrane
N_{water}	water flux through the HFRO membrane
P_F	feed pressure into interceptor
P_R	reject pressure from interceptor
q_P	permeate flowrate per HFRO module
TAC	total annualized cost for interceptor (RON)
π_{RO}	osmotic pressure at HFRO reject side

Binary Variables

Y_a (so,si)	piping interconnection between source stream to sink unit operation
$Y_{b,perm}$ (int,si)	piping interconnection between interceptor permeate to sink unit operation
$Y_{b,rej}$ (int,si)	piping interconnection between interceptor reject to sink unit operation
Y_d (so,int)	piping interconnection between source stream to interceptor

CHAPTER 1
INTRODUCTION

1.1 BACKGROUND OF STUDY

Water is an essential component in refineries due to its characteristic of being a good heat and mass transfer agent without causing hazards to the processes. However, currently its cost is increasing while the quality is becoming worse which lead to an increase in the costs associated to water and wastewater treatment. The shortages in freshwater affected the industry to find an optimal alternatives in order to minimize the use of water supply and also to follow the stringent rules of environmental regulations on wastewater discharged. Besides, an implementation of sustainable development plays an important role in an engineering project.

The application of water reuse, regeneration and recycle (W3R) technique in minimization of water and wastewater becomes crucial in recent years in order to solve the problem of water supply in line with environmental awareness. The main reasons of such situation to be occurred are due to limited resources of freshwater, high cost of freshwater supply and also more strict regulations on discharge of wastewater. Besides that, the increase in wastewater treatment cost, environmental awareness and plant efficiency requirements also contributes to the importance of this approach. The concept of water reuse, regeneration and recycle (W3R) technique is explained further in the following.

1.2 PROBLEM STATEMENT

A requirement to determine the possible options for optimization of water network structure which allows the minimization of freshwater used with the presence of the following constraints:

- a set of water-producing streams process sources with known flowrate and contaminant concentration

- a set of water-using operations of process sinks with known inlet flowrate and maximum allowable contaminant concentration
- a set of water-treatment technologies interception units (RO)
- a set of freshwater sources with known contaminant concentration

An optimal design of water network system needs to be determined with the following criteria:

- minimum freshwater used and wastewater discharged
- optimum allocation of sources to sinks
- optimum duties of source interception

1.3 OBJECTIVES

The objectives of the study are listed below:

i. To develop a source-interceptor-sink superstructure representation for water network design consisting the concept of water reuse, regeneration and recycle (W3R).

ii. To formulate the optimization model derived from the superstructure representation which consists:
   - nonlinear mass balances with bilinear terms that result from multiplication of variable stream flowrates and compositions;
   - constraints of the design and structural specifications which is the relationship of interconnectivity between the units and streams inflicting the choice of W3R alternatives;
   - specifications of water content such as total suspended solids (TSS) and other related parameters based on Malaysian Environmental Quality Act 1974.

iii. To solve the mixed-integer nonlinear program (MINLP) optimization model by using GAMS modeling language with the application of Piecewise Linear Relaxation solution strategy to give fast computational time.

1.4 SCOPES OF STUDY AND OVERVIEW OF MAIN CHAPTERS

This study concerns on the development of source-interceptor-sink superstructure for that includes feasible alternative structures for potential water reuse, regeneration, and recycle (W3R) for water using and wastewater treatment units of a petroleum refinery. It also deals with the formulation of a mathematical model with optimization procedure based on the developed superstructure. Besides, the techniques of determining the best solution for optimization model by application of Piecewise Linear Relaxation as the solution strategy in handling bilinear variables also will be considered in the study.

The notion of water network design and the concept of water reuse, regeneration and recycle (W3R) will be explained in Chapter 2. Besides, an overview of superstructure representation of water network design proposed by several authors and the concept of partitioning regenerator units which is applied in RO are introduced. The idea of PLR as the solution strategy in approximation of bilinear terms is also discussed in Chapter 2.

The proposed methodology is given in Chapter 3. This section also covers the gantt chart and tool used in this study.

Chapter 4 explains the superstructure representation and the formulation of the model optimization for sources, interceptors and sinks as well as PLR formulation. Formulation of the model for sources, interceptors and sinks adopted in this work is largely based on the work of Ismail (2010) and Tjun (2009). Additionally, two revised formulations are proposed, mainly on the interceptors, for the following purposes: (1) to reduce the number of bilinear terms in the model; and (2) to incorporate the constraint on feed pressure to a membrane-based interceptor.

On the other hand, Chapter 5 presents the computational results for four case studies which involve seven sources, an interceptor and seven sinks. The difference between these case studies is the application of PLR in the problem as the solution strategy to handle bilinearities in the model formulation. This chapter also discussed and proved that PLR can be applied in a large-scale problem.

Last but not least, the conclusion and recommendation for this project is highlighted in Chapter 6 where a few ideas are proposed in order to improve this work in future.

CHAPTER 2

LITERATURE REVIEW

2.1 CONCEPT OF WATER REUSE, REGENERATION AND RECYCLE

2.1.1 Water Reuse

Water reuse involves the flow of used water from the outlet of a process unit to the other process unit. Figure 2.1 illustrates the used water from Operation 2 flows to Operation 1 where the contaminant level at the outlet of Operation 2 must be acceptable at the inlet of Operation 1. The amount of both freshwater and wastewater can be reduced by this technique because the same water is used twice (Smith, 2005).

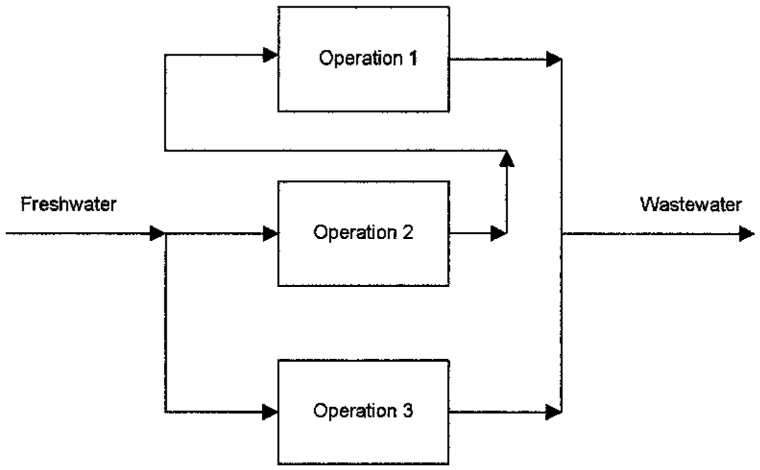

Figure 2.1 Flow Representation of Water Reuse

2.1.2 Water Regeneration-Reuse

The used water from a process unit flows to a treatment process for regeneration of water quality so that it is acceptable in other process unit. This arrangement reduces the amount of both freshwater and wastewater and removes part of effluent load. It also eliminates the contaminant load which should be removed in the final treatment before discharge (Smith, 2005). The regeneration-reuse arrangement is shown in Figure 2.2.

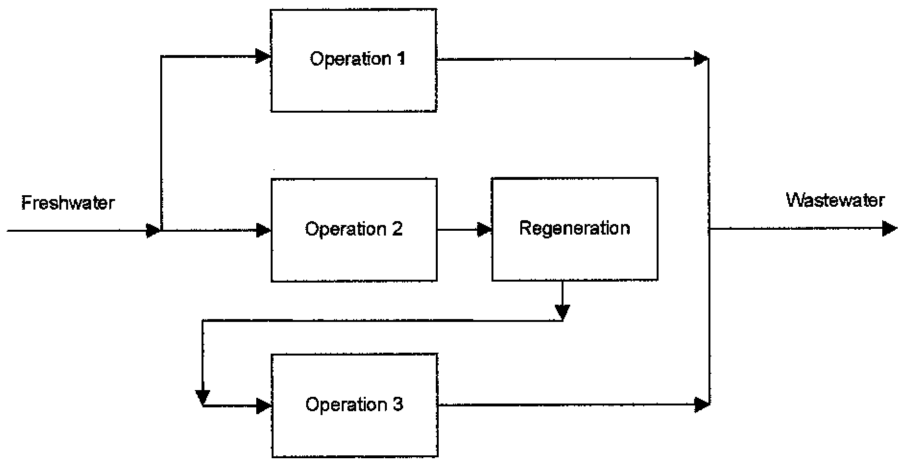

Figure 2.2 Flow Representation of Water Regeneration-Reuse

2.1.3 Water Regeneration-Recycling

This arrangement shows by Figure 2.3 where a regeneration process takes place at the outlet of all operations and then is recycled back to the same process. It reduces the amount of freshwater and wastewater. It decreases the effluent load which can be achieved by regeneration process taking up part of required effluent treatment load. The difference between regeneration-recycling and regeneration-reuse is that the water flows to the same operation many times in latter technique whereas the water only used once in the former technique (Smith, 2005).

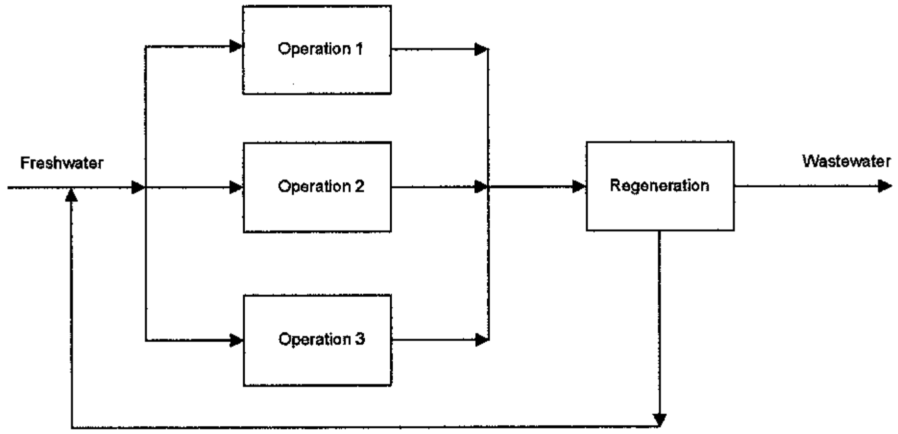

Figure 2.3 Flow Representation of Water Regeneration-Recycling

2.2 SUPERSTRUCTURE REPRESENTATION

Gabriel and El-Halwagi (2005) proposed a superstructure representation as source-interceptor-sink framework for reuse and recycling process. The authors claimed that interception may be used to remove selected pollutants from the process streams by using separation devices or interceptors. Optimization model was formulated based on the developed superstructure with the presence of MINLP model formulation which consists of minimum cost of freshwater supply and interceptor that meet the process requirement. Figure 2.4 shows several stream interconnections between source to interceptor and interceptor to sink.

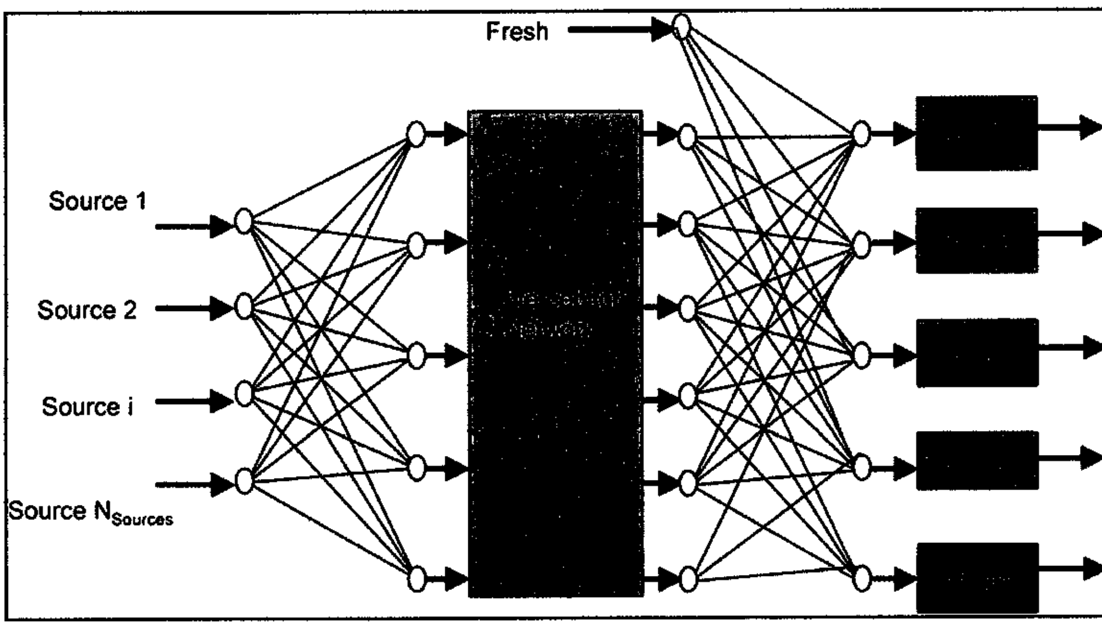

Figure 2.4 Source-Interceptor-Sink Superstructure Representation of a Problem (Gabriel and El-Halwagi, 2005)

A petroleum refinery can be considered as generalized pooling problem due to its significant mathematical programming problem. Superstructure proposed by Meyer and Floudas (2006) shows the existing source streams, treatment units that is interceptor and process units. Interconnections between source to interceptor (treatment unit), source to sink, interceptor to sink and interceptor to other interceptor are shown in Figure 2.5.

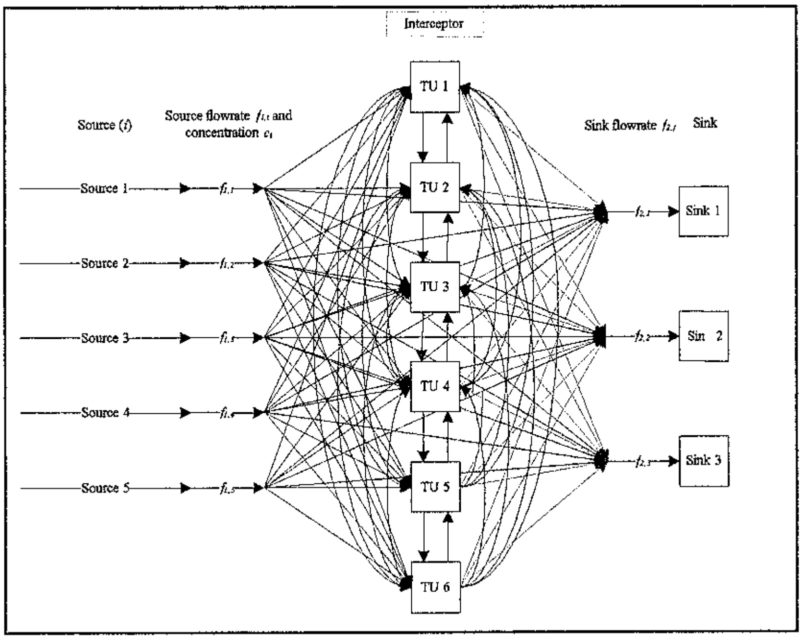

Figure 2.5 Superstructure Representation for Generalized Pooling Problem (Meyer and Floudas, 2006)

2.3 PARTITIONING REGENERATOR UNIT

Tan et al. (2009) discussed about integration of partitioning regenerator units in a source-sink superstructure representation model. Partitioning regenerator unit can be defined as splitting a contaminated water stream into a regenerated permeate stream and a low-quality reject stream. This can be described in membrane separation-based processes such as reverse osmosis (RO) and ultrafiltration. According to Tan et al. (2009), both permeate and rich streams are potentially to be reused or recycle within plant.

Several criteria are considered in formulation of the optimization model problem. Some parts of the sources that have fixed flowrate and contaminant concentration can be reused or recycled, flowed to regenerator (interceptor) or discharged to the environment. On the other hand, there is a demand for specific flowrate of water at below identified concentration maximum value for sinks. The mixed water produced by different sources will be fed into a single partitioning regenerator unit where both permeate and reject streams that discharged by the regenerator are potentially to be reused or recycled within plant itself. An assumption is made on regenerator unit that is fixed ratio of flowrates for permeate and rich streams and fixed contaminant removal ratio.

2.4 PIECEWISE LINEAR RELAXATION

Relaxation involves outer-approximating the feasible region of a given problem and underestimating (overestimating) the objective function of a minimization (maximization) problem (Wicaksono and Karimi, 2008). It is achieved by applying boundary on the complicating variables, that is for this case is bilinear variables, in the original problem by means of under-, over- and/or outer-estimating the specific variables. Based on the review done on several authors, it is shown that Piecewise Linear Relaxation (PLR) is potentially can be a solution strategy in handling bilinear variables in the optimization modelling problem.

Bilinear variable is a multiplication of two linear variables. Generally, it exhibits multiple local optimal solutions and high degree of difficulty to locate its global solution, especially for larger industrial scale problems. Due to its non-convexity, there is no guarantee of global optimal solution that obtained from the potential local solutions. As for water network design problems, bilinear variables are given by multiplication of an unknown contaminant concentration term and an unknown flowrate term in concentration balances which mostly occurs in concentration balances.

Relaxation does not replace the whole original problem but offers guaranteed bounds on the solutions of the problem. Bilinear enveloped proposed by McCormick (1976) involves the substitution of additional variable, z into bilinear term, xy in the original problem. The notion of relaxation includes the ab initio partitioning of search domain and combining the continuous convex-to-convex relaxations based on convex envelope of particular partitions into overall combined relaxation. The tightness of overall discrete relaxation is improved due to convex relaxation of nonconvex functions over smaller partitions of the feasible region.

Three ways in partitioning the search domain are big-M formulation, convex combination formulation and incremental cost formulation. Computational comparison of PLR had been conducted by Gounaris et al. (2009). It shows that Big-M formulation always failed in obtaining the solutions for particular problem. On the other hand, convex combination formulation provides major improvement but with occurrence of failures in high-N regime only. In this work, incremental cost formulation is chosen as the solution strategy due to the incremental nature of problem. The comparison on solution strategy in handling bilinear variables is given in Table 2.1.

Table 2.1 Comparison on Solution Strategy in Handling Bilinear Variables

Author	Type of Model	Solution Strategy to Handle Bilinear Variables	Findings from Applying the Solution Strategy
Hasan and Karimi (in press)	NA	• Piecewise Linear Relaxation (PLR) • Univariate and bivariate partitioning	• Extensive numerical comparison between univariate and bivariate partitioning
Gounaris et al. (in press)	Pooling problem	• Piecewise Linear Relaxation (PLR) • Ab initio uniform (identical) univariate partitioning using convex envelopes	• Suitable for large-scale problems • Fast computational time
Pham et al. (2009)	Pooling problem	• Piecewise Linear Relaxation • Discretization of quality variables	• Suitable for large-scale problems • Fast computational time • Near-global optimal solution
Wicaksono and Karimi (2008)	MILP on global mathematical optimization problem	• Piecewise Linear Relaxation (PLR) • Univariate and bivariate partitioning	• Improved relaxation quality with bivariate partitioning • Solution time to obtain Piecewise Linear Relaxation varies with MILP relaxation scheme
Saif et al. (2008)	MINLP on reverse osmosis network (RON)	• Convex relaxation on branch-and-bound algorithm • Piecewise underestimators and overestimators	• Give very tight lower bound • Large solution time
Meyer and Floudas (2006)	MINLP on generalized pooling problem for wastewater treatment network	• Augmented Reformulation–linearization technique (RLT) • Smooth piecewise quadratic perturbation function • Piecewise discretization of quality variables	• Give very tight lower bound • large solution time
Karuppiah and Grossmann (2006)	Nonconvex GDP Integrated water network systems	• Piecewise Linear Relaxation (PLR) in branch-and-bound algorithm • Branch-and-contract	• Discretization of flow variables • Low solution time
Androulakis et al. (1995)	NLP on general constrained nonconvex problem	• Convex quadratic NLP relaxation named αββ underestimator	• Poor tightness of relaxation • Improved by Meyer and Floudas (2006) with smooth piecewise quadratic perturbation function
Sherali and Alameddine (1992)	NA	• Reformulation–linearization technique (RLT)	• Longer computational time
McCormick (1976)	Rectangle	• Convex and concave underestimators	• Characterized as convex envelopes for bilinear terms by Al-Khayyal and Falk

CHAPTER 3
METHODOLOGY

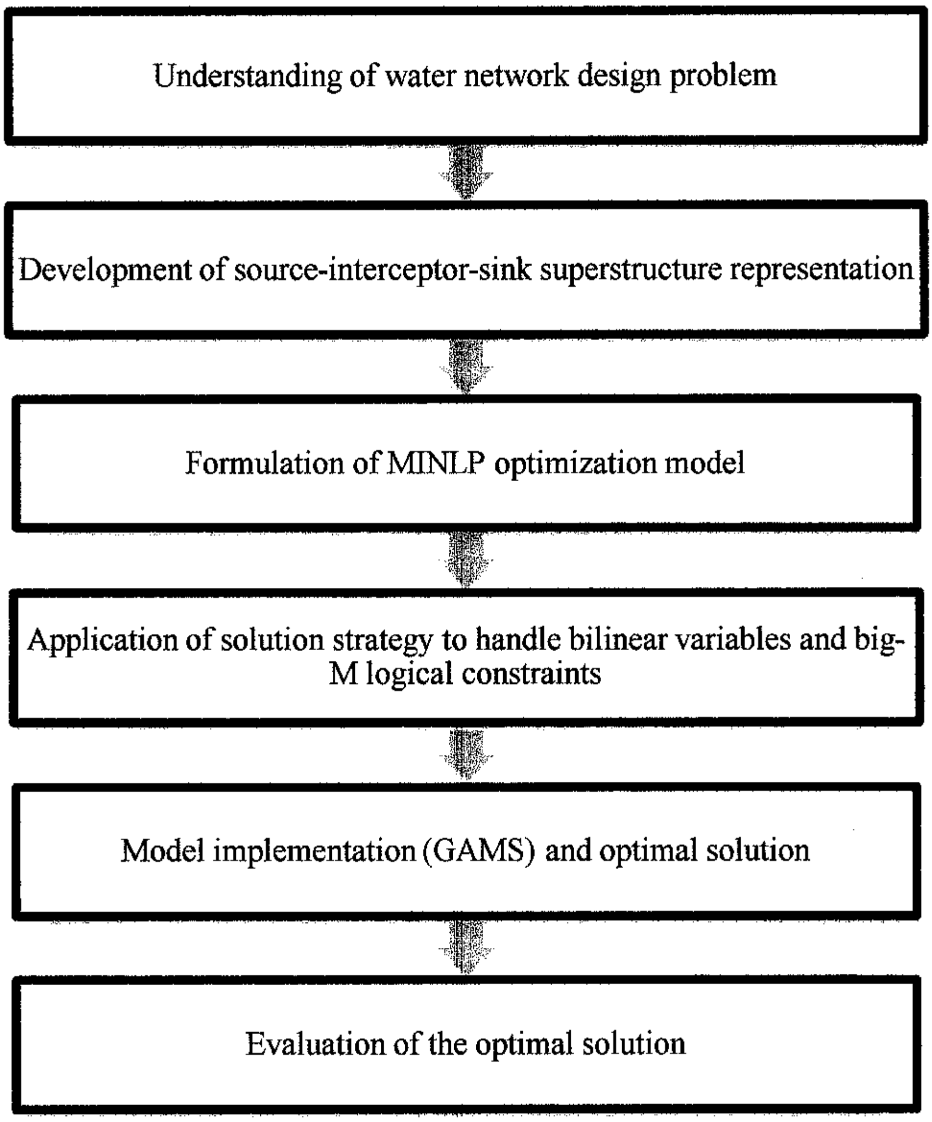

Figure 3.1 Methodology Chart

The method in this study starts with the understanding of the problem of water network design for a petroleum refinery with the presence of water reuse, regeneration and recycles (W3R) technique. Data for identified flowrates and concentration of contaminants are collected from a refinery plant in Malacca. Then, a superstructure representation is developed which includes all possible interconnections between sources, a single interceptor that is reverse osmosis network (RON), and sinks.

After that, the mixed-integer nonlinear programming (MINLP) optimization model is formulated with the specified constraints and objective function which is to minimize the usage of freshwater, wastewater discharged as well as the total cost for RON. The model consists of bilinear variables that are the major problem in optimization model which will be handled by Piecewise Linear Relaxation (PLR) as its solution strategy. On the other hand, another problem occurs in optimization is Big-M logical constraints which will be solved by specification of tighter upper and lower bound.

The next step involves the implementation of optimization model in General Algebraic Modeling System (GAMS) modeling language to determine the feasible optimal solution for the problem. GAMS modeling language software will be used for this project. It is a high-level modeling system for mathematical programming and optimization. It consists of a language compiler and a stable of integrated high-performance solvers. GAMS is tailored for complex, large scale modeling applications, and allows to build large maintainable models that can be adapted quickly to new situation. Lastly, the solution will be evaluated based on the real-world petroleum refinery practical features. The proposed key milestone for FYP II is shown below.

Detail/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Research Progress - Literature Review - Objective Function - Logical constraint formulation - Revised formulation														
Submission of Progress Report I														
Research Progress - Solution strategy - Obtain optimal solution														
Submission of Progress Report II														
Pre-EDX														
EDX														
Submission of Final Report														

Figure 3.2 Gantt Chart of FYP II

CHAPTER 4

OPTIMIZATION MODEL FORMULATION

4.1 SUPERSTRUCTURE REPRESENTATION

A superstructure is developed based on an actual operating refinery with multiple sources, multiple interceptor units, and multiple sinks.

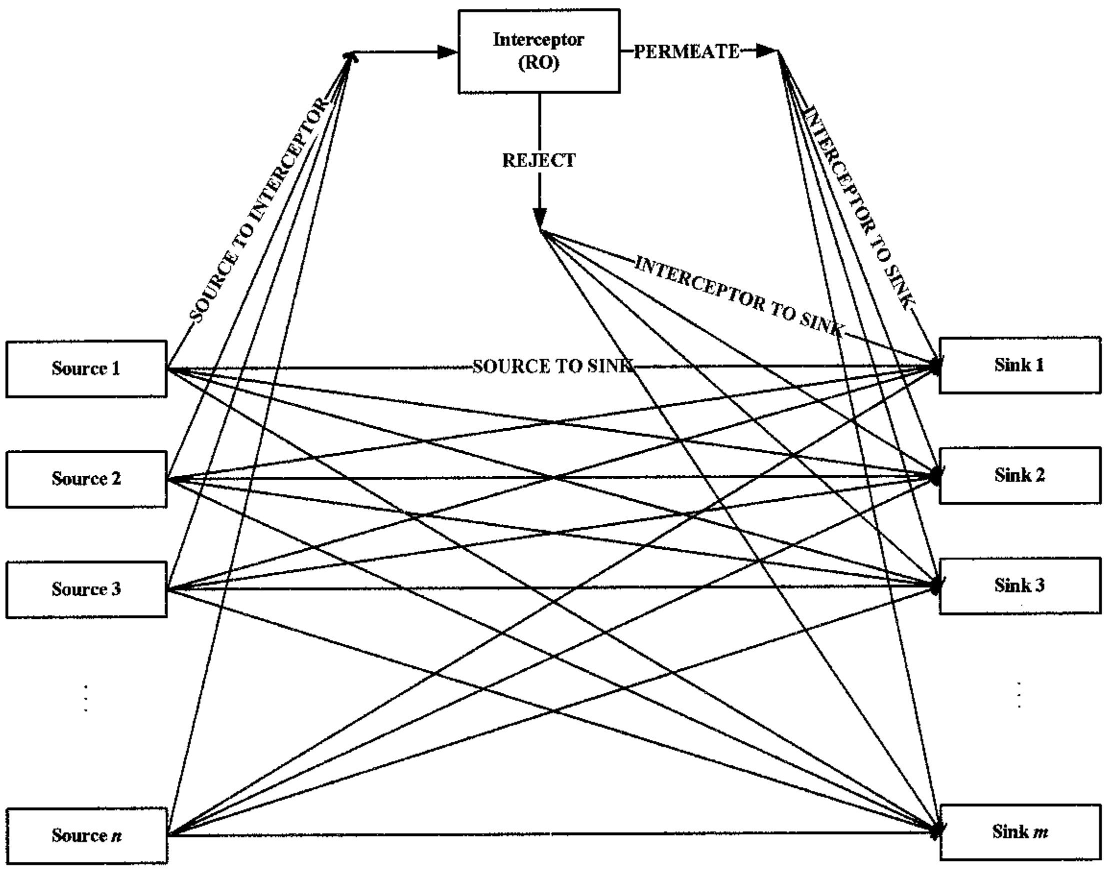

Figure 4.1 Superstructure Representation of Possible Interconnections between Source-Interceptor-Sink

The superstructure representation of source-interceptor-sink had been proposed based on a local refinery plant water management as illustrated in Figure 4.1. The problem representation is useful for developing material balances and other constraints associated with the optimization model formulation. In this project, only single stage reverse osmosis network is considered as the interceptor for the detailed design parametric optimization, latter incorporates into the main optimization problem. Figure 4.2 shows the general representation of source-interceptor-sink structure.

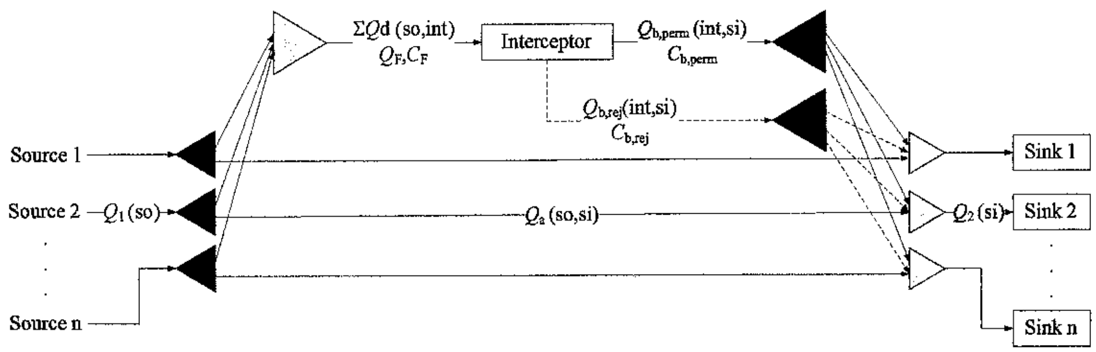

Figure 4.2 General Representation of Source-Interceptor-Sink

4.2 OPTIMIZATION MODEL FORMULATION

We consider two types of variables in our optimization model formulation that is (1) continuous variables on the water flowrates and contaminant concentrations; and (2) 0–1 variables (or binary variables) on the piping interconnections that involve interconnections between the following entities:

- between a source and a sink,
- between a source and an interceptor,
- between a permeate stream (of an interceptor) and a sink,
- between a reject stream (of an interceptor) and a sink,

The binary variables are also employed to model the existences of the streams of an interceptor, namely:

- the inlet stream to an interceptor,
- the outlet streams from an interceptor that comprises the concentrated reject stream and the diluted permeate stream.

Material balances for the source-interceptor-sink superstructure representation are developed for water flowrates and contaminant concentrations based on optimization model formulations proposed by Tan et al. (2009), Meyer and Floudas (2006), and Gabriel and El-Halwagi (2005). The identified values included are outlet flowrates of sources, outlet concentrations of sources, inlet flowrate of sinks and maximum allowable inlet concentration of sinks. Besides, liquid phase recovery, α and removal ratio, RR are also considered for a single interceptor unit. The objective function and material balances are described in the following sections.

4.2.1 Objective Function

The objective function of the problem is to minimize the overall cost which is represented by the minimization of freshwater use and wastewater discharges, piping interconnections cost, and reverse osmosis network cost (Ismail, 2010).

$$
\begin{aligned}
\min \text{obj}_{\text{cost}} = {} & \text{cost of freshwater per year} \\
& + \text{cost of effluent treatment (discharge) per year} \\
& + \text{operating and capital cost of interceptor per year} \\
& + \text{operating and capital cost of pipelines per year}
\end{aligned}
$$

$$
\begin{aligned}
\min \text{obj}_{\text{cost}} = {} & \left[C_{\text{water}} \times \text{load of freshwater} \times \text{AOT}\right] \\
& + \left[C_{\text{discharge}} \times \text{load of discharge} \times \text{AOT}\right] \\
& + \left[\text{Total annualized cost of interceptor from detail design}\right] \\
& + \left[D \times \begin{bmatrix} (\text{operating cost parameter of pipeline} \times \text{load of the pipeline}) + \\ (\text{capital cost parameter of pipeline} \times \text{existence of the pipeline}) \end{bmatrix} \times \text{Annualizing Factor}\right]
\end{aligned}
$$

The complete objective function formulation is shown in equation **(1).**

$$
\begin{aligned}
\min \text{obj}_{\text{cost}} = {} & \underbrace{\left[C_{\text{water}} \sum_{\text{si} \in \text{SI}} Q_{\text{a}}(\text{freshwater}, \text{si}) + C_{\text{discharge}} Q_2(\text{discharge})\right] \text{AOT}}_{\text{Annualized cost of freshwater use and wastewater discharge treatment}} \\
& + \underbrace{\sum_{\text{co} \in \text{CO}} \text{TAC}(\text{CO})}_{\substack{\text{Annualized cost of interceptor} \\ \text{from the parametric optimization problem in detailed design}}} \\
& \underbrace{+ D \left\{ \begin{aligned}
& \left[p \sum_{\text{so} \in \text{SO}} \sum_{\text{int} \in \text{INT}} \frac{Q_{\text{d}}(\text{so}, \text{int})}{3600 v} + q \sum_{\text{so} \in \text{SO}} \sum_{\text{int} \in \text{INT}} Y_{\text{d}}(\text{so}, \text{int}) \right] \\
& + \left[p \sum_{\text{int} \in \text{INT}} \sum_{\text{si} \in \text{SI}} \frac{Q_{\text{b,perm}}(\text{int}, \text{si})}{3600 v} + q \sum_{\text{so} \in \text{SO}} \sum_{\text{int} \in \text{INT}} Y_{\text{b,perm}}(\text{int}, \text{si}) \right] \\
& + \left[p \sum_{\text{int} \in \text{INT}} \sum_{\text{si} \in \text{SI}} \frac{Q_{\text{b,rej}}(\text{int}, \text{si})}{3600 v} + q \sum_{\text{so} \in \text{SO}} \sum_{\text{int} \in \text{INT}} Y_{\text{b,rej}}(\text{int}, \text{si}) \right] \\
& + \left[p \sum_{\text{so} \in \text{SO}} \sum_{\text{si} \in \text{SI}} \frac{Q_{\text{a}}(\text{so}, \text{si})}{3600 v} + q \sum_{\text{so} \in \text{SO}} \sum_{\text{int} \in \text{INT}} Y_{\text{a}}(\text{so}, \text{si}) \right]
\end{aligned} \right\} \frac{m(1-m)^n}{(1+m)^n - 1}}_{\text{Annualized cost of operating and capital piping interconnections}}
\end{aligned}
\qquad \textbf{(1)}
$$

4.2.2 Material Balances

4.2.2.1 Material Balances for Sources

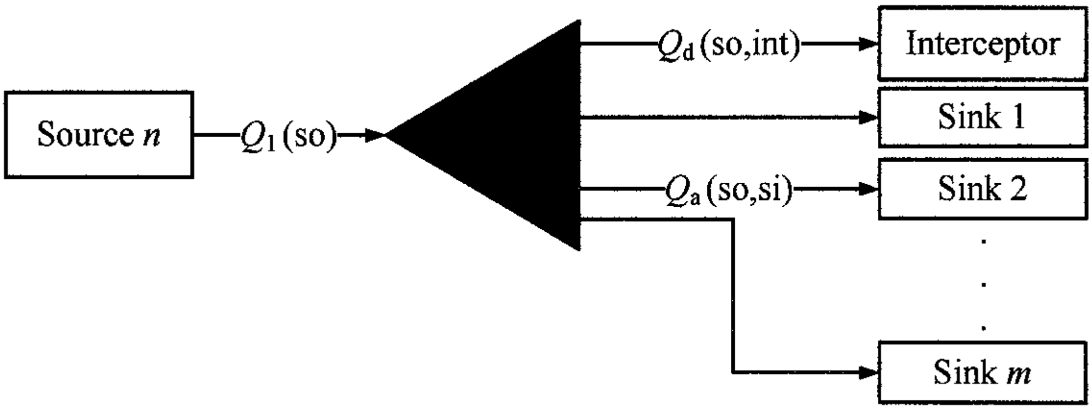

Figure 4.3 Representation of Material Balance for a Source

Figure 4.3 shows the flow representation of a source stream which can be splitted into several streams for direct reuse to the sinks, and/or for regeneration (to the interceptors) before the reuse. This representation is useful to develop the flow and concentration balances for source.

(a) Flow balances for sources

$$Q_1(\text{so}) \geq \sum_{\text{int}\in\text{INT}} Q_d(\text{so},\text{int}) + \sum_{\text{si}\in\text{SI}} Q_a(\text{so},\text{si}) \qquad \forall \text{so} \in \text{SO} \qquad \textbf{(2)}$$

The flow balances for sources as given by **(2)** indicates that the flowrate of a source Q_1(so) is greater than the sum of the flowrate splits from the source to the interceptor units for regeneration $\sum_{\text{int}\in\text{INT}} Q_d(\text{so,int})$ and from the source to the sinks for direct reuse or recycle $\sum_{\text{si}\in\text{SINK}} Q_a(\text{so,si})$. The flow balance is applied to each source. It is written as an inequality instead of an equality (as is typical of a flow balance) to account for discharging any excess source of water directly into the environment (Tan et al., 2009). It is noteworthy that if this flow balance is represented as equality, the model is likely to return an infeasible solution.

(b) Concentration balances for sources

$$Q_1(\text{so}) \cdot C_{\text{so}}(\text{so,co}) \geq C_{\text{so}}(\text{so,co}) \cdot \sum_{\text{int} \in \text{INT}} Q_d(\text{so,int}) + C_{\text{so}}(\text{so,co}) \cdot \sum_{\text{si} \in \text{SI}} Q_a(\text{so,si})$$

$$\forall \text{so} \in \text{SO}, \forall \text{co} \in \text{CO} \qquad \textbf{(3)}$$

The concentration balance for a source **(3)** represents that the multiplication of the contaminant concentration in the source stream C_{so}(so,co) with Q_1(so) is equivalent to the total of multiplication between C_{so}(so,co) and $\sum_{\text{int} \in \text{INT}} Q_d(\text{so,int})$ and multiplication between C_{so}(so,co) and $\sum_{\text{si} \in \text{SINK}} Q_a(\text{so,si})$.

Since C_{so}(so,co) in all terms can be canceled out, equation **(3)** is thereby equivalent to equation **(2)**, as shown below, thus equation **(3)** is negligible.

$$Q_1(\text{so}) \cdot \cancel{C_{\text{so}}(\text{so,co})} \geq \cancel{C_{\text{so}}(\text{so,co})} \cdot \sum_{\text{int} \in \text{INT}} Q_d(\text{so,int}) + \cancel{C_{\text{so}}(\text{so,co})} \cdot \sum_{\text{si} \in \text{SI}} Q_a(\text{so,si})$$

$$\forall \text{so} \in \text{SO}, \cancel{\forall \text{co} \in \text{CO}}$$

$$Q_1(\text{so}) \geq \sum_{\text{int} \in \text{INT}} Q_d(\text{so,int}) + \sum_{\text{si} \in \text{SI}} Q_a(\text{so,si}), \qquad \forall \text{so} \in \text{SO}$$

4.2.2.2 Material Balances for Interceptors

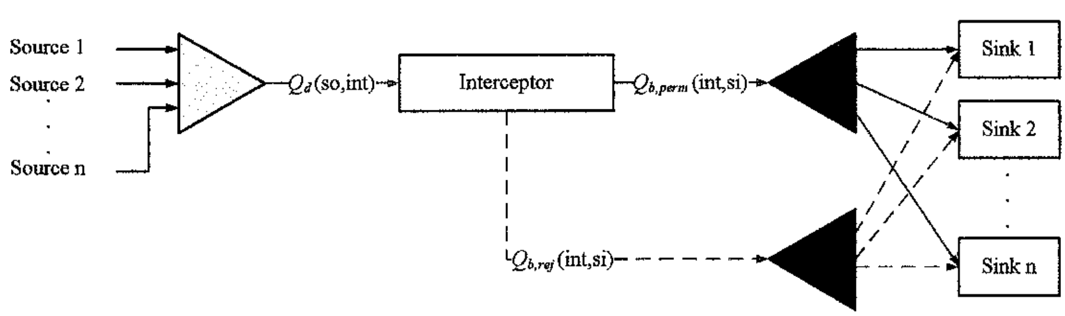

Figure 4.4 Representation of Material Balance for an Interceptor

Figure 4.4 shows the representation of an interceptor that receives the mixing of source streams and generates the permeate and reject streams that are further splitted to each sink. This representation is useful to develop the flow and concentration balances for an interceptor.

(a) Flow balance for an interceptor:

$$\sum_{so \in SO} Q_{d}(so,int) = \sum_{si \in SINK} Q_{b,perm}(int,si) + \sum_{si \in SI} Q_{b,rej}(int,si) \qquad \forall\, int \in INT \tag{4}$$

The flow balance for an interceptor **(4)** insists on the sum of the mixed (or combined) flowrate of multiple sources to a partitioning interceptor $\sum_{so \in SO} Q_{d}(so,int)$ is equivalent to the following:

- sum of flowrate of the stream splits from the permeate stream of a partitioning interceptor to each of the sinks $\sum_{si \in SI} Q_{b,perm}(int,si)$;
- sum of flowrate of the stream splits from the reject stream of a partitioning interceptor to each of the sinks $\sum_{si \in SI} Q_{b,perm}(int,si)$.

(b) Concentration balance for an interceptor:

$$\begin{aligned} \sum_{so \in SO} \left(Q_{d}(so,int) \cdot C_{so}(so,co)\right) = C_{perm}(int,co) \cdot \sum_{si \in SI} Q_{b,perm}(int,si) \\ + C_{rej}(int,co) \cdot \sum_{si \in SI} Q_{b,rej}(int,si) \end{aligned} \tag{5}$$

$$\forall\, int \in INT,\ \forall co \in CO$$

The concentration balance for an interceptor **(5)** for a partitioning interceptor can be described as equality between the sum of the multiplication of component flowrate and contaminant concentration from each source to the interceptor $\sum_{so \in SO} \left(Q_{d}(so,int) \cdot C_{so}(so,co)\right)$ with the total of the following:

- multiplication of the term $\sum_{si \in SI} Q_{b,perm}(int,si)$ and contaminant concentration generated by the interceptor in the permeate stream $C_{perm}(int,co)$;

- multiplication of the term $\sum_{si \in SI} Q_{b,perm}(\text{int,si})$ and contaminant concentration generated by the interceptor in the permeate stream C_{perm}(int,co);

Liquid phase recovery

The parameter liquid phase recovery α represents a fixed fraction of a regenerator inlet flowrate that exits in the permeate stream, which yields the water balance across the regenerator. The equation further implies that the complement of the fraction of the inlet water (as given by (1−α)) is discharged as the regenerator reject stream (Tan et al., 2009). They are expressed by the following relations:

$$\alpha(\text{int}) \cdot Q_F = \sum_{si \in SI} Q_{b,perm}(\text{int,si}), \quad \forall \text{int} \in \text{INT}$$
$$\Rightarrow \alpha(\text{int}) = \frac{\sum_{si \in SI} Q_{b,perm}(\text{int,si})}{Q_F} \tag{6}$$
$$\Rightarrow 1 - \alpha(\text{int}) = \frac{\sum_{si \in SI} Q_{b,rej}(\text{int,si})}{Q_F}$$

Since these two relations are not independent (i.e., redundant) of each other, only one of them is included as a model constraint in the computational exercise.

Removal ratio

Removal ratio is defined as the fraction of mass load in a regenerator inlet stream that exits in its reject stream (Tan et al., 2009). The fixed-value parameter RR(int,co) in constraint **(7)** represents the removal ratio of a contaminant (co) for an interceptor (int).

$$RR(\text{int,co})\left(\sum_{so \in SO} Q_d(\text{so,int}) \cdot C_{so}(\text{so,co})\right) = C_{rej}(\text{int,co}) \sum_{si \in SI} Q_{b,rej}(\text{int,si})$$
$$RR(\text{int,co}) = \frac{C_{rej}(\text{int,co}) \sum_{si \in SI} Q_{b,rej}(\text{int,si})}{\left(\sum_{so \in SO} Q_d(\text{so,int}) \cdot C_{so}(\text{so,co})\right)} \tag{7}$$
$$\forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO}$$

Alternatively, RR can be defined in terms of the parameters of the reject stream of an interceptor as follows:

$$RR(\text{int,co})\left(\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int})\cdot C_{\text{so}}(\text{so,co})\right)=C_{\text{rej}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})$$

$$RR(\text{int,co})\left(Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})\right)=C_{\text{rej}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})$$

$$RR(\text{int,co})=\frac{C_{\text{rej}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})}{Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})} \quad \textbf{(8)}$$

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

Accordingly, RR can be defined in terms of the parameters of the permeate stream of an interceptor:

$$RR(\text{int,co})=\frac{Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})\ -\ C_{\text{perm}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si})}{Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})}$$

$$RR(\text{int,co})=1-\frac{C_{\text{perm}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si})}{Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})}$$

$$1-RR(\text{int,co})=\frac{C_{\text{perm}}(\text{int,co})\cdot\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si})}{Q_{\text{F}}(\text{int, co})\cdot C_{\text{F}}(\text{int, co})} \quad \textbf{(9)}$$

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

4.2.2.3 Material Balances for Sinks

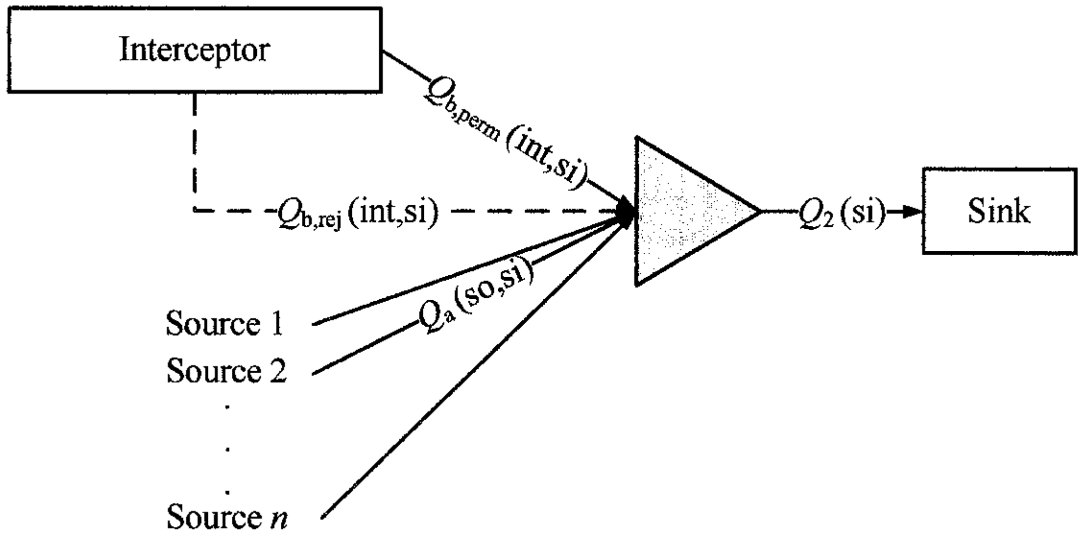

Figure 4.5 Representation of Material Balance for a Sink

Figure 4.5 shows the flow representation of a sink which receives the mixing of either permeate or reject streams from an interceptor and the mixed source streams. This representation is useful to develop the flow and concentration balances for a sink.

(a) Flow balances for sinks

$$Q_2(\mathrm{si}) = \sum_{\mathrm{so}\in\mathrm{SO}} Q_a(\mathrm{so,si}) + \sum_{\mathrm{int}\in\mathrm{INT}} \left(Q_{b,\mathrm{perm}}(\mathrm{int,si}) + Q_{b,\mathrm{rej}}(\mathrm{int,si})\right) \quad \forall \mathrm{si} \in \mathrm{SI} \qquad \textbf{(10)}$$

The flow balance for a sink **(10)** is associated with the equality between the inlet flowrate of a sink, Q_2(si) with the summation of $\sum_{\mathrm{so}\in\mathrm{SO}} Q_a(\mathrm{so,si})$ and total of both $Q_{b,perm}$(int,si), and $Q_{b,rej}$(int,si). Equation **(10)** is applied to each sink.

(b) Concentration balances for sinks

$$\left(\sum_{so\in SO} Q_a(\text{so,si})\cdot C_{so}(\text{so,co})\right)+\sum_{int\in INT}\left(C_{perm}(\text{int,co})\cdot Q_{b,perm}(\text{int,si})+C_{rej}(\text{int,co})\cdot Q_{b,rej}(\text{int,si})\right)$$
$$=Q_2(\text{si})\cdot C(\text{si,co}) \tag{11}$$

$\forall \text{si}\in \text{SI}, \forall \text{co}\in \text{CO}$

The concentration balance for a sink **(11)** is depicted as above, where the summation of $\sum_{so\in SO} Q_a(\text{so,si})C_{so}(\text{so,co})$ and $\sum_{int\in INT}\left(C_{perm}(\text{int,co})Q_{b,perm}(\text{int,si})+C_{rej}(\text{int,co})Q_{b,rej}(\text{int,si})\right)$ is equivalent to multiplication of Q_2(si) and the contaminant concentration into the sink C(si,co).

Since there are specific values for maximum allowable contaminant concentration to each sink, the term C(si,co) is changed to C_{max} (si,co) and the inequality is taking place. The term Q_2(si) in equation **(11)** can be replaced by the equation **(10)**. The final formulation derivation of concentration balance for a sink is shown in equation **(12)**.

$$\left(\sum_{so\in SO} Q_a(\text{so,si})\cdot C_{so}(\text{so,co})\right)+C_{perm}(\text{int,co})\cdot Q_{b,perm}(\text{int,si})+C_{rej}(\text{int,co})\cdot Q_{b,rej}(\text{int,si})$$
$$\leq\left(\sum_{so\in SO} Q_a(\text{so,si})+\sum_{int\in INT}\left(Q_{b,perm}(\text{int,si})+Q_{b,rej}(\text{int,si})\right)\right)C_{max}(\text{si,co}) \tag{12}$$

$\forall \text{si}\in \text{SI}, \forall \text{co}\in \text{CO}$

(c) Restrictions on mixing of permeate and reject streams in sinks

The previous flow and concentration balances for a sink allow mixing of the permeate and reject streams of a membrane-based interceptor at the inlet of a sink. However, we ought to forbid such a mixing because the function of this type of interceptor is to separate (or partition) its outlets into a concentrated stream (i.e., the reject stream) and a diluted stream (permeate stream) before entering the sinks. This constraint **(13)** is applicable to each sink as follows:

$$Y_{\text{perm}}(\text{int,si}) + Y_{\text{rej}}(\text{int,si}) \leq 1, \quad \forall \text{si} \in \text{SI}, \forall \text{int} \in \text{INT} \tag{13}$$

The forbidden mixing constraint specifies that for a sink operation, only one of either the permeate stream or the reject stream from each interceptor is allowed to enter the sink.

The less-than-or-equal-to inequality allows none of the piping interconnections from either a permeate or a reject stream to a sink to be selected for minimizing the objective function value. In other words, the optimizer is susceptible to not selecting any of the permeate and reject streams because the cost-minimization objective function would tend to select as few piping interconnections (as modeled by 0–1 variables) as possible. But a solution without the presence of the outlet streams of an interceptor would not be reasonable, hence we reformulate this constraint in the form of an equality, as follows:

$$Y_{\text{perm}}(\text{int,si}) + Y_{\text{rej}}(\text{int,si}) = 1, \quad \forall \text{si} \in \text{SI}, \forall \text{int} \in \text{INT} \tag{14}$$

The final form of this constraint ensures that at least one of either the permeate or the reject stream is selected. But note that the constraint does not ensure that at least one of the piping interconnections involving a permeate stream and at least one such piping interconnection for a reject stream must be selected. This might not be a concern because if the reject stream concentration of an interceptor is lower than the maximum allowable concentration (or $C_{\max}$ value) of a sink, then the reject stream can be sent to the sink, and the corresponding permeate stream of that interceptor can also be accepted into the sink, thus ensuring that both the permeate and reject streams of an interceptor are selected.

4.2.3 Revised Formulation on Material Balances for Interceptors to Reduce Bilinearities

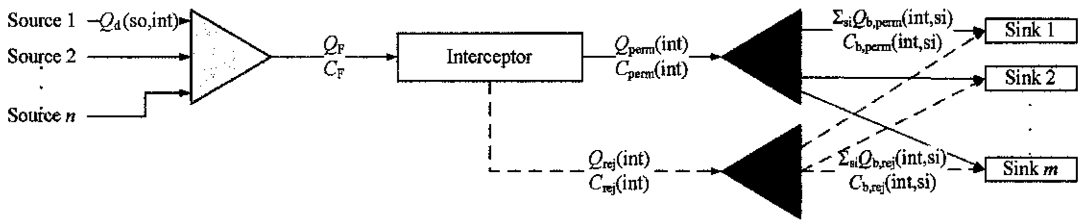

Figure 4.6 Revised Subsuperstructure Representation of Interceptors

Figure 4.6 shows the revised subsuperstructure representation of an interceptor that receives the mixing of source streams and generates the permeate and reject streams that are further splitted to each sink. This representation is useful to develop flow and concentration balances before the interceptors, for the interceptors and after the interceptors.

(a) Flow balances for mixers before interceptors

$$\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int}) = Q_{\text{F}}, \quad \forall \text{int} \in \text{INT} \tag{15}$$

The flow balances for mixers before interceptors **(15)** enforces that the mixed or combined flowrate of multiple sources to a partitioning interceptor $\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int})$ is equivalent to the feed flowrate to the interceptor Q_F.

(b) Concentration balances for mixers before interceptors

$$\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int}) \cdot C_{\text{so}}(\text{so,co}) = Q_{\text{F}}(\text{int,co}) \cdot C_{\text{F}}(\text{int,co}), \quad \forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO} \tag{16}$$

The concentration balances for mixers before interceptors **(16)** for a partitioning interceptor can be described as the equality between the multiplication

$\sum_{so \in SO} Q_d(\text{so,int}) \cdot C_{so}(\text{so,co})$ with multiplication of Q_F(int,co) and contaminant concentration of feed to the interceptor C_F(int,co).

Note the following simple analysis to determine the number of bilinear terms:

$$\underbrace{\sum_{so \in SO} \left(Q_d(\text{so,int}) \cdot \overbrace{C_{so}(\text{so,co})}^{\substack{\text{known} \\ \text{parameter}}} \right)}_{\text{no bilinear term}} = \underbrace{Q_F(\text{int,co}) \cdot C_F(\text{int,co})}_{\text{1 bilinear term}}, \quad \forall \text{int} \in \text{INT}, \forall \text{co} \in \text{CO}$$

(c) Flow balances for interceptors

$$Q_F = Q_{perm}(\text{int}) + Q_{rej}(\text{int}), \quad \forall \text{int} \in \text{INT} \qquad \textbf{(17)}$$

The flow balance for interceptor **(17)** represents Q_F is equivalent to the summation of flowrate of permeate stream of a partitioning interceptor Q_{perm}(int) and flowrate of reject stream of a partitioning interceptor Q_{rej}(int).

(d) Concentration balances for interceptors

$$Q_F C_F(\text{int,co}) = Q_{perm}(\text{int}) C_{perm}(\text{int,co}) + Q_{rej}(\text{int}) C_{rej}(\text{int,co}), \quad \forall \text{int} \in \text{INT} \qquad \textbf{(18)}$$

The concentration balance for interceptor **(18)** corresponds to the term $Q_F C_F(\text{int,co})$ which is equivalent to the summation of multiplication between the term Q_{perm}(int) with contaminant concentration generated in the permeate stream C_{perm}(int,co) and multiplication between the term Q_{rej}(int) with contaminant concentration generated in the reject stream C_{rej}(int,co). However, the relations in equation **(16)** and **(17)** are replaced into equation **(18)** and solved for C_{rej} **(19)**.

$$
\begin{aligned}
C_{\text{rej}} &= \frac{Q_{\text{F}}C_{\text{F}} - Q_{\text{perm}}C_{\text{perm}}}{Q_{\text{rej}}} \\
&= \frac{Q_{\text{F}}C_{\text{int}} - \alpha Q_{\text{F}}(1-RR)C_{\text{F}}}{(1-\alpha)Q_{\text{F}}} \\
&= \frac{\cancel{Q_{\text{F}}}C_{\text{F}} - \alpha \cancel{Q_{\text{F}}}(1-RR)C_{\text{F}}}{(1-\alpha)\cancel{F_{\text{in}}}} \\
&= \frac{C_{\text{F}}(1-\alpha(1-RR))}{(1-\alpha)} \\
&= \frac{(1-\alpha+\alpha RR)}{(1-\alpha)}C_{\text{F}} \\
&= \left(\frac{1-\alpha}{(1-\alpha)} + \frac{\alpha}{(1-\alpha)}RR\right)C_{\text{F}} \\
&= \left(\frac{1-\cancel{\alpha}^{1}}{(\cancel{1}-\alpha)} + \frac{\alpha}{(1-\alpha)}RR\right)C_{\text{F}} \\
\therefore & \boxed{C_{\text{rej}} = \left(1 + RR\frac{\alpha}{(1-\alpha)}\right)C_{\text{F}}}
\end{aligned}
\tag{19}
$$

At inlet to an interceptor, consider the following revised formulation of bilinear concentration balances for interceptors, in which, we utilize the variable Q_{F} and C_{F}.

$$
\underbrace{\sum_{\text{so}\in\text{SO}}\left(Q_{\text{d}}(\text{so,int})\overbrace{C_{\text{so}}(\text{so,co})}^{\text{known}}\right)}_{\text{no bilinear term}} = \underbrace{Q_{\text{F}}(\text{int,co})\cdot C_{\text{F}}(\text{int,co})}_{\text{1 bilinear term}}
\tag{20}
$$

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

Concentration balance at the outlet of an interceptor is modeled after that of a splitter concentration balance, which does not involve any bilinear term, as follows:

$$
(1-RR(\text{int,co}))\cdot C_{\text{F}}(\text{int,co}) = C_{\text{b,perm}}(\text{int,co})
\tag{21}
$$

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

$$
\left(1 + RR\frac{\alpha}{(1-\alpha)}\right)\cdot C_{\text{F}}(\text{int,co}) = C_{\text{b,rej}}(\text{int,co})
\tag{22}
$$

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

Thus, this alternative formulation of concentration balances for interceptor **(21)** and **(22)** only involves one bilinear term.

Nevertheless, note that equation **(22)** utilizes a different relation for the removal ratio physical parameter as given by $C_{\text{rej}} = \left(1 + RR\dfrac{\alpha}{(1-\alpha)}\right)C_{\text{F}}$. This relation holds true even for the case of $RR(\text{int,co}) = 0$, in which an interceptor does not remove a certain contaminant.

(e) Flow balances for splitters after interceptors

$$Q_{\text{perm}}(\text{int}) = \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si}), \quad \text{int} \in \text{INT} \tag{23}$$

The flow balance of permeate stream for splitter after interceptor is represented by equation **(23)** where $Q_{\text{perm}}(\text{int})$ equals to total flowrate for the stream splits from the permeate stream of a partitioning interceptor to each of the sinks $\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si})$.

$$Q_{\text{rej}}(\text{int}) = \sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si}), \quad \forall\,\text{int} \in \text{INT} \tag{24}$$

The flow balance of reject stream for splitter after interceptor is represented by equation **(24)** where $Q_{\text{rej}}(\text{int})$ equals to total flowrate for the stream splits from the reject stream of a partitioning interceptor to each of the sinks $\sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})$.

(f) Concentration balances for splitters after interceptors

$$Q_{\text{perm}}(\text{int}) \cdot C_{\text{perm}}(\text{int,co}) = \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si}) \cdot C_{\text{b,perm}}(\text{int,co}), \quad \forall\,\text{int} \in \text{INT} \tag{25}$$

The concentration balance of permeate stream for splitter after interceptor is indicated by equation **(25)** where multiplication of $Q_{\text{perm}}(\text{int})$ with contaminant concentration generated in the permeate stream $C_{\text{perm}}(\text{int,co})$ is equivalent to multiplication of the term $\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{int,si})$ and $C_{\text{perm}}(\text{int,co})$.

$$Q_{\text{rej}}(\text{int})\cdot C_{\text{rej}}(\text{int,co}) = \sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})\cdot C_{\text{b,rej}}(\text{int,co}), \quad \forall\,\text{int}\in\text{INT} \qquad \textbf{(26)}$$

The concentration balance of reject stream for splitter after interceptor is indicated by equation **(26)** where multiplication of $Q_{\text{rej}}(\text{int})$ with contaminant concentration generated in the reject stream $C_{\text{rej}}(\text{int,co})$ is equivalent to multiplication of the term $\sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{int,si})$ and $C_{\text{rej}}(\text{int,co})$.

4.2.4 Detailed Design of Interceptor Model Formulation

The model formulation of RO detailed design that serves as offline parametric optimization problem is based on El-Halwagi (1997). Such single-stage RON synthesis problem can be described in Figure 4.7.

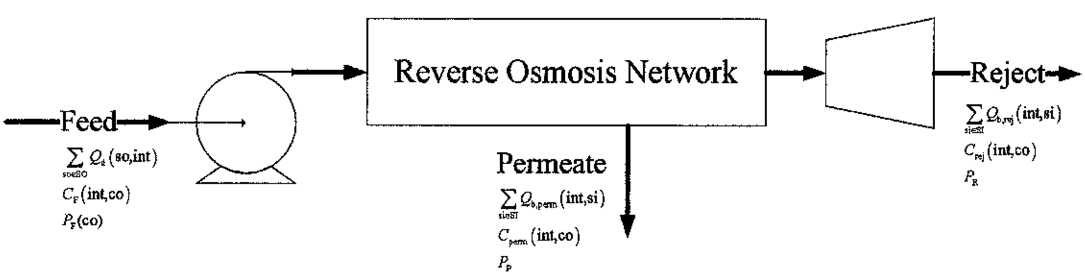

Figure 4.7 Reverse Osmosis Network Synthesis Problem (El-Halwagi, 1997)

We consider the detailed design of a single-stage hollow fiber reverse osmosis (HFRO) type module as our case study. We assume that the RON consists of three (3) different types of unit operations (Saif et al., 2008):

1. pump to increase the pressure of the source streams;
2. RO modules that separate the feed into a concentrated stream (i.e., the reject stream) and a diluted stream (permeate stream);
3. turbine to recover kinetic energy from high-pressure stream.

Equation **(27)** shows the derivation for total annualized cost (TAC) of the single-stage RON consisting of the fixed costs for RO modules, pump, and turbine, and the operating costs for pump and pretreatment chemicals. The TAC also considers the operating value of turbine, as represented by the subtraction term in the function.

$$\begin{aligned}\text{TAC} = & \left(\text{Annualized fixed cost of modules}\right) + \left(\text{Annualized fixed cost of pump}\right) \\ & + \left(\text{Annualized fixed cost of turbine}\right) + \left(\text{Annual operating cost of pump}\right) \\ & + \left(\text{Annual operating cost of pre-treatment chemicals}\right) \\ & - \left(\text{Operating value of turbine}\right)\end{aligned}$$

Mathematically, the expression of the TAC function for HFRO is shown below.

$$\begin{aligned}\text{TAC} = & \left(C_{\text{module}} \times \text{no of modules}\right) + \left(C_{\text{pump}} \times \text{inlet load of pump}\right) \\ & + \left(C_{\text{turbine}} \times \text{inlet load of turbine}\right) + \left(\frac{C_{\text{electricity}} \times \text{inlet load of pump}}{\eta_{\text{pump}}}\right) \\ & + \left(C_{\text{chemicals}} \times \text{amount of chemicals needed}\right) \\ & - \left(C_{\text{electricity}} \times \text{inlet load of turbine} \times \eta_{\text{turbine}}\right)\end{aligned}$$

$$\begin{aligned}\text{TAC} = & \left(C_{\text{module}} \times \frac{\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}(\text{RO,si})}{q_{\text{P}}}\right) + \left(C_{\text{pump}} \times \left(\text{power of pump}\right)^{0.65}\right) \\ & + \left(C_{\text{turbine}} \times \left(\text{power of turbine}\right)^{0.43}\right) \\ & + \left(\frac{\left(\text{power of pump}\right)}{\eta_{\text{pump}}} \times \left(C_{\text{electricity}} \times \text{AOT}\right)\right) \\ & + \left(\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,RO})\left(C_{\text{chemicals}} \times \text{AOT}\right)\right) - \left(\left(\text{power of turbine}\right) \times \eta_{\text{turbine}} \times \left(C_{\text{electricity}} \times \text{AOT}\right)\right)\end{aligned} \quad \textbf{(27)}$$

where

$$q_{\text{P}} = S_m A\left(P_{\text{F}} - \left(\frac{\Delta \text{P}_{\text{shell}}}{2} + P_{\text{P}}\right) - \frac{\pi_{\text{F}}}{2}\left(1 + \frac{C_{\text{rej}}(\text{RO,co})}{C_{\text{F}}(\text{RO,co})}\right)\right)\gamma, \qquad \text{(El-Halwagi, 1997)}$$

$$\text{power of pump} = \sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,RO})\left(P_{\text{F}} - P_{\text{atm}}\right)\left(1.01325 \times 10^5\right), \text{ and}$$

$$\text{power of turbine} = \sum_{\text{si}\in\text{SI}} Q_{\text{b,rej}}(\text{RO,si})\left(P_{\text{R}} - P_{\text{atm}}\right)\left(1.01325 \times 10^5\right).$$

Reformulation of total annualized cost of reverse osmosis network to eliminate dependence on the type of contaminants

El-Halwagi (1997) defines the osmotic pressure of the RO at the feed side π_F as a constant. Since the contaminant concentration of the permeate is very much lower than that on the feed side, the osmotic pressure of the RO at the permeate side can be neglected. Hence, to obtain a more detailed model that covers the representative range encountered in the optimization procedure, the following relation is adopted, as proposed by Saif et al. (2008), for the osmotic pressure at the reject side π_{RO}:

$$\pi_{\mathrm{RO}} = \mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{F,average}}(\mathrm{RO,co}) \tag{28}$$

where OS is a proportionality constant between the osmotic pressure and average solute concentration on the feed side (Saif et al., 2008) whose value is in the range between 0.006 to 0.011 psi/(mg/L) based on Parekh (1988). $C_{\mathrm{F,average}}(\mathrm{RO,co})$ is the average concentration for a contaminant (co) on the feed side, which is rewritten in terms of the contaminant concentration on the permeate side as follows:

$$\sum_{\mathrm{co}} C_{\mathrm{F,average}}(\mathrm{RO,co}) = \frac{\sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A(\Delta P - \Delta\pi_{\mathrm{RO}})\gamma}{K_c} \tag{29}$$

Where

K_c = the solute or contaminants permeability coefficient (1.82×10^{-8} m/s)

$\Delta P = P_{\mathrm{F}} - \left(\frac{\Delta \mathrm{P_{shell}}}{2} + P_{\mathrm{P}} \right).$

Hence, the relation for π_{RO} becomes:

$$\pi_{\mathrm{RO}} = \frac{\mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A(\Delta P - \Delta\pi_{\mathrm{RO}})\gamma}{K_c} \tag{30}$$

Saif et al. (2008) proposed that the relation for the permeate flowrate from RO as:

$$Q_{\mathrm{P}} = (\text{no of modules}) \cdot A \cdot S_m \cdot \gamma(\Delta P - \pi_{\mathrm{RO}})$$

Therefore,

$$\text{no of modules} = \frac{Q_{\mathrm{P}}}{q_{\mathrm{P}}} = \frac{Q_{\mathrm{P}}}{A \cdot S_m \cdot \gamma(\Delta P - \pi_{\mathrm{RO}})} \tag{31}$$

Substituting π_{RO} and ΔP into the above relation gives:

$$\begin{aligned}\frac{\sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,perm}}(\mathrm{RO,si})}{q_{\mathrm{P}}} &= \frac{\sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,perm}}(\mathrm{RO,si})}{A \cdot S_m \cdot \gamma\left(\Delta P - \dfrac{\mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A(\Delta P - \Delta\pi_{\mathrm{RO}})\gamma}{K_c}\right)} \\ &= \frac{\sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,perm}}(\mathrm{'RO',si})}{A \cdot S_m \cdot \gamma\left(P_{\mathrm{F}} - \left(\dfrac{\Delta \mathrm{P}_{\mathrm{shell}}}{2} + P_{\mathrm{P}}\right) - \dfrac{\mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A\left(P_{\mathrm{F}} - \left(\dfrac{\Delta \mathrm{P}_{\mathrm{shell}}}{2} + P_{\mathrm{P}}\right) - \Delta\pi_{\mathrm{RO}}\right)\gamma}{K_c}\right)}\end{aligned} \tag{32}$$

The final derivation of TAC from **(27)** until **(32)** is represented as **(33)**:

$$\mathrm{TAC} = \underbrace{\left[C_{\mathrm{module}} \times \left(\frac{\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}}\right) \sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,perm}}(\mathrm{RO,si})}{A \cdot S_m \cdot \gamma \left(P_{\mathrm{F}} - \left(\frac{\Delta P_{\mathrm{shell}}}{2} + P_{\mathrm{P}} \right) - \frac{\mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A \left(P_{\mathrm{F}} - \left(\frac{\Delta \mathrm{P}_{\mathrm{shell}}}{2} + P_{\mathrm{P}} \right) - \Delta\pi_{\mathrm{RO}} \right) \gamma}{K_c} \right)} \right) \right]}_{\text{annualized fixed cost of module}}$$

$$+ \underbrace{\left[C_{\mathrm{pump}} \left(\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}} \right) \left(\sum_{\mathrm{so}\in\mathrm{SO}} Q_{\mathrm{d}}(\mathrm{so,RO}) \right) (P_{\mathrm{F}} - P_{\mathrm{atm}}) \left(1.01325 \times 10^5 \right) \right)^{0.65} \right]}_{\text{annualized fixed cost of pump}}$$

$$+ \underbrace{\left[C_{\mathrm{turbine}} \left(\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}} \right) \left(\sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,rej}}(\mathrm{RO,si}) \right) \left(\overbrace{(P_{\mathrm{F}} - \Delta P_{\mathrm{shell}})}^{P_{\mathrm{R}}} - P_{\mathrm{atm}} \right) \left(1.01325 \times 10^5 \right) \right)^{0.43} \right]}_{\text{annualized fixed cost of turbine}}$$

$$+ \underbrace{\left[\frac{\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}} \right) \left(\sum_{\mathrm{so}\in\mathrm{SO}} Q_{\mathrm{d}}(\mathrm{so,RO}) \right) (P_{\mathrm{F}} - P_{\mathrm{atm}}) \left(1.01325 \times 10^5 \right) C_{\mathrm{electricity}} \cdot \mathrm{AOT}}{\eta_{\mathrm{pump}} \left(10^3\ \frac{\mathrm{W}}{\mathrm{kW}} \right)} \right]}_{\text{annual operating cost of pump}}$$

$$+ \underbrace{\left[\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}} \right) \left(\sum_{\mathrm{so}\in\mathrm{SO}} Q_{\mathrm{d}}(\mathrm{so,RO}) \right) \cdot C_{\mathrm{chemicals}} \cdot \mathrm{AOT} \right]}_{\substack{\text{annual operating cost} \\ \text{of chemicals}}}$$

$$- \underbrace{\left[\frac{\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}} \right) \left(\sum_{\mathrm{si}\in\mathrm{SI}} Q_{\mathrm{b,rej}}(\mathrm{RO,si}) \right) \left(\overbrace{(P_{\mathrm{F}} - \Delta P_{\mathrm{shell}})}^{P_{\mathrm{R}}} - P_{\mathrm{atm}} \right) \left(1.01325 \times 10^5 \right) \eta_{\mathrm{turbine}} \cdot C_{\mathrm{electricity}} \cdot \mathrm{AOT}}{\left(10^3\ \frac{\mathrm{W}}{\mathrm{kW}} \right)} \right]}_{\text{Operating value of turbine}}$$

$$\forall \mathrm{co} \in \mathrm{CO} \tag{33}$$

The constraint on RO operating condition as associated with the feed pressure P_{F} in **(33)** is then given by:

$$\Delta P = \frac{P_{\mathrm{F}} + P_{\mathrm{R}}}{2} - P_{\mathrm{P}} = \frac{P_{\mathrm{F}} + P_{\mathrm{F}} - \Delta P_{\mathrm{shell}}}{2} - P_{\mathrm{P}} = P_{\mathrm{F}} - \left(\frac{\Delta P_{\mathrm{shell}}}{2} + P_{\mathrm{P}} \right)$$
$$P_{\mathrm{F}} = \Delta P + \left(\frac{\Delta P_{\mathrm{shell}}}{2} + P_{\mathrm{P}} \right) \tag{34}$$

where

$$\Delta P = \frac{N_{\text{water}}}{A\gamma} + \frac{\pi_{\text{F}}}{C_{\text{F}}(\text{RO,co})} C_{\text{S}},$$

$$N_{\text{water}} = \frac{N_{\text{solute}}}{C_{\text{perm}}(\text{RO,co})},$$

$$N_{\text{solute}} = \left(\frac{D_{2M}}{K\delta}\right) C_{\text{S}}, \text{ and}$$

while we adopt the following relation for C_S in order to express P_{F} in terms of $C_{\text{F}}(\text{RO,co})$ and $C_{\text{perm}}(\text{RO,co})$ (for the purpose of writing clarity, the indices have been omitted here):

$$\begin{aligned}
C_S &= \frac{C_{\text{F}} + C_{\text{R}}}{2} \\
&= \frac{\left(\cancel{Q_{\text{P}}C_{\text{F}}} + \cancel{Q_{\text{R}}}C_{\text{F}}\right) + \cancel{Q_{\text{R}}}C_{\text{R}} - \cancel{Q_{\text{P}}C_{\text{F}}}}{2\cancel{Q_{\text{R}}}} \\
&= \frac{\left(Q_{\text{P}} + Q_{\text{R}}\right)C_{\text{F}} + Q_{\text{R}}C_{\text{R}} - Q_{\text{P}}C_{\text{F}}}{2Q_{\text{R}}} \\
&= \frac{Q_{\text{F}}C_{\text{F}} + Q_{\text{R}}C_{\text{R}} - Q_{\text{P}}C_{\text{F}}}{2Q_{\text{R}}} \\
&= \frac{Q_{\text{F}}C_{\text{F}} + \left(Q_{\text{F}}C_{\text{F}} - Q_{\text{P}}C_{\text{P}}\right) - Q_{\text{P}}C_{\text{F}}}{2Q_{\text{R}}} \\
C_S &= \frac{2Q_{\text{F}}C_{\text{F}} - Q_{\text{P}}C_{\text{P}} - Q_{\text{P}}C_{\text{F}}}{2\left(Q_{\text{F}} - Q_{\text{P}}\right)}
\end{aligned}$$

However, the above relation for CS contains bilinearities, hence we propose to utilize the following alternative expression for CS:

$$C_{\text{S}} = \frac{C_{\text{F}}(\text{RO,co}) + C_{\text{rej}}(\text{RO,co})}{2}$$

$$C_{\text{S}} = \frac{C_{\text{F,RO,co}} + C_{\text{rej}}(\text{RO,co})}{2}$$

which yields:

$$P_F = "\left(\frac{D_{2M}}{K\delta}\right)\frac{\left(2Q_F C_F - Q_P C_P - Q_P C_F\right)}{2C_P A\gamma\left(Q_F - Q_P\right)} + \frac{\pi_F\left(2Q_F C_F - Q_P C_P - Q_P C_F\right)}{2C_F\left(Q_F - Q_P\right)} + \left(\frac{\Delta P_{\text{shell}}}{2} + P_P\right)"$$

$$P_F = \text{SFC}\left(\frac{1}{A\gamma}\right)\frac{\left(2C_F \sum_{\text{so}\in\text{SO}} Q_d - C_{\text{perm}}\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}} - C_F \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}\right)}{2C_{\text{perm}}\left(\sum_{\text{so}\in\text{SO}} Q_d - \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}\right)}$$

$$+\frac{\pi_F\left(2C_F \sum_{\text{so}\in\text{SO}} Q_d - C_{\text{perm}}\sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}} - C_F \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}\right)}{2C_F\left(\sum_{\text{so}\in\text{SO}} Q_d - \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}\right)}$$

$$+\left(\frac{\Delta P_{\text{shell}}}{2} + P_P\right)$$

where

$$Q_F = \sum_{\text{so}\in\text{SO}} Q_d$$

$$Q_P = \sum_{\text{si}\in\text{SI}} Q_{\text{b,perm}}$$

$$C_P = C_{\text{perm}}$$

and $\text{SFC} = \frac{D_{2M}}{K\delta}$ is the salt flux constant.

Finally, P_F is derived as **(35)** with the substitution of C_S .

$$
\begin{aligned}
P_{\mathrm{F}} &= \Delta P + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right) \\
&= \left(\frac{N_{\text{water}}}{A\gamma} + \frac{\pi_{\mathrm{F}}}{\mathrm{C}_{\mathrm{F}}(\mathrm{RO,co})} C_{\mathrm{S}}\right) + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right) \\
&= \left(\frac{\left(\frac{N_{\text{solute}}}{C_{\mathrm{P}}(\mathrm{RO,co})}\right)}{A\gamma} + \frac{\pi_{\mathrm{F}}}{\mathrm{C}_{\mathrm{F}}(\mathrm{RO,co})} C_{\mathrm{S}}\right) + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right) \\
&= \left(\frac{\left(\frac{\left(\frac{D_{2M}}{K\delta}\right) C_{\mathrm{S}}}{C_{\mathrm{P}}(\mathrm{RO,co})}\right)}{A\gamma} + \frac{\pi_{\mathrm{F}}}{\mathrm{C}_{\mathrm{F}}(\mathrm{RO,co})} C_{\mathrm{S}}(\mathrm{RO,co})\right) + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right) \\
&= \frac{D_{2M}\left(C_{\mathrm{F}}(\mathrm{RO,co}) + C_{\mathrm{R}}(\mathrm{RO,co})\right)}{2K\delta A\gamma C_{\mathrm{P}}(\mathrm{RO,co})} + \frac{\pi_{\mathrm{F}}}{\mathrm{C}_{\mathrm{F}}(\mathrm{RO,co})}\left(\frac{C_{\mathrm{F}}(\mathrm{RO,co}) + C_{\mathrm{R}}(\mathrm{RO,co})}{2}\right) \\
&\quad + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right)
\end{aligned} \tag{35}
$$

Hence, equation **(35)** can be simplified as follows:

$$
P_{\mathrm{F}} = \frac{\mathrm{SFC}\left(C_{\mathrm{F}}(\mathrm{RO,co}) + C_{\mathrm{R}}(\mathrm{RO,co})\right)}{A\gamma C_{\mathrm{P}}(\mathrm{RO,co})} + \frac{1}{2}\pi_{\mathrm{F}}\left(1 + \frac{C_{\mathrm{R}}(\mathrm{RO,co})}{\mathrm{C}_{\mathrm{F}}(\mathrm{RO,co})}\right) + \left(\frac{\Delta P_{\text{shell}}}{2} + P_{\mathrm{P}}\right) \tag{36}
$$

Constant γ in **(12)** to **(21)** is defined as:

$$
\gamma = \left(\frac{\eta}{1 + \dfrac{16 A \mu r_{\mathrm{o}} L L_{\mathrm{s}} \eta}{1.0133 \times 10^{5} r_{\mathrm{i}}^{4}}}\right) \tag{37}
$$

where

$$\eta = \frac{\tanh\theta}{\theta}$$

$$\tanh\theta = \frac{e^{\theta} - e^{-\theta}}{e^{\theta} + e^{-\theta}} = \frac{e^{2\theta} - 1}{e^{2\theta} + 1}$$

$$\theta = \left(\frac{16A\mu r_o}{1.0133\times 10^5 r_i^2}\right)^{1/2} \frac{L}{r_i}$$

4.2.5 Big-*M* Logical Constraints

Big-M logical constraints relate continuous variables to 0–1 binary variables. For water network problem, it represents a stream flowrate to existence of stream or pipe connection. This constraint ensures non-zero flowrate when stream is selected in optimal solution or vice versa. For instance, a binary variable of 1 implies the existence of a stream that indicates there is a flowrate to operate the stream. For the case of dealing with such logic constraints that involve continuous variables as corresponded to this work, the conversion of that logic into mixed-integer constraints is applied by using the "big-*M*" constraints (Biegler et al., 1997). The "big-*M*" parameters associated with these constraints are denoted as the upper and lower bounds for the related continuous variables. Formulations of big-M logical constraints on flowrates balances for this problem are shown in equations **(38)** until **(45)**.

$$Q_{\mathrm{a}}(\mathrm{so,si}) \le \overline{M_{\mathrm{a}}}(\mathrm{so,si})\, Y_{\mathrm{a}}(\mathrm{so,si}) \tag{38}$$

$$Q_{\mathrm{b,perm}}(\mathrm{int,si}) \le \overline{M_{b,perm}}(int,si)\, Y_{\mathrm{b,perm}}(\mathrm{int,si}) \tag{39}$$

$$Q_{\mathrm{b,rej}}(\mathrm{int,si}) \le \overline{M_{b,rej}}(int,si)\, Y_{\mathrm{b,rej}}(\mathrm{int,si}) \tag{40}$$

$$Q_{\mathrm{d}}(\mathrm{so,int}) \le \overline{M_{d}}(so,int)\, Y_{\mathrm{d}}(\mathrm{so,int}) \tag{41}$$

$$Q_{\mathrm{a}}(\mathrm{so,si}) \ge \underline{M_{a}}(so,si)\, Y_{\mathrm{a}}(\mathrm{so,si}) \tag{42}$$

$$Q_{\mathrm{b,perm}}(\mathrm{int,si}) \ge \underline{M_{b,perm}}(int,si)\, Y_{\mathrm{b,perm}}(\mathrm{int,si}) \tag{43}$$

$$Q_{\mathrm{b,rej}}(\mathrm{int,si}) \ge \underline{M_{b,rej}}(int,si)\, Y_{\mathrm{b,rej}}(\mathrm{int,si}) \tag{44}$$

$$Q_{\mathrm{d}}(\mathrm{so,int}) \ge \underline{M_{d}}(so,int)\, Y_{\mathrm{d}}(\mathrm{so,int}) \tag{45}$$

From the computational experiments, the lower bound for big-M constraints and larger values of upper bound for big-M tend to give a poorer relaxation during solution phase which leads to infeasible solution. Thus, specifications of tighter lower and upper bounds for big-M constraints are required in order to solve this problem.

Table 4.1 Specification on Upper Bound of Big-M Logical Constraints

Origin	**Destination**	**Upper bound**
Source	Sink	The smaller (minimum) value between the two
Source	Interceptor	Follows source flowrate
Interceptor	Sink	Follows sink flowrate
Source and interceptor	Discharge	Summation of all sources

4.2.6 Model Tightening Constraints

The following constraints are enforced in the MINLP model for a complete representation of the problem:

a) Lower and upper bounds on the variable flowrate of feed, $Q_F(\text{int})$ into the RO interceptor

$$Q_F^L(\text{int}) \le Q_F(\text{int}) \le Q_F^U(\text{int}) \qquad \textbf{(46)}$$

where

$$Q_F(\text{int}) = \sum_{so \in SO} Q_d(so,\text{int}) \qquad \forall \text{int} \in \text{INT}$$

In the computational experiments on the TAC minimization problem for offline parametric optimization, the variable $Q_F(\text{int})$ into the RO interceptor tends to assume the specified lower bound value. Therefore, a good lower bound value has to be chosen for this purpose.

b) Lower and upper bounds on variable pressure of feed, P_F into RO interceptor

$$P_F^L \le P_F \le P_F^U \qquad \textbf{(47)}$$

It is noteworthy that equation **(29)** tends to give numerical difficulties in the computational experiment arising from division with a zero value. Although this can be overcome by specifying a non-zero lower bound value of $Q_{b,perm}$, the model solution still tends to be infeasible. Therefore, the lower and upper bound values of variable P_F are enforced in the model based on the common range specified by El-Halwagi (1997).

c) Lower and upper bounds on variable osmotic pressure of RO interceptor, $\Delta\pi_{RO}$ at the reject side

$$\Delta\pi_{RO}^L \le \Delta\pi_{RO} \le \Delta\pi_{RO}^U \qquad \textbf{(48)}$$

The osmotic pressure tends to return as an illogical value (more than 1000 atm) as the model is solved without specifying the upper and lower bounds on the osmotic pressure. Therefore, both the upper and lower bound values have to be incorporated into the model. However, it is also observed that the variable $\Delta\pi_{RO}$ tends to assume the specified upper bound value as they are incorporated. A good upper bound value has to be chosen for this purpose.

d) Forbidden interconnection between the freshwater stream to RO interceptor

$$Q_1(\text{'freshwater'}) = \sum_{si \in SINK} Q_a(\text{'freshwater'}, si) \qquad \textbf{(49)}$$

To avoid the freshwater from going directly into the RO interceptor, the above constraint **(49)** is enforced so that the freshwater will only directly consumed by the sinks. The contaminant concentrations in the freshwater shall be low enough where the treatment of freshwater is not practical.

4.2.7 Solution Strategy in Handling Bilinearities by Piecewise Linear Relaxation

A possible relaxation of bilinear variables would be to substitute every occurrence of these variables by a new variable, z. They are restricted by adding the following linear constraints:

$$\begin{aligned}
&\text{convex envelope:} \\
&\qquad \text{(a)}\quad z \geq y^L x + x^L y - x^L y^L \\
&\qquad \text{(b)}\quad z \geq y^U x + x^U y - x^U y^U \\
&\text{concave envelope:} \\
&\qquad \text{(a)}\quad z \leq y^U x + x^L y - x^L y^U \\
&\qquad \text{(b)}\quad z \leq y^L x + x^U y - x^U y^L
\end{aligned} \tag{50}$$

where in this case, variable flowrate,Q is represented by x while variable contaminant concentration,C is indicated by y.

Applying the incremental cost formulation to model partitioning the search domain, the use of $\theta(n)$ as binary variables is occupied.

$$\theta(n) = \mathrm{mu}(n, rr) = \begin{cases} 1, & \text{if } x \geq x(n) \\ 0, & \text{otherwise} \end{cases} \qquad 1 \leq n \leq (N-1) \tag{51}$$

First, we use the local incremental variable in (3)

$$\begin{aligned}
&Q = Q^L + \sum_{n=1}^{N} \left(d(n) \cdot \delta u(n)\right) \qquad 0 \leq \delta u(n) \leq 1 \\
&\text{where} \\
&\qquad \delta u(n) \geq \theta(n) \\
&\qquad \delta u(n) \leq \theta(n-1)
\end{aligned} \tag{52}$$

Note that the following constraints are added in each partition (Wicaksono and Karimi, 2008)

$$\begin{aligned}
&\theta(1) \leq \delta u(1) \\
&\delta u(n) \leq \theta(n-1)
\end{aligned} \tag{53}$$

Next, multiplying **(52)** by δC and defining $\delta w(n) = \delta u(\mathrm{n})\cdot \delta y$ where $\delta C = C\text{-}C^L$ give us:

$$
\begin{aligned}
&Q\cdot\delta C = Q^L\cdot\delta C + \delta C\sum_{n=1}^{N}\left(d(n)\cdot\delta u(n)\right)\\
&Q\left(C-C^{\mathrm{L}}\right) = Q^{\mathrm{L}}\left(C-C^{\mathrm{L}}\right) + \left(C-C^{\mathrm{L}}\right)\sum_{n=1}^{N} d(n)\cdot\delta u(n)\\
&\underbrace{QC}_{z} - QC^{\mathrm{L}} = Q^{\mathrm{L}}C - Q^{\mathrm{L}}C^{\mathrm{L}} + \sum_{n=1}^{N} d(n)\cdot\underbrace{\left(\delta u(n)\left(C-C^{\mathrm{L}}\right)\right)}_{\delta w(n)}\\
&z = QC^{\mathrm{L}} + Q^{\mathrm{L}}C - Q^{\mathrm{L}}C^{\mathrm{L}} + \sum_{n=1}^{N} d(n)\cdot\delta w(n)
\end{aligned}
\qquad \textbf{(54)}
$$

The hard bounds of $\delta u(\mathrm{n})$ is taken into consideration compared to the tighter bounds of $\delta u(\mathrm{n})$ which involves the variable θ. The convex and concave envelope can be tighten up by replacing the following relations into **(50)**.

$$
\begin{aligned}
&z = QC\\
&Q = \delta u(n)\\
&C = C - C^{\mathrm{L}}\\
&Q^{\mathrm{L}} = 0\\
&Q^{\mathrm{U}} = 1\\
&C^{\mathrm{L}} = 0\\
&C^{\mathrm{U}} = C^{\mathrm{U}} - C^{\mathrm{L}}
\end{aligned}
$$

The derivations are represented by **(55)** – **(58)**.

convex envelope (a):

$$
\begin{aligned}
&z \ge C^L Q + Q^L C - Q^L C^L\\
&QC \ge 0\cdot\delta u(n) + 0\cdot(C - C^{\mathrm{L}}) - 0\cdot 0\\
&\delta u(n)\cdot(C - C^{\mathrm{L}}) \ge 0\\
&\delta w(n) \ge 0 \qquad \text{(eliminated)}
\end{aligned}
\qquad \textbf{(55)}
$$

convex envelope (b):

$$\begin{aligned} & z \geq C^U Q + Q^U C - Q^U C^U \\ & QC \geq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) + 1 \cdot (C - C^{\mathrm{L}}) - 1 \cdot (C^U - C^{\mathrm{L}}) \\ & \delta u(n) \cdot (C - C^{\mathrm{L}}) \geq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) + C - C^U \\ & \delta w(n) \geq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) + C - C^U \end{aligned} \qquad \textbf{(56)}$$

concave envelope (a):

$$\begin{aligned} & z \leq C^U Q + Q^L C - Q^L C^U \\ & QC \leq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) + 0 \cdot (C - C^{\mathrm{L}}) - 0 \cdot (C^U - C^{\mathrm{L}}) \\ & \delta u(n) \cdot (C - C^{\mathrm{L}}) \leq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) \\ & \delta w(n) \leq (C^U - C^{\mathrm{L}}) \cdot \delta u(n) \end{aligned} \qquad \textbf{(57)}$$

concave envelope (b):

$$\begin{aligned} & z \leq C^L Q + Q^U C - Q^U C^L \\ & QC \leq 0 \cdot \delta u(n) + 1 \cdot (C - C^{\mathrm{L}}) - 1 \cdot 0 \\ & \delta u(n) \cdot (C - C^{\mathrm{L}}) \leq (C - C^{\mathrm{L}}) \\ & \delta w(n) \leq (C - C^{\mathrm{L}}) \end{aligned} \qquad \textbf{(58)}$$

CHAPTER 5

RESULTS AND DISCUSSION

5.1 PROBLEM DATA FOR MODEL

Table 5.1 Fixed Flowrates for Sources

Source	Flowrate (m^3/h)
PSR-1_ProcessArea	23
BW1	1.8
BD3	3.5
OWe-RG2	25
BDBLs2	72.3
SW2	2

Table 5.2 Fixed Flowrates for Sinks

Sink	Flowrate (m^3/h)
FIREWATER	3
OSW-SB	144
BOILER	128.3
HPU2	29.7
PSR1_SW	2
BDBLu	56.3333

Table 5.3 Maximum Inlet Concentration to the Sources

Source	Maximum Allowable Inlet Concentration for TSS (mg/L)
PSR-1_ProcessArea	40
BW1	37
BD3	1.00
OWe-RG2	12
BDBLs2	0.129
SW2	10
FRESHWATER	300
Note: Standard B Limit	100

Table 5.4 Maximum Inlet Concentration to the Sinks

Sink	Maximum Allowable Inlet Concentration for TSS (mg/L)
FIREWATER	25
OSW-SB	20
BOILER	20
HPU2	25
PSR1_SW	25
BDBLu	25
Discharge	100
Note: Standard B Limit	100

Table 5.5 Liquid Phase Recovery α and Removal Ratio *RR* for Reverse Osmosis Interceptor

Parameters	Fixed Values
Liquid Phase Recovery, α	0.7
Removal Ratio of TSS Contaminant	0.975

Table 5.6 Economic Data, Physical Constants, and Other Model Parameters (mainly for objective function formulation)

Parameters	**Fixed Values**
Annual operating time, AOT	8760 hr/yr
Unit cost for discharge (effluent treatment), $C_{discharge}$	\$0.22/ton
Unit cost for freshwater, C_{water}	\$0.13/ton
Manhattan distance, D	100 m
Fractional interest rate per year, m	5% = 0.05
Number of years, n	5 years
Parameter for piping cost based on CE plant index, p	7200 (carbon steel piping at CE plant index = 318.3)
Parameter for piping cost based on CE plant index, q	250 (carbon steel piping at CE plant index = 318.3)
Velocity, v	1 m/s

Table 5.7 Economic Data for Detailed Design of HFRO Interceptor

Parameters	**Fixed Values**
Viscosity of water μ	0.001 kg/m.s
Water permeability coefficient, A	5.573×10^{-8} m/s.atm
Annual operating time, AOT	8760 hr/yr
Cost of pretreatment chemicals, $C_{chemicals}$	\$0.03/m^3
Cost of electricity, $C_{electricity}$	\$0.06/kW.hr
Cost per module of HFRO membrane, C_{module}	\$2300/yr.module
Cost coefficient for pump, C_{pump}	\$6.5/yr.W$^{0.65}$
Cost coefficient for turbine, $C_{turbine}$	\$18.4/yr.W$^{0.43}$

Table 5.8 Geometrical Properties and Dimensions for Detailed Design of HFRO Interceptor

Module Property	**Value**
Solute (contaminant) flux constant, $D_{2M}/K\delta$	1.82×10^{-8} m/s
HFRO fiber length, L	0.750 m
HFRO seal length, L_s	0.075 m
Permeate pressure from interceptor, P_p	1 atm
Inside radius of HFRO fiber, r_i	21×10^{-6} m
Outside radius of HFRO fiber, r_o	42×10^{-6} m
Membrane area per module S_m	180 m^2 per module

Table 5.9 Physical Properties for Detailed Design of HFRO Interceptor

Module Property	**Value**
Shell side pressure drop per HFRO membrane module, ΔP_{shell}	0.4 atm
Pump efficiency, η_{pump}	0.7
Turbine efficiency, $\eta_{turbine}$	0.7
Osmotic pressure coefficient at HFRO, OS	0.006 psi/(mg/L) = 4.0828×10^{-4} atm
Solute (contaminant) permeability coefficient, K_C	$1.82\ 10^{-8}$ m/s

5.2 COMPUTATIONAL RESULTS

We consider four case studies that are simplified variants of an actual real-world industrial-scale water network design problem to demonstrate the proposed model formulation and modeling approach in general. The cases involve seven sources, one interceptor of reverse osmosis treatment technology, seven sinks, and one quality parameter of contaminant concentrations. The comparisons between these case studies are illustrated below.

Table 5.10 Comparison between Case Study 1, 2, 3 and 4

Case Study	**Model Formulation**	**Solution Strategy**
Case Study 1	Conventional mass balances (Tan et al., 2009; Meyer and Floudas, 2006; and Gabriel and El-Halwagi, 2005)	Without PLR
Case Study 2	Revised formulation on material balances for interceptors and on expression for CF	Without PLR
Case Study 3	Conventional mass balances	Convex relaxation based on PLR
Case Study 4	Revised formulation on material balances for interceptors and on expression for CF	Convex relaxation based on PLR

Table 5.11 Comparisons of Computational Results to Determine the Optimal Design and Suitable Solution Strategies

No	**Item**	**Case Study 1**	**Case Study 2**	**Case Study 3**	**Case Study 4**
1	**Economic parameters**				
a	Total cost for water integration and retrofit (dollar per year)	466 800	470 300	615 300	554 100
b	Total annualized cost (TAC) of RO	96 290	96 290	96 290	18 850
2	**Design parameters of RO**				
a	Feed pressure into interceptor, P_F (atm)	56.812	56.812	56.812	1.400
b	Reject pressure from interceptor, P_R (atm)	56.412	56.412	56.412	1.000
c	Osmotic pressure at reject side, $\Delta\pi_{RO}$	55.000	32.500	10.000	21.250
d	Optimal duties of RON				
	Power of pump (kW)	62 840	62 840	113 600	814.0
	Power of turbine (kW)	18 720	18 720	445 600	0
3	**Water flowrates**				
a	Total freshwater with reuse, regeneration and recycle (m^3/hr)	243.033	241.033	285.736	253.262
b	Total inlet flow into RO Q_F (m^3/h)	40.000	40.000	40.000	40.000
c	Total permeate stream outlet flow of RO Q_P (m^3/h)	28.000	28.000	39.900	28.000
d	Total reject stream outlet flow of RO Q_R (m^3/h)	12.000	12.000	0.100	12.000
4	**Contaminant concentrations**				
a	Feed concentration into RO interceptor C_F(RO,co) (mg/L)	0.129	0.129	0.0004	6.107
b	Permeate concentration from RO interceptor C_{perm}(RO,co) (mg/L)	0.005	0	0	0.153
c	Reject concentration from RO interceptor C_{rej}(RO,co) (mg/L)	0.419	0.430	0	20.000

Note: All values are reported to the nearest 4 significant values. Any flowrate value smaller than 0.05 m^3/h is taken to be zero (which indicate that the associated piping interconnection is not operated).

Table 5.12 Model Sizes and Computational Statistics

Case Study	**Case Study 1**	**Case Study 2**	**Case Study 3**	**Case Study 4**
Type of model	MINLP	MINLP	MINLP	MINLP
Solver	GAMS/BARON	GAMS/BARON	GAMS/BARON	GAMS/BARON
No. of continuous variables	162	164	809	802
No. of discrete binary variables	70	70	87	87
No. of constraints	107	110	1027	1043
No. of iterations	0	0	0	0
CPU time (s) (resource usage)	3369.250	3592.940	15.760	19.840
Remarks	Integer Solution	Integer Solution	Integer Solution	Integer Solution

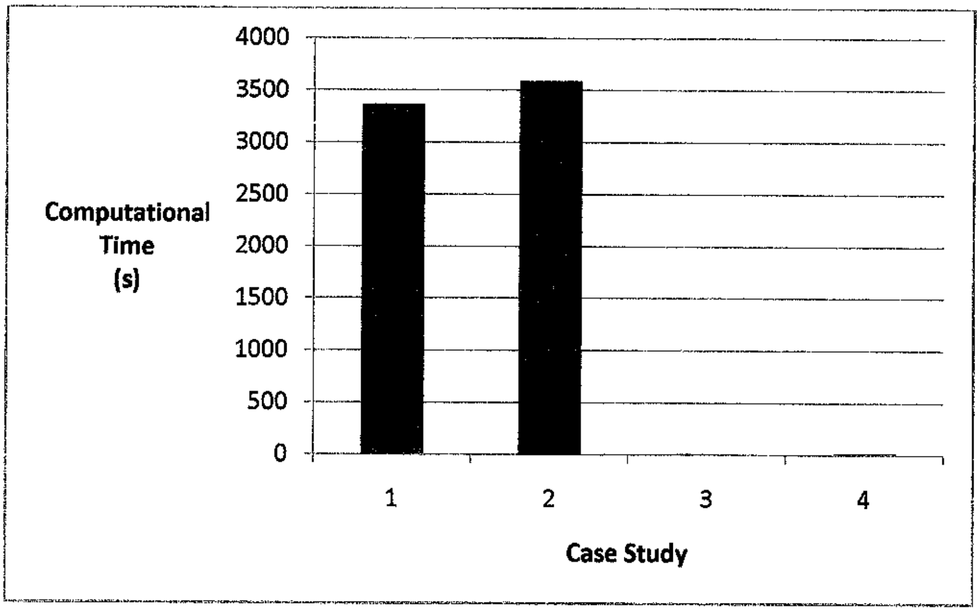

Figure 5.1 Comparison on Computational Time for 4 Case Studies

5.2.1 Calculation for percentage of reduction on computational time

Take average time (s) for case study without PLR and with PLR, we get:

$$\text{Reduction (\%)} = \frac{3480-17}{3480} \times 100 = 99.51\%$$

5.2.2 Optimum Allocation of Source-Interceptor-Sink

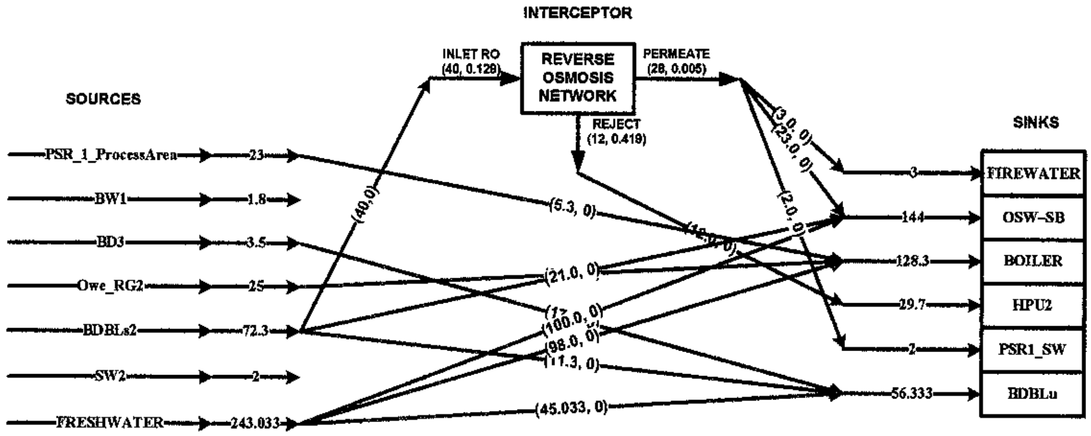

Figure 5.2 Optimal Network Structure for Case Study 1

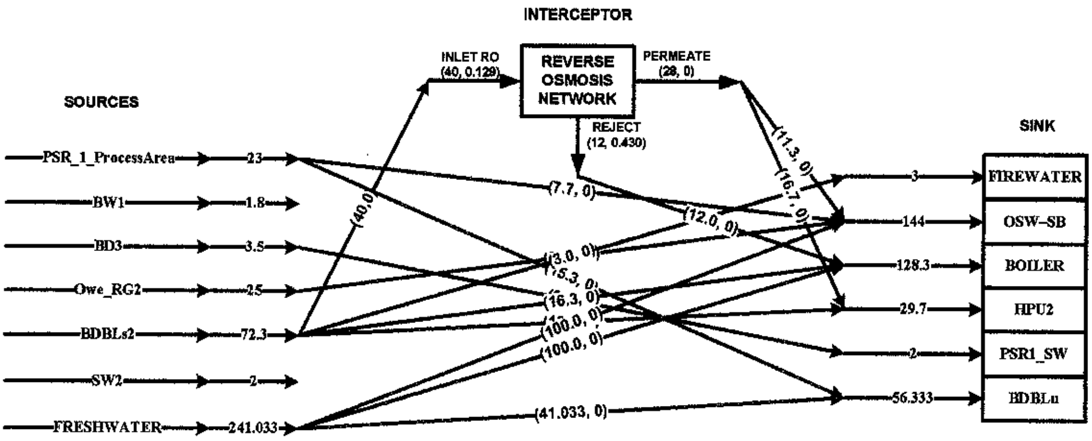

Figure 5.3 Optimal Network Structure for Case Study 2

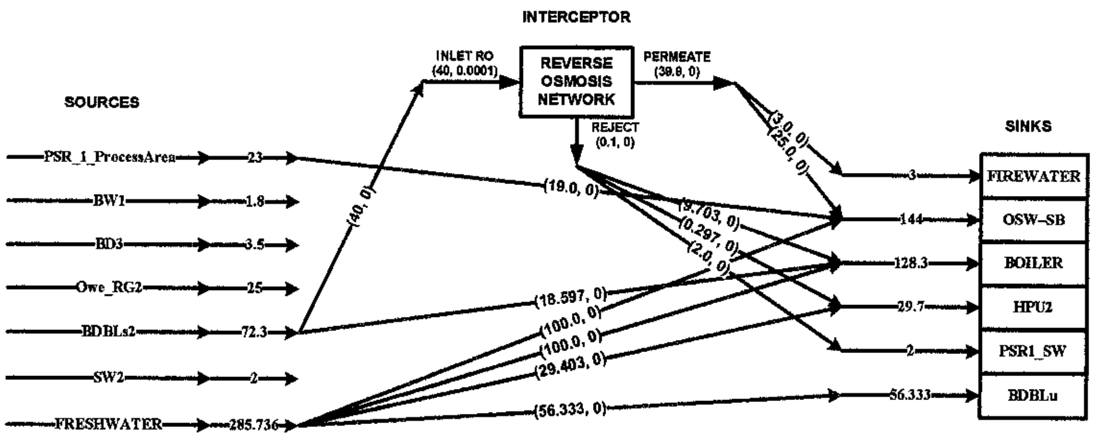

Figure 5.4 Optimal Network Structure for Case Study 3

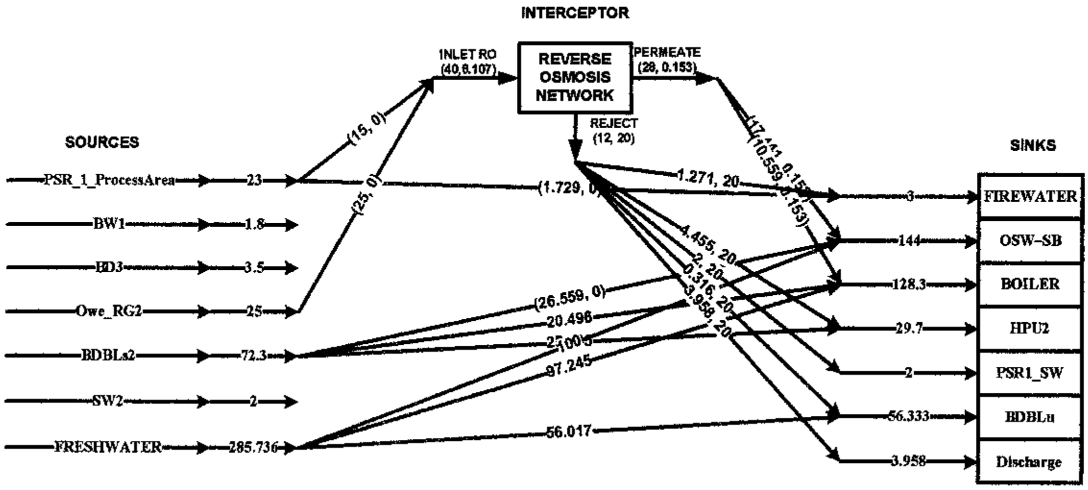

Figure 5.5 Optimal Network Structure for Case Study 4

Note: values in parentheses on stream lines indicate water flowrates in m^3/h, contaminant concentration in mg/L

5.3 DISCUSSION

Based on the comparison of computational results for case study 1, 2, 3 and 4 that is explained in previous section, it shows that the formulation with convex relaxation based on Piecewise Linear Relaxation (PLR) gives a much lower computational time which is proposed by Gounaris, Misener and Floudas (2009). The notion proposed by Pham et al. (2009) is proven which stated that this solution strategy can give fast computational time for a large-scale problem. The results demonstrated that PLR can improve the results in terms of the tightness of lower bound in such a way the original domain of one of the two variables in bilinear terms is partitioned into many subdomains and the principles of bilinear relaxation are applied for each of them (Gounaris et al., 2009).

The optimum structure of source-interceptor-sink for these case studies mostly involves water regeneration-reused as its water minimization technique. Case Study 4 represents a better possible freshwater usage as well as the interconnections between interceptor and the sinks since it supplies to more sinks compared to the other case studies. Although Case Study 1 registers the lowest cost, this may not be the global optimal solution. The formulation with reduced bilinearities in Case Study

4 represents a more attractive solution, which to some extent proves the benefit of avoiding nonconvexities due to bilinearities.

The formulation with reduced bilinearities offers a more cost-effective design, presents a better design that involves generally lower pressure and requires less pumping power that leads to a lower cost. Besides, the formulation with reduced bilinearities presents an optimal design that omits the use of turbine as a final energy recovery stage because the reject stream is at a relatively low pressure.

In general, the formulation with reduced bilinearities proposes an optimal design that is competitive against the designs presented by the other approaches. Despite involving the highest concentrations, the formulation with reduced bilinearities is still within the regulatory limits.

CHAPTER 6
CONCLUSION AND RECOMMENDATION

6.1 CONCLUSION

All in all, this work proves that Piecewise Linear Relaxation can give fast computational time for a large-scale optimization problem. It can be applied as a solution strategy in handling the bilinearities in this case. The revised formulation for interceptor where the bilinear terms in this problem are reduced with the presence of PLR technique proposes the best global optimal solution. The development of these techniques and tools are significant in order to deal with the integrated water management problem at petroleum refineries, which become the main concern and interest associated with the shortage of freshwater supply within our country.

6.2 RECOMMENDATION

It is recommended to apply Piecewise Linear Relaxation in the actual real-world industrial-scale water network design problem which is very much a larger problem compared to the case studies. Besides, multiple contaminants can also be considered along with the complex detailed design of other interception technologies model formulation. Despite problem for a petroleum refinery, the application of PLR should be explored in various problems such as for a chemical plant or heat integration network problem.

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