Optimization with Integrated Offline Parametric Optimization of Detailed Process Model of an Interceptor Unit for Water Network Synthesis and Retrofit Design

by

Norafidah binti Ismail (8401)

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

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CERTIFICATION OF APPROVAL

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Approved by,

(Khor Cheng Seong)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

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SAMPLE OF CERTIFICATION OF ORIGINALITY

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.

NORAFIDAH BINTI ISMAIL

ACKNOWLEDGEMENT

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ABBREVIATIONS

W3R	water reuse, regeneration, and recycle
GAMS	general algebraic modeling system
BARON	branch and reduce optimization navigator
LP	linear programming
MILP	mixed-integer linear programming
MINLP	mixed-integer nonlinear programming
NLP	nonlinear programming
RO	reverse osmosis
RON	reverse osmosis network
HFRO	hollow fiber reverse osmosis
COD	chemical oxygen demand
OnG	oil and grease
TSS	total suspended solids

NOTATION AND NOMENCLATURE

Sets and Indices

SOURCE	set of sources *so*
SINK	set of sinks *si*
INTERCEPTOR	set of interceptor *int* (in this project, it represents only a single-stage reverse osmosis network)

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*
$M_{b,\text{perm}}$ (int,si)	big-M parameter for interconnection between interceptor *int* permeate *perm* to sink unit operation *si*
$M_{b,\text{rej}}$ (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 *co* in feed *F* of interceptor *int*
C_{perm} (int,co)	contaminant concentration *co* in interceptor *int* permeate *perm*
C_{rej} (int,co)	contaminant concentration *co* in interceptor *int* reject *rej*
Q_a (so,si)	flowrate of source stream *so* to sink unit operation *si*
$Q_{b,perm}$ (int,si)	flowrate of interceptor *int* permeate *perm* to sink unit operation *si*
$Q_{b,rej}$ (int,si)	flowrate of interceptor *int* reject *rej* to sink unit operation *si*
Q_d (so,int)	flowrate of source stream *so* to interceptor *int*
Q_F (int)	total feed flowrate into interceptor *int*
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 *so* to sink unit operation *si*
$Y_{b,perm}$ (int,si)	piping interconnection between interceptor *int* permeate *perm* to sink unit operation *si*
$Y_{b,rej}$ (int,si)	piping interconnection between interceptor *int* reject *rej* to sink unit operation *si*
Y_d (so,int)	piping interconnection between source stream *so* to interceptor *int*

ABSTRACT

Petroleum refineries is a prime example of industrial plants that demand high quantities of water for process consumption and generate volumes of highly contaminated industrial effluents and wastewaters. Scarcity of freshwater resources and increasingly stringent environmental regulations on industrial effluents have motivated refineries to develop water reuse technologies for sustainability of plant operations. The technology concept can be characterized into three (3) strategies: reuse, regeneration, and recycle (W3R). The major contribution of this work is to consider the design of alternative refinery water network structures that incorporate the detailed design of wastewater treatment technology (or interceptor) in an optimization-based modeling framework as an offline parameter optimization problem. For this purpose, a source–interceptor–sink superstructure representation is adopted that embeds many feasibly possible alternative water network configurations. A mixed-integer nonlinear programming (MINLP) optimization model is formulated based on the superstructure with the objective of minimizing freshwater import, wastewater generation, piping interconnections, and the total cost of installing and operating the treatment technology. The parametric optimization problem comprising of material balances and the detailed phenomena model for interceptor, specifically for a single-stage hollow fiber reverse osmosis (HFRO) membrane module, is incorporated in the overall MINLP framework. The modeling approach is developed in conjunction with its implementation into general algebraic modeling system (GAMS), using data of a real operating refinery situation. The model is solved iteratively by branch and reduce optimization navigator (BARON), resulting in freshwater consumption requirements to be 296.2 m^3/h at the optimal refinery water network structure and operating conditions, which accounts for nearly 61% of water recovery compared to current operating requirements (before the integration and retrofit initiatives based on W3R).

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CHAPTER 1

INTRODUCTION

1 BACKGROUND OF STUDY

1.1 Motivation for Optimizing Water Network Design and Retrofitting

Water consumption in a petroleum refinery generally demands high quantities for steam generation, process cooling system, and other purposes. Four (4) major processes in which that steam generation is playing significant role are distillation, desulfurization, alkylation, and hydrogen production. Since steam cannot be directly reused as returned condensate in the refining process, requirements for make-up water normally are high. Similar condition takes place to the process cooling system, characterized by make-up water required by cooling towers.

Simultaneously, refinery as well is the major contributor for large volumes of highly contaminated industrial effluents and wastewaters. The contaminants associated are such as biochemical oxygen demand (BOD) and chemical oxygen demand (COD) contributed by hydrogen sulphide, ammonia, phenol, sulphides, suspended solids, dissolved solids, etc., emulsified oil, benzene, benzo(a)pyrene, heavy metals, and other pollutants. **Table 1.1** in the next page shows the qualitative evaluations on general petroleum refinery wastewater flow and characteristics.

Globally, the water resources in various regions and countries are expected to face unprecedented pressures in the coming decades as a result of continuing population growth and uneven distributions of population and water (Asano et al., 2007). This can be described by urbanization development, in which that imbalance between water demands and sources may be resulted due to population growth.

Table 1.1: Qualitative evaluation of refinery wastewater flow and characteristics (Wang et al., 2004)

Source of waste	Flow	BOD	COD	Phenol	Sulfide	Free Oil	Emulsified Oil	pH	Temperature	Ammonia	Chloride	Acidity	Alkalinity	Suspended Solids
Crude oil and product storage	xx	x	xxx	x		xxx	xx	o	o	o	n/a	o	n/a	xx
Crude desalting	••	••	••	•	•••	•	•••	•	•••	••	•••	o	•	•••
Crude distillation	•••	•	•	••	•••	••	•••	•	••	•••	•	o	•	•
Thermal cracking	•	•	•	•	•	•		••	••	•	•	o	••	•
Catalytic cracking	•••	••	••	•••	•••	•	•	•••	••	•••	•	o	•••	•
Hydrocracking	•	n/a	n/a	••	••	n/a	n/a	n/a	••	••	n/a	n/a	n/a	n/a
Polymerization	•	•	•	o	•	•	o	•	•	•	•	•	o	•
Alkylation	••	•	•	o	••	•	o	••	•	•	••	••	o	••
Isomerization	•	n/a.	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Reforming	•	o	o	•	•	•	o	o	•	•	o	o	o	o
Solvent refining	•	n/a.	•	•	o	n/a	•	•	o	n/a	n/a	o	•	n/a
Asphalt blowing	•••	•••	•••	•	n/a	•••	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Dewaxing	•	•••	•••	•	o	•	o	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Hydrotreating	•	•	•	n/a	••	o	o	••	n/a	••	o	o	•	o
Drying and sweetening	•••	•••	•	••	o	o	•	••	o	•	o	•	•	••

Indicators:

xxx	major contribution
xx	moderate contribution
x	minor contribution
o	insignificant
n/a	not applicable

In addition to the scarcity of freshwater sources, stringent environmental regulations on wastewater discharges, increasing in environmental awareness, high cost of freshwater supply, and increasing in requirements for plant efficiency and optimization had driven a local refinery plant to implement the principle of sustainability of water supply to the plant operations. The goal of sustainable water resources development and management is to meet water needs reliably and equitably for current and future generations by designing integrated and adaptable systems, optimizing water-use efficiency, and making continuous efforts towards preservation and restoration of natural ecosystems (Asano et al., 2007). In addition, profitability of the industry or organization has to be maintained simultaneously with the development of water resources sustainability and environmental performance, which lead to the needing of process integration and optimization strategy to achieve such aspiration.

1.2 Definition of Reuse, Regeneration, and Recycle

For the purpose of process integration and optimization to sustain freshwater supply and minimize environmental impact from wastewater generation, a local refinery plant has included water reuse concept as part of its technology agenda. Consider the supply of fresh water to all operations in the plant without process integration and optimization, as depicted by a simple configuration in **Figure 1.1**. The explanation on reuse, regeneration, and recycle will be then utilizing the same representation throughout this section.

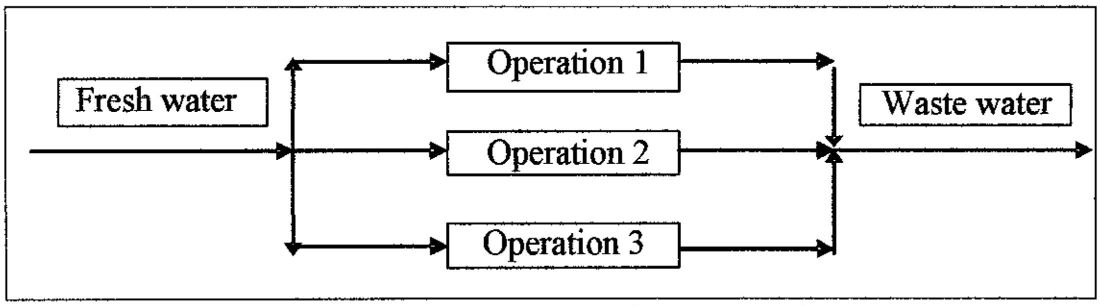

Figure 1.1: Freshwater Used in All Operations (Smith, 2005)

The concept of water reuse is characterized by reusing wastewater effluent from one operation, back into that similar operation or to other operation(s). The aims of this reuse technology as described previously can be achieved through the approaches of three (3) strategies as below and in the subsequent pages.

1. Water reuse

   Water reuse solely is a direct reuse of water to other operation(s) without any treatments, in which that the water effluent condition is insignificantly contaminated and exceed water purity requirement of the operation(s) to be fed. There are many examples when water with some level of certain contaminants is acceptable for use rather than using the highest quality water (Smith, 2005). The schematic of reuse strategy is represented below **(Figure 1.2)**.

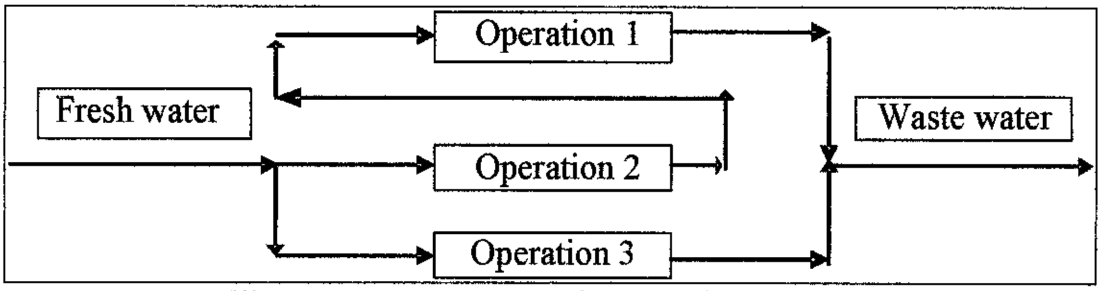

Figure 1.2: Water Reuse Scheme (Smith, 2005)

1. Water regeneration (i.e., treatment).

   Water regeneration can be as well referred as water treatment. Regeneration is a term used to describe any treatment process that regenerates the quality of water such that it is acceptable for further use (Smith, 2005). In addition, part of the contaminant loads is able to be removed or otherwise removed in the final effluent treatment before discharge as wastewater. Regeneration reuse strategy can be characterized as treating the water effluent before reusing it into the other operation(s). **Figure 1.3** below shows the schematic representation of regeneration reuse strategy.

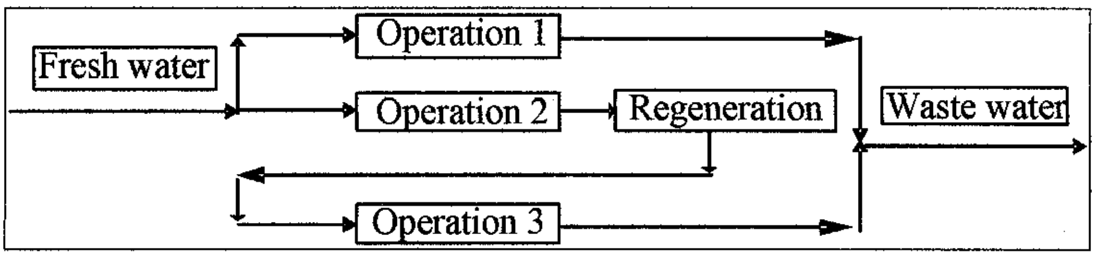

Figure 1.3: Water Regeneration Reuse Scheme (Smith, 2005)

2. Water recycle

The treated water effluent, which is recycled back into the similar operation or process in which it has been used previously, is called regeneration recycle strategy. Even though both regeneration reuse and regeneration recycle are producing similar outcomes, regeneration recycling allows larger reductions in the freshwater use and wastewater generation (Smith, 2005). However, major problem may be encountered characterized by the buildup of undesired contaminants in the recycle, such as microorganisms or products of corrosion. The buildup to the extent might create problems to the process. Schematic representation showing the configuration of the regeneration recycle strategy is depicted in **Figure 1.4** below.

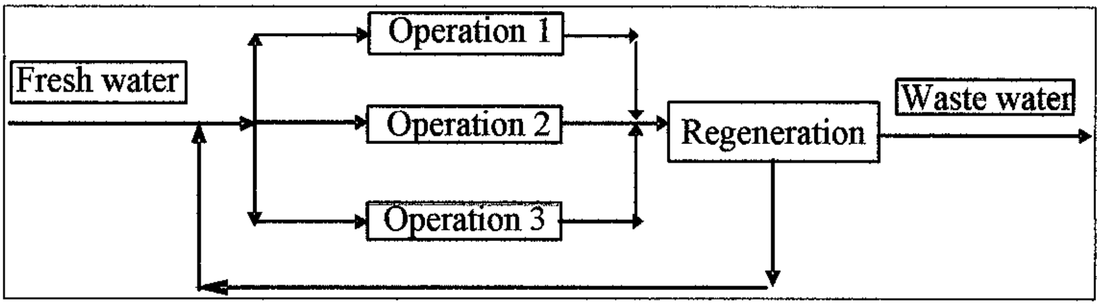

Figure 1.4: Water Regeneration Recycle Scheme (Smith, 2005)

All of the three (3) strategies mentioned are capable to minimize both freshwater usages and wastewater discharges that subsequently sustain the freshwater supply and minimize environmental impact from the wastewater generation.

1.3 Definition of Sources, Interceptors, and Sinks

Definition of sources, interceptors, and sinks are as below:

1. Sources are any streams whose water can be reused, regenerated, or recycled. Consider **Figure 1.2** previously, it is observed that Operation 2 is the source stream for Operation 1. **Figure 1.3** shows that apart of having the freshwater stream as the source for Operation 1 and 2, the stream from Operation 2 itself is the source for regeneration or treatment unit. **Figure 1.4** again shows that the streams coming out from all the three (3) operations are the source streams of the regeneration unit;

2. Interceptors are water treatment technologies that represent the regeneration strategy. **Figure 1.3** and **1.4** show the existence of interceptor in the strategy scheme;
3. Sinks are any units that can accept the reuse, regeneration, or recycle of water. Since Operation 1 in **Figure 1.2** accepts the stream from Operation 2, Operation 1 is therefore considered as the sink. In **Figure 1.3**, Operation 3 is a sink which accepts the regenerated water.

2 PROBLEM STATEMENT

From the previous mentioned driving motivations, the aim is to determine the possible options of optimized water network structure that allow for minimization of freshwater supply and wastewater generation. These can be developed given sets of data below, for the main optimization problem:

1. A set of process sources with flowrates and contaminant concentrations of their wastewater effluents that can be reused;
2. A set of process sinks with specific inlet flowrate which accept the reused and regenerated water;
3. A single interception unit or regeneration technology for wastewater treatment to remove the targeted species from the sources (note that in this work, the following terms are used interchangeably to refer to an interception unit: "interceptor", "regeneration technology", "regeneration unit", "regenerator", "treatment technology", and "treatment unit"). Particularly in this work, a single-stage RON is considered as the interception unit;
4. Maximum allowable contaminant concentrations of the sinks (maximum concentrations of sinks) for reused and regenerated water acceptance;
5. Freshwater source with known contaminant concentrations that can be purchased to supplement the use of process sources.

This main optimization problem is performed in conjunction with an offline unconstrained parameter optimization problem for the detailed design of a regeneration unit, for example, a reverse osmosis network (RON). This parametric optimization problem is a phenomena model of the detailed design of RO, in which that such model is developed in the form of a single parametric curve representing the minimum cost (in this case, the TAC). The functions governing the TAC are such as:

1. Inlet-outlet flows and concentrations;
2. Membrane types, sizes, number, and arrangement;
3. Optimal operating conditions, for example, the reject pressure of RO;
4. The type, size, and number of pump and turbine.

The cost minimization parametric curve is then incorporated into the main optimization problem.

Based on the given sets of data for the main optimization problem, and minimization of regeneration unit total cost for parametric optimization problem, the objective now is to determine the optimal design of water network structure that meets the following criteria:

1. Minimum freshwater use and wastewater generation;
2. Optimum allocation of sources to sinks, sources to interceptor, and interceptor to sinks as represented by their piping interconnections;
3. Optimum duties of source interception or regeneration which allow for minimum fixed and operating cost of interception unit.

The following assumptions are used in this work in conjunction with the problem representation (Leong, 2009):

1. The total flowrate of a stream is taken to be constant and equal to that of pure water in that stream since the level of individual contaminant flows is so slow and is therefore negligible (that is, the contaminants are at the concentration level of parts per million);
2. Water flow demands of the utility units are assumed to be fixed (for systems all data for the limiting water profiles is available and is certain);
3. The number of water using and water treatment operations is fixed;
4. The removal ratios *RR* and α for the treatment unit are independent of the inlet concentration to the particular unit;
5. Heat integration is not allowed, hence isothermal network operation is assumed;
6. The network operates under constant pressure (but for parametric optimization problem in determining the regeneration unit detailed design, the assumption is not implemented);
7. The contaminant load is fixed and is independent of the flowrate; although this assumption can be challenged conceptually and even practically in some cases, it has been considered adequate for most of the systems analyzed.

3 OBJECTIVES AND SCOPE OF STUDY

3.1 Objectives of Study

The main objective of this study is to formulate and solve for mathematical optimization modeling of water network design and retrofit in a local refinery plant. The models involve methodologies as below:

1. Superstructure representation: Identification of sources, interceptors, and sinks;
2. Optimization model formulation for a refinery water network that mainly consists of:
    - Material balances on water flowrates and contaminant concentrations, representing the parameters and continuous variables associated with the source-interceptor-sink interconnections;
    - Detailed design of the regeneration unit or water treatment technology that considers the operating conditions as described by flows, temperatures, and pressures of the unit;
    - Consideration of a mixed-integer nonlinear program (MINLP) model formulation that allows for explicit determination of optimal piping interconnections among sources, interceptor, and sinks, in conjunction with the optimal continuous variables (binary integers of mixing and/or splitting of streams, direct water reuse/recycle without regeneration, etc.);
3. Solution of the MINLP optimization models using GAMS modeling language;
4. Finally, validation of the model solution in terms of the optimal refinery water network structure/configuration design based on real-world practical features.

3.2 Scopes of Study

The MINLP model will be solved with the assistance of computer, specifically using GAMS software language that has several advantages over Water Pinch Analysis method. The advantages are (Leong, 2009):

1. It provides automated optimal solution (provided that the model formulation has been verified for correctness);
2. It is able to accommodate a large number of variables consisting of flowrates and multiple contaminant concentrations;
3. It provides ease of incorporating various constraints, for example, concentration limits to meet regulatory discharge requirements, in an effort to accurately model real-world situation;
4. It allows simultaneous considerations of multiple alternatives or options for water reuse, regeneration, and recycle opportunities.

A number of works on the optimization modelling have been developed previously to integrate the refinery plant water network structure. **Table 1.2** below shows the comparisons between the previous and current work approaches.

Table 1.2: Comparison between the Previous and the Current Work

Previous Works	Current Work
1. Retrofitted the existing water network structure.	1. Employs binary 0–1 variables to explicitly consider new alternative structures and designs.
2. Solved using non-linear programming (NLP) formulation.	2. Solved using mixed-integer nonlinear programming (MINLP) formulation
3. Did not incorporate detailed design for the regeneration or water treatment technology units	3. Incorporating the detailed design of water treatment technologies for water regeneration
4. Represented the structural representation using State-Task Network, STN representation	4. Representing the structural representation using Source-Interceptor-Sink superstructure representation

CHAPTER 2

LITERATURE REVIEW AND THEORY

Most of the studies published in literature have dealt with the issue of minimizing freshwater supply in water-using processes separately from the design of effluent treatment systems (Leong, 2009). It means that some of the previous studies did not take into consideration the regeneration units to be incorporated in the problem framework and be solved simultaneously.

1 GRAPHICAL TARGETTING METHOD

Other than graphical method proposed by Wang and Smith (1994) to find the target of minimum freshwater consumption, rigorous graphical targeting had also been presented by El-Halwagi et al. (2003). The paper presents a systematic, single-stage or noniterative, and graphical method for rigorously targeting minimum usage of fresh resources by using segregation, mixing, and direct recycle/reuse strategies. They had introduced the improvised version of graphical targeting method over the previous works that can be broadly classified as iterative targeting and detailed network design. Both iterative targeting and detailed network design characteristics can be eliminated by implementing the methodologies proposed by El-Halwagi et al. (2003) as below:

1. Describe the problem through optimization formulation.
2. Use dynamic programming techniques to determine the mathematical conditions and characteristics of an optimal solution strategy.
3. The conditions and characteristics are transformed into a graphical technique that can be readily used to identify rigorous targets for minimum usage of fresh resources.
4. The devised visualization tool is a novel graph of load versus flow rate constructed in a way that yields the rigorous target without iterations.
5. The minimum usage of freshwater, the minimum discharge of waste, and the maximum recycle/reuse of process streams can be determined from the devised visualization tool.

Even though the method had been proven easy and applicable, it does not take into account for optimal solution when incorporating regeneration strategy or effluent treatment systems into the problem representation, which will require more complex formulation and probably cannot be solved by graphical targeting method solely.

2 SOURCE SHIFTS

With the same purpose and satisfaction on targeting minimum freshwater, concept of source shifts to design many different water networks had been introduced by Prakash and Shenoy (2005). The concept is intended to allow the designer to explore many other possible alternative networks that satisfy minimum freshwater consumption in quick and systematic manner. Evolution of water networks to simpler practical designs may be as well achieved by using the source shift concept but at the cost of some penalty in freshwater usages. The paper basically shows how many different minimum freshwater networks may be designed and evolved to yield simpler designs with acceptable freshwater and wastewater penalties, all of which by using three-source and two-source shifts respectively.

Three-source shifts done in the paper is based on the concept of equivalent sources, for example "A water source S_j is equivalent to two (2) other sources S_i and S_k, if the two sources when mixed in a particular ratio have the same flowrate and effective concentration as the source S_j" (Prakash and Shenoy, 2005). Source S_j then can be shifted from a demand say D1 to another demand D2, and given fixed ratio fs_i of sourse S_i and $1-fs_i$ of source S_k that equivalently can be shifted from demand D2 to D1. New network designs can be generated then for minimum freshwater. Two-source shifts are able to eliminate few matches and lead to simplification of the networks but incurring freshwater penalty.

Even though the concept is very useful to evolve water network designs, regeneration strategy is still not included for the implementation purpose.

3 SOURCE-INTERCEPTOR-SINK REPRESENTATION

It is observed that earlier work only focused on the design issues concerning either one of the two subsystems to avoid handling the complex interactions between water using and wastewater-treatment networks (Leong, 2009). However, there are several literatures that provide the incorporation of regeneration strategy, and involve those complex interactions with water using operations for integrating the overall water network design. Those interactions are commonly represented as source-interceptor-sink framework, rather than only source-sink representations as per the proposals that had been discussed in Section 1 and 2 earlier. In many cases, direct recycling/reuse of process and waste streams may not be feasible because of intolerable levels of contaminants that can detrimental to the process performance or can build up to unacceptable levels. Therefore, interception may be used to selectively remove pollutants from the process streams using separation devices or interceptors (Gabriel and El-Halwagi, 2005). However, global optimization may not be able to guarantee for such complex interactions, for example the presence of bilinear terms that contribute to the nonconvexity.

4 GLOBAL OPTIMIZATION SOLUTION APPROACH

4.1 Problem Reformulation into a Linear Program

Gabriel and El-Halwagi (2005) had introduced a systematic procedure for material recovery and pollution prevention through simultaneous recycling/reuse and interception, by first represent the problem as the source-interception-sink structural representation. Based on the developed source-interception-sink framework, optimization formulation then can be described, resulting in development of MINLP formulation to determine the following:

1. Minimum cost of the fresh resources and interception units that satisfy the process requirements
2. Optimum allocation of sources to sinks
3. Optimum selection of interception devices
4. Optimum duties of source interception

The proposal states that reformulating the program into a linear program (LP) is needed, since global solution cannot be guaranteed by commercial software because of the nonconvexity of the objective function and the bilinearity of several constraints described in the literature. The global optimization procedure that is based on the problem reformulation can be developed by invoking several simplifying assumptions as follow:

1. No mixing of sources is allowed before interception; mixing is used primarily after interception and before entering the sinks
2. Each interceptor is discretized into a number of interceptors with given removal efficiencies
3. The total annualized cost of the interceptor is proportional to the removed load of the targeted species in the interceptor

Figure 2.1 and 2.2 show the source-interceptor-sink representations before and after the problem reformulation respectively.

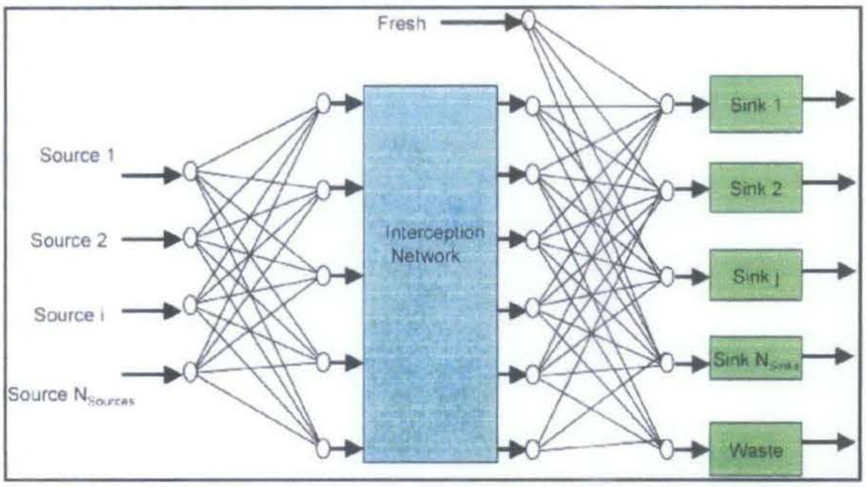

Figure 2.1: Structural Representation of the Problem (Gabriel and El-Halwagi, 2005)

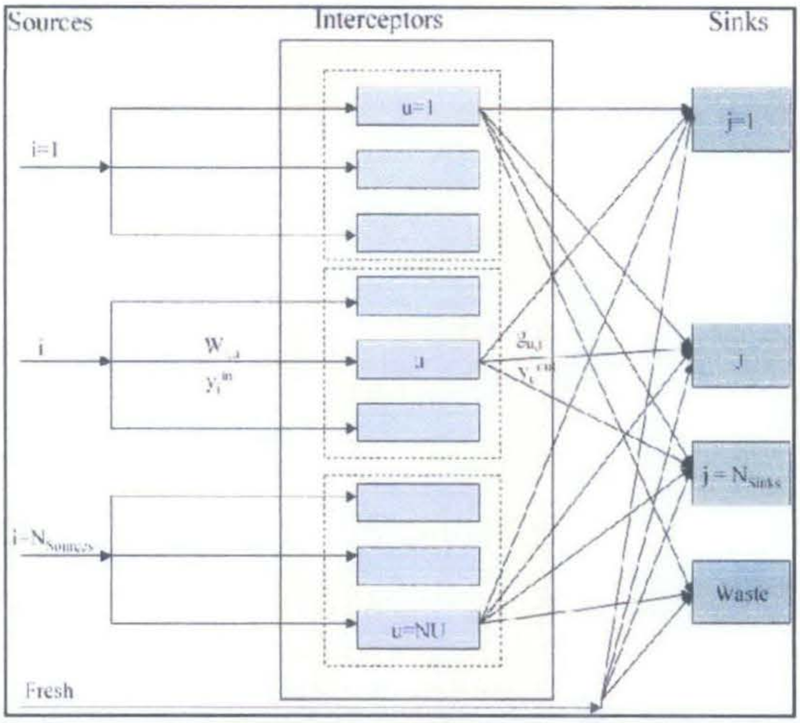

Figure 2.2: Structural Representation of the Reformulated Problem (Gabriel and El-Halwagi, 2005)

The problem reformulation into a linear program (LP) method had significantly contributed to the global optimization solution. However, through observation at the formulated constraints in the literature, the source that being allocated to the available sinks is only fresh water instead of considering the reuse from other source streams into the sinks. This phenomenon is clearly shown in **Figure 2.1 and 2.2** even though the problem statement of the literature says otherwise.

4.2 Piecewise Linear Reformulation Linearization Technique

Pooling problem is an industrially significant mathematical programming problem that originates from the petroleum refinery sector because of the various blending attributes in conjunction with the refined process streams (Meyer and Floudas, 2006). Meyer and Floudas (2006) propose for the three methodologies of convex relaxation to approach global optimization solution for the pooling problem, as follow:

1. The bilinear product convex envelope formulation
2. The Reformulation Linearization Technique, RLT formulation by reformulating the MINLP as the MILP.
3. The piecewise linear RLT by partitioning the original domain of the variables involved and application of the bilinear relaxation principles.

These approaches seem very useful for pooling problems characterized by the determination of various interceptor technologies and interconnection between them for regeneration strategy. Besides, the integrated piecewise linear RLT method is also being discussed thoroughly by Gounaris et al. (2009).

4.3 Convex Hull Discretization Approach

Another approach to cater for pooling problem in achieving global or near global optimal solution is the convex hull discretization approach as proposed by Pham, Laird, & El-Halwagi (2009). The additional advantage of this method is that it can actually produce the results in a reasonable computational time, since it is capable of reducing the problem size. There are three (3) concepts as the basis for this approach, which are:

1. Discretization of qualities or contaminant concentrations for each pool or interceptor.
2. Application of integer cuts for the pools or interceptors.
3. Convex hull search by invoking physical limits on the possible combinations of interceptor contaminant concentrations in the convex hull construction.

This approach is difficult to be implemented with GAMS program. It has been only proven applicable by LINGO program, which is the other available optimization software. Better insight on the literature is needed to implement this approach on GAMS.

5 SYNTHESIS OF WATER NETWORKS WITH PARTITIONING REGENERATORS

The incorporation of partitioning regenerators in a source-sink superstructure model had been discussed by Tan et al (2009). Partitioning regenerator function by splitting a contaminated water stream into a regenerated lean stream and a low-quality reject stream, which can be associated with membrane separation-based processes or technologies. They had proposed that both lean and reject stream are potentially to be reused/recycle within plant. Other model characteristics for the optimization model problem in the literature are:

1. Fixed flowrate and concentration of the sources. Part of the sources may be reused/recycled, sent to a centralized regenerator (interceptor) and/or discharged as effluent.
2. Sinks that demand for specific flowrate of water at or below a specified concentration limit.
3. Mixed water from different process sources is fed into a single partitioning regenerator. Both lean and reject stream discharged by the regenerator are potentially to be reused/recycle within plant.
4. The regenerator is assumed to be characterized by a fixed ratio of lean and rich stream flowrates and fixed contaminant removal ratio.

The literature by Tan et al (2009) is significantly contributing to the current progress of this research study. Material balances constraints for optimization model formulation in this work are mainly based on the model problem discussed by Tan et al (2009), due to the relevancy of the reverse osmosis unit with the partitioning regenerator.

6 INTER-PLANT WATER INTEGRATION

Inter-plant water integration is proposed to achieve the desire of integrating the groups of water network in accordance to the different geographical locations or the different business entities. Chew et al (2008) propose for both direct and indirect interplant water network synthesis for this purpose. The regeneration unit implementation is represented as the centralized hub for the indirect integration, modeled by MINLP formulation and solved using RLT. Another inter-plant water integration is discussed by Chew & Foo (2009) using the pinch analysis concept for network targetting. Both literatures analyze the incorporation of pipeline cost into the objective function formulation. Such detailed objective function formulation is being mainly refered for the implementation into the model of the research project.

7 DETAILED DESIGN OF REVERSE-OSMOSIS UNIT

Reverse osmosis has shown itself to be a viable technology for the treatment and minimization of industrial and domestic wastewater streams (Saif, Elkamel, &

Pritzker, 2008). In this research, a single-stage Reverse Osmosis technology is considered as the interceptor. The detailed design of this technology has to be performed as the offline parametric optimization problem, to minimize the cost of interceptor simultaneously with the minimization of freshwater and wastewater.

The literature that is made as reference in this project for designing a single-stage Reverse Osmosis network is from El-Halwagi (1997). A Reverse Osmosis network is composed of multiple Reverse Osmosis modules, pumps, and turbines. The network detailed design proposes for determination of minimum total annualized cost (TAC) of the RON interceptor to optimize the parameters and variables associated, corresponding to the main optimization problem.

Another literature that proposes for the detailed design of the reverse osmosis is associated with seawater desalination. Marcovecchio et al (2005) had solved for nonconvex problem by using global optimization algorithm to find the global optimal design of reverse osmosis networks for seawater desalination. Seawater is proposed to be purified using this technology due to the scarcity of natural fresh water supplies. The main scopes of the work are to formulate a detailed optimization problem for the design of reverse osmosis networks including an accuracy model for the transport phenomena across the membrane and a complete cost function, and to solve the problem for global optimization by the algorithm which is deterministic. The design proposed in this literature is more complex than the one from El-Halwagi (1997), even for its single-stage RO because of the emphasis on model accuracy for the transport phenomena.

Another complex detailed design of RON model is proposed by (Saif, Elkamel, & Pritzker, 2008). The complexity in the model proposed by them comes from the determination for optimum configuration of the multiple stages RON unit operations, which are the modules, pumps, and turbines.

Other literature reviews are summarized in **Appendix A**.

CHAPTER 3

METHODOLOGY

1 METHODOLOGY CHART

Figure 3.1 and **3.2** respectively show the general mathematical programming approach to process synthesis and design problem, and the chart of methodology sequences used in this research project.

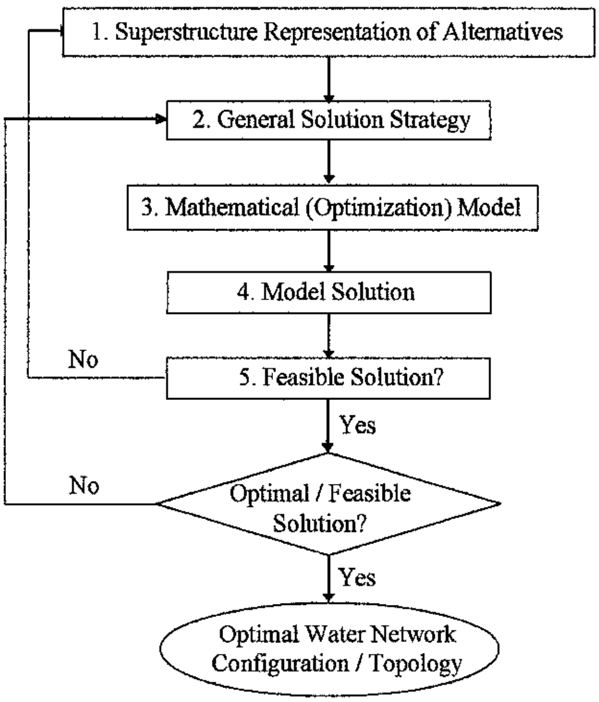

Figure 3.1: Mathematical Programming Approach to Process Synthesis and Design Problem

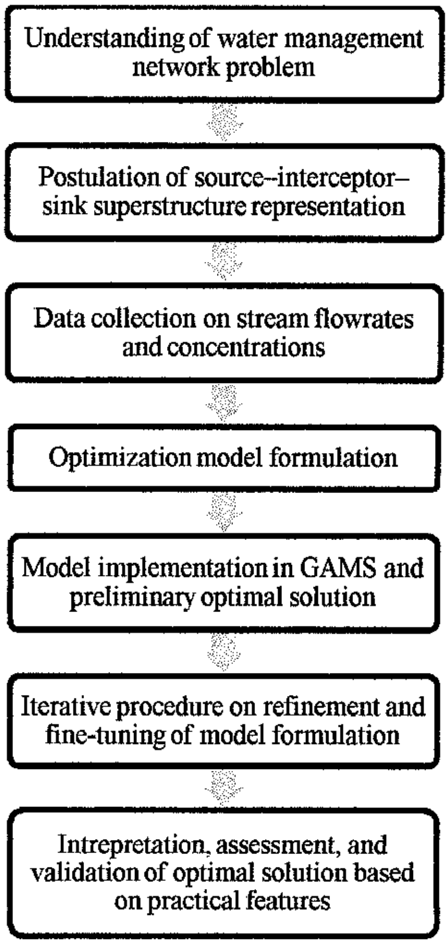

Figure 3.2: Methodology of the Research Project

2 EXPLANATION ON THE METHODOLOGY

After the understanding on the physics of problem associated with the design and retrofit of a water management network in local refinery, a draft of source-interceptor-sink superstructure representation is postulated. All of the feasibly possible alternative interconnections between the sources, interceptor, and sinks are configured out, but for consideration only a single interception unit, which is single-stage reverse osmosis for this project. The superstructure representation is shown as **Figure 4.1** in Chapter 4.

In conjunction with the optimization model formulation, plant data collection is performed to define the parameters on stream flowrates and concentrations based on the postulated superstructure representation. The objective function of such the MINLP model is to minimize freshwater import into the system for consumption and to minimize the total flow of wastewater generation for either further effluent treatment or discharging directly to the environment. These objectives are represented as the minimization of the total cost of water integration, which others include the installation and operating costs of reverse osmosis unit and piping interconnections between sources, interceptor, and sinks. The model constraints are comprising the following:

1. Material balances or water balances on water flows and contaminant concentrations
2. Maximum inlet contaminant concentrations of certain operations
3. Structural considerations of interconnections of material streams and units for water reuse, regeneration, and recycle (piping interconnections between sources, interceptor, and sinks)
4. Wastewater treatment technology that is modeled in terms of performance efficiency as represented by the fixed removal ratios of each particular contaminant, liquid phase recovery, operating conditions, and other variables associated.

Preliminary optimal solution is obtained to determine the continuous decision variables of flowrates and contaminant compositions, and the discrete decisions of the interconnections between the streams and operation and/or regeneration units (source – interceptor – sink) for water reuse, regeneration, and recycle. Subsequently, iterative procedure of refinement and fine-tuning of the optimization model formulation is taking place, to obtain the optimal solutions. Further interpretation, assessment, and validation of the rigorous optimal solutions are worked out to the context of a real-world refinery water network design and retrofit problem.

The key activity milestone of this research project is shown in **Figure 3.3**.

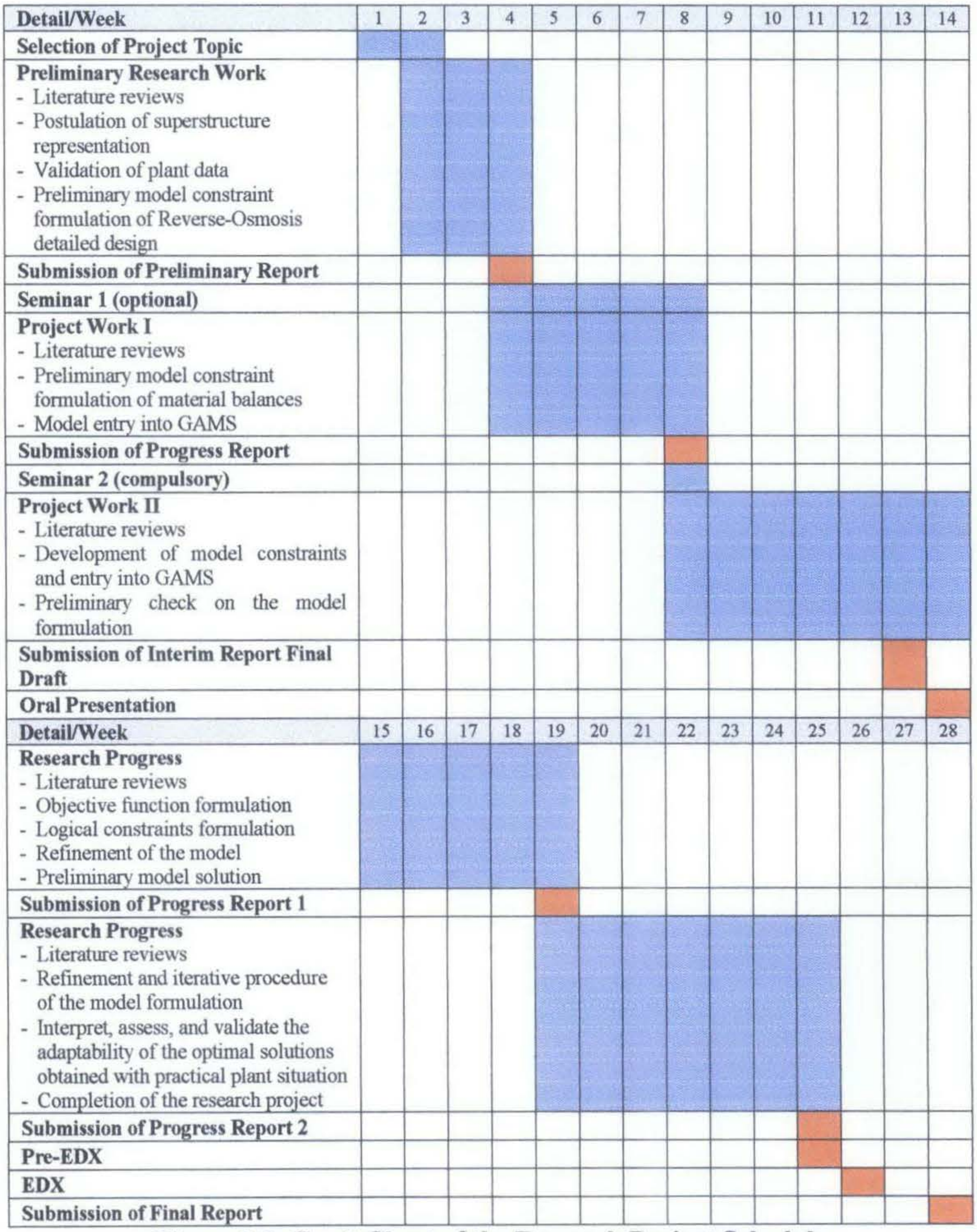

Figure 3.3: Gantt Chart of the Research Project Schedule

CHAPTER 4

OPTIMIZATION MODEL FORMULATION

1 SUPERSTRUCTURE REPRESENTATION

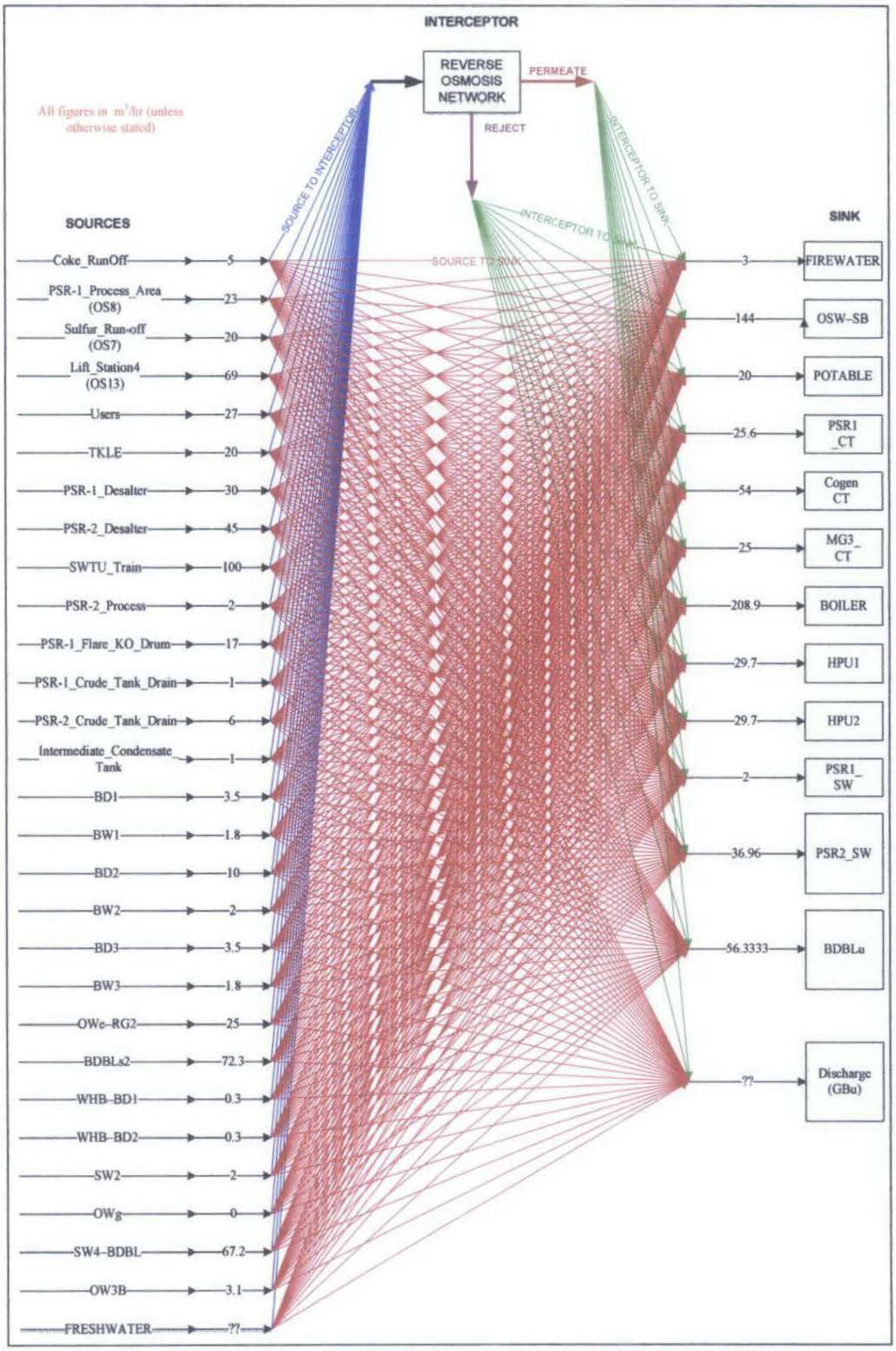

Figure 4.1: Source-Interceptor-Sink Superstructure Problem Representation

A source-interceptor-sink superstructure representation had been postulated based on a local refinery plant water management network for design and retrofit as in **Figure 4.1**. The problem representation is very 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** clarifies the general representation of source-interceptor-sink structure.

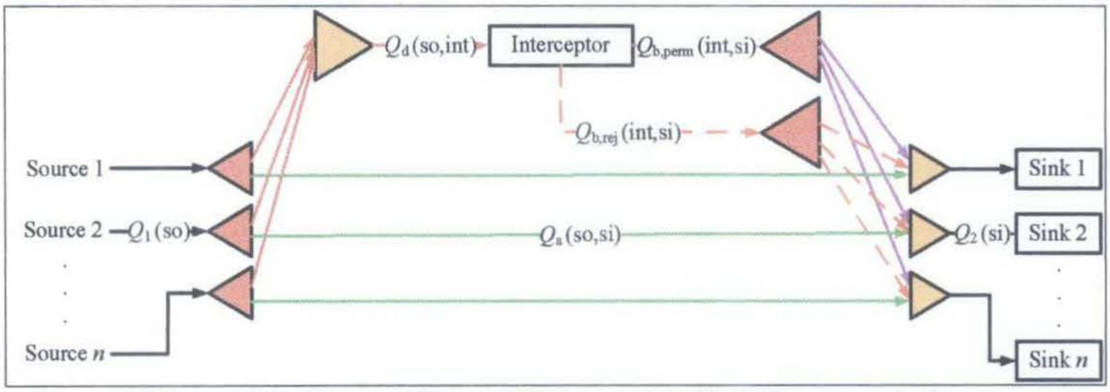

Figure 4.2: General Source-Interceptor-Sink Representation

2 OPTIMIZATION MODEL FORMULATION

2.1 Objective Function Formulation

The objective function of the project is to minimize the overall cost, represented by the minimization of freshwater use and wastewater discharges, piping interconnections cost, and reverse osmosis network cost. The objective function for this model is shown below (Chew & Foo, 2009) (Chew et al., 2008):

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

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

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

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

Several assumptions are made on the parameters in the objective function **(1)**, as shown in **Table 5.4** of Chapter 5. It is also assumed that all the pipelines share the same properties of parameter p and q, Manhattan distance D, and stream velocity v.

To be precise, this objective function is subjected to the following constraints, which will be elaborated throughout the subsequent sections:

1. Material balances (flow and concentration balances) incorporating the liquid phase recovery α and removal ratio RR, plus the forbidden mixing constraint for permeate and reject streams into each sink;
2. Detail design of reverse osmosis network;
3. Logical constraints utilizing big-M parameters for binary or mixed-integer model;

4. Additional constraints for bounded values (model tightening constraints).

2.2 Material Balances Formulation

Based on the source-interceptor-sink superstructure representation in **Figure 4.1**, several material balances that serve as the constraints in the optimization model had been developed. The model characteristics are assumed similar to the model problem discussed by Tan et al (2009), accept that the detail design of the partitioning regenerator is included as the parametric optimization problem and/or constraint to the main problem. These material balances formulation can be shown in the subsequent paragraphs.

2.2.1 Material Balance for Sources

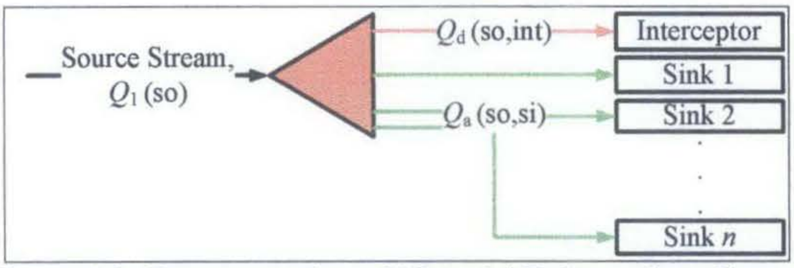

Figure 4.3: Representation of Material Balance for a Source

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 very useful to develop the flow balance and concentration balance for a source.

2.2.1.1 Flow balance for a source

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

The flow balance **(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 $\sum_{\text{int}\in\text{INT}} Q_d(\text{so,int})$ for regeneration, and from the source to the sinks $\sum_{\text{si}\in\text{SINK}} Q_a(\text{so,si})$ for direct reuse/recycle. 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 returns an infeasible solution.

2.2.1.2 Concentration balance for a source

$$Q_1(\text{so})C_{\text{so}}(\text{so,co}) \geq C_{\text{so}}(\text{so,co}) \sum_{\text{int}\in\text{INT}} Q_d(\text{so,int}) + C_{\text{so}}(\text{so,co}) \sum_{\text{si}\in\text{SINK}} Q_a(\text{so,si}) \qquad \textbf{(3)}$$
$$\forall \text{so} \in \text{SOURCE}, \forall \text{co} \in \text{CONTAMINANT}$$

The concentration balance for a source **(3)** represents that the multiplication of the contaminant concentration in the source stream C_{so}(so,co) with the flowrate of the source stream Q_1(so) is equivalent to the total of the following:

- Multiplication between contaminant concentration in the source stream C_{so}(so,co) and the sum of the flowrate splits from the source to interceptors $\sum_{\text{int}\in\text{INT}} Q_d(\text{so,int})$;
- Multiplication between contaminant concentration in the source stream C_{so}(so,co) and the sum of the flowrate splits from the source to sinks $\sum_{\text{si}\in\text{SINK}} Q_a(\text{so,si})$.

Since the contaminant concentration in a source stream C_{so}(so,co) in all terms can be canceled out, the concentration balance **(3)** is thereby equivalent to the flow balance **(2)**, as represented below. The concentration balance for a source **(3)** is therefore negligible.

$$Q_1(\text{so})\cancel{C_{\text{so}}(\text{so,co})} \geq \cancel{C_{\text{so}}(\text{so,co})} \sum_{\text{int}\in\text{INT}} Q_d(\text{so,int}) + \cancel{C_{\text{so}}(\text{so,co})} \sum_{\text{si}\in\text{SINK}} Q_a(\text{so,si})$$
$$\forall \text{so} \in \text{SOURCE}, \cancel{\forall \text{co} \in \text{CONTAMINANT}}$$

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

2.2.2 Material Balances for Interceptors

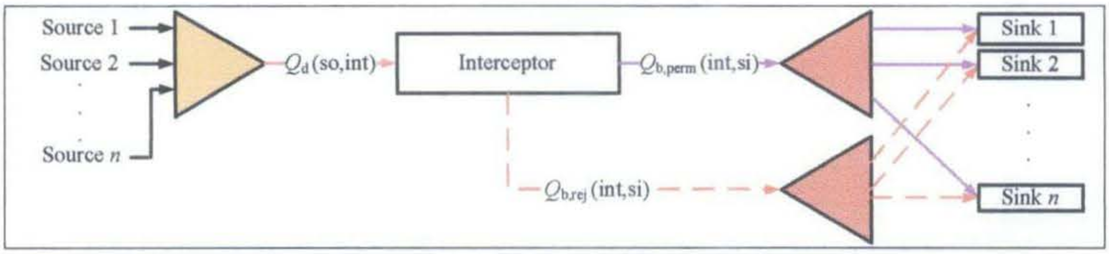

Figure 4.4: Representation of Material Balance for an Interceptor

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

2.2.2.1 Flow balances for interceptors

$$\sum_{so \in SO} Q_d(so, int) = \sum_{si \in SINK} Q_{b,perm}(int, si) + \sum_{si \in SINK} Q_{b,rej}(int, si) \quad \forall int \in INTERCEPTOR \qquad (4)$$

The flow balance constraint **(4)** enforces that the sum of the mixed flowrate of multiple sources to a partitioning interceptor $\sum_{so \in SO} Q_d(so,int)$ is equivalent to the summation of the following:

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

2.2.2.2 Concentration balances for interceptors

$$\sum_{\text{so}\in\text{SO}} \left(Q_{\text{d}}(\text{so,int})C_{\text{so}}(\text{so,co})\right) = C_{\text{perm}}(\text{int,co}) \sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int,si}) + C_{\text{rej}}(\text{int,co}) \sum_{\text{si}\in\text{SINK}} Q_{\text{b,rej}}(\text{int,si}) \quad (5)$$

$$\forall\,\text{int} \in \text{INTERCEPTOR}, \forall\,\text{co} \in \text{CONTAMINANT}$$

Concentration balance **(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 $\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int})C_{\text{so}}(\text{so,co})$, with the total of the following:

- Multiplication of the term $\sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int,si})$ and contaminant concentration generated in the permeate stream $C_{\text{perm}}(\text{int,co})$;
- Multiplication of the term $\sum_{\text{si}\in\text{SINK}} Q_{\text{b,rej}}(\text{int,si})$ and contaminant concentration generated in the reject stream $C_{\text{rej}}(\text{int,co})$.

2.2.2.3 Liquid phase recovery

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

$$\alpha \sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int}) = \sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int,si}) \qquad \forall\text{int} \in \text{INTERCEPTOR}$$

$$\Rightarrow \alpha = \frac{\sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int,si})}{\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int})} \qquad \forall\text{int} \in \text{INTERCEPTOR} \quad (6)$$

and

$$1-\alpha = \frac{\sum_{si \in SINK} Q_{b,rej}(\text{int,si})}{\sum_{so \in SO} Q_d(\text{so,int})} \qquad \forall \text{int} \in \text{INTERCEPTOR} \qquad (7)$$

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.

2.2.2.4 Removal ratio

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

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

$$RR(\text{int,co}) = \frac{C_{rej}(\text{int,co}) \sum_{si \in SINK} Q_{b,rej}(\text{int,si})}{\left(\sum_{so \in SO} Q_d(\text{so,int})C_{so}(\text{so,co})\right)} \qquad (8)$$

$\forall \text{int} \in \text{INTERCEPTOR}, \forall \text{co} \in \text{CONTAMINANT}$

where C_{rej}(int,co) is the contaminant concentration of the reject stream generated by the interceptor, $\sum_{si \in SINK} Q_{b,rej}(\text{int,si})$ is the summation of the reject flowrate splits from an interceptor to each of the sinks, and $\sum_{so \in SO} Q_d(\text{so,int})C_{so}(\text{so,co})$ is the summation of multiplication component between flowrate and contaminant concentration of each respective source to the interceptor.

Note that the concentration balances for the permeate and reject streams of an interceptor can be completely derived from equations **(5)**, **(6)**, and **(8)**, as illustrated in the following for the permeate stream by substituting the definition for α of constraint **(6)** into constraint **(5)**:

$$\left(\sum_{so\in SO} Q_d(so,int)C_{so}(so,co)\right) = C_{perm}(int,co)\cdot\left(\alpha\sum_{so\in SO} Q_d(so,int)\right) + C_{rej}(int,co)\sum_{si\in SINK} Q_{b,rej}(int,si)$$

followed by substituting the definition of *RR* for the reject stream from constraint **(8)**:

$$\left(\sum_{so\in SO} Q_d(so,int)C_{so}(so,co)\right) = C_{perm}(int,co)\cdot\left(\alpha\sum_{so\in SO} Q_d(so,int)\right) + RR(int,co)\left(\sum_{so\in SO} Q_d(so,int)C_{so}(so,co)\right)$$

$$\Rightarrow (1-RR(int,co))\left(\sum_{so\in SO} Q_d(so,int)C_{so}(so,co)\right) = C_{perm}(int,co)\alpha\sum_{so\in SO} Q_d(so,int) \quad \textbf{(9)}$$

$$\forall int \in \text{INTERCEPTOR}, \forall co \in \text{CONTAMINANT}$$

which yields the definition of *RR* for the permeate stream, indicating that this is a redundant constraint. Hence, the interceptor model can be completely defined by constraints **(4)**, **(5)**, **(6)**, and **(8)**.

2.2.3 Material Balances for Sinks

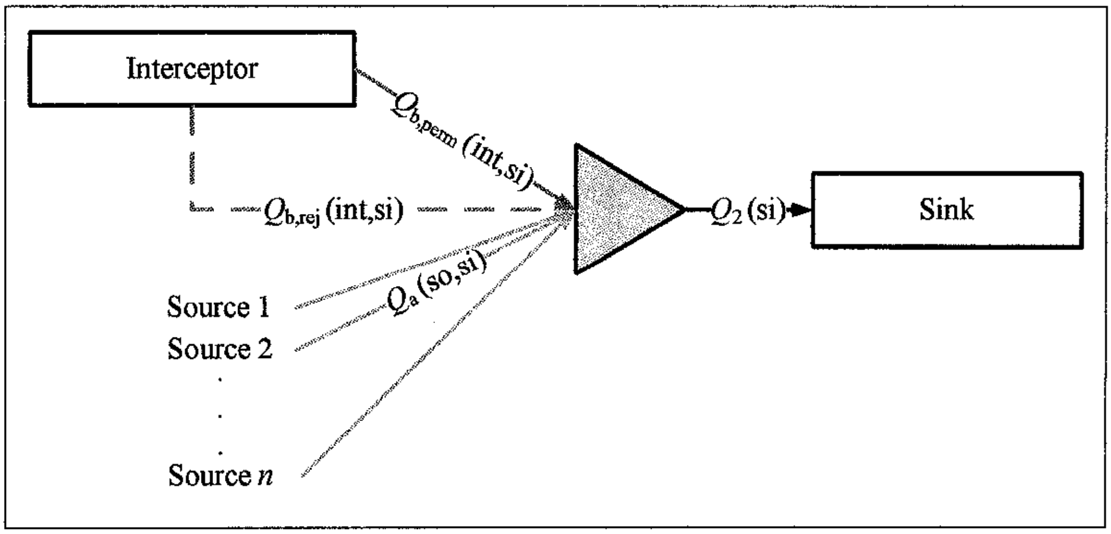

Figure 4.5: Representation of Material Balances for Sinks

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 very useful to develop for flow balance and concentration balance for a sink.

2.2.3.1 Flow balances for sinks

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

Flow balance **(10)** for a sink is associated with the equality between the inlet flowrate of a sink, $Q_2(\text{si})$ with the total of the following:

- Sum of the mixed flowrate from different sources to the sink $\sum_{\text{so}\in\text{SO}} Q_a(\text{so,si})$;
- Total of both the permeate flowrate from interceptor to sink $Q_{\text{b,perm}}(\text{int,si})$, and the reject flowrate from interceptor to sink $Q_{\text{b,rej}}(\text{int,si})$.

The equation balance is applied to each sink.

2.2.3.2 Concentration balance for a sink

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

The concentration balance **(11)** for a sink is depicted as above, where

- $\sum_{\text{so}\in\text{SO}} Q_a(\text{so,si})C_{\text{so}}(\text{so,co})$ is a sum of multiplication component between the flowrate and contaminant concentration of each respective source to the sink
- $\sum_{\text{int}\in\text{INT}} \left(C_{\text{perm}}(\text{int,co})Q_{\text{b,perm}}(\text{int,si}) + C_{\text{rej}}(\text{int,co})Q_{\text{b,rej}}(\text{int,si})\right)$ is the total of multiplication component between the permeate contaminant concentration and its flowrate $C_{\text{perm}}(\text{int,co})Q_{\text{b,perm}}(\text{int,si})$, and the reject contaminant concentration and its flowrate $C_{\text{rej}}(\text{int,co})Q_{\text{b,rej}}(\text{int,si})$

- Q_2(si) is the inlet flowrate of a sink and C(si,co) is the contaminant concentration into the sink.

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

$$\left(\sum_{so\in SO} Q_a(so,si)C_{so}(so,co)\right)+C_{perm}(int,co)Q_{b,perm}(int,si)+C_{rej}(int,co)Q_{b,rej}(int,si)$$
$$\leq\left(\sum_{so\in SO} Q_a(so,si)+\sum_{int\in INT}\left(Q_{b,perm}(int,si)+Q_{b,rej}(int,si)\right)\right)C_{max}(si,co)$$
$$\forall si\in SINK, \forall co\in CONTAMINANT$$

(12)

2.2.3.3 Forbidden mixing of permeate and reject stream into the sink

The previous flow and concentration balances for a sink seem to allow the permeate and reject streams from the interceptor to be mixed when entering each sink. Restriction has to be made to avoid the mixing, or else there is no point of having the interceptor at the first place. Another constraint is therefore added for this purpose.

$$Q_{b,perm}(int,si)\times Q_{b,rej}(int,si)=0 \qquad \forall si\in SINK \qquad \textbf{(13)}$$

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

2.3 Formulation of Parameter Optimization Model for Detailed Design of the Reverse Osmosis Network Interceptor

The preliminary 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 4.6**.

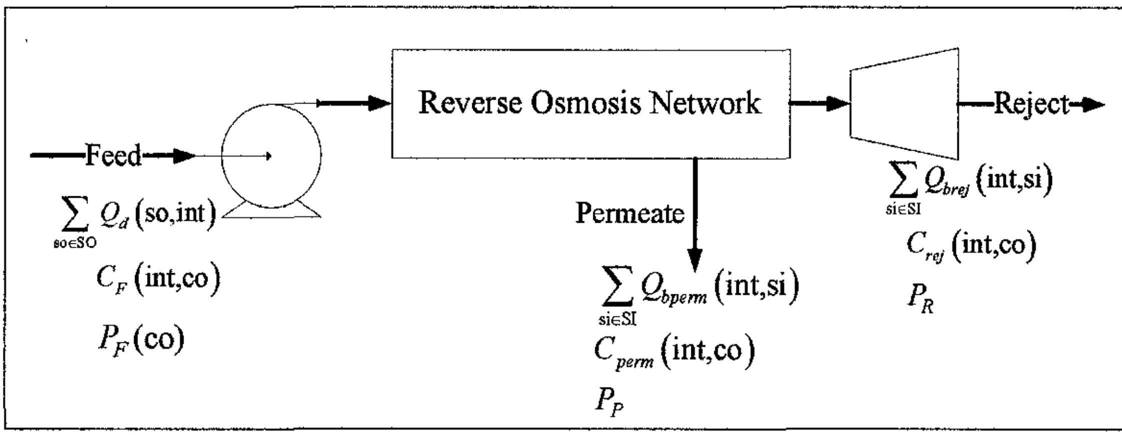

Figure 4.6: Reverse Osmosis Network Synthesis Problem (El-Halwagi, 1997)

Detailed design of single-stage Hollow Fiber Reverse Osmosis (HFRO) type module is considered as the case study. It is assumed 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 (reject stream) and a diluted stream (permeate stream);
3. Turbine to recover kinetic energy from high-pressure stream.

(14) shows the derivation for total annualized cost of the single-stage RON consisting the fixed costs of RO modules, pump, and turbine, and operating costs of pump and pre-treatment 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.

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

$$\begin{aligned}\text{TAC} = &\left(C_{\text{module}} \times \frac{\sum_{si\in SI} Q_{\text{b,perm}}(\text{RO,si})}{q_{\text{P}}}\right) + \left(C_{\text{pump}} \times (\text{power of pump})^{0.65}\right) \\ &+ \left(C_{\text{turbine}} \times (\text{power of turbine})^{0.43}\right) \\ &+ \left(\frac{(\text{power of pump})}{\eta_{\text{pump}}} \times \left(C_{\text{electricity}} \times \text{AOT}\right)\right) \\ &+ \left(\sum_{so\in SO} Q_{\text{d}}(\text{so,RO})\left(C_{\text{chemicals}} \times \text{AOT}\right)\right) - \left((\text{power of turbine}) \times \eta_{\text{turbine}} \times \left(C_{\text{electricity}} \times \text{AOT}\right)\right)\end{aligned} \quad \textbf{(14)}$$

Where

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

$$\text{power of pump} = \sum_{so\in SO} Q_{\text{d}}(\text{so,RO})\left(P_{\text{F}} - P_{\text{atm}}\right)\left(1.01325\times10^5\right), \text{ and}$$

$$\text{power of turbine} = \sum_{si\in SI} Q_{\text{b,rej}}(\text{RO,si})\left(P_{\text{R}} - P_{\text{atm}}\right)\left(1.01325\times10^5\right).$$

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}:

$$\pi_{\text{RO}} = \text{OS} \cdot \sum_{co} C_{\text{F,average}}(\text{RO,co}) \qquad \textbf{(15)}$$

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:

$$\sum_{\mathrm{co}} C_{\mathrm{F,average}}(\mathrm{RO,co}) = \frac{\sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A(\Delta P - \Delta\pi_{\mathrm{RO}})\gamma}{K_c} \tag{16}$$

where K_c is the solute or contaminants permeability coefficient (1.82×10^{-8} m/s) and $\Delta P = P_{\mathrm{F}} - \left(\frac{\Delta \mathrm{P_{shell}}}{2} + P_{\mathrm{P}}\right)$. So, the relation for π_{RO} becomes:

$$\pi_{\mathrm{RO}} = \frac{\mathrm{OS} \cdot \sum_{\mathrm{co}} C_{\mathrm{perm}}(\mathrm{RO,co}) \cdot A(\Delta P - \Delta\pi_{\mathrm{RO}})\gamma}{K_c} \tag{17}$$

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

$$Q_{\mathrm{P}} = (\text{no of modules}) \cdot A \cdot S_m \cdot \gamma(\Delta P - \pi_{\mathrm{RO}}) \tag{18}$$

Therefore,

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

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

$$\frac{\sum_{si\in SI} Q_{b,perm}(RO,si)}{q_P} = \frac{\sum_{si\in SI} Q_{b,perm}(RO,si)}{A\cdot S_m\cdot\gamma\left(\Delta P - \frac{OS\cdot\sum_{co} C_{perm}(RO,co)\cdot A(\Delta P - \Delta\pi_{RO})\gamma}{K_c}\right)}$$

$$= \frac{\sum_{si\in SI} Q_{b,perm}('RO',si)}{A\cdot S_m\cdot\gamma\left(P_F - \left(\frac{\Delta P_{shell}}{2} + P_P\right) - \frac{OS\cdot\sum_{co} C_{perm}(RO,co)\cdot A\left(P_F - \left(\frac{\Delta P_{shell}}{2} + P_P\right) - \Delta\pi_{RO}\right)\gamma}{K_c}\right)}$$

(19)

The final derivation of TAC from **(14)** and **(19)** is represented as **(20)**:

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

$$+\underbrace{\left[C_{pump}\left(\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}}\right)\left(\sum_{so\in SO} Q_d(so,RO)\right)(P_F - P_{atm})\left(1.01325\times10^5\right)\right)^{0.65}\right]}_{\text{annualized fixed cost of pump}}$$

$$+\underbrace{\left[C_{turbine}\left(\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}}\right)\left(\sum_{si\in SI} Q_{b,rej}(RO,si)\right)\left(\overbrace{(P_F - \Delta P_{shell})}^{P_R} - P_{atm}\right)\left(1.01325\times10^5\right)\right)^{0.43}\right]}_{\text{annualized fixed cost of turbine}}$$

$$+\underbrace{\left[\frac{\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}}\right)\left(\sum_{so\in SO} Q_d(so,RO)\right)(P_F - P_{atm})\left(1.01325\times10^5\right)C_{electricity}\cdot \mathrm{AOT}}{\eta_{pump}\left(10^3\ \frac{\mathrm{W}}{\mathrm{kW}}\right)}\right]}_{\text{annual operating cost of pump}}$$

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

$$-\underbrace{\left[\frac{\left(\frac{1\ \mathrm{h}}{3600\ \mathrm{s}}\right)\left(\sum_{si\in SI} Q_{b,rej}(RO,si)\right)\left(\overbrace{(P_F - \Delta P_{shell})}^{P_R} - P_{atm}\right)\left(1.01325\times10^5\right)\eta_{turbine}\cdot C_{electricity}\cdot \mathrm{AOT}}{\left(10^3\ \frac{\mathrm{W}}{\mathrm{kW}}\right)}\right]}_{\text{Operating value of turbine}}$$

$\forall co \in \mathrm{CONTAMINANT}$

(20)

The constraint on RO operating condition as associated with the feed pressure P_F in **(20)** is then given by:

$$\Delta P = \frac{P_F + P_R}{2} - P_P = \frac{P_F + P_F - \Delta P_{shell}}{2} - P_P = P_F - \left(\frac{\Delta P_{shell}}{2} + P_P\right)$$
$$P_F = \Delta P + \left(\frac{\Delta P_{shell}}{2} + P_P\right) \qquad \textbf{(21)}$$

Where

$$\Delta P = \frac{N_{water}}{A\gamma} + \frac{\pi_F}{C_F(\mathrm{RO,co})} C_S,$$

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

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

$$C_S = \frac{C_F(\mathrm{RO,co}) + C_{rej}(\mathrm{RO,co})}{2}$$

Finally, the P_F is derived as **(22)**.

$$P_F(\mathrm{co}) = \left(\frac{D_{2M}}{K\delta}\right)\left(\frac{1}{A\gamma}\right) \frac{\left(2C_F(\mathrm{RO,co}) \sum_{so \in SO} Q_d(\mathrm{so,RO}) - C_{perm}(\mathrm{RO,co}) \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si}) - C_F(\mathrm{RO,co}) \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si})\right)}{2C_{perm}(\mathrm{RO,co})\left(\sum_{so \in SO} Q_d(\mathrm{so,RO}) - \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si})\right)}$$
$$+ \frac{\pi_F\left(2C_F(\mathrm{RO,co}) \sum_{so \in SO} Q_d(\mathrm{so,RO}) - C_{perm}(\mathrm{RO,co}) \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si}) - C_F(\mathrm{RO,co}) \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si})\right)}{2C_F(\mathrm{RO,co})\left(\sum_{so \in SO} Q_d(\mathrm{so,RO}) - \sum_{si \in SINK} Q_{b,perm}(\mathrm{RO,si})\right)}$$
$$+ \left(\frac{\Delta P_{shell}}{2} + P_P\right)$$
$$\forall \mathrm{co} \in \mathrm{CONTAMINANT} \qquad \textbf{(22)}$$

Constant γ in **(14)** to **(22)** is defined as:

$$\gamma = \left(\frac{\eta}{1 + \frac{16A\mu r_o L L_s \eta}{1.0133 \times 10^5 r_i^4}} \right) \tag{23}$$

where

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

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

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

2.4 Big-*M* Logical Constraints

Binary 0-1 variables in the mixed-integer optimization methods are very much associated with the logic constraints. For the case of dealing with such logic constraints that involve continuous variables as corresponded to this research project, 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. The formulations for the "big-*M*" logical constraints are shown as **(24)** – **(31)**.

$$Q_a(so,si) \le \overline{M_a}(so,si)\, Y_a(so,si) \tag{24}$$

$$Q_{b,perm}(int,si) \le \overline{M_{b,perm}}(int,si)\, Y_{bperm}(int,si) \tag{25}$$

$$Q_{b,rej}(int,si) \le \overline{M_{b,rej}}(int,si)\, Y_{brej}(int,si) \tag{26}$$

$$Q_d(so,int) \le \overline{M_d}(so,int)\, Y_d(so,int) \tag{27}$$

$$Q_a(so,si) \ge \underline{M_a}(so,si)\, Y_a(so,si) \tag{28}$$

$$Q_{b,perm}(int,si) \ge \underline{M_{b,perm}}(int,si)\, Y_{bperm}(int,si) \tag{29}$$

$$Q_{b,rej}(int,si) \ge \underline{M_{b,rej}}(int,si)\, Y_{brej}(int,si) \tag{30}$$

$$Q_d(so,int) \ge \underline{M_d}(so,int)\, Y_d(so,int) \tag{31}$$

From the computational experiments, the lower bound for "big-M" constraints tends to give infeasible solution. The upper bound for "big-M" is sufficient to give the logic piping interconnections represented by the binary variables, as corresponding to the involved continuous variables. That upper bound value is chosen based on the maximum allowable flowrate capacity that can pass through the piping interconnections.

2.5 Model Tightening Constraints

The following additional constraints are stipulated in the MINLP model for a more complete representation of the problem:

1. Lower and upper bounds on variable feed flowrate into RO interceptor

$$Q_F^L(\text{int}) \leq Q_F(\text{int}) \leq Q_F^U(\text{int}) \qquad \textbf{(32)}$$

Where

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

In the computational experiment on the TAC minimization problem for offline parametric optimization, the feed flowrate 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.

2. Lower and upper bounds on variable feed pressure into RO interceptor

$$P_F^L \leq P_F \leq P_F^U \qquad \textbf{(33)}$$

It is noteworthy that equation **(22)** 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 $Q_{b,\text{perm}}$, the model solution still tends to be infeasible in the computational experiments that is conducted. Therefore, the lower and upper bound values of feed pressure P_F

are enforced in the model based on the common range specified by El-Halwagi (1997).

3. Lower and upper bounds on variable osmotic pressure of RO interceptor at the reject side

$$\Delta\pi_{\mathrm{RO}}^{\mathrm{L}} \leq \Delta\pi_{\mathrm{RO}} \leq \Delta\pi_{\mathrm{RO}}^{\mathrm{U}} \qquad \textbf{(34)}$$

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 osmotic pressure variable tends to assume the specified upper bound value as they are incorporated. A good upper bound value has to be chosen for this purpose.

4. Forbidden interconnection between the freshwater stream to RO interceptor

$$Q_1(\text{'freshwater'}) = \sum_{\text{si}\in\text{SINK}} Q_{\text{a}}(\text{'freshwater'}, \text{si}) \qquad \textbf{(35)}$$

To avoid the freshwater from going directly into the RO interceptor, the above constraint **(35)** is enforced so that the freshwater will only directly consumed by the sinks. By right, the contaminant concentrations in the freshwater shall be low enough where the treatment of freshwater is not practical.

2.6 The Complete Model Formulation

Objective function:

$$\min \text{obj}_{\text{cost}} = \underbrace{\left[C_{\text{water}} \sum_{\text{si}\in\text{SINK}} Q_{\text{a}}(\text{freshwater},\text{si}) + C_{\text{discharge}} Q_2(\text{discharge})\right]\text{AOT}}_{\text{Annualized cost of freshwater use and wastewater discharge treatment}}$$

$$+ \underbrace{\sum_{\text{co}\in\text{CONT}} \text{TAC}(\text{CO})}_{\substack{\text{Annualized cost of interceptor}\\ \text{from the detail design}}}$$

$$+ \underbrace{D\left\{\begin{aligned}&\left[p\sum_{\text{so}\in\text{SO}}\sum_{\text{int}\in\text{INT}}\frac{Q_{\text{d}}(\text{so,int})}{3600v}+q\sum_{\text{so}\in\text{SO}}\sum_{\text{int}\in\text{INT}}Y_{\text{d}}(\text{so,int})\right]\\&+\left[p\sum_{\text{int}\in\text{INT}}\sum_{\text{si}\in\text{SINK}}\frac{Q_{\text{b,perm}}(\text{int,si})}{3600v}+q\sum_{\text{so}\in\text{SO}}\sum_{\text{int}\in\text{INT}}Y_{\text{b,perm}}(\text{int,si})\right]\\&+\left[p\sum_{\text{int}\in\text{INT}}\sum_{\text{si}\in\text{SINK}}\frac{Q_{\text{b,rej}}(\text{int,si})}{3600v}+q\sum_{\text{so}\in\text{SO}}\sum_{\text{int}\in\text{INT}}Y_{\text{b,rej}}(\text{int,si})\right]\\&+\left[p\sum_{\text{so}\in\text{SO}}\sum_{\text{si}\in\text{SINK}}\frac{Q_{\text{a}}(\text{so,si})}{3600v}+q\sum_{\text{so}\in\text{SO}}\sum_{\text{int}\in\text{INT}}Y_{\text{a}}(\text{so,si})\right]\end{aligned}\right\}\frac{m(1-m)^n}{(1+m)^n-1}}_{\text{Annualized cost of operating and capital piping interconnections}}$$

subject to:

s.t $\quad Q_1(\text{so}) \geq \sum_{\text{int}\in\text{INT}} Q_{\text{d}}(\text{so},\text{int}) + \sum_{\text{si}\in\text{SINK}} Q_{\text{a}}(\text{so},\text{si}) \qquad \forall \text{so}\in\text{SOURCE}$

$$\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so},\text{int}) = \sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int},\text{si}) + \sum_{\text{si}\in\text{SINK}} Q_{\text{b,rej}}(\text{int},\text{si}) \qquad \forall \text{int}\in\text{INTERCEPTOR}$$

$$\left(\sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int}) C_{\text{so}}(\text{so,co})\right) = C_{\text{perm}}(\text{int},\text{co}) \sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int},\text{si}) + C_{\text{rej}}(\text{int},\text{co}) \sum_{\text{si}\in\text{SINK}} Q_{\text{b,rej}}(\text{int},\text{si})$$
$\forall \text{int}\in\text{INTERCEPTOR}, \forall \text{co}\in\text{CONTAMINANT}$

$$\alpha \sum_{\text{so}\in\text{SO}} Q_{\text{d}}(\text{so,int}) = \sum_{\text{si}\in\text{SINK}} Q_{\text{b,perm}}(\text{int,si}) \qquad \forall \text{int}\in\text{INTERCEPTOR}$$

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

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

$$\left(\sum_{\mathrm{so}\in\mathrm{SO}} Q_a(\mathrm{so},\mathrm{si}) C_{\mathrm{so}}(\mathrm{so},\mathrm{co})\right) + C_{\mathrm{perm}}(\mathrm{int},\mathrm{co}) Q_{\mathrm{b,perm}}(\mathrm{int},\mathrm{si}) + C_{\mathrm{rej}}(\mathrm{int},\mathrm{co}) Q_{\mathrm{b,rej}}(\mathrm{int},\mathrm{si})$$
$$\le \left(\sum_{\mathrm{so}\in\mathrm{SO}} Q_a(\mathrm{so},\mathrm{si}) + \sum_{\mathrm{int}\in\mathrm{INT}} \left(Q_{\mathrm{b,perm}}(\mathrm{int},\mathrm{si}) + Q_{\mathrm{b,rej}}(\mathrm{int},\mathrm{si})\right)\right) C_{\max}(\mathrm{si},\mathrm{co})$$
$$\forall \mathrm{si} \in \mathrm{SINK}, \forall \mathrm{co} \in \mathrm{CONTAMINANT}$$

$$Q_{\mathrm{b,perm}}(\mathrm{int},\mathrm{si}) \times Q_{\mathrm{b,rej}}(\mathrm{int},\mathrm{si}) = 0 \qquad \forall \mathrm{si} \in \mathrm{SINK}$$

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

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

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

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

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

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

$$\forall \mathrm{co} \in \mathrm{CONTAMINANT}$$

$$P_R = P_F - \Delta P_{shell}$$

$$Q_a(so,si) \le \overline{M_a}(so,si) Y_a(so,si) \qquad \forall so \in SOURCE, \forall si \in SINK$$

$$Q_{b,perm}(int,si) \le \overline{M_{b,perm}}(int,si) Y_{b,perm}(int,si) \qquad \forall int \in INTERCEPTOR, \forall si \in SINK$$

$$Q_{b,rej}(int,si) \le \overline{M_{b,rej}}(int,si) Y_{b,rej}(int,si) \qquad \forall int \in INTERCEPTOR, \forall si \in SINK$$

$$Q_d(so,int) \le \overline{M_d}(so,int) Y_d(so,int) \qquad \forall so \in SOURCE, \forall int \in INTERCEPTOR$$

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

$$Q_F^L(int) \le Q_F(int) \le Q_F^U(int)$$

$$C_F(int,co) \sum_{so \in SO} Q_d(so,int) = \left(\sum_{so \in SO} Q_d(so,int) C_{so}(so,co) \right)$$
$\forall int \in INTERCEPTOR, \forall co \in CONTAMINANT$

$$P_F^L \le P_F \le P_F^U$$

$$\Delta\pi_{RO}^L \le \Delta\pi_{RO} \le \Delta\pi_{RO}^U$$

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

$$Y_a(so,si), Y_{b,perm}(int,si), Y_{b,rej}(int,si), Y_d(so,int) = \{0,1\}$$

$$TAC(co), Q_a(so,si), Q_{b,perm}(int,si), Q_{b,rej}(int,si), Q_d(so,int),$$
$$C_F(int,co), C_{perm}(int,co), C_{rej}(int,co), Q_F(int), P_F \ge 0$$

2.7 Additional Remarks

Only one interceptor is considered in this work (that is, the reverse osmosis treatment technology) because considering more than one interceptor will cause the problem to be quite tedious. While it is certainly possible to model more than one interceptor technology, for instance, to consider two treatment technologies, the complexity will arise from the arrangement of these two technologies and the determination of the intermediate compositions. While for a single technology, it is straightforward to discretize the inlet and outlet compositions and derive an optimal policy for each of the scenarios to be considered. It will give much more cumbersome and difficulty (to do so) with multiple technologies because the derivation of the optimal policy has to be performed for each of the technologies considered.

CHAPTER 5

COMPUTATIONAL RESULTS AND DISCUSSIONS

1 PROBLEM DATA FOR MODEL

Table 5.1: Fixed flowrates and fixed contaminant concentrations for sources based on actual refinery data

	Flowrate (m^3/h)	OnG (mg/L)	TSS (mg/L)	COD (mg/L)	Chloride (mg/L)	Phosphate (mg/L)
Coke_RunOff	5	2	127	167	n/a	n/a
PSR-1_ProcessArea	23	2	40	52	n/a	n/a
Sulfur_RunOff	20	0	16	86	n/a	n/a
Lift_Station4	69	24 100	6774	178	n/a	n/a
Users	27	0	10	22.2	n/a	n/a
TKLE	20				n/a	n/a
PSR-1_Desalter	30	1430	1945	2234	n/a	n/a
PSR-2_Desalter	45	0	0	0	n/a	n/a
SWTU_Train	100	0	0	844	n/a	n/a
PSR-2_Process	2	99	13	231	n/a	n/a
PSR-1_Flare_KO_Drum	17	2	14	28	n/a	n/a
PSR-1_Crude_Tank_Drain	1	439	228	667	n/a	n/a
PSR-2_Crude_Tank_Drain	6	5	6081	299	n/a	n/a
Intermediate_Condensate_Tank	1	544	108	8610	n/a	n/a
BD1	3.5	1	37	81	152.00	18.52
BW1	1.8	1	37	81	152.00	18.52
BD2	10	3	5	30	108.00	19.09
BW2	2	n/a	n/a	n/a	n/a	n/a
BD3	3.5	3.60	1.00	48.00	65.83	19.34
BW3	1.8	n/a	n/a	n/a	n/a	n/a
OWe-RG2	25	0	12	47	n/a	n/a
BDBLs2	72.3	0	0.129	4.974	n/a	n/a
WHB-BD1	0.3	0	3	116	n/a	n/a
WHB-BD2	0.3	0	3	116	n/a	n/a
SW2	2	0	10	22.2	n/a	n/a
OWg	0	0	10	22.2	n/a	n/a
SW4-BDBL	67.2	0	10	22.2	n/a	n/a
OW3b	3.1	n/a	n/a	n/a	n/a	n/a
FIREWATER	3	n/a	n/a	n/a	n/a	n/a
OSW-SB	144	n/a	n/a	n/a	n/a	n/a
POTABLE	20	n/a	n/a	n/a	n/a	n/a
PSR1_CT	25.6	n/a	n/a	n/a	n/a	n/a
Cogen_CT	54	n/a	n/a	n/a	n/a	n/a
MG3_CT	25	n/a	n/a	n/a	n/a	n/a
BOILER	208.9	n/a	n/a	n/a	n/a	n/a
HPU1	29.7	n/a	n/a	n/a	n/a	n/a
HPU2	29.7	n/a	n/a	n/a	n/a	n/a
PSR1_SW	2	n/a	n/a	n/a	n/a	n/a
PSR2_SW	36.96	n/a	n/a	n/a	n/a	n/a
BDBLu	56.3333	n/a	n/a	n/a	n/a	n/a

Table 5.2: Maximum Inlet Concentration to the Sinks

Wastewater Streams		Oily Water	Oily Surface Water	Standard B Limits
Flow (m3/h)	Design Ave	260		n/a
	Design Max	424		n/a
pH		7.5	7	5.5 – 9
BOD (mg/l)		232	10	50
COD (mg/l)		613	20	100
Oil & Grease (mg/l)		350	50	10
Suspended Solids (mg/l)		162	20	100
Chloride (mg/l)		500	-	-
Phenol (mg/l)		10	-	1
Temperature, oC		38 oC	25 oC oC	40 oC
Sulphide (mg/l)		15	-	0.5

Table 5.3: 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
Removal Ratio of COD Contaminant	0.9
Removal Ratio of Chloride Contaminant	0.94
Removal Ratio of Phosphate Contaminant	0.97

Table 5.4: Economic data, physical constants, and other model parameters (mainly for objective function formulation)

Parameters	Fixed Values
AOT	8760 hr/yr
$C_{discharge}$	\$0.22/ton
C_{water}	\$0.13/ton
D	100 m
m	5% = 0.05
n	5 years
p	7200 (carbon steel piping at CE plant index = 318.3)
q	250 (carbon steel piping at CE plant index = 318.3)
v	1 m/s

Table 5.5: Economic data for HFRO Cost Modeling (Interceptor Detailed Design)

Parameters	Fixed Values
μ	0.001 kg/m.s
A	5.573×10^{-8} m/s.atm
AOT	8760 hr/yr
$C_{chemicals}$	$0.03/m^3
$C_{electricity}$	$0.06/kW.hr
C_{module}	$2300/yr.module
C_{pump}	$6.5/yr.W$^{0.65}$
$C_{turbine}$	$18.4/yr.W$^{0.43}$
$D_{2M}/K\delta$	1.82×10^{-8} m/s
L	0.750 m
L_s	0.075 m
P_p	1 atm
r_i	21×10^{-6} m
r_o	42×10^{-6} m
S_m	180 m^2
ΔP_{shell}	0.4 atm
η_{pump}	0.7
$\eta_{turbine}$	0.7
OS	0.006 psi/(mg/L) = 4.0828×10^{-4} atm
K_C	1.82×10^{-8} m/s

Table 5.6: Variable Bounds

Variables	Lower Bound	Upper Bound
Q_F(int)	40 m^3/hr	120 m^3/hr
P_F	10 atm	70 atm
$\Delta\pi_{RO}$	0 atm	55 atm
$\overline{M_a}$(so,si)	-	100 m^3/hr
$\overline{M_{b,perm}}$(int, si)	-	50 m^3/hr
$\overline{M_{b,rej}}$(int, si)	-	50 m^3/hr
$\overline{M_d}$(so, int)	-	50 m^3/hr

2 COMPUTATIONAL RESULTS

The computational results using GAMS/BARON can be shown as the following:

- Total cost for water integration and retrofit = **$ 769,435/yr**
- Total freshwater **without** reuse, regeneration, and recycle (without water integration) = 750 m^3/h
- Total freshwater **with** reuse, regeneration, and recycle = 296.169 m^3/h or **296.2 m^3/h**
- Percentage of water recovery = $\frac{750-296.169}{750} \times 100\% = 60.51\%$ or **61%**
- Total annualized cost of RO = **$ 94,926/yr**
- $Q_F(\text{int}) = \sum_{so \in SO} Q_d(\text{so,int}) =$ **40 m^3/hr**
- $P_F =$ **56.395 atm**
- $P_R = P_F - \Delta P_{shell} =$ **55.995 atm**
- $\Delta\pi_{RO} =$ **55 atm**
- $$\text{no of modules} = \frac{\left(\frac{1\ \text{h}}{3600\ \text{s}}\right)\sum_{si \in SI} Q_{b,perm}(\text{RO,si})}{A \cdot S_m \cdot \gamma \left(P_F - \left(\frac{\Delta P_{shell}}{2} + P_P\right) - \frac{OS \cdot \sum_{co} C_{perm}(\text{RO,co}) \cdot A\left(P_F - \left(\frac{\Delta P_{shell}}{2} + P_P\right) - \Delta\pi_{RO}\right)\gamma}{K_c} \right)}$$
  $$= 23.851 \approx \mathbf{24\ modules}$$
- Power of pump and turbine representing the optimum duties of RON:

  $$\text{power of pump} = Q_F (P_F - P_{atm})(1.01325 \times 10^5)$$
  $$= \left(\frac{1\ \text{h}}{3600\ \text{s}}\right)\left(\sum_{so \in SO} Q_d(\text{so,RO})\right)(P_F - P_{atm})(1.01325 \times 10^5)$$
  $$= \left(\frac{1\ \text{h}}{3600\ \text{s}}\right)(30)(56.395-1)(1.01325 \times 10^5)$$
  $$= \mathbf{46.774\ kW}$$

$$\text{power of turbine} = Q_R \left(P_R - P_{atm}\right)\left(1.01325\times10^5\right)$$
$$= \left(\frac{1\ \text{h}}{3600\ \text{s}}\right)\left(\sum_{si\in SI} Q_{b,rej}(\text{'RO'},si)\right)\left(P_R - P_{atm}\right)\left(1.01325\times10^5\right)$$
$$= \left(\frac{1\ \text{h}}{3600\ \text{s}}\right)(30)(55.995-1)\left(1.01325\times10^5\right)$$
$$= \underline{\mathbf{46.436\ kW}}$$

Table 5.7: Computational Results on Contaminant Concentration Variables

	OnG	TSS	COD	Chloride	Phosphate
Feed concentration into RO interceptor $C_F(\text{RO},co)$ in mg/L	223.086	55.153	19.268	22.436	3.235
Permeate concentration from RO interceptor $C_{perm}(\text{RO},co)$ in mg/L	318.694	1.970	2.753	1.923	0.139
Reject concentration from RO interceptor $C_{rej}(\text{RO},co)$ in mg/L	-	179.246	57.803	70.299	10.461

Table 5.8: Model Sizes and Computational Statistics

Type of model	Mixed-Integer Nonlinear Program (MINLP)
Solver	GAMS/BARON
No. of continuous variables	926
No. of discrete binary variables	432
No. of constraints	573
No. of iterations	1801
CPU time (s) (resource usage)	1000.01

3 OPTIMUM SOURCE-INTERCEPTOR-SINK ALLOCATIONS

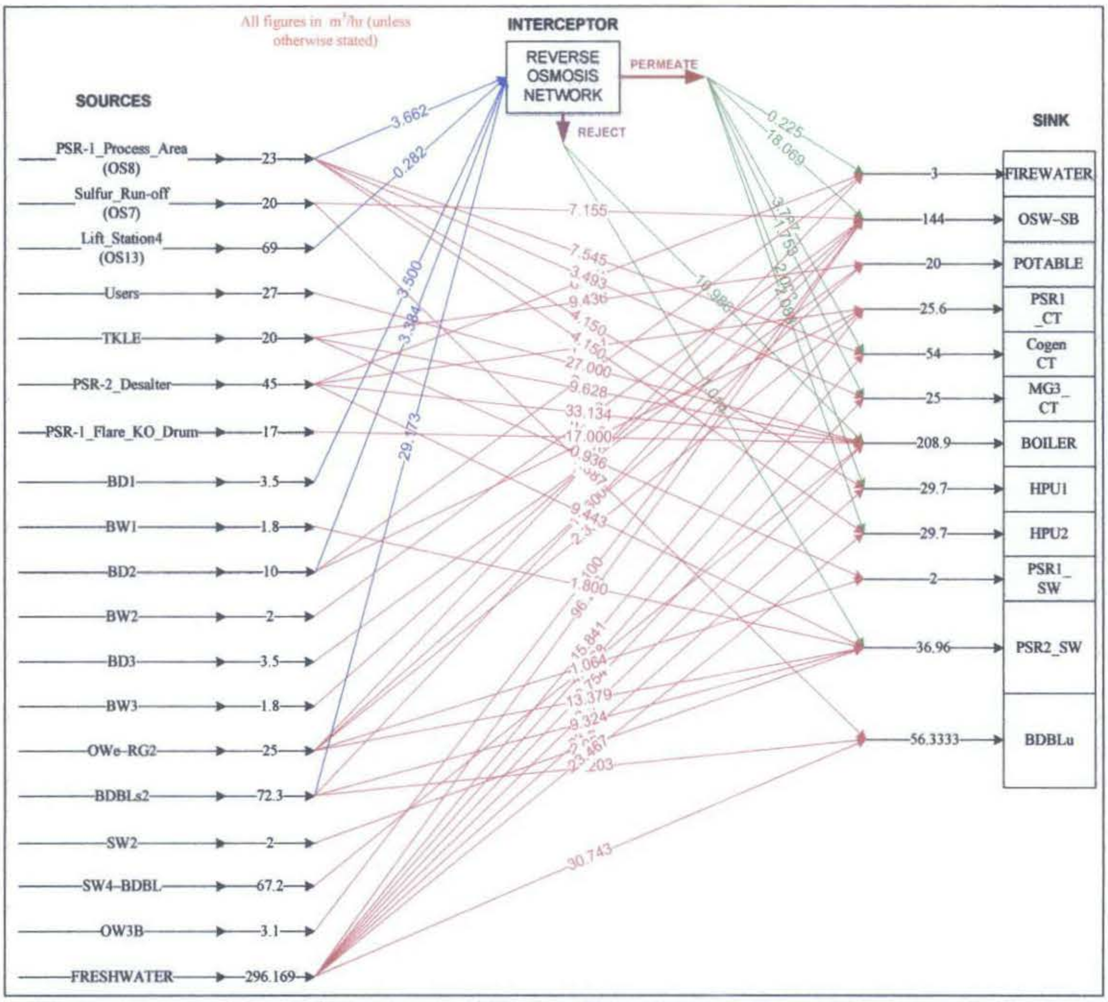

Figure 5.1: Optimal Structure of Piping Interconnection Allocations between Sources, Interceptors, and Sinks

Table 5.9: GAMS Solutions for Flowrate Continuous Variables

VARIABLE Qa.L flowrate of source to sink	FIREWATER	OSW-SB	POTABLE	PSR1_CT
Sulfur_RunOff		7.155		
TKLE			9.436	
PSR-2_Desalter	0.942			1.481
BD2	0.690			5.926
BW2		2.000		
BD3			3.500	
BW3		1.800		
OWe-RG2	1.142		7.064	2.352
BDBLs2		15.600		
OW3b		3.100		
FRESHWATER		96.276		15.841
	Cogen_CT	MG3_CT	BOILER	HPU1
PSR-1_ProcessArea	7.545	3.493		4.150
Users			27.000	
TKLE			9.628	
PSR-2_Desalter			33.134	
PSR-1_Flare_KO_Drum			17.000	
SW4-BDBL			67.200	
FRESHWATER	42.668	19.754	43.953	23.467
	HPU2	PSR1_SW	PSR2_SW	BDBLu
PSR-1_ProcessArea	4.150			
Sulfur_RunOff				7.387
TKLE		0.936		
PSR-2_Desalter			9.443	
BW1			1.800	
OWe-RG2		1.064	13.379	
BDBLs2			9.324	18.203
SW2			2.000	
FRESHWATER	23.467			30.743

VARIABLE Qb_perm.L flowrate of permeate to sink	FIREWATER	OSW-SB	Cogen_CT	MG3_CT	HPU1	HPU2
RO	0.225	18.069	3.787	1.753	2.083	2.083

VARIABLE Qb_rej.L flowrate of reject to sink	BOILER	PSR2_SW
RO	10.986	1.014

VARIABLE Qd.L flowrate from source to interceptor	RO
PSR-1_ProcessArea	3.662
Lift_Station4	0.282
BD1	3.500
BD2	3.384
BDBLs2	29.173

Table 5.10: GAMS Solutions for Piping Interconnection Binary Variables

VARIABLE Qa.L flowrate of source to sink	FIREWATER	OSW-SB	POTABLE	PSR1_CT
Sulfur_RunOff		1.000		
TKLE			1.000	
PSR-2_Desalter	1.000			1.000
BD2	1.000			1.000
BW2		1.000		
BD3			1.000	
BW3		1.000		
OWe-RG2	1.000		1.000	1.000
BDBLs2		1.000		
OW3b		1.000		
FRESHWATER		1.000		15.841
	Cogen_CT	MG3_CT	BOILER	HPU1
PSR-1_ProcessArea	1.000	1.000		1.000
Users			1.000	
TKLE			1.000	
PSR-2_Desalter			1.000	
PSR-1_Flare_KO_Drum			1.000	
SW4-BDBL			1.000	
FRESHWATER	1.000	1.000	1.000	1.000
	HPU2	PSR1_SW	PSR2_SW	BDBLu
PSR-1_ProcessArea	1.000			
Sulfur_RunOff				1.000
TKLE		1.000		
PSR-2_Desalter			1.000	
BW1			1.000	
OWe-RG2		1.000	1.000	
BDBLs2			1.000	1.000
SW2			1.000	
FRESHWATER	1.000			1.000

VARIABLE Qb_perm.L flowrate of permeate to sink	FIREWATER	OSW-SB	Cogen_CT	MG3_CT	HPU1	HPU2
RO	1.000	1.000	1.000	1.000	1.000	1.000

VARIABLE Qb_rej.L flowrate of reject to sink	BOILER	PSR2_SW
RO	1.000	1.000

VARIABLE Qd.L flowrate from source to interceptor	RO
PSR-1_ProcessArea	1.000
Lift_Station4	1.000
BD1	1.000
BD2	1.000
BDBLs2	1.000

3 DISCUSSIONS

The GAMS computational results can be generally interpreted as below:

1. There is no oil and grease contaminant in the reject stream of RO since the membrane modules are not meant to remove that type of contaminant. This is represented by the non-existence of removal ratio data of oil and grease removal by RO. RO is generally applicable for desalination process, and for salts, organics, and ions heavy metals removal (El-Halwagi, 1997).
2. There are no piping interconnections to the discharge sink. This can be due to the inequality representation of the flow balance for sources. The remaining wastewater flow from the sources can be assumed to be either discharged directly to the environment or going through the wastewater treatment process before the discharge. Based on the manual calculations on the remaining source stream flows, the discharge is 219.776 m^3/hr.
3. It is important to stipulate the upper bound on freshwater use. A loose upper bound is not only tends to give a slightly higher freshwater amount required, but also some inconsistencies between the binary and continuous variables associated with the big-M logical constraints (i.e., flowrate variable returns a zero-value which corresponds to no piping interconnection, but its associated binary variable returns otherwise). The reported computational results (from GAMS) are based on freshwater upper bound of 300 m^3/h.
4. It is important to stipulate the bounds for the variable Q_F, especially the lower bound because the solution for Q_F tends to assume the lower bound value. This is explained in Section 2.5 of Chapter 4.
5. It is important to stipulate the lower and upper bounds for the variable P_F, which contributes to the determination of TAC. This is explained in Section 2.5 of Chapter 4.
6. It is important to stipulate the lower and upper bounds for the variable $\Delta\pi_{RO}$, which contributes to the determination of number of RO membrane modules and TAC. This is explained in Section 2.5 of Chapter 4.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The objective function of this model is associated with the minimization of the total cost for water network integration, which can be characterized by the minimum consumption of freshwater, minimum wastewater discharge for further effluent treatment, minimum cost of pipelines, and minimum cost of the interceptor. Material balances that serve as the constraints in this model are formulated for the partitioning regenerator, which is single-stage reverse osmosis technology in this case. The developed detailed design of interceptor, specifically HFRO module is very useful for determining the minimum cost of interceptor to represent the parametric optimization problem. The optimum parameters and variables associated are incorporated into the main optimization problem, and the iterative procedure to solve simultaneously for the minimum cost of interceptor, minimum freshwater and wastewater, and minimum cost of pipeline interconnections are taking place in GAMS tool. The simultaneous procedure for determining the cost of pipelines is very much associated with the binary 0-1 variables and logical constraints, for the existence of the interconnections within the optimized continuous variables. The development of these techniques and tools are important to address the integrated water management problem at petroleum refineries, which become the particular interest and concern associated with the alarming of scarcities of freshwater availabilities within our country.

For future work, it is recommended that multiple stage of RON with multiple possible configurations of the unit operations (modules, pumps and turbines) is considered as the interceptor as proposed by Saif, Elkamel, & Pritzker (2008) to increase the treatment efficiency. Additionally, other multiple interconnected treatment technologies with each of their complex detailed designs can be expanded as the interceptor network in the proposed modeling framework of an integrated refinery water network structure. For more accurate representation of the problem, detailed design of homogenizer prior to the interceptor unit can be considered in the future work.

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APPENDICES

APPENDIX A : LITERATURE REVIEWS

Author (year)	General description	Optimization model type	Modeling technique	Solution strategy
Putra and Amminudin (2008)	Integrated water management network of water using and wastewater treatment units	Mixed-integer linear programming (MILP) and NLP	Considers practical design concerns and user (engineer) preferences, e.g., sizes and complexity of piping interconnections	Two-step approach of structural (via MILP) and parametric optimization (via NLP)
Karuppiah and Grossmann (2006)	Integrated water management network	NLP and MINLP	• Superstructure with all possible interconnections of process units and treatment units using mixers and splitters • Accounts for mass load of contaminants	• Bound strengthening cuts based on overall contaminant flow balances • Logic cuts • Global optimization algorithm
Chang and Li (2005)	Integrated water management network	NLP	• Superstructure incorporates additional design options and a fixed number of repeated treatment units • Inequality constraints on concentrations to account for possible existence of unrecoverable contaminants	• Method to produce a good initial guess to enhance convergence efficiency • Techniques to manipulate structural properties of water networks
Huang et al. (1999)	Integrated water usage and distributed wastewater treatment network	NLP	• Extended version of Takama et al.'s (1980) superstructure by incorporating multiple water	Initial feasible points are generated through water pinch analysis or by solving

Author (year)	General description	Optimization model type	Modeling technique	Solution strategy
			sources and sinks, water losses, and repeated water treatment units • Uses the strategy/heuristic/technique of "repeated water treatment units" to represent effect of recycling wastewater requiring further treatment (i.e., another "round" of treatment using the same treatment technology)	nonlinear system of equations resulting from fixing several key design variables at reasonable levels in the NLP
Alva-Argáez et al. (1998)	Industrial water systems	MINLP	Superstructure includes all possibilities for water reuse, regeneration, recycling, and treatment	• Incorporate insights from water pinch • decomposition of original nonconvex MINLP into a sequence of MILP relaxation models to obtain a feasible solution (similar approach to Galan and Grossmann's LP relaxation) • objective function is augmented with an increasing penalty term that pursues a reduction of the problem infeasibilities
Takama et al. (1980)	Optimal allocation of water in oil refineries	NLP (nonconvex)	Superstructure embeds high connectivity for reuse and treatment configurations	The complex method to develop optimal network design

APPENDIX B : MODEL IMPLEMENTATION IN GAMS

```
$TITLE: PP(M)SB WATER NETWORK
$EOLCOM #
*Base Case


SETS

SO    source (stream)
/
Coke_RunOff
PSR-1_ProcessArea
Sulfur_RunOff
Lift_Station4
Users

*OWSinlet
TKLE
PSR-1_Desalter
PSR-2_Desalter
SWTU_Train
PSR-2_Process
PSR-1_Flare_KO_Drum
PSR-1_Crude_Tank_Drain
PSR-2_Crude_Tank_Drain
Intermediate_Condensate_Tank

BD1
BW1
BD2
*BD2-BDBL3
BW2
BD3
BW3
OWe-RG2
BDBLs2
WHB-BD1
WHB-BD2
SW2
OWg
```

SW4-BDBL

OW3b

FRESHWATER

/

INT interceptor or regeneration or treatment unit

/

RO

*UF

/

SI sink (process unit)

/

FIREWATER

OSW-SB

POTABLE

PSR1_CT

Cogen_CT

MG3_CT

BOILER

HPU1

HPU2

PSR1_SW

PSR2_SW

BDBLu

Discharge

/

CO contaminant

/

OnG

TSS

COD

CHLORIDE

PHOSPHATE

$ontext

SULPHIDE

```
TDS
$offtext
/

;

ALIAS (INT,INT2)

;

SCALARS

Cmodule     cost per module of membrane (in $ per yr.module)   /2300/
Cpump       cost per power of pump (in $ per yr.W**0.65)       /6.5/
Cturbine    cost per power of turbine (in $ per yr.W**0.43)    /18.4/
Cchemicals  cost of pretreatment chemicals (in $ per m**3)     /0.03/
Celectricity   cost of electricity (in $ per kW.h)             /0.06/
AOT         annual operating time (in h per yr)                /8760/
Sm          membrane area per module (in m**2 per module)      /180/
A           permeability (in m per s.atm)                      /0.00000005573/
SFC         salt flux constant (in m per s)                    /0.0000000182/
miu         viscosity (in kg per m.s)                          /0.001/
ro          outside radius of fiber (in m)                     /0.000042/
ri          inside radius of fiber (in m)                      /0.000021/
L           fiber length (in m)                                /0.750/
Ls          seal length (in m)                                 /0.075/
deltaPshell shell side pressure drop per module (in atm)       /0.4/
piF         osmotic pressure of feed (in atm)                  /1.57/
OS          proportionality constant between osmotic pressure and average solute concentration on feed
side        /0.00040828/
Kc          solute permeability coefficient                    /0.0000000182/
Patm        atmospheric pressure (in atm)                      /1/

*QF         feed flowrate (in m**3 per second)                 /26/
NETApump    pump efficiency                                    /0.7/
PP          permeate pressure (in atm)                         /1/
NETAturbine turbine efficiency                                 /0.7/
```

ALPHA a fixed fraction of the inlet flowrate of the interceptor RO that is present in the permeate (lean) stream with range of value = (0.6 - 0.8) /0.7/

Cwater freshwater unit cost (in $ per m3) /0.13/
Cdischarge effluent treatment unit cost (in $ per m3) /0.22/
D cross plant pipelines distance (in m) /100/
p cost parameter of carbon steel pipe (CE plant index=318.3) /7200/
q cost parameter of carbon steel pipe (CE plant index=318.3) /250/
v stream flowrate velocity (in m per s) /1/
m fractional interest rate per year /0.05/
n number of years /5/
;

PARAMETERS

Ma(SO,SI) big-M parameters
Mb_perm(INT,SI)
Mb_rej(INT,SI)
Md(SO,INT)
Me(INT)

Ma_lo(SO,SI) big-M parameters
Mb_lo(INT,SI)
Md_lo(SO,INT)
Me_lo(INT)

nRO no. of RO modules

RR(INT,CO) removal ratio for RO
/
RO.TSS 0.975
RO.COD 0.9
RO.CHLORIDE 0.94
*RO.SULPHIDE 0.97
RO.PHOSPHATE 0.97
*RO.TDS 0.99

/

* RO can remove: (1) aqueous salts, (2) metal ions, more??

Cmax(SI,CO) maximum allowable concentration in sink in mg per L

Cso(SO,CO) outlet concentration of source in mg per L

/

Coke_RunOff.OnG 2
PSR-1_ProcessArea.OnG 2
Sulfur_RunOff.OnG 0
Lift_Station4.OnG 24100
Users.OnG 0
TKLE.OnG 0
PSR-1_Desalter.OnG 1430
PSR-2_Desalter.OnG 0
SWTU_Train.OnG 0
PSR-2_Process.OnG 0
PSR-1_Flare_KO_Drum.OnG 0
PSR-1_Crude_Tank_Drain.OnG 439
PSR-2_Crude_Tank_Drain.OnG 0
Intermediate_Condensate_Tank.OnG 544
BD1.OnG 1
BW1.OnG 1
BD2.OnG 3
BW2.OnG 3
BD3.OnG 3.6
BW3.OnG 3.6
OWe-RG2.OnG 1
BDBLs2.OnG 72.3
WHB-BD1.OnG 0.3
WHB-BD2.OnG 0.3
SW2.OnG 2
OWg.OnG 20
SW4-BDBL.OnG 1
OW3B.OnG 4
FRESHWATER.OnG 3

Coke_RunOff.TSS 127

PSR-1_ProcessArea.TSS	40
Sulfur_RunOff.TSS	16
Lift_Station4.TSS	6774
Users.TSS	10
PSR-2_Crude_Tank_Drain.TSS	6081
TKLE.TSS	0
PSR-1_Desalter.TSS	1945
PSR-2_Desalter.TSS	0
SWTU_Train.TSS	0
PSR-2_Process.TSS	13
PSR-1_Flare_KO_Drum.TSS	14
PSR-1_Crude_Tank_Drain.TSS	228
Intermediate_Condensate_Tank.TSS	108
BD1.TSS	37
BW1.TSS	37
BD2.TSS	5
BW2.TSS	0
BD3.TSS	1
BW3.TSS	0
OWe-RG2.TSS	12
BDBLs2.TSS	0.129
WHB-BD1.TSS	3
WHB-BD2.TSS	3
SW2.TSS	10
OWg.TSS	10
SW4-BDBL.TSS	10
OW3B.TSS	0
FRESHWATER.TSS	10

Coke_RunOff.COD	167
PSR-1_ProcessArea.COD	52
Sulfur_RunOff.COD	86
Lift_Station4.COD	178
Users.COD	22.2
PSR-2_Crude_Tank_Drain.COD	299
TKLE.COD	0
PSR-1_Desalter.COD	2234
PSR-2_Desalter.COD	0
SWTU_Train.COD	844

PSR-2_Process.COD	231
PSR-1_Flare_KO_Drum.COD	28
PSR-1_Crude_Tank_Drain.COD	667
Intermediate_Condensate_Tank.COD	8610
BD1.COD	81
BW1.COD	81
BD2.COD	30
BW2.COD	0
BD3.COD	48
BW3.COD	0
OWe-RG2.COD	47
BDBLs2.COD	4.974
WHB-BD1.COD	116
WHB-BD2.COD	116
SW2.COD	22.2
OWg.COD	22.2
SW4-BDBL.COD	22.2
OW3B.COD	0
FRESHWATER.COD	22.2

BD1.CHLORIDE	152
BW1.CHLORIDE	152
BD2.CHLORIDE	108
BD3.CHLORIDE	65.83

BD1.PHOSPHATE	18.52
BW1.PHOSPHATE	18.52
BD2.PHOSPHATE	19.09
BD3.PHOSPHATE	19.34

/

;

FREE VARIABLE

OBJ

```
;
BINARY VARIABLES

Ya(SO,SI)

* do not need to differentiate between Yb_perm and Yb_rej because
*Yb(INT,SI)
Yb_perm(INT,SI)
Yb_rej(INT,SI)



Yd(SO,INT)
Ye(INT)
;
POSITIVE VARIABLES

TAC   total annualized cost for a certain contaminant

Q1(SO)
Q2(SI)    flowrate of sink (in m**3 per hour)

Qa(SO,SI)      flowrate of source to sink

*Qb(INT,SI)     flowrate of interceptor to sink
Qb_perm(INT,SI) flowrate of permeate to sink
Qb_rej(INT,SI)  flowrate of reject to sink

Qd(SO,INT)     flowrate from source to interceptor

CF(INT,CO)
Cperm(INT,CO)   concentration of permeate
Crej(INT,CO)    concentration of reject
QF(INT)
qqF(INT)

PF
PR
deltapiF
;
```

EQUATIONS

OBJ_FNC

FLOW_BAL_SO
FRESH_SPLIT
FORBID_FRESH_TO_DISCHARGE

TOTAL_FLOW_INT_OUTLET
FLOW_BAL_INT
CONC_BAL_INT
EQ_INT

RR_DEFINITION
FLOW_BAL_INTperm
CONC_BAL_INTperm
FLOW_BAL_INTrej
CONC_BAL_INTrej

FLOW_BAL_SI
CONC_BAL_SI

FORBIDDEN_MIXING
EQ_QF

EQ_RO
EQ_PF
EQ_PR

BIG_Ma
BIG_Mb_perm
BIG_Mb_rej
BIG_Md
BIG_Me

BIG_Ma_lo
BIG_Mb_lo
BIG_Md_lo
BIG_Me_lo

```
;

*OBJ_FNC..    OBJ =E= Q1('FRESHWATER')+Q2('Discharge');
*OBJ_FNC..    OBJ =E= Q1('FRESHWATER')+SUM(CO,TAC(CO))+Q2('Discharge');
*$ontext
OBJ_FNC..          OBJ  =E=  (Cwater*  SUM  (  SI,  Qa('FRESHWATER',SI)  )  +
Cdischarge*Q2('Discharge')) * AOT + TAC
            + D * ( ( p * SUM ( (SO,INT),Qd(SO,INT) ) * POWER(3600*v,-1) + q*SUM(
(SO,INT),Yd(SO,INT) ) )
            +  (  p*SUM(  (INT,SI),Qb_perm(INT,SI)  )*POWER(3600*v,-1)  +  q*SUM(
(INT,SI),Yb_perm(INT,SI) ) )
            +  (  p*SUM(  (INT,SI),Qb_rej(INT,SI)  )*POWER(3600*v,-1)  +  q*SUM(
(INT,SI),Yb_rej(INT,SI) ) )
            + ( p*SUM( (SO,SI),Qa(SO,SI) )*POWER(3600*v,-1) + q*SUM( (SO,SI),Ya(SO,SI) )
) )
            * (m*((1+m)**n))*POWER((1+m)**n-1,-1) ;
*$offtext

$ontext
OBJ_FNC..          OBJ  =E=  (Cwater*  SUM  (  SI,  Qa('FRESHWATER',SI)  )  +
Cdischarge*Q2('Discharge')) * AOT + SUM(CO,TAC(CO))
            + D * ( p * SUM ((SO,INT),Qd(SO,INT) ) * POWER(3600*v,-1)
            + (p*SUM((INT,SI),Qb(INT,SI))*POWER(3600*v,-1) )
            + (p*SUM((SO,SI),Qa(SO,SI))*POWER(3600*v,-1) ))
            * (m*((1+m)**n))*POWER((1+m)**n-1,-1) ;

$offtext


FLOW_BAL_SO(SO)..    Q1(SO) =G= SUM(INT,Qd(SO,INT)) + SUM(SI, Qa(SO,SI))
;
FRESH_SPLIT..    Q1('FRESHWATER') =E= SUM(SI, Qa('FRESHWATER',SI))
;

FORBID_FRESH_TO_DISCHARGE..  Qa('FRESHWATER','Discharge')=E=0;


*TOTAL_FLOW_INT_OUTLET(INT)..    SUM(SI,Qb(INT,SI)) =E= SUM(SI,Qb_perm(INT,SI)) +
SUM(SI,Qb_rej(INT,SI));
```

```
*NOT INCLUDED:
FLOW_BAL_INT(INT)..          SUM(SO,Qd(SO,INT)) =E= SUM(SI,Qb_perm(INT,SI)) +
SUM(SI,Qb_rej(INT,SI));

CONC_BAL_INT(INT,CO)..          SUM(SO,    Qd(SO,INT)*Cso(SO,CO))     =E=
Cperm(INT,CO)*SUM(SI,Qb_perm(INT,SI))+ Crej(INT,CO)*SUM(SI,Qb_rej(INT,SI));


EQ_INT(INT,CO)..          CF(INT,CO)*SUM(SO,Qd(SO,INT))     =E=
SUM(SO,Qd(SO,INT)*Cso(SO,CO));


RR_DEFINITION(INT,CO)..     RR(INT,CO)*(SUM(SO,   Qd(SO,INT)*Cso(SO,CO)))   =E=
Crej(INT,CO)*SUM(SI, Qb_rej(INT,SI));


FLOW_BAL_INTperm(INT)..  ALPHA*SUM(SO, Qd(SO,INT)) =E= SUM(SI, Qb_perm(INT,SI));


CONC_BAL_INTperm(INT,CO)..   ( 1 - RR(INT,CO) ) * SUM(SO, Qd(SO,INT)*Cso(SO,CO))
=E= Cperm(INT,CO)*ALPHA*SUM(SO, Qd(SO,INT));


FLOW_BAL_INTrej(INT)..  (1-ALPHA)*SUM(SO, Qd(SO,INT)) =E= SUM(SI, Qb_rej(INT,SI));

CONC_BAL_INTrej(INT,CO) ..    RR(INT,CO) * SUM(SO, Qd(SO,INT)*Cso(SO,CO)) =E=
Crej(INT,CO)*(1 - ALPHA) * SUM(SO, Qd(SO,INT));


FLOW_BAL_SI(SI)..    Q2(SI) =E= SUM(SO, Qa(SO,SI)) + SUM ( INT, Qb_perm(INT,SI) +
Qb_rej(INT,SI) )
;

CONC_BAL_SI(SI,CO)..          SUM(SO,   Qa(SO,SI)*Cso(SO,CO))   +   SUM
(INT,Cperm(INT,CO)*Qb_perm(INT,SI)+     Crej(INT,CO)*Qb_rej(INT,SI)     )    =L=    (
SUM(SO,Qa(SO,SI))+ SUM ( INT, Qb_perm(INT,SI)+ Qb_rej(INT,SI) ) ) * Cmax(SI,CO)
;
```

*When the 2 outlet streams of a partitioning regenerator is fed to the same sink, either one of the stream flowrates will be zero. Or else it defeat the purpose of the separation (because in the first place, we are separating the permeate and reject streams). However, when you have more than 1 sink, then both outlet streams can have different flowrate.

```
FORBIDDEN_MIXING(SI)..    Qb_perm('RO',SI)*Qb_rej('RO',SI) =E= 0;

EQ_QF(INT)..    QF(INT)=E= SUM(SO, Qd(SO,INT));
*Cmax(SI,CO)=20;
Cmax(SI,CO) = 25;
Cmax('OSW-SB','OnG') = 50;
Cmax('OSW-SB','TSS') = 20;
Cmax('OSW-SB','COD') = 20;

Cmax('BOILER','OnG') = 1;
Cmax('BOILER','TSS') = 20;
Cmax('BOILER','COD') = 20;


$ontext
Cmax(SI,CO)=25;

*Cperm.UP(INT,CO)=0.0012;
Cmax('OSW-SB','OnG') = 50;
Cmax('OSW-SB','TSS') = 20;
Cmax('OSW-SB','COD') = 20;
$offtext
*Cperm.LO(INT,CO) = 0.00001;
*Cperm.UP(INT,CO) = 0.0012;
*CF.LO(INT,CO)=1E-4;
*CF.UP(INT,CO)=50;
PF.LO=10;
PF.UP=70;
*Qb_perm.LO(INT,SI)=0.1;
*Qb_perm.UP(INT,SI)=100;

*CF.FX('RO','OnG')=0.00001;
*CF.FX('RO','TSS')=0.00001;
*CF.FX('RO','COD')=0.00001;

QF.LO(INT) = 40;
QF.UP(INT) = 120;
```

```
deltapiF.UP = 55;
deltapiF.LO = 0;


Ma(SO,SI) = 100;
Mb_perm(INT,SI) = 50;
Mb_rej(INT,SI) = 50;
Md(SO,INT) = 50;
Me(INT) = 200;

*lower bounds must not be zero
Ma_lo(SO,SI) = 0.1;
Mb_lo(INT,SI) = 0.1;
Md_lo(SO,INT) = 0.1;
Me_lo(INT) = 0.01;


Q1.FX('Coke_RunOff') = 5;
Q1.FX('PSR-1_ProcessArea') = 23;
Q1.FX('Sulfur_RunOff') = 20;
Q1.FX('Lift_Station4') = 69;
Q1.FX('Users') = 27;
Q1.FX('TKLE') = 20;
Q1.FX('PSR-1_Desalter') = 30;
Q1.FX('PSR-2_Desalter') = 45;
Q1.FX('SWTU_Train') = 100;
Q1.FX('PSR-2_Process') = 2;
Q1.FX('PSR-1_Flare_KO_Drum') = 17;
Q1.FX('PSR-1_Crude_Tank_Drain') = 1;
Q1.FX('PSR-2_Crude_Tank_Drain') = 6;
Q1.FX('Intermediate_Condensate_Tank') = 1;
Q1.FX('BD1') = 3.5;
Q1.FX('BW1') = 1.8 ;
Q1.FX('BD2') = 10;
Q1.FX('BW2') = 2;
Q1.FX('BD3') = 3.5;
Q1.FX('BW3') = 1.8;
Q1.FX('OWe-RG2') = 25;
Q1.FX('BDBLs2') = 72.3;
Q1.FX('WHB-BD1') = 0.3;
```

```
Q1.FX('WHB-BD2') = 0.3;
Q1.FX('SW2') = 2;
Q1.FX('OWg') = 0;
Q1.FX('SW4-BDBL') = 67.2;
Q1.FX('OW3b') = 3.1;

*maximum allowable freshwater
Q1.UP('FRESHWATER') = 300;

*$ontext
Q2.FX('FIREWATER') = 3;
Q2.FX('OSW-SB') = 144;
Q2.FX('POTABLE') = 20;
Q2.FX('PSR1_CT') =25.6;
Q2.FX('Cogen_CT')=54;
Q2.FX('MG3_CT')=25;
Q2.FX('BOILER')=208.9;
Q2.FX('HPU1')=29.7;
Q2.FX('HPU2')=29.7;
Q2.FX('PSR1_SW')= 2;
Q2.FX('PSR2_SW')=36.96;
Q2.FX('BDBLu')= 56.3333;
*$offtext



EQ_RO..    TAC =E= (Cmodule*SUM(SI,Qb_perm('RO',SI)*POWER(3600,-1)))/(Sm*A*( PF -
(0.5*deltaPshell)- PP - ((OS*SUM(CO,Cperm('RO',CO))*A*(PF - (0.5*deltaPshell)- PP - deltapiF)
        *(((    (exp    (2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-
1)/(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1))
        /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))

/(1+(16*A*miu*ro*L*LS*(((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-
1))))-1)
        /(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+ 1))
        /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
        /(1.0133e5*(ri**4))))))*POWER(Kc,-1)))
        *(((    (exp    (2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-
1)/(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1))
        /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
```

```
/(1+(16*A*miu*ro*L*LS*(((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-1)
           /(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+ 1))
           /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
           /(1.0133e5*(ri**4))))))
           + Cpump*((SUM(SO,Qd(SO,'RO')*POWER(3600,-1))*(PF - Patm)*1.01325E5)**0.65)
           + Cturbine*((SUM(SI,Qb_rej('RO',SI)*POWER(3600,-1))*((PF - deltaPshell) - Patm)*1.01325E5)**0.43)
           + SUM(SO, Qd(SO,'RO')*POWER(3600,-1))*(PF - Patm)*1.01325E5*Celectricity*AOT*POWER(NETApump,-1)*0.001
           + SUM(SO, Qd(SO,'RO')*POWER(3600,-1))*Cchemicals*AOT
           - SUM(SI,Qb_rej('RO',SI)*POWER(3600,-1))*((PF - deltaPshell) - Patm)*1.01325E5*NETAturbine*Celectricity*AOT*0.001
;


*$ontext
EQ_PF(CO)..            PF =E= SFC * (2*SUM(SO, Qd(SO,'RO'))*CF('RO',CO) - SUM(SI,Qb_perm('RO',SI))*Cperm('RO',CO) - SUM(SI,Qb_perm('RO',SI))*CF('RO',CO)) * POWER (2*Cperm('RO',CO)*A*(SUM(SO,Qd(SO,'RO'))-SUM(SI,Qb_perm('RO',SI)))
          *(((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-1)
          *POWER(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1,-1)
          *POWER(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1)),-1))
          *POWER(1 + ( (16*A*miu*ro*L*Ls*((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-1)
          *POWER(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1,-1)
          *POWER(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1)),-1)))
          *POWER(1.0133e5*(ri**4),-1)),-1)),-1)
          + piF*(2*SUM(SO, Qd(SO,'RO'))*CF('RO',CO) - SUM(SI,Qb_perm('RO',SI))*Cperm('RO',CO) - SUM(SI,Qb_perm('RO',SI))*CF('RO',CO))*POWER(2*CF('RO',CO)*(SUM(SO,Qd(SO,'RO')) - SUM(SI,Qb_perm('RO',SI))),-1)
          + (0.5 * deltaPshell + PP)
;

EQ_PR..   PR =E= PF - deltaPshell;

*$offtext
*BIG-M LOGICAL CONSTRAINTS (UPPER BOUNDS)
```

```
BIG_Ma(SO,SI)..    Qa(SO,SI) =L= Ma(SO,SI)*Ya(SO,SI)
;
BIG_Mb_perm(INT,SI)..    Qb_perm(INT,SI) =L= Mb_perm(INT,SI)*Yb_perm(INT,SI)
;
BIG_Mb_rej(INT,SI)..    Qb_rej(INT,SI) =L= Mb_rej(INT,SI)*Yb_rej(INT,SI)
;
BIG_Md(SO,INT)..    Qd(SO,INT) =L= Md(SO,INT)*Yd(SO,INT)
;
BIG_Me(INT)..    SUM ( SO, Qd(SO,INT) ) =L= Me(INT)*Ye(INT)
;


*BIG-M LOGICAL CONSTRAINTS (LOWER BOUNDS)

*$ontext
BIG_Ma_lo(SO,SI)..    Qa(SO,SI) =G= Ma_lo(SO,SI)*Ya(SO,SI)
;
*BIG_Mb_lo(INT,SI)..    Qb(INT,SI) =G= Mb_lo(INT,SI)*Yb(INT,SI)
;
BIG_Md_lo(SO,INT)..    Qd(SO,INT) =G= Md_lo(SO,INT)*Yd(SO,INT)
;
BIG_Me_lo(INT)..    SUM ( SO, Qd(SO,INT) ) =G= Me_lo(INT)*Ye(INT)
;
*$offtext
MODEL WATER
/
OBJ_FNC

FLOW_BAL_SO



FRESH_SPLIT
*FORBID_FRESH_TO_DISCHARGE



FLOW_BAL_INT
*TOTAL_FLOW_INT_OUTLET
```

CONC_BAL_INT

EQ_INT
RR_DEFINITION

FLOW_BAL_INTperm
*CONC_BAL_INTperm
*FLOW_BAL_INTrej
*CONC_BAL_INTrej

FLOW_BAL_SI
CONC_BAL_SI

*MIN_CF
EQ_RO
*LOWER_BOUND_QF
*UPPER_BOUND_QF

**QF_EQUIVALENT
FORBIDDEN_MIXING
EQ_QF

*BIG_Ma
*BIG_Mb
*BIG_Md

*EQ_PF
*EQ_PR

BIG_Ma
BIG_Mb_perm
BIG_Mb_rej
BIG_Md

```
*BIG_Me

*BIG_Ma_lo
*BIG_Mb_lo
*BIG_Md_lo
*BIG_Me_lo
/
;

*WATER.reslim = 100000;

OPTION
LIMROW = 10000
LIMCOL = 10000
*OPTCA = 0.7
*OPTCR = 0.7
*MINLP = DICOPT
MINLP = BARON
;


SOLVE WATER USING MINLP MINIMIZING OBJ
;

nRO = SUM(SI,Qb_perm.L('RO',SI)*POWER(3600,-1))/(Sm*A*( PF.L - (0.5*deltaPshell)- PP -
OS*SUM(CO,Cperm.L('RO',CO))*A*(PF.L - (0.5*deltaPshell)- PP - deltapiF.L)
            *(((     (exp      (2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-
1)/(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1))
            /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))

/(1+(16*A*miu*ro*L*LS*(((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-
1))))-1)
            /(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+ 1))
            /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
            /(1.0133e5*(ri**4)))))*POWER(Kc,-1))
            *(((     (exp      (2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-
1)/(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+1))
            /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
```

```
/(1+(16*A*miu*ro*L*LS*(((exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))-1)
        /(exp(2*(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))+ 1))
        /(SQRT((16*A*miu*ro)/(1.0133e5*(ri**2)))*(L*POWER(ri,-1))))
        /(1.0133e5*(ri**4))))))
;

DISPLAY
Qa.l,
Qb_perm.l,
Qb_rej.l,
Qd.l,
Ya.l,
Yb_perm.l,
Yb_rej.l,
Yd.l
nRO

;

*concentration balance
```