GENERIC CASCADE ANALYSIS TECHNIQUE FOR SETTING THE MINIMUM TARGETS FOR RESOURCE CONSERVATION

FOO CHWAN YEE

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To my beloved wife Cecilia Cheah Choon Shiuan, parents and siblings

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ABSTRACT

The current drive towards environmental sustainability and the rising costs of raw material and waste treatment have encouraged the process industry to find new ways to reduce resource consumption and waste generation. Concurrently, the development of systematic techniques for resource conservation and recycling within a process plant has seen extensive progress. The advent of process integration technique based on pinch analysis as a tool for the synthesis of optimal resource conservation networks (RCNs) has been one of the most significant advances in the area of pollution prevention over the last decade. However, most of the work on setting targets for resource conservation have been carried out using graphical tools. There is a clear need to develop a numerical technique to quickly and accurately establish the minimum resource targets for a RCN. This thesis presents a new targeting tool called the *cascade analysis* technique to locate the minimum fresh feed and discharge flowrate targets, pinch location(s) and the resource allocation target for various types of RCNs. The RCNs cases covered in this thesis include continuous and batch water networks, utility gas network as well as property-based network. In the synthesis of water network, water cascade analysis (WCA) is the first numerical technique that is able to handle both mass transfer and non-mass transfer-based water-using processes simultaneously. A new concept to achieve zero discharge via the use of regeneration unit optimisation in water network is also presented. Gas cascade analysis (GCA) and property cascade analysis (PCA) techniques are the first non-iterative numerical targeting tools for the synthesis of utility gas and property-based networks. The appropriate placement of resource regeneration/purification unit(s) and other process changes options were also assessed using these newly developed cascade analysis techniques.

ABSTRAK

Keprihatinan terhadap pemuliharaan alam sekitar dan kenaikan harga bahan mentah serta kos rawatan sisa telah menggesa industri proses untuk mencari penyelesaian baru dalam usaha mengurangkan penggunaan sumber serta penjanaan sisa. Pada masa yang sama, penyelidikan yang meluas telah dilaksanakan dalam pembangunan teknik sistematik yang melibatkan kitar semula dan penjimatan sumber dalam sesebuah loji proses. Dewasa ini, teknik integrasi proses berdasarkan analisa jepitan untuk sintesis jaringan penjimatan sumber (RCNs) optima merupakan antara teknik yang terpenting dalam penyelidikan pencegahan pencemaran. Walau bagaimanapun, penyelidikan yang meluas dalam penetapan sasaran penjimatan sumber telah bertumpu kepada kaedah grafik. Oleh itu, adalah amat penting untuk membangunkan satu kaedah berangka yang pantas, jitu dan berkesan untuk mencapai sasaran penggunaan sumber yang minima. Tesis ini membentangkan satu kaedah baru untuk penetapan sasaran rekabentuk yang dikenali sebagai teknik analisa lata untuk menetapkan sasaran kadaralir suapan segar dan pembuangan sisa, lokasi jepitan dan sasaran peruntukan sumber bagi pelbagai jenis RCNs. Kes-kes RCNs yang dibincangkan dalam tesis ini merangkumi jaringan air sistem berterusan dan kelompok, jaringan gas utiliti dan jaringan sifat. Dalam jaringan air, analisa lata air (WCA) adalah kaedah berangka pertama yang boleh menangani kedua-dua jenis proses penggunaan air yang berdasarkan pindah jisim dan bukan pindah jisim. Satu konsep baru untuk mencapai sisa sifar dalam jaringan air melalui pengoptimuman unit penjanaan telah dibangunkan. Untuk jaringan gas utiliti dan jaringan sifat, analisa lata gas (GCA) dan analisa lata sifat (PCA) merupakan kaedah berangka pertama yang tidak melibatkan pengiraan iteratif. Penempatan alat penjanaan semula dan penulenan sumber serta skema pengubahsuaian proses juga dianalisa melalui teknik baru analisa lata telah dibangunkan.

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Symbols in Roman

C - impurity concentration

C_i - impurity concentration of process sinks *j*

C_{in} - inlet concentration of regeneration unit

C_j - impurity concentration of process source *i*

C_k - impurity concentration at level *k*

C_{M} - impurity concentration of make-up stream

C_{P} - impurity concentration of purge stream

C_{R} - impurity concentration of recycle stream

C_{out} - outlet concentration of regeneration unit

Cum. Δm - cumulative load

ΔC_{RG} - inlet and outlet concentration of regeneration unit

Δm - mass/property load

Δm_j^{in} - inlet mass/property load of process sinks *j*

$\Delta m_j^{\mathrm{min}}$ - minimum mass/property load of process sinks *j*

$\Delta m_j^{\mathrm{max}}$ - maximum mass/property load of process sinks *j*

$\Delta m_{\mathrm{S},i}$ - mass load removed from a water source *i*

Δy - driving force difference

Δt - duration of time interval

F_{C} - cumulative flowrate

F_{D} - discharge flowrate

F_{F} - fresh feed flowrate

$F_{\mathrm{F},\,k}$ - interval fresh feed flowrate

F_i - flowrate of process sinks *j*

F_j - flowrate of process source *i*

F_{M} - flowrate of make-up stream

F_{P} - flowrate of purge stream

F_{R} - flowrate of recycle stream

$F_{\mathrm{RG},\, i}$ - flowrate sent for regeneration from water source i

F_{reg} - total regeneration flowrate

l - time interval

M - material content

M_{FW} - flow of fresh water (batch process)

$M_{\mathrm{FW},\, k}$ - interval fresh water flowrate (batch process)

M_i - flow of process sinks j (batch process)

M_j - flow of process source i (batch process)

$M_{i,\, j}$ - flow fed from source i to sink j (batch process)

M_{ST} - water storage capacity

M_{WW} - flow of wastewater (batch process)

N_{SK} - number of process sink

N_{SR} - number of process source

n - number of driving force levels

p - property

$\overline{p}$ - mean property

p_j^{in} - inlet property of sink j

p_j^{min} - minimum property of sink j

p_j^{max} - maximum property of sink j

q - number of time intervals

RVP - Reid vapour pressure

R - resistivity

R_∞ - reflectivity

RP - removal percentage

SK - process sink

SR - process source

$\Sigma_i\, F_i$ - summation of process source flowrate

$\Sigma_j\, F_j$ - summation of process sink flowrate

$\Sigma_i\, M_i$ - summation of process source flow (batch process)

$\Sigma_j\, M_j$ - summation of process sink flow (batch process)

t - time

t^s - start time

t^t - end time

x_i - fractional contribution of source i

y - driving force

y_k - driving force at level k

Greek letter

Δ - difference

Σ - summation

μ - viscosity

ρ - density

ψ - property operator

ψ_i - property operator of source i

ψ_j - property operator of sink j

ψ_j^{in} - inlet property operator of sink j

$\psi_j^{\min}$ - minimum property operator of sink j

$\psi_j^{\max}$ - maximum property operator of sink j

Superscript

in - inlet

min - minimum

max - maximum

s - start

t - end

out - outlet

Subscripts

C - cumulative
F - fresh feed
D - waste discharge
i - process source
in - inlet
j - process sink
k - number of driving force level
M - make-up
out - outlet
P - purge
R - recycle
RG - regeneration
reg - regeneration
SK - sink
SR - source

CHAPTER 1

INTRODUCTION

1.1 Background problem

The current drive towards environmental sustainability and the rising costs of resources and waste treatment have encouraged the process industry to find new ways to reduce its resource consumption and waste generation. Process plants are now taking more serious steps towards minimising resource consumption via in-plant reuse and recycle. This corresponds to reduced waste generation as a mean to reduce production cost and to ensure sustainable growth of business activities. Recently, significant progress has been made in the optimisation of material recycle and reuse. In particular, *process integration* technique has emerged as an effective tool in handling the many waste minimisation (also often called as *pollution prevention*) problems in the process industries.

1.2 Process integration and process synthesis

Process integration is defined as the holistic approach to process design, retrofitting and operation which emphasises the unity of the process (El-Halwagi, 1997). In the context of pollution prevention, process integration element that plays the more important role in providing systematic solution is that of *process synthesis*.

Process synthesis is the step to determine the optimum interconnection of different processing units to form a flowsheet that meets the process design requirement (Westerberg, 1980). It has been an active research area since the late 1960s (Nishida *et al.*, 1981). Since then, process synthesis has been an active research area and the review on its development can now be found in many review papers (Hendry *et al.*, 1973; Hlaváček, 1978; Westerberg, 1980, 1987; Stephanopoulos, 1981; Nishida *et al.*, 1981; Gundersen and Naess, 1988; Linnhoff, 1993; Manousiouthakis and Allen, 1995; El-Halwagi, 1998; El-Halwagi and Spriggs, 1998; Johns, 2001; Dunn and El-Halwagi, 2003; Li and Kraslawski, 2004) and textbooks (Rudd *et al.*, 1973; Linnhoff *et al.*, 1982; Douglas, 1988; Smith, 1995, 2005; Shenoy, 1995; Mann and Liu, 1999; El-Halwagi, 1997, 2006).

Manousiouthakis and Allen (1995) had broadly classified process synthesis into seven major areas:

i. Material synthesis
ii. Reaction path synthesis
iii. Reactor network synthesis
iv. Separation network synthesis
v. Heat exchanger network synthesis
vi. Mass exchanger network synthesis
vii. Total flowsheet network synthesis

Among these many process synthesis areas, two of the most well developed areas are the synthesis of heat exchanger network synthesis (HEN, or commonly know as *heat integration*) and mass exchanger network (MEN, commonly known as *mass integration*). Both of the heat and mass integration areas have been widely accepted as practical design tools and have been included in almost all process design textbooks lately (e.g. see Douglas, 1988; Biegler *et al.*, 1997; Turton *et al.*, 1998; Allen and Shonnard, 2002; Seider *at al.*, 2003; Smith, 1995, 2005). Heat, mass and the recent established property integration (Shelley and El-Halwagi, 2000; Vasiliki and El-Halwagi, 2005) techniques together become the three subsets of process integration techniques.

In the context of pollution prevention, various special cases of mass and property integration has received much attention from both the academic and industrial practitioners. This includes the synthesis of water and hydrogen (special cases of mass integration) as well as the property-based networks. These special cases can be generally categorised under the main framework of material reuse/recycle, or more specifically *resource conservation networks* (RCNs).

1.3 Problem statement

Most of the works on the synthesis of RCNs based on process integration technique have been carried out using graphical tools. Many limitations have been associated with these graphical tools, such as inaccuracy and cumbersomeness. Clearly, a more efficient tool based on numerical technique is needed to handle the minimum fresh resource and waste discharge targeting step in these RCNs and overcome the limitations of graphical approaches.

1.4 Objective

The objective of this research is to develop a generic systematic technique to efficiently and accurately locate the minimum fresh feed and discharge targets in a RCN. This includes continuous and batch water networks, property-based network and utility gas network.

1.5 Scopes of research

This research is divided into four main parts:

i. Flowrate targeting for water network in continuous mode

Minimum fresh water and wastewater flowrates targeting based on pinch analysis concept is the first stage of the water network synthesis. It is carried out prior to water network design. A new targeting technique is to be developed to locate the minimum water flowrates, covering both mass transfer-based and non-mass transfer-based water-using processes. Options for process changes are to be assessed using the new targeting technique.

ii. Synthesis of a batch water network

A two-stage procedure for the synthesis of batch water network will be developed. In the first stage, the targeting technique developed for continuous water network will be extended to the batch water network problem. The time dimension is taken as a primary constraint in this adaptation. In the second stage, a systematic design procedure for a water network utilising the newly introduced batch network representation will be presented.

iii. Targeting for utility gas network

Targeting technique developed in earlier chapters will be applied to nitrogen, oxygen and hydrogen gas networks. Beside, appropriate placement of gas purification units will be assessed using the targeting tool.

iv. Synthesis of property-based network

A two-stage procedure for the synthesis of property-based network is to be developed. New graphical and numerical targeting tools will be developed to locate the various network targets prior to network design.

1.6 Contributions of the work

This thesis offers significant contributions in the area of RCNs synthesis. The key contributions are summarised as follows:

i. A generic non-iterative numerical technique for locating minimum fresh and discharge flowrate targets in a RCN called the *cascade analysis technique* has been developed. It has been applied to various kind RCN problems with different characteristics (e.g. driving force, multiple pinches, etc.).
ii. For the synthesis of water network, *water cascade analysis* (WCA) technique is the first numerical technique that is able to handle both mass transfer and non-mass transfer-based water-using processes simultaneously. A new concept to achieve zero discharge in water network is also presented, i.e. with the use of regeneration unit optimisation.
iii. For the synthesis of batch water network, the two-step approach presented in this thesis is the first work to handle both mass transfer and non-mass transfer-based water-using processes, as can be found in the open literature.
iv. *Gas cascade analysis* (GCA) technique is the first non-iterative numerical targeting tool for utility gas network synthesis. New application of utility gas network synthesis has also been firstly extended into oxygen and nitrogen gas networks. Besides, problem involving multiple pinches for utility gas network has also been addressed and solved for the first time.
v. The *property cascade analysis* (PCA) technique is the first numerical targeting tool for property-based network.

1.7 Summary of this thesis

Cascade analysis technique is non-iterative and can quickly yield rigorous targets prior to detailed network design. The developed methodologies are described in depth in each chapter using various literature and industrial case studies.

Chapter 2 provides a review of the relevant theories and literatures of this thesis related to the development in process integration for the synthesis of RCNs. The development of a systematic targeting procedure is initiated here.

The methodology for setting minimum fresh feed and discharge targets for RCNs using cascade analysis technique is described in Chapter 3. The generic representation of the cascade analysis technique that is applicable to various RCN problems is presented here.

In Chapter 4, cascade analysis technique is applied to maximum water recovery (MWR) network problem. Hence, it is called the WCA technique. WCA handles both mass transfer-based and non-mass transfer-based water-using operations and is applicable to a wide range of water network (e.g. multiple pinches). WCA also helps in the assessment of various options for process changes, including water regeneration, equipment modifications and optimisation towards zero discharge.

A new extension of WCA technique, i.e. *time-dependent water cascade analysis* (TDWCA) technique is next applied to the synthesis of a batch water network, as discussed in Chapter 5. A new network representation called the *time-water network* is also introduced in this chapter to synthesis the batch MWR network to achieve the established fresh water and wastewater targets.

Chapter 6 describes the application of cascade analysis technique in utility gas network, i.e. the GCA technique. Different industrial processes involving the integration of nitrogen, oxygen and hydrogen gases are used to demonstrate the GCA technique. Appropriate placement of gas purification units is also being assessed.

Cascade analysis technique is next applied to the property-based network in Chapter 7. Two new tools are developed here. With the introduction of a new graphical tool called the *property surplus diagram*, a basic framework for the determination of the minimum fresh feed and discharge targets is provided. The PCA technique is next established to set targets via a tabular approach. A network design technique is also presented to synthesise a maximum resource recovery (MRR) network that achieves the various established targets.

Chapter 8 concludes the thesis by summarising the main points discussed and exploring the potential areas for future development of RCNs synthesis. Figure 1.1 summarises the conceptual links between the chapters in this thesis.

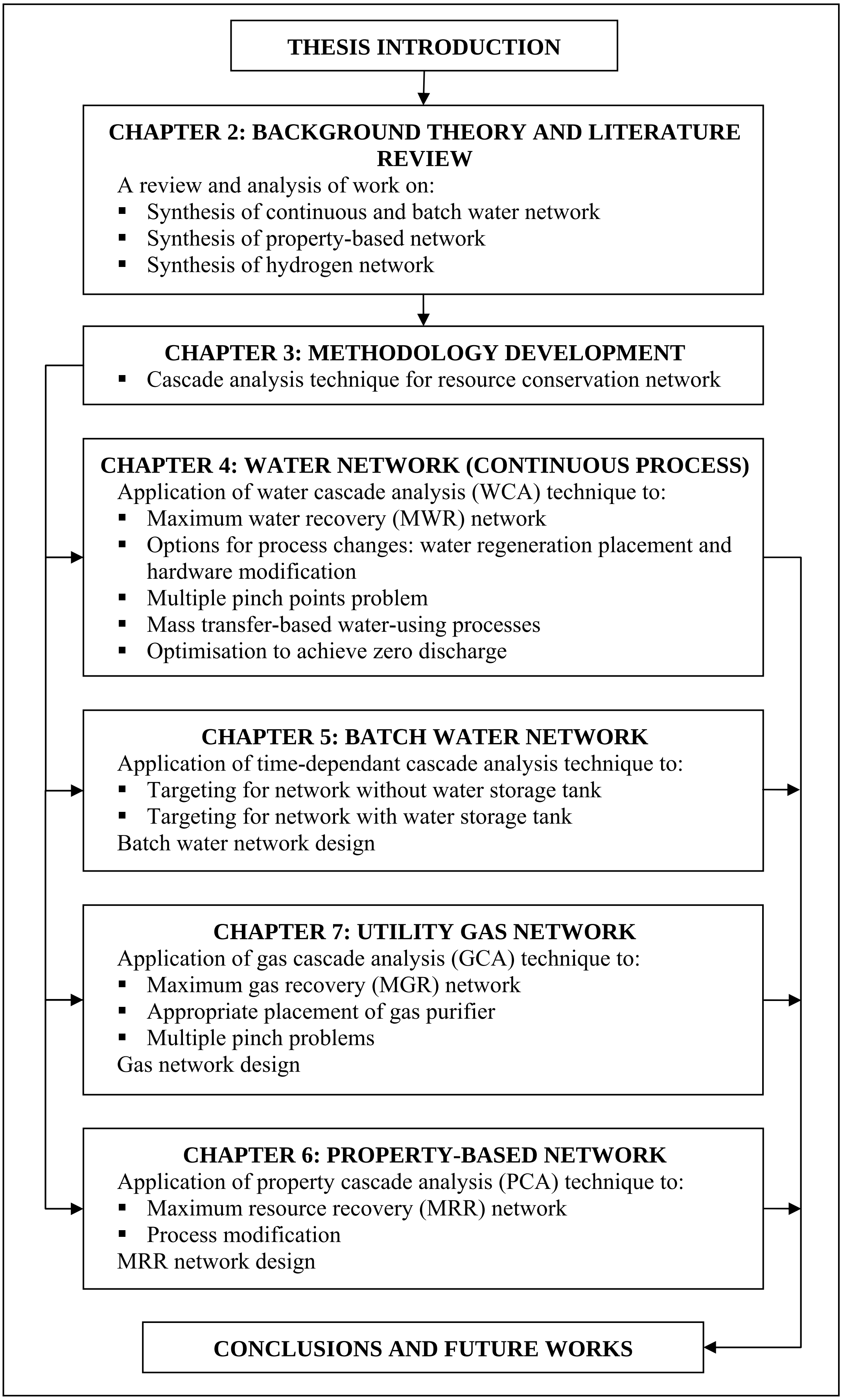

Figure 1.1 A flow diagram illustrating the conceptual links between the chapters

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