A NEW ALGEBRAIC TOOL FOR SIMULTANEOUS TARGETING AND DESIGN OF MASS EXCHANGER NETWORK

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ABSTRACT

Process effluent recovery can be a potential source of revenue as well as an effective way to reduce the environmental footprint for industrial processes. In addition to sustaining business profitability, modern day industries have to fulfil their social responsibility by contributing toward environmental conservation and sustainable development. Mass (or materials) integration is a methodology for systematic and efficient reuse and recycling of materials in a closed loop within a mass exchange network (MEN). The integration of systems and processes promotes manufacturing synergy and minimises waste generation, disposal, and reduces the use of fresh materials and mass separating agents. Methodologies for MEN design and targeting include insight-based graphical and algebraic techniques as well as mathematical programming approaches. This study presents a new algebraic tool for simultaneous targeting and design of mass exchanger network that overcomes the limitations of previously developed mass integration approaches such as composition interval table (CIT), graphical composite curves (CCs) and grid diagram for MEN. The current CIT and CC cannot completely map individual rich and lean process streams, or individual process and utility streams. Hence, the mass separating agent (MSA) targeting results cannot be used to simultaneously design the MEN. Although pinch-based tools have been established for MEN design, the procedure is typically done in two sequential stages. The first stage involves MSA targeting using CIT. Once the targeting stage is completed the MEN design to achieve the MSA target is done using grid diagram. As the CIT cannot be used to visualise the MEN, repetitive stream-wise composition and mass load balance calculations have to be done in order to achieve the minimum MSA and number of mass exchange units. The aforementioned significant limitations of the conventional pinch-based approach have been overcomed by the newly developed segregated composition interval table (SECIT) proposed in this research. SECIT represents mass cascade along composition intervals for lean and rich individual streams. SECIT can help identify pinch point(s), determine utility targets and conduct SECIT mass allocation (SMA). The SMA can be converted to a SECIT network diagram that represents the MEN in terms of mass exchange quality and quantity, on the interval composition scale. Economic analysis study showed that the total capital cost target for MEN based on the newly developed SECIT is USD 752,539. This total capital cost target agrees with those obtained using conventional composite curves. However, sensitivity analysis study carried out using various minimum composition differences showed an optimal total cost of USD 448,945 and was found at minimum composition difference of 0.0001. Furthermore, sensitivity analysis study based on selection of materials of construction showed that 303 stainless steel type is the best material of construction for the newly SECIT network design. Four case studies, including an industrial application had been presented to demonstrate the validity and advantages of the proposed approach. This study shows that the SECIT and segregated network design can be an essential blend of algebraic and graphical visualisation tools for simultaneous MEN targeting and design of simple and complex processes and for retrofit cases involving threshold problems, stream splitting and multiple pinches.

ABSTRAK

Proses pemulihan efluen berpotensi menyumbang hasil pendapatan selain amat berkesan untuk mengurangkan jejak alam sekitar bagi proses industri. Disamping mencapai keuntungan, industri masa kini perlu memenuhi tanggungjawab sosialnya dengan menyumbang kepada pemuliharaan alam sekitar dan pembangunan mapan. Integrasi jisim (atau bahan) adalah kaedah penggunaan sisa buangan secara sistematik dan cekap dalam sebuah rangkaian penukaran jisim (MEN). Integrasi sistem dan proses menggalakkan sinergi pengeluaran, meminimakan penjanaan sisa, pelupusan, mengurangkan penggunaan bahan segar dan agen pemisahan jisim. Kaedah rekabentuk dan sasaran MEN merangkumi tatacara berasaskan grafik dan teknik algebra, serta kaedah pengaturcaraan matematik. Kajian ini membentangkan perkakas algebra baharu bagi penetapan sasaran serta reka bentuk rangkaian penukar jisim secara serentak, yang mengatasi kekangan kaedah integrasi jisim yang terdahulu seperti jadual interval komposisi (CIT), lengkuk komposit grafik (CCs) dan rajah grid MEN. CIT dan CC tidak dapat memetakan aliran individu proses yang kaya dengan aliran bersih, atau aliran proses individu dan aliran utiliti. Oleh itu, hasil sasaran ejen pemisah jisim (MSA) tidak boleh digunakan untuk merekabentuk MEN secara serentak. Meskipun kaedah berasaskan jepitan telah lama digunakan bagi merekabentuk MEN, prosedur jepitan biasanya dilaksanakan dalam dua langkah yang berturutan. Langkah pertama melibatkan penyasaran MSA menggunakan CIT. Setelah tahap penyasaran selesai, rajah grid digunakan untuk rekabentuk MEN bagi mencapai sasaran MSA. Oleh kerana CIT tidak boleh digunakan bagi visualisasi MEN, imbangan komposisi aliran serta jisim perlu dilakukan secara berulang bagi mencapai MSA minimum dan bilangan unit penukaran jisim. Keterbatasan pendekatan berasaskan kaedah konvensional jepitan telah diatasi melalui jadual interval komposisi segregasi (SECIT) yang baharu dibangunkan dalam kajian ini. SECIT mewakili profil aliran jisim merentasi komposisi bagi aliran kaya dan aliran bersih. Ia digunakan untuk mencari titik jepitan, mengira sasaran utiliti dan peruntukan jisim SECIT (SMA). SMA boleh ditukar kepada rajah rangkaian SECIT bagi mempamerkan rangkaian penukaran jisim dan juga jumlah penukaran jisim pada skala interval komposisi. Kajian analisis ekonomi menunjukkan bahawa jumlah sasaran kos modal untuk MEN berdasarkan SECIT yang baharu dibangunkan adalah USD 752,539. Keseluruhan sasaran kos modal ini menghasilkan keputusan yang sama jika dibandingkan dengan kaedah konvensional yang menggunakan lengkuk komposit. Bagaimanapun, kajian analisis sensitiviti yang dijalankan dengan menggunakan pelbagai perbezaan komposisi minimum menunjukkan bahawa jumlah kos tahunan yang optimum ialah USD 448,945 dan keputusan ini dihasilkan pada perbezaan komposisi minimum iaitu 0.0001. Selain itu, analisis sensitiviti berdasarkan pemilihan bahan pembinaan menunjukkan bahawa jenis keluli tahan karat 303 adalah bahan pembinaan terbaik untuk reka bentuk rangkaian SECIT yang baharu dibangunkan. Empat kajian kes, termasuklah aplikasi industri telah dibentangkan bagi membuktikan kelebihan pendekatan ini. Kajian ini menunjukkan bahawa SECIT dan rekabentuk rangkaian segregasi merupakan kombinasi penting untuk perkakas visualisasi algebra dan grafik bagi menyasarkan MEN secar serentak dan merekabentuk proses-proses yang ringkas dan kompleks, termasuk kes-kes berbilang jepitan, pemecahan aliran dan masalah ambangan.

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LIST OF ABBREVIATIONS

ACC	-	Annualized Capital Cost
AX	-	Arabionoxylan
AXOS	-	Arabionoxylan Oligosaccharides
b	-	constant
CC	-	Composition Curves
CIT	-	Composition Interval Table
COG	-	Coke Oven Gas
CO_2	-	Carbon (IV) oxide
CO	-	Cabon (II) oxide
DFP	-	Driving Force Plot
EMU	-	External Mass Utility
ETD	-	Energy Transfer Diagram
ExtMSA	-	External Mass Separating Agent
GA	-	Generic Algorithm
GCC	-	Grand Composite Curve
GD	-	Grid Diagram
HEN	-	Heat exchange Network
LP	-	Linear Programming
LSCMP	-	Lean Stream Composition Mass Plot
ME	-	Mass Exchanger
MEN	-	Mass Exchange Network
MILP	-	Mixed Integer Linear Programming
MINLP	-	Mixed Integer Non-Linear programming
MMR	-	Maximum Mass Recovery
MSA	-	Mass Separating Agent
NPV	-	Net Present Value
OTGD	-	Overall Time Grid Diagram
PDM	-	Pinch Design Method
RSCMP	-	Rich Stream Composition Mass Plot
SCMP	-	Stream Composition Mass Plot

SECIT	-	Segregated Composition Interval Table
SePTA	-	Segregated Problem Table Algorithm
SMA	-	Segregated CIT Mass Allocation
SND	-	Segregated CIT Network Diagram
S&TBS	-	Supply and Target Based Superstructure
SWS	-	Step- Wise Superstructure
TAC	-	Total Annual Cost
TGD	-	Time Grid Diagram
T&SBS	-	Target and Supply Based Superstructure
UTM	-	Universiti Teknologi Malaysia
USD	-	United State Dollar

LIST OF SYMBOLS

A - Absorption factor
c - constrain value
C_{min} - Minimum cost of MSA
C_{pinch} - Composition pinch
C_{T} - Cost of installed tray
C_{BT} - Base Cost
D - Column diameter
F_{n} - Tray number factor
F_{NT} - Tray factor
F_{TM} - Material factor
F_{TT} - Type of Tray
G - Gas mass flow rate
G_{L} - Mass flow rate of lean stream
G_{net} - Net Mass flow rate
G_{R} - Mass flow rate of lean stream
H - Column height
i - Rich stream number
j - Lean stream number
L^{c} - Maximum mass flow rate of lean stream
M - Mass load
ΔM_{casi} - Mass cascade at interval i
ΔM_{casi-1} - Mass cascade at interval *i-1*
$\Delta M_{int,i}$ - Net mass change at interval *i*
ΔM - Change in Mass load
m_i - Mass transfer coefficient
Ne - Equilibrium stage
N_{i} - Number of independent sub-problem
N_{R} - Number of Rich stream
Ns - Number of lean stream
Nr - Number of real tray

N_T - Number of tray
R - Set of rich streams
S - Set of lean streams
s - Tray spacing
SE - External MSA
SP - Process MSA
ΔT_{min} - Minimum temperature difference
U_{max} - Maximum superficial gas velocity
U_{min} - Minimum number of units
$U_{overall}$ - Overal minimum number of units
Uv - Actual superficial gas velosity
x_{lim} - Limiting composition of lean stream
x^s - Supply composition for lean stream
x^t - Target composition for lean stream
x^{max} - Maximum practical solute compositon
y - Composition of rich streams
y^s - Supply composition for rich stream
y^t - Target composition of lean stream
Δy - Composition difference
y_{mod} - Modified rich steram composition

Greek
ε - Mimnimum composition difference
$\propto$ - Start stream interval for number of stages
β - End stream interval for number of stages
ρ_l - Density of liquid (kg/m^3)
ρ_v - Density of gas (kg/m^3)
π - Constant
η_o - Overall efficiency

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CHAPTER 1

INTRODUCTION

1.1 Research Background

Growing global concern on environmental sustainability, rising costs of energy, raw materials and waste treatment as well as increasingly stringent emission regulations, are among the factors that encourage process industry to employ process integration for resource conservation. The optimal design of solvent utilisation and recovery networks based on mass integration concept can help conserve valuable material resources while reducing environmental emissions. The industrial solvent market size was over USD 23.5 billion in 2017 and industries expect solvent consumption globally to remain at over 28 million tons in 2024 (Ahuja and Deb, 2018).

Mass Exchange Networks (MEN) are widely used in process industry to cost-effectively treat liquid wastes generated by a plant to an acceptable level. Mass integration can involve removal of pollutants/contaminants from process streams, or recovery of waste before being discharged to the environment. The design of a mass integration system, or more widely known as MEN, requires a combination of systematic conceptual approach and powerful computational tools.

Mass exchange has a key role to play in minimising hazardous wastes from processes. This is made possible through the optimal design of mass exchange networks that involve the transfer of pollutants or contaminants from a set of pollutant-rich streams to a set of pollutant-lean streams. The MEN are systems of direct contact mass transfer units, which use process streams of external mass separation agents (MSA, lean streams) to selectively remove pollutants from waste process streams (rich streams). Examples of mass-exchange operations include absorption, adsorption, stripping, solvent extraction, leaching, and ion exchange.

Practical industrial applications of mass exchange systems are concerned with aspects of design, operation and optimisation of single and multiple mass exchangers with the goal of operating cost-effectively through the minimum use of mass separating agents (MSA, or solvent) as lean streams to remove contaminants from the "rich streams". A systematic methodology for MEN design can therefore yield ample technical and economic benefits.

Over the past 40 years, pinch analysis has been established as a systematic tool for optimal design of resource utilization networks including heat (Linnhoff and Hindmarsh, 1982), mass pinch (El-Halwagi and Manousiouthakis, 1989), water (Wang and Smith, 1994), total site heat integration (Klemes *et al*.,1997), oxygen pinch (Zhelev, 1999), hydrogen pinch (Towler, 2002), CO_2 emission pinch (Tan *et al.*, 2012), power pinch (Wan Alwi *et al.*, 2013), bio-refinery integration (Shenoy and Shenoy, 2014), sustainable power generation planning (Jia *et al*., 2016), pinch analysis to determine policies for health care delivery system (Basu *et al*., 2017), waste management pinch analysis (Ho *et al*., 2017), managing finance for energy conservation (Roychaudhuri and Bandyopadyay, 2018) and Iterative pinch analysis (Arya and Bandyopadyay, 2019).

El-Halwagi and Manousiouthakis (1989) proposed an MEN targeting and design methodology for minimising mass separating agents (MSA) that is analogous to pinch analysis approach for heat exchange network synthesis. Following the success of heat pinch analysis, the MEN synthesis approach has also found practical industrial applications. Later advances in MEN techniques have included capital cost target, capital-energy cost trade-off targeting as well as retrofit targeting among other developments based on pinch analysis.

Numerous insight-based algebraic and graphical MEN synthesis approaches have been developed over the years. In general, MEN synthesis tasks for the algebraic and graphical approaches are typically performed in two sequential stages covering MSA flowrate targeting and network design. Research on MEN synthesis using mathematical programming approaches that is well-suited for handling large and complex MEN problems has also seen extensive progress. All in all, both the insight-based and mathematical programming approaches complement one another in addressing varieties of practical industrial problems. The algebraic and graphical approaches provide essential visualisation tools for practitioners who typically appreciates the insights and understanding it provides in solving of manageable scale, while mathematical programming approaches provides the computing power that is essential to address larger and more complex problems.

The fundamentals of MEN was first introduced by (El-Halwagi and Manousiouthakis, 1989). El-Halwagi and Manousiouthakis (1989) applied pinch technique for MEN synthesis through targeting and design sequentially. The minimum composition difference (ε) is presented to pinpoint thermodynamic bottleneck (pinch) that limits the extent of mass exchange. They introduced the algebraic tool, composition interval table (CIT) and graphical tool termed as mass composite curves (CCs) which maps composite rich and lean streams on a composition versus mass load diagram (y-M) to achieve maximum possible mass exchange, thus achieving minimum external MSA requirement.

However, the minimum number of unit target is also achieved by using the number of streams information. They also introduced Grid Diagram (GD) as an interface for MEN design with several design rules. The author stated that stream-matching should begin from the pinch to ensure that no mass transfer across the pinch takes place for minimum MSA target to be achieved in the design.

A key limitation of the CIT is that, it is based on the composite stream profile. As the CIT does not show the profile of individual rich and lean stream mass cascade, it cannot guide individual process to process and process to utility stream matching. As a result, the CIT also cannot be used for MEN design. The need for a systematic, interactive, insight-based simultaneous MEN targeting and synthesis approach have motivated this work. This research proposes the Segregated CIT (SECIT) as a new algebraic technique that allows the MSA targeting and MEN network design to be simultaneously performed. The SECIT technique enables matches between each rich and lean stream to be readily be used to generate the final MEN configuration. Hence, repetitive stream-wise composition and mass load balance calculations can be avoided during the MEN synthesis.

1.2 Problem Statement

Raw materials are vital resources to chemical and process industries. Synthesis of MEN involves the transfer of waste materials from rich streams to lean streams (Mass Separating Agent (MSA)). For the purpose of targeting, the minimum MSA flowrates, composition interval table (CIT) and composite curves (CCs) have been among the most widely used pinch analysis algebraic and graphical tools. The targets for the minimum flowrate of MSA can be determined using CIT and the MEN, designed using the grid diagram (GD).

As the CIT cannot be used to visualise the MEN, repetitive stream-wise composition and mass load balance calculations have to be done to achieve the minimum MSA and number of mass exchange units. There is the need to develop an algebraic technique for simultaneous MEN targeting and design. Ideally, the new technique should be based on profiles of mass cascade across composition intervals for lean and rich individual MSA streams. This new algebraic approach will overcome the limitations of CIT and CCs.

Follow is the problem statement of this work:

Given a number of pollutant-rich streams (N_R) and a number of MSAs (pollutant-lean streams, N_S). Also given are the flowrate of each rich stream, the rich stream's supply (inlet) composition and its target (outlet) composition, where i = 1, 2 ..... N_R. In addition, each MSA's supply and target compositions, and, are given; where j = 1, 2 ..... N_S. The flowrate of each MSA is unknown, and is to be determined so as to minimise the network cost. The candidate lean streams can be classified into N_{SP} process MSAs and N_{SE} external MSAs (where $N_{SP}+N_{SE}=N_S$). Process MSAs that is available on site can be used to remove pollutants/contaminants at a low cost, or at almost no cost. Each MSA flowrate that is available for mass exchange is limited by *its availability within the plant, and is bounded by the value. The flowrates of externally purchased MSAs shall be dictated by economic considerations.*

The goal of this research is to develop a new algebraic technique to simultaneously target the minimum MSA, maximise mass recovery and identify the pinch point for mass exchange. The methodology should also allow the lean and rich streams to be individually mapped in the form of an MEN design that satisfies the minimum flowrates of MSA at the minimum total cost. The trade-off between capital and operating costs and sensitivity analysis shall be performed to establish the optimal MEN design that yields the minimum network cost.

1.3 Research Objectives

The overall objective of the study is to develop a new algebraic approach for simultaneous targeting and design of mass exchanger networks. The specific objectives of the research are to:

1. Develop a new pinch-based algebraic approach for simultaneous MEN targeting and design for single, multiple pinch problems with stream splitting and threshold problem based on individual streams approach.
2. Apply the new technique to illustrative and industrial case studies.
3. Analyse economics and sensitivity analysis to assess the profitability of mass exchanger network.
4. Compare the new targeting method and network design results with other MEN methods.

1.4 Research Scope

Below is the research scope to accomplish the aforementioned objectives:

(a) State-of-the-art analysis of MEN targeting and synthesis techniques.

(b) Identification of the interaction between MEN targeting and network design, and the different types of MEN which includes single, multiple pinch problems, stream splitting and threshold cases.

(c) Development of MEN targeting and network design algorithm method for single pinch problem with no stream splitting based on individual stream approach using Microsoft excel tool version 365.

(d) Development of MEN targeting and network design algorithm method for multiple pinch problem with stream splitting based on individual stream approach.

(e) Development of MEN targeting and network design algorithm method for threshold cases.

(f) Application of the new algebraic technique to illustrative and industrial case studies to validate the effectiveness of the approach.

(g) Analyse the economics and sensitivity analysis to assess the profitability of the proposed mass exchanger network.

(h) Comparison of the results of the new developed algebraic technique with other mass integration targeting techniques such as CIT and CCs.

1.5 Research Contributions

Five new contributions have emerged from this research work as follows:

(a) A new algebraic technique for MEN design known as Segregated Composition Interval Table (SECIT) have been developed to provide designers with valuable insights for simultaneous MEN targeting and design.

(b) A new SECIT mass allocation technique based on individual, as opposed to composite process streams to assist designers visualize the mass exchange network on a segregated composition interval table.

(c) Designers do not need to undergo the feasibility criteria checking and repetitive mass balance calculations throughout the process of network design since the targeting stage can be translated directly to network design stage.

(d) This research aid in the development of mass exchange recovery (MER). Industries that consume huge amount of MSA and have multiple mass exchangers can optimise the MER and minimise their MSA.

(e) A new method have been developed for capital cost target and optimum minimum composition difference based on individual stream matches for optimal MEN design to yield minimum network cost.

1.6 Thesis Outline

This thesis comprises five chapters. Chapter 1 introduces the research background, presents the problem statement, research objectives, research scope and research contributions. Chapter 2 provides a review of the state of the art for synthesis of MEN which includes introduction to pinch analysis, fundamentals of MEN design and synthesis, MEN targeting and network design using pinch analysis, review of STEP and SEPTA, supertargeting for MEN, MEN using mathematical programming,

, multicomponent transfer of MEN,   simultaneous targeting and design of MEN. The chapter concludes by highlighting the research gap on current simultaneous targeting and design for MEN synthesis.

Chapter 3 describes the step-wise research methodology to accomplish the stated objectives. It provides an overall summary of the methodology,describe the single pinch problem, multiple pinch problem with stream splitting scenario and threshold problem, Segregated Composition Interval Table (SECIT), Segregated CIT Mass Allocation (SMA), Segregated CIT Network design (SND) and economic and sensitivity analysis methodology. Chapter 4 presents the industrial application case study that illustrate the applicability of the new approach, analyse economics and sensitivity analysis to assess the profitability of the proposed mass exchanger network and compare the results with other MENs methods. Finaly, Chapter 5 concludes the overall research study and recommends possible future work to be explored.

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