CRANFIELD UNIVERSITY

SALIHU ADAMU GIREI

OPTIMAL DESIGN AND OPERATION OF HEAT EXCHANGER NETWORK

SCHOOL OF ENGINEERING
Process Systems Engineering

PhD
Academic Year: 2011 - 2015

Supervisor: Dr Yi Cao
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ABSTRACT

Heat exchanger networks (HENs) are the backbone of heat integration due to their ability in energy and environmental managements. This thesis deals with two issues on HENs. The first concerns with designing of economically optimal Heat exchanger network (HEN) whereas the second focus on optimal operation of HEN in the presence of uncertainties and disturbances within the network. In the first issue, a pinch technology based optimal HEN design is firstly implemented on a 3–streams heat recovery case study to design a simple HEN and then, a more complex HEN is designed for a coal-fired power plant retrofitted with CO_2 capture unit to achieve the objectives of minimising energy penalty on the power plant due to its integration with the CO_2 capture plant. The benchmark in this case study is a stream data from (Khalilpour and Abbas, 2011). Improvement to their work includes: (1) the use of economic data to evaluate achievable trade-offs between energy, capital and utility cost for determination of minimum temperature difference; (2) redesigning of the HEN based on the new minimum temperature difference and (3) its comparison with the base case design. The results shows that the energy burden imposed on the power plant with CO_2 capture is significantly reduced through HEN leading to utility cost saving maximisation. The cost of addition of HEN is recoverable within a short payback period of about 2.8 years. In the second issue, optimal HEN operation considering range of uncertainties and disturbances in flowrates and inlet stream temperatures while minimizing utility consumption at constant target temperatures based on self-optimizing control (SOC) strategy. The new SOC method developed in this thesis is a data-driven SOC method which uses process data collected overtime during plant operation to select control variables (CVs). This is in contrast to the existing SOC strategies in which the CV selection requires process model to be linearized for nonlinear processes which leads to unaccounted losses due to linearization errors. The new approach selects CVs in which the necessary condition of optimality (NCO) is directly approximated by the CV through a single regression step. This work was inspired by Ye et al., (2013) regression based globally optimal CV selection with no model linearization and Ye et al., (2012) two steps regression based data-driven CV selection but with poor optimal results due to regression errors in the two steps procedures. The advantage of this work is that it doesn’t require evaluation of derivatives hence CVs can be evaluated even with commercial simulators such as HYSYS and UNISIM from among others. The effectiveness of the proposed method is again applied to the 3-streams HEN case study and also the HEN for coal-fired power plant with CO_2 capture unit. The case studies show that the proposed methodology provides better optimal operation under uncertainties when compared to the existing model-based SOC techniques.

Keywords:

Heat exchanger network, Design, Optimal operation, Data-driven, Self-optimizing control

ACKNOWLEDGEMENTS

I sincerely wish to thank my supervisor Dr Yi Cao who beyond the scope of supervision has been a source of encouragement and guidance throughout the course of the study. His critical assessment at all stages of this work was invaluable in reshaping and giving it a novel outlook. I am moreover indebted to my co-supervisor Prof Antonis Kokossis for his contributions at some stage in my research. I would also like to thank all the staff of Oil and Gas Centre especially our distinguished Mrs S. Skears among others.

I wish to thank the Federal Government of Nigeria for funding my doctorate degree study through its Petroleum Technology Development Fund (PTDF) overseas scholarship scheme.

I am also grateful to my parents for their continuous spiritual and moral support and to my wife Zainab who with patience and determination, managed to endure as a mother, a wife and then a student, in all circumstances that we had to face during the course of this study. And to my lovely kids Abdur-Rahman and Abdur-Raheem, I will say thank you for putting up with Daddy's stay-up-late routine and agreeing to leave the University Park early while other kids were playing because Daddy had only few minutes to spend with you at the Park.

I also wish to acknowledge the assistance of my brothers; Alhaji Abdurrahman Halilu Girei and Alhaji Idris Salihu Girei, without which this study would not have been possible. Both of them encourage me to apply for further studies in the UK and Cranfield University.

In the last three years, I have met a number of people and I immensely benefited from interactions with them both academically and otherwise. I am obliged to all of them, particularly to these close friends; Aminu Hamisu, Dr Chechet Biliyok, Dawid Hanak, John Melchizedek Britto, Mohammed Dahiru Aminu, Dr Mubarak Muhammad, Dr Shehu Grema, and Yahaya Baba among others.

Finally and above all, I thank Allah SWT for sparing my life and for His divine guidance to this very moment in my study.

DEDICATION

To the love and memory of Fadimatu (Adda) Usman Babbani Girei, my late stepmother, who died from primary liver cancer on 17th January 2004, May her soul rest in peace.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS

AMTD	Average Mean Temperature Difference
CAPEX	Capital Expenditures
CDU	Crude Distillation Unit
CVs	Control Variables
DOF	Degree of Freedom
HE	Heat Exchanger
HENs	Heat Exchanger Networks
HENS	Heat Exchanger Network Synthesis
HPS	High Pressure Steam
HPT	High Pressure Turbine
HRAT	Heat Recovery Approach Temperature
LMTD	Log Mean Temperature Difference
LP	Linear Programming
LPS	Low Pressure Steam
LPT	Low Pressure Turbine
MINLP	Mixed integer Nonlinear Programming
MPS	Medium Pressure Steam
MPT	Medium Pressure Turbine
NCO	Necessary Condition of Optimality
NLP	Nonlinear Programming
NTU	Number of Transfer Unit
OPEX	Operating Expenditures
PCC	Post Combustion Capture
PFD	Process Flow Diagram
PT	Pinch Technology
RTO	Real Time Optimization
SOC	Self-optimizing Control
TAC	Total Annualized Cost
VDU	Vacuum Distillation Unit

1 INTRODUCTION

1.1 Background

Heat exchanger networks (HENs) has gradually developed into a field of research on energy management in chemical and process industries. Most literatures in this field are either tailored towards developing a HEN with minimum utility consumption, heat exchanger (HE) areas and numbers of HE units or they are aimed at synthesizing networks with reasonable trade-offs between annualized capital and operating cost.

Basically, the methodologies for synthesis of HEN are, according to Smith et al. (2010), categorized as shown in Figure 1-1 below:

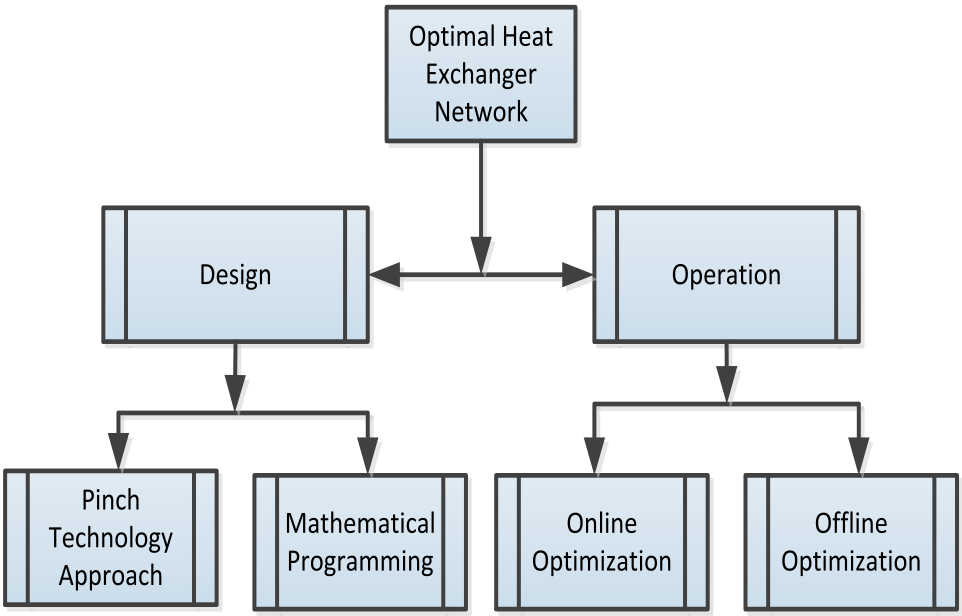

Figure 1-1 HEN Methodologies

A detailed annotated review on HEN methods can be found in the work of Furman and Sahinidis (2002) and in an earlier work by Gundersen and Naess (1988). In their work on HEN operations, Glemmestad and co-workers (1999) categorized the existing research on HENs into: (i) nominal design, (ii) flexibility and controllability, and (iii) operation. The nominal design is usually achieved using pinch technology or mathematical programming methods. It involves designing of HEN with fixed process stream data without taking into account any changes that may take place as a result of disturbances or uncertainties in process stream variables. The flexibility and controllability which, purely, is a mathematical or stochastic method require designing of HEN that works satisfactorily within a specified range of operating conditions such as the heat capacity flowrates and stream target temperatures. The third and last category which covers the operations of HEN required designing of control systems to operate and maintain efficiency of HEN operation within acceptable design specifications.

Despite considerable progress in category (i) and (ii) above, development in category (iii); the operation and control of HEN is limited when compared to numerous literatures that investigate various HEN problems. It is obvious that changes in environmental conditions, changes in stream temperatures, flowrates and heat transfer properties due to leakages or fouling in heat exchangers can give rise to unusual scenarios that affect the performance of the entire network; thus the need for a different look into the control and operation of HEN systems becomes imperative. HEN design without considerations for operational mode changes are bound to operate at temperatures higher or lower than the specified target temperatures depending upon the type and nature of the disturbances.

The contributions of Mathisen et al. (1992), Mathisen et al. (1994), Boyaci et al. (1996), Aguilera and Marchetti (1998), Glemmestad et al. (1999), Lersbamrungsuk et al. (2008), and most recently the work of Jaschke and Skogestad (2012) have all presented different ideas for achieving optimal HEN operation and control. Their method proposed different model-based control variables (CVs) selection procedures for achieving economically optimal operation in the presence of uncertainties and disturbances.

The key challenge is however the tendency to choose the candidate CVs for plantwide controls structure implementation and where process model is not available, CV selection is impossible. Traditionally, CVs for optimal process operations are kept at the desired setpoint using model online; CVs are chosen from measurements based on experience and process knowledge (Jaschke and Skogestad 2011) and in real time optimization (RTO) using model based approaches to reduce the frequency at which setpoints updates itself whenever disturbances occurred making traditional RTO relatively expensive and difficult to implement (Jaschke and Skogestad, 2012a).

To overcome this disadvantage, Skogestad (2000) proposed a control structure design where CVs are selected offline to give optimal or near-optimal plant operations at constant setpoint in the presence of disturbances. The approach is termed self-optimizing control (SOC) method. The CVs are usually selected as single measurement or combination of measurements by linearizing the process model around its nominal operating point (Ye et al., 2013). This procedure has been implemented on several models including distillation column (Alstad and Skogestad, 2007), CSTR (Jaschke and Skogestad, 2012b), reactor (Kariwala, 2007), and heat exchanger network (Jaschke and Skogestad, 2012a). In all cases, the solution relies heavily on availability of process models, ability to solve optimization problem offline and linearization of the process model if the model is nonlinear which results in local solutions. These factors render existing SOC method unsuitable for practical situations, where model equations are not available.

In an attempt to overcome the localness associated with the existing SOC methods, Ye et al., (2013) suggests selecting CVs based on the concept of Necessary conditions on optimality (NCO) approximation. The NCO approximation technique can be used to overcome the localness associated with linearization procedure in the existing SOC approaches. The CVs in the NCO method are selected to approximate unmeasured NCO over the entire operation region with zero set point to achieve near global optimal operations. Although the NCO approximation achieved global solution, a disadvantage to the NCO method is that process model is an explicit requirement.

Recently, Ye et al. (2012), pioneered a new method of CV selection which relies solely on process data to select CVs in a two-step regression procedure. The method is entirely data-driven and uses regression to approximate the NCO or reduced gradient from measurement function. The two steps procedure was shown to achieve near optimal control in a much wider operation range, however, large errors arising in both regression steps are a limitation in this approach.

1.2 Research Motivation

The refocusing on economic and environmentally benign designs has compelled many industries to revamp their design and operational requirements to attain the objective of satisfying both environmental regulations and minimum energy consumptions. For example, to decrease CO_2 emissions into the environment, existing power plants must be integrated with CO_2 capture plant while new ones are not build without CO_2 capture unit; crude distillation unit (CDU) and vacuum distillation unit (VDU) are also integrated to minimize cost of production.

Although integration introduced the benefit of energy saving, integration in general leads to increased interactions between hitherto separate plant units (such as reactors, separators, distillation columns and furnaces) resulting into changes in characteristics and behaviours of the overall plant operations whenever the nominal operating conditions such as inlet temperatures, flowrates etc., are altered due to disturbances or changes in the manipulative inputs. For example, in HENs, these disturbances may propagate downstream paths of the network and to the whole-length of the HEN causing changes in stream target temperatures and setpoints thereby resulting into suboptimal plant operation.

This work is also inspired by the need to develop a data-based CV selection SOC procedure that may be applicable to complex industrial process through the use of historical process data collected overtime during plant operation. Currently, existing SOC method depend heavily on good process model and where model information is not sufficient due to complexity of the original plant structure or the model became complex due to integration, a good SOC-CV cannot be achieved. The SOC procedure developed in this work is completely data-driven CV obtained from process measurement collected during operation with this new method, CVs can be selected using commercial simulators such as ASPEN HYSYS©, ASPEN PLUS© and UniSim© among other numerous commercial simulators available.

The choice of HEN for coal-fired power plant retrofitted with CO_2 capture unit as a case study is significantly important to the energy industry due to increasing number of interest in HEN because of its ability to reduce energy penalty as well as CO_2 emission. Many power plants are nowadays integrated with CO_2 capture unit to satisfy environmental regulations thus making the plant more complex with adverse effect on design, operation and plant economy.

1.3 Aim, Objective and Novelty

The aim of this study is to introduce a data-driven methodology for CV selection based on the concept of SOC and to implement the new procedure on HEN to achieve optimal operation at constant set-points target temperatures in the presence of uncertainties and disturbances while minimizing energy consumption. Based on these aim, the research objectives are as follows:

1. Develop a novel regression based data-driven control variable selection based on SOC methods without and with equality constraints.
2. Implement the new method on a simple case three streams HEN problem.
3. Compare the newly developed data-based SOC with existing model based SOCs.
4. Design HEN for coal-fired power plant retrofitted with CO_2 capture and demonstrates the proposed data-driven method.

The novelties of the proposed study include:

(a) The use of historical process data to drive self-optimizing control variable in a single-regression based method has not been reported in any available literature. Ye et al., (2012) reported a two-step regression method which approximates economic objectives using operational data, in the first step and evaluate the CV in the second step following NCO approximation method.

(b) Most literatures consider HEN operation problem as an LP problem with bypass mixing evaluated arbitrary, in this work bypass mixing is explicitly considered resulting into HEN problem becoming an NLP problem.

(c) Aside from simple HEN case study, this work has been implemented on a HEN designed for super-critical coal-fired power plant with CO_2 capture.

1.4 Scope of the Research

The concept of data-driven self-optimizing control is entirely a new method developed in this thesis. The idea involves driving SOC variables which gives optimal operation based on historical data collected overtime during process operations. This method is particularly important where it is difficult or very expensive to obtain a good mathematical model describing process operations.

The data-driven approach select CVs from operational data in a single regression step, in line with the method of necessary condition of optimality (NCO) reported in Ye et al. (2012) and Ye et al. (2013) where in the former obtained globally optimal CVs using NCO without the usual linearization of process model associated with CVs selections, the later uses data to select CVs in two regression steps by approximating the NCO leading large regression errors from the two steps.

ASPEN ENERGY ANALYZER© is used to design the HENs given stream data before redesign and implementation on ASPEN HYSYS© to allow addition of bypasses on each of the process-to-process exchanger because of limitation to the use of bypasses on ENERGY ANALYZER©. The bypassed HEN will be used to demonstrate the effectiveness of the proposed approach using specified range of disturbances introduced into the HEN. Two HENs are selected for use as case study in this thesis: (i) the famous 3-streams simple HEN case study reported in many literatures, (ii) HEN design for coal-fired power plant retrofitted with CO_2 capture unit. In addition to ENERGY ANALYZER© and ASPEN HYSYS©, MATLAB© is used to develop the data-based control structure design procedure.

It is important to note that, the data-driven method is not tailored to HEN operations only; it is a general methodology that can be applied to any process plant. HEN was chosen as the case study for implementing the data-driven SOC procedure because of the limited number of research considering ‘Operation of HEN’ compared to research on ‘design of HEN’ despite its significance in energy cost savings.

1.5 Outline of this Work

Chapter two encompasses a detailed literature review on various approaches for HEN design and operation, the critical development and progress in the areas of optimal operation of HEN, brief overview of review of HEN for power plant and CO_2 capture. A description of several methodologies proposed in these literatures is discussed while highlighting their individual shortcomings.

In chapter three, a step by step procedure for nominal HEN design based on pinch technology, optimization, design and economic trade-off is discussed.

Chapter four implements the design of HEN for the 3-simple HEN and HEN for coal-fired power plant retrofitted with CO_2 capture.

Chapter five introduces HEN operations and optimization, the steady state models when considering HEN problem as LP or an NLP problem. Various LMTD approximations and DOF analysis for HEN problems

Chapter six presents the overview of plantwide operation using different SOC procedures developed overtime; the local, the exact the brute force as related to this work is highlighted. The global SOCs such as the NCO approximation method and our newly developed data-driven SOC will also be discussed.

Chapter seven presents the detailed data-driven technique on the simple case study and on the HEN for coal fired power plant with CO_2 capture unit. Monte Carlo simulation and loss evaluation is also presented in detail.

Finally Chapter eight presents conclusions and recommendations for further studies.

1.6 Publications

List of published and publication(s) in progress part of this thesis are:

1.6.1 Published

Chapter Four

Girei, S. A., Wang, M., Hamisu, A. A., (2013), “Heat exchanger network design and economic analysis for coal-fired power plant retrofitted with CO_2 capture”**,** in: *24rd European Symposium on Computer Aided Process Engineering,* vol. 32, p. 433-438

Chapter Seven

Girei, S. A., Cao, Y., Grema, A. S., Lingjian, Y., Kariwala, V. (2014). “Data-driven self-optimizing control”, in: *24rd European Symposium on Computer Aided Process Engineering*, vol. 33, p. 649-654

Girei, S. A., Cao, Y., Kokossis, A. (2014). “A Data-driven self-optimizing control with equality constraints”, in: *20th International conference on automation and computing*, Article 6935495, pp. 248-253

1.6.2 In progress

Chapter Six

Girei, S. A., Cao, Y., Kokossis, A. (2015). “Optimal operation of heat exchanger network for coal-fired power plant retrofitted with CO_2 Capture Unit”, *Journal of Process Control* (in progress)

2 LITERATURE REVIEW

2.1 Introduction

This chapter is divided into two sections, section one described some basic concepts of HEN design. Different HEN design approaches are briefly discussed and the benefits and fundamentals of using Pinch Technology are elaborated. Stages of pinch design, energy targeting, synthesis and optimization of HEN were discussed.

In the later part of the chapter, Heat exchanger network operation was introduced. Various contributions on HEN operations and the choice of manipulating variables, degree of freedom and bypass selections were highlighted.

2.2 Heat Exchanger Network Design

The synthesis of heat exchanger networks (HEN) is an important aspect of chemical process design (Linnhoff and Hindmarsh, 1983) and has been a subject of a considerable amount of research for the past 40 years (Furman and Sahinidis, 2002).

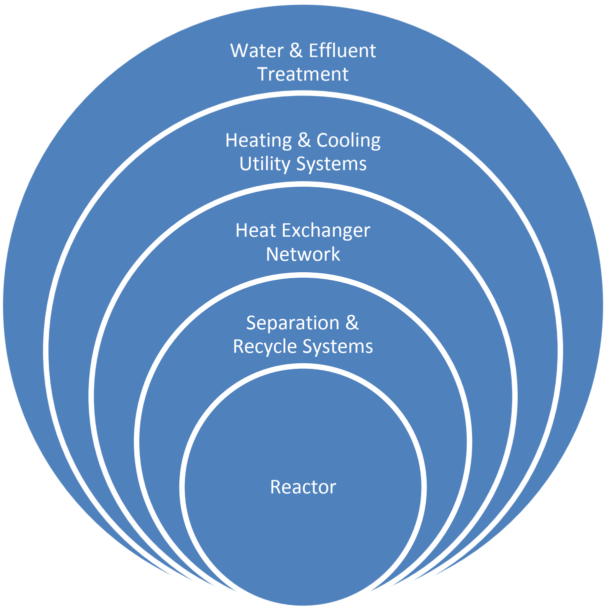

Figure 2-1 Onion model of process design synthesis (Biegler et al., 1997)

In a process design hierarchy, HEN design comes third in order of importance on the onion layers diagram (Figure 2-1). The onion layer begins with a reactor which dictates the product requirements followed by separation and recycle system before the HEN design, Figure 2-1. The HE duties which cannot be satisfied by heat recovery systems are supplemented through external utility systems –layer four. The HEN on onion diagram is often referred to as heat recovery systems.

HEN design exchanges heat energy between process streams in a more economical way by matching hot and cold streams in order to recover unutilized heat from the process with make-up demand for heating or cooling supplemented through heating and cooling utilities.

The design approach undertaken by most researchers can be grouped into two major categories namely: *the pinch analysis methods and the mathematical programming methods* (though sometimes *the stochastic programming* is often referred to as the third category) (Smith et al., 2010). Because of inadequate mathematical formulations to handle the effect of changes in operational modes, maintaining optimality in the HEN operating conditions becomes a trial-and-error procedure. Hence, optimal operation of HEN design is compromised and the overall profitability of the plant reduced (Rodera et al., 2003).

2.2.1 Pinch Technology

The Pinch Technology (PT) design method is the most developed technique for HENS (Sieniutycz and Jezowski, 2009) due to its simplicity and sufficient physical insight. Floudas (1995) reported that, the work of Hofmann (1971) which received less attention in the early 1970s and the work of Linnhoff and Flower (1978a; 1978b) are the brainchild of PT, since then, PT has been successful over scales of industrial problems due to its thermodynamic and heuristics insight which made it to remain the industrial standard (Shenoy, 1995), although mathematical programming offer advantages in many cases. Its potential in explaining economic trade-offs has maintained a convincing edge amongst practitioners and engineers (Tantimurata, 2001), Even though, the industrial integrity of PT has been well established over the years, it is, however, not without some major drawbacks. PT design does not account for changes in design parameters. The maximum amount of energy recovery in pinch technology is limited by thermodynamic driving force (ΔT_{min}) which prevents further integration whenever the pinch rules are violated. An interesting feature of PT method is its necessity for redesign to evaluate and improve the HEN through minimization of total annualized cost (TAC) by improving trade-off: number of matches –cost of utilities (Ahmad et al, 1990).

Although design emphasis shifted from single task pinch to multitask such as decomposition and simultaneous HEN, Pinch analysis is more preferred technology for HEN especially in retrofitting due to the following reasons (Rossiter & Associate, 2015):

1. It provides a systematic procedure which guarantees optimum design without relying on luck and guesses.
2. The design is based on thermodynamics and can be applicable to all processes and technologies be it continuous or batch, new design or retrofit design.
3. PT has proven energy savings. About 15 % or more energy cost reduction is even where process has already been optimized by "conventional" methods.
4. Automatic pollution prevention. Reduced CO_2, SOx and NO_x emissions are the natural consequence of better energy efficiency.
5. Lower cost debottlenecking. Pinch analysis shows us how to make better use of existing equipment and systems, and thus minimizes new equipment requirements in capacity upgrades.

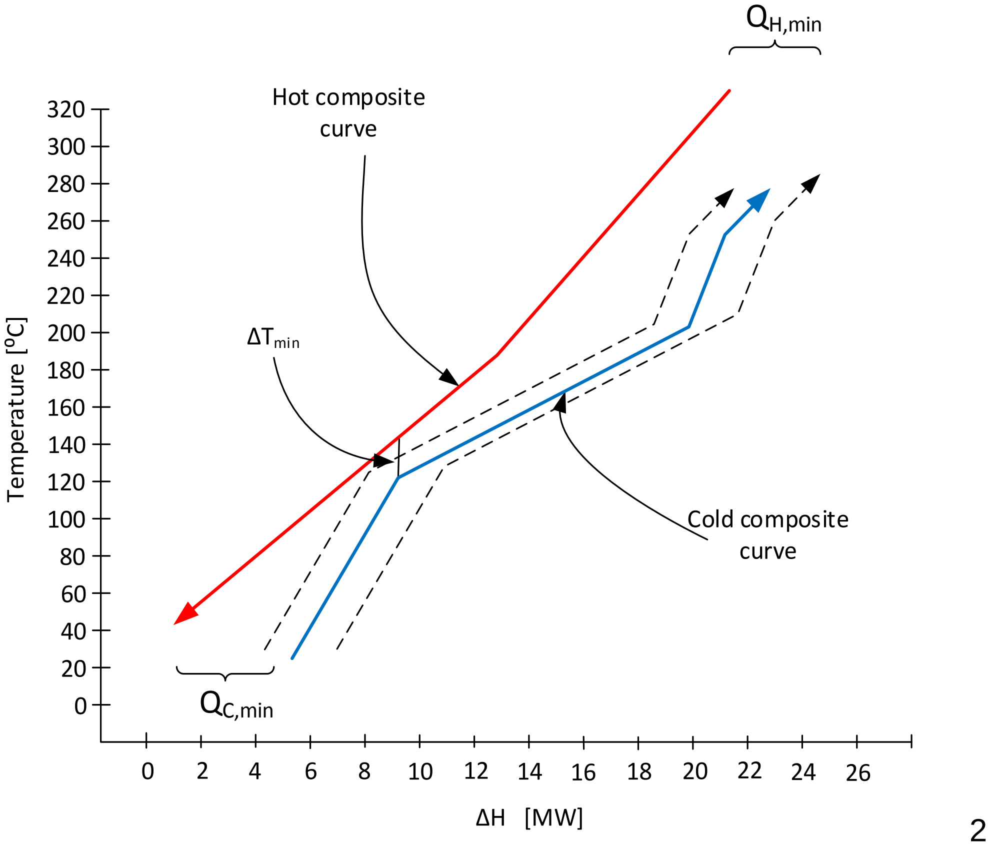

Figure 2-2 Overview of Pinch Composite Curve (Glemmestad, 1999)

2.2.1.1 Energy Targeting

Energy targeting is crucial to any PT (Shenoy, 1995; Smith, 2005). It determines the minimum amount of energy consumptions in the overall process (Linnhoff, 1998). The first step in energy targeting is to identify the sources of heat (hot streams) and sink (cold streams) from material and energy balance stream. These streams are then transformed into hot and cold composite curves as shown on the temperature-enthalpy (T-H) plot in Figure 2-2 above. The ΔT_{min} represents the driving force for heat transfer between the two curves. The higher the value of ΔT_{min} means the lesser the amount of process energy recovery and vice versa. At $\Delta T_{min} = 0$, i.e the hot and cold composite curves touches each other, infinite heat transfer area is required, the design become infeasible. Increasing the value of ΔT_{min} decreased the heat transfer area requirement and increased the utilities consumption. On the other hand, decreasing the value of ΔT_{min} decreased the utilities requirement and increased the heat transfer area, thus signifying the desirability for trade-off optimization in order to achieve optimum HEN design.

The intersection of ΔT_{min} on the cold and hot composite curves refers to as the 'pinch point'. It is a point where the curves constrict the most. The $Q_{H,min}$ and $Q_{C,min}$ are the extra heating and cooling utilites that must be supplied to balance the heating and cooling requirements of the HEN design.

2.2.1.2 Synthesis

Following energy targeting which specified the ΔT_{min}, $Q_{H,min}$ and $Q_{C,min}$, and the amount of energy recovery from the process, the synthesis begins at the pinch points. The design is usually divided into area above the pinch point and area below the pinch point. For below the pinch point is the heat source and above the pinch point is the heat sink.

The matching of streams to construct HEN is done separately between these areas by adopting certain 'tick-off' pinch rules highlighted in Linnhoff 1998 and also in Smiths, 2005. In most cases, PT design has single pinch points, however if there are more pinches, subtasking between pinch is necessary. Jezowski (1992a) and Trivedi et al., (1989a) have suggested an alternate approach for handling multiple pinch problems.

This PT rule minimizes the number of HEs in the design with maximum duty on each of the exchangers in the network. Any stream with deficient heating or cooling requirement is supplemented by utility exchangers at the end of the stream in question to meet the target requirement of that stream.

2.2.1.3 Optimization

The final step in the sequence of pinch HEN design is to optimize the network to achieve cost optimal HEN with maximum possible energy recovery and minimum utility consumptions. The objective is to minimize the total cost annualized cost in the entire network, which is defined by the minimum temperature difference. The optimization results are directly influenced by the selected ΔT_{min} in evaluating the annualized cost. What this means is that the smaller the ΔT_{min} the higher the amount of energy recovery and the larger the HE area, capital and operating cost of the overall network and vice versa. The degree of freedom for manipulating the HEN capital cost are the loops, utility paths and splits streams (Smith, 2005).

The design optimization is formulated as a multivariable optimization subject to

1. Nonnegative heat duty in each match.
2. Positive temperature difference from each exchanger.
3. Stream split, branch flowrates are positive.
4. Total enthalpy change within tolerant limit.

2.2.2 Mathematical Programming

2.2.2.1 Decomposition Approach

Heat exchanger network design based on decomposition approach simplifies the design problem into sub-tasks based on pinch point which can be treated with much ease than the single-task approach. In this case, the original HEN design problem is decomposed into three subproblems with each step being considered as a separate unit namely;

(i) Minimum utility cost: This concept was first introduced by Hohmann (1971) and Linnhoff and Flowers (1978). It involves recovering the maximum amount of energy from the system using fixed heat recovery approach temperature (HRAT) without first compromising the network structure. Any non-energy-efficient structures are eliminated from the network in the later step of the design. Important contributions in this area are the LP transportation model of Cerda et al. (1983) and its improvement by Papoulias and Grossmann (1983).

(ii) Minimum number of matches: These steps determine the minimum number of matches between hot and cold stream which returns energy-efficient number of exchanger networks for the fixed utility target. A rigours approach in the form of mixed integer linear programming (MILP) transportation model was presented by Cerda and Westerberg (1983) an as MILP transhipment model by Papoulias and Grossmann (1983).

(iii) Minimum investment cost: Given the targets (i) and (ii), the network configuration that gives the minimum investment cost (Capital cost and Operating Cost) are determined in this stage. Floudas (1986) formulated and optimized and NLP problem for the minimum annualized cost of the network.

The main disadvantage of decomposition approach is that the effectiveness of each step relies on the decision of the previous steps, hence the likelihood that the trade-offs between utility costs, the number of matches, the area requirement and the minimum investment cost cannot be accounted for appropriately. As a result, HEN design based on decomposition may result into a sub-optimal network because the minimum utility may not be the exact representation of the original HEN problem.

2.2.2.2 Simultaneous Approach

The simultaneous synthesis was aimed at finding optimal solution to HEN problem without recourse to decomposition into sub-networks. Unlike in the decomposition approach where the trade-offs between various costs are not adequately accounted for, simultaneous optimization accounts for total annual costs comprising of utility cost, area cost as well as fixed charge for exchanger units within a reasonable computational expense. Formulations on simultaneous approach are very complex and usually results into MINLP optimization problems based on simplifying assumptions.

Floudas and Ciric (1986) proposed a generalized match-network MINLP formulations for overcoming uncertainties associated with selection of optimal HE matching and network configuration for minimum investment cost. The approach simultaneously optimized the best network configuration using a selection procedure based on transshipment model of Papoulias and Grossmann (1983) for selection of stream matches and heat loads. This procedure may be considered inefficient for optimal network due to pre-selection of HRAT at the early stage of the design. Further modifications of this work was presented in Ciric and Floudas (1991), this includes approximation technique for estimating utility consumption as a piecewise linear function of HRATs.

A simultaneous formulation which has advantage of not relaying on HRAT or exchanger minimum approach temperature (EMAT) was presented by Yee and Grossmann (1990). This model was based on stage-wise superstructure formulations in Yee et al. (1990a). The superstructure is divided into stages with cooling and heating utility supplied at both end of the stages. The model was formulated based on the following assumptions:

i. Isothermal mixing

ii. No split stream flowing through more than one exchanger

iii. Utilities located at the ends of the superstructure

iv. No stream bypass

These assumptions simplified the HEN problem into having linear constraints with the objective function assuming nonlinear nonconvex form. A preliminary screening procedure for the MINLP synthesis of HEN, an improvement to Yee and Grossmann (1990) model was presented in series of work by Daichendt and Grossmann (1994 a; 1994b). They suggested a procedure for selecting number of stages within the network and eliminating unnecessary units of exchangers.

Marselle et al. (1982) first introduce the concept of resilience in HEN design through introduction of a network which will tolerate uncertainties in temperature and flowrates within a range of acceptable maximum energy efficiency. The proposed network is known to be structurally resilient within a bound of specified disturbances, meaning, the HEN allows for maximum energy recovery for this disturbance range. The study relies on heuristic method to identify number of worst-case scenarios such as maximum heating and cooling, and maximum heat recovery approach temperature. The method requires manual combination of the individual worst-cases to give resilient network which adjusts flow distributions in the network to meet temperature constraints with minimum utility usage. Because their method independently accounts for the network uncertainties, its application on an industrial size problem becomes practically impossible due to nonlinearity in an exchanger problem.

Swaney and Grossmann (1985a) introduced a framework for systematic examination of flexibility in process plant using a flexibility index which identifies the maximum region outside processes operating under uncertainty in inlet parameter remains practically infeasible. The study identifies a bound which guaranteed feasible operating condition through manipulation of control variable and the critical points (worst-case scenarios) which limit flexibility of the process. In a later series of their work, Swaney and Grossmann (1985b) presented a direct search procedure and implicit enumeration scheme for numerical computation of flexibility index. Similarly, Saboo et al. (1985) defines resilience index (RI) for inlet and target temperature changes in HEN and went further to present an approach for calculating resilience index.

Floudas and Grossmann (1986) proposed a strategy for HEN network synthesis based on multiperiod MILP and LP transshipment model of Poupolias and Grossmann (1983). The model was illustrated to account for the change in pinch points which is as a result of different period of operation. It also accounts for minimum utility cost for each of the period and requires few numbers of units matching for optimal network configuration. A further extension of the work which involves an NLP formulations based on automatic generation of multiperiod heat exchanger network configuration was presented in Floudas and Grossmann (1987). The superstructure features all possible structural options for generating network which gives minimum investment cost, number of units and utility cost for each period.

Tantimuratha and Kokossis (2004) proposed a dual approach method established on hypertarget framework of Broines and Kokossis (1999a, b, c) for conceptual screening of cost effective primal matches at the same time assessing the flexibility of the design options. Both the model and procedure are employed to assess trade-offs between energy cost, exchanger area cost and flexibility potential of the network. The model employs graphical technique to enhance decision-making during network selection. However, despite enhanced energy management, the design requires more number of unnecessary units to achieve a flexible network in most cases while incurring significant economic penalties.

Aaltola J. (2002) presented a framework for the design of a flexible HEN for multiperiod operations based on stage-wise superstructure of Yee et al. (1990). The study minimized the total annual cost through a system which combines MINLP model and search algorithms for synthesis of a simultaneous Multiperiod network that operates over a range of stream flowrates and temperatures without losing the desired target while maintaining the network economy. The model works satisfactorily for networks with stream splits and bypasses, and it does not rely on sequential decomposition of problem into sub-problems, nor does it consider pinch point. The model uses LP/NLP search algorithms to overcome the limitations imposed by MINLP model. However, despite simplifying assumptions, the model cannot guarantee network feasibility for a relatively large size problem.

Chen and Hung (2004) proposed a three steps decomposition procedure for synthesis of HEN that involves specified uncertainties in the source-stream temperatures and flow rates. The three steps formulations involves (i) MINLP formulation for the network design, (ii) flexibility analysis to determine the feasibility of the network over specified range of disturbances (iii) integer cuts for exclusion of disqualified networks. The proposed model was demonstrated using some numerical examples, however, for a single problem, several iterations are required to identify the final network which is major concern for industrial scale problem. Another major concern is the increase in number of continues variable which left the designer with no option than to tradeoff between number of variable and search space.

Verheyen and Zhang (2006) developed a network of combined MINLP-NLP model for multiperiod HEN which is a modification of Yee et al. (1990) and Aaltola (2002). The NLP part of the model improves the solution and allow for non-isothermal mixing. The introduction of maximum area cost per period in the objective function equation and the removal of slack variable and weighted parameters are the main modifications compared to the previous work. The increasingly large size of the problem owing to non-linear terms in the constraint equation made the model more complex and more difficult to solve.

Chen and Hung (2007) further extended the scope of previous work by Chen and Hung (2004) to include mass exchanger network covering specified disturbances in flow rates and temperature or compositions of the inlet process streams. Like the previous work, the stage-wise superstructure base MINLP formulation of Yee et al. (1990) was applied to network synthesis with minimum total annualized cost (TAC). The problem in this case was also decomposed into three iteration steps namely; the synthesis, flexibility testing and size restrain consideration. Moreover, numerical example using GAMS/SBB and GAMS/CONOPT3 shows that several iteration steps are required to obtain satisfied network configurations. A large search space due number of continues variable is also a subject of concern for industrial scale problems.

Gorji-Bandpy et al. (2011) propose network optimization techniques base on genetic algorithms and sequential quadratic programming for establishing network fitness and determination of thermal load respectively. The method proves superior to the traditional pinch technology; however, no comparison of the resulting network generated in this optimization with a literature established case study to test the feasibility of the HEN structure. Moreover, the possibility of operational changes was not considered in their study. The network also uses Meta-heuristic optimization methods which is a disadvantage when handling industrially large problem.

El-Temtemy and Gabr (2011) used sensitivity table to design flexible HEN for multiperiod operations. A two steps approach for selecting and generating a base case HEN model, and for targeting temperature and utilities using sensitivity table was use for synthesis of HEN with flexible and optimum properties. The method works fine for two hot, two cold streams exchanger network, however, the suitability of the method in handling large size problem is questionable.

An interesting MINLP work presented based on superstructure of Yee and Grossmann (1990) was those of Drobez et al. (2012). It involves simultaneous synthesis of energy efficient biogas process with HEN superstructure. The result is a combined synthesis involving the biogas process, process streams and the

HEN. Such overall synthesis of entire process is unrealistic and challenging to solve for complex processes.

2.3 Heat Exchanger Network Operation

In HEN operation, the control objective is to minimize utility consumptions while satisfying the stream outlet temperatures (target temperatures). It is assumed that the heat exchanger areas are fixed during operation. Each process exchangers or utility exchangers have one degree of freedom for control whereas the exchanger outlet temperatures on either cold or hot side are regarded as measurements. The utility duty is manipulated by adjusting the hot or cold stream inlet flowrate depending on the process requirement. On the other hand, each process exchanger is fitted with bypass stream for manipulating the exchanger duty.

In general, given a HEN with constant area, supply and target temperature, heat capacity flowrate, the optimal operation requires satisfying:

i. Stream target temperature.

ii. Utility minimization.

iii. Dynamic stability.

These objectives were classified as primary, secondary and tertiary objectives respectively (Glemmestad, 1997). The first requirement for achieving optimal operation of HEN is to meet the stream outlet temperature requirement. This is because the target streams variables are inlet specification to adjoining process units such as reactor, absorber, and separator among others. The secondary objective requires providing the exchanger stream with minimum possible amount to utilities while ensuring that the streams are feasible.

2.3.1 Manipulative Variables

The most common strategies for the control of streams target temperature in any given network are via manipulation of bypass placement on process-to-process exchangers, manipulation of duties of process-utility exchangers and lastly but less desired flowrate manipulation through stream splitters. Each of these manipulations is briefly introduced.

2.3.2 Bypass Flow Manipulation

In Figure 2-3, manipulation of the exchanger EX-100 duty is achieved through bypass placement on the supply stream H1 by splitting and mixing the stream with the corresponding exchanger exit stream (point S_{h1} and M_{h1} on Hot stream H1 in Figure 2-3). The bypass is used to reject disturbances in supply temperature or supply stream heat capacity flowrates.

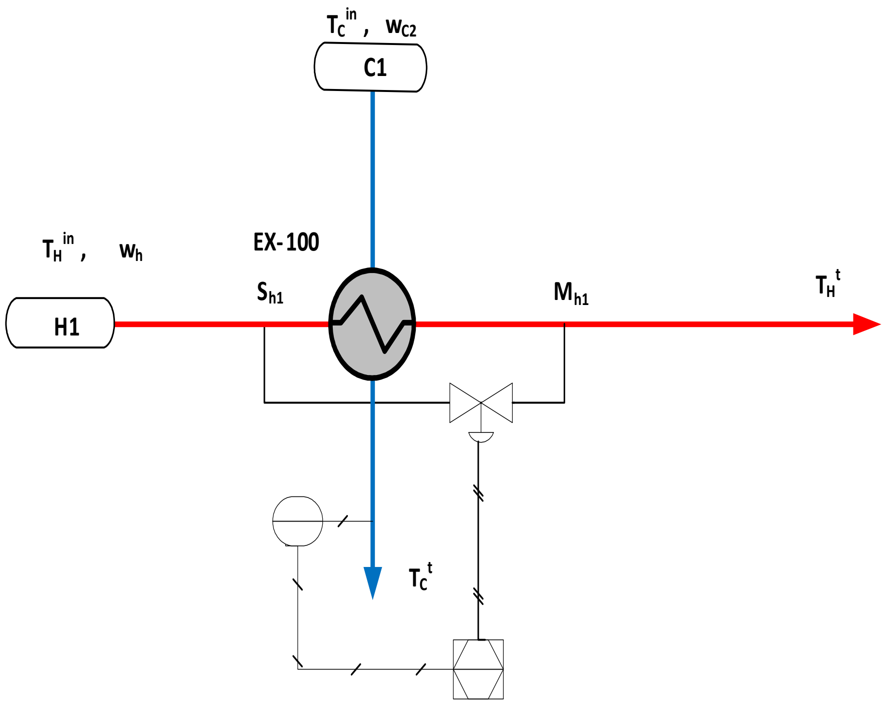

Figure 2-3 Bypass controlled Exchanger

Bypass placement can either be placed on inlet cold stream supply temperature or hot temperature supply streams. Mathisen (1992) have shown that for steady state process, the choice of bypass placement on either hot or cold stream is insignificant when controlling a steady state HEN, however, these bypass placement are different dynamically.

In many cases, the bypass streams are used to keep the stream target at their setpoint. When this happens, the bypass stream is usually attached to the last process heat exchanger on the stream (either hot or cold stream).

2.3.3 Utility Flow Manipulation

The utility-to-process exchangers provides heat balance to satisfy the target temperatures in the form of cooling utilities on the hot streams side or heating utilities on the cold streams side depending on the type of streams considered. The utility-to-process exchangers are usually placed at the end of the stream to maintain the target temperature at their setpoints. Figure 2-4 is a typical utility-to-process exchanger of a cooling located on a hot stream exit for keeping the target T_H^t at its setpoint value.

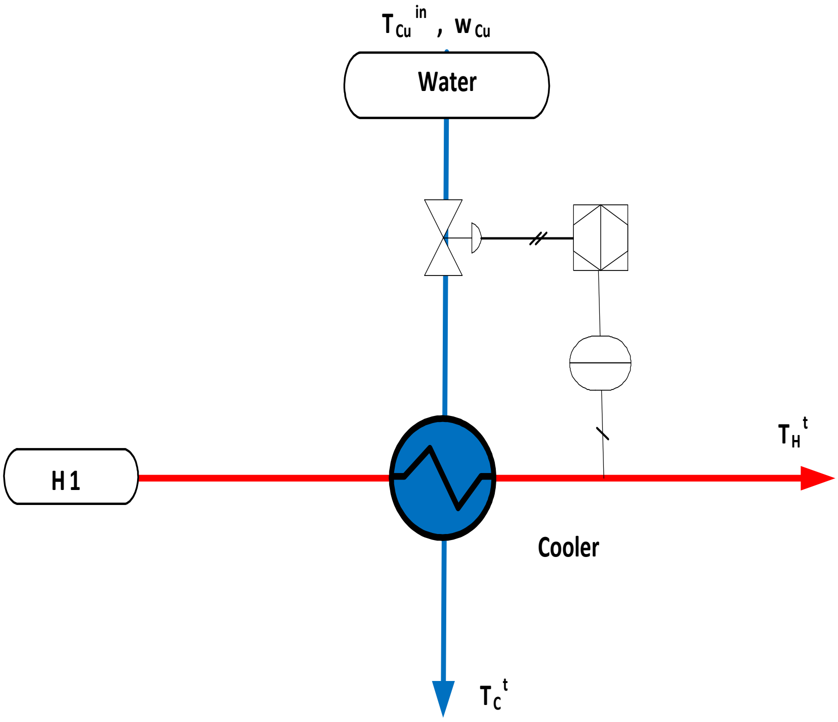

Figure 2-4 Utility controlled Process-utility Exchanger

During manipulation of utility-to-process exchangers, it is always assumed that the process plant has sufficient heating and cooling supplies to meet the demand during operation. This means that there are sufficient heat duties to keep the stream target at their setpoints. These allow room for direct manipulation of utility exchanger duty instead of utility stream inlet flowrates. The assumption significantly reduced the complexity of HEN simulation by making it easier to compute the exchanger exiting temperature from utility duty without accounting for utility exit temperature and inlet flowrates.

2.3.4 Split Stream Ration

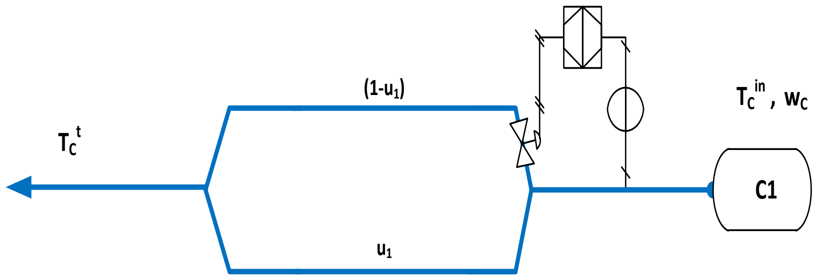

Figure 2-5 Stream Split Controlled

The stream split in Figure 2-5, is one of the seldom considered manipulations in theory of HEN operation. Streams are split during HEN design so that the population of hot streams exactly equals the population of cold streams.

When steam split is considered as manipulation, it is assumed that the split fraction varies, however, in most scenarios, stream split is used for optimization purpose than for regulatory control because the controlled variable (target temperature) does not change monotonically with the manipulated variable, (Young et al., 2006) (flow rate of a branch). This perhaps explains why most literatures reported the preference of fixed split stream fraction over variable split stream during process operation.

2.4 Summary

A detailed review of various methodologies for development of HEN from a given stream data have been presented. The design categories include the pinch technology, mathematical programming as well as stochastic programming methods. The pinch technology method is the most established due to its thermodynamics and physical insight. The HENs designed using pinch methods are nominal design and does not accommodate changes in streams properties. Mathematical programming on the other hand can handle large size problem and is capable of accommodating disturbances. Mathematical programming is also divided into decomposition where large size problem are decomposed into subtasks for ease computational difficulties, and the simultaneous approach which considered the HEN problem as a whole with no decomposition. The most prominent research in these areas is the transhipment model and superstructure of Papoulias and Grossman (1983) and Yee and Grossmann (1992) respectively.

The pinch design begins with energy targeting where the process is evaluated to ascertain the potentials of recovering waste or unused heat from any given plant. This usually achieved through the design of composite curves to conceptualize the entire heat recovery and utility requirements for the whole process plant. Utility targeting is conducted using grand-composite curves followed by areas targeting for network synthesis. Having achieved all the targets, the HEN is design and optimized to obtain a final network minimum HEN area and number of units. This is usually accomplished in a network with best matching that gives same output target requirement.

The number of literatures investigating operation of HEN is not too many compared to those that study design of HEN. Operation is usually carried out to control the effect of disturbances and uncertainness in the network while achieving optimum operation with minimum utility consumption and constant target temperatures. There are total of three manipulative variables; (i) the bypass, (ii) the utility exchangers (iii) the split streams. Several literatures consider bypasses and utility exchanges as manipulation while stream split is used for optimization rather than regulatory control due to its monotonic effect.

3 HEAT EXCHANGER NETWORK DESIGN

3.1 Introduction

A detailed nominal HEN design methodology based on the pinch technology approach is presented in this chapter. The basic essential steps leading to pinch design including energy targeting which allows the designer to assess the energy management opportunities in a given process plant prior to the proper design; how much cooling and heating can be recovered from the entire plant; the composite curves and HEN trade-off between capital and utility cost and finally selection of best driving for ΔT_{min} during design are described using illustrative examples.

3.2 Energy and Utility Targeting

Energy targeting is key in identifying potential energy savings in a given process plant without necessary carrying out the pinch design. This is possible through simple material and energy balance across the plant to evaluate the total energy that can be recovered from the process and the amount of additional external heating and cooling needed in the overall process. The targeting is carried out by using the composite curves technique as reported in Linnhoff, (1998), or by using problem table algorithms method as presented in Hohman (1971) and Linnhoff and Flower (1978). Through targeting, both capital and energy cost for the design of HEN can be assessed (Smith, 2005). The advantage of targeting is that it allows for plantwide screening of processes to asses energy saving opportunities prior to HEN design and retrofitting. This is one of the remarkable abilities of pinch technology.

3.2.1 Composite Curves Energy Target

The composite curves are a temperature-enthalpy (T-H) graphical representation of energy recovery between process streams. It comprises of the cold-composite-curves (heat demand) and the hot-composite-curves (heat supply) plotted on the same T-H diagram. Once the thermal data which contain supply and target temperatures, the heat capacity flowrates and the enthalpies of each streams are identified and extracted from process flowsheets, composite curves can be generated to assess energy saving opportunities in the whole process even prior to the HEN design.

The construction begins with plotting temperature against enthalpy for the individual streams, for either hot or cold stream type. Each stream is identified by its heat capacity flowrate CP in all intervals. The enthalpies of streams within the same intervals are added into single stream with CP equals to the sum total of the individual CPs within same interval bracket. Both the cold and hot composite curves are constructed in a similar manner involving the combination of the streams T-H curves and summing up their respective heat capacity flowrates in each case.

3.2.1.1 Illustration Example

The energy targeting using composite curves is explained in the illustrative example below using a simple 3-stream process data in Table 3-1. The streams consist of 1-Hot stream and 2-Cold streams with their CPs, supply and target temperatures $\boldsymbol{T_S}$ and $\boldsymbol{T_T}$ respectively.

Table 3-1 Three Streams Heat Recovery Problem

Stream	**Type**	T_S **[ºC]**	T_T **[ºC]**	CP **[kW/ºC]**
1	Hot	190	30	1.0
2	Cold	80	160	1.5
3	Cold	20	130	0.5

Figures 3-1 (a) and (b) are plots for hot and cold process streams represented on the T-H diagrams. The hot composite curve plot in Figure 3-1 (a) is a single hot stream with 190 ºC supply and 30 ºC target temperature as indicated in Table 3-1.

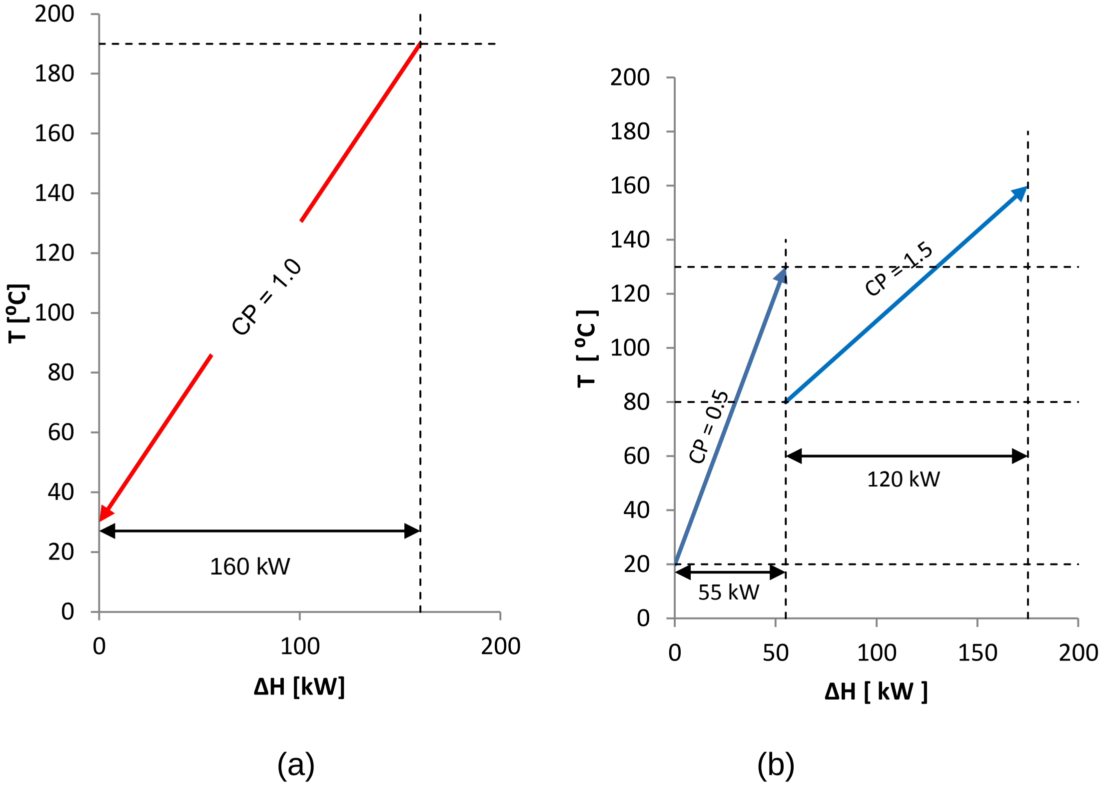

Figure 3-1 (a) Hot stream plot, (b) Cold stream plot

Figure 3-1 (b) on the other hand, shows a T-H profile of the two cold streams population from the same Table 3-1 plotted individually on same graph. For each stream, change in enthalpy (ΔH) is evaluated as $\Delta H = \mathrm{CP}\Delta T$, where CP is the heat capacity flowrate and ΔT is the interval temperature change. By combining the streams in the given temperature range Hoffman (1971), Linnhoff et al., (1979) shows how the streams behave individually on the T-H graph. The temperature axis is divided into intervals defined by the supply and target temperature of each stream as shown in Figure 3-1.

The heat capacity flowrate CP within a given interval are added into a single stream with CP equivalent to the sum total of the CPs of individual streams in same interval. For example, two streams form interval 2 on the temperature axis, the CP on that interval is the sum total of the CPs confined in the interval i.e. $CP = 0.5 + 1.5 = 2.0$ as shown in Figure 3-2, the cold composite stream.

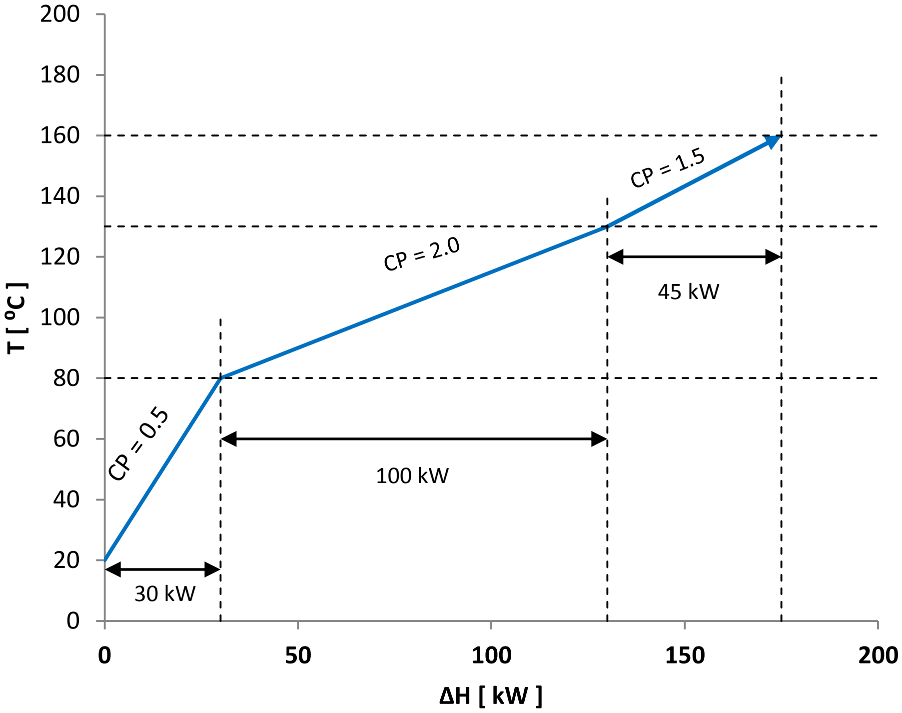

Figure 3-2 Cold composite stream

Both the composite hot and cold curves are then plotted on the same T-H graph to give composite curves with $\Delta T_{min} = 10\,℃$ as the minimum temperature difference indicated in Figure 3-3. Heat transfer is carried out from the hot composite curves to the cold composite curves, i.e. heat energy recovered from the hot composite stream is utilized to heat-up the cold composite streams. The smaller the value of ΔT_{min}, the greater the amount of heat recovery and the lower the additional external heating and cooling requirement in the overall process. In this example, for $\Delta T_{min} = 10$ ºC, the heat recovery is 100 kW with 30 kW of external cooling and 45 kW of external heating requirements.

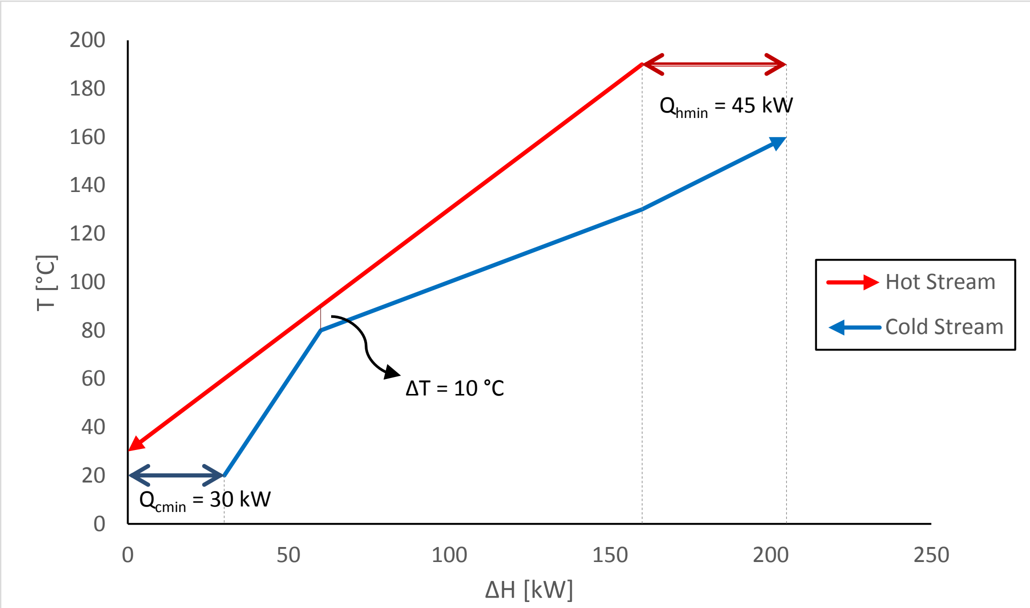

Figure 3-3 Construction of Composite Curves

3.2.2 Problem Table Energy Target

The problem table algorithm avoids the use of graphs to target energy and utility requirements of a given process (Linnhoff and Flowers, 1978), instead, the method calculates energy targets directly from thermal data without graphical construction. The process is divided into intervals in similar manner to what is obtainable in the composite curve in Figure 3-2. To construct the problem table algorithm, the hot stream temperature is shifted to be $\Delta T_{min}/2$ colder than its original value while the cold stream is increased to be hotter than the original value by the same amount. This shifting is necessary to prevent infeasible heat transfer process and cross-pinching in the design.

In Smith (2005), three simplified procedure for energy recovery/targeting based on problem table algorithms method are presented as follows:

1. By subtracting $\Delta T_{min}/2$ from hot stream temperatures and adding $\Delta T_{min}/2$ to cold stream temperatures, the shifted temperatures interval is setup.

2. From each shifted interval, a simple energy balance is obtained in this form:

$$\Delta H_i = \left[\sum_{Cold\ Streams} CP_c - \sum_{Hot\ Streams} CP_H \right] \Delta T_i \tag{3-1}$$

where i is the shifted interval, ΔH_i and ΔT_i are heat balance and temperature difference across the intervals.

3. ΔH value equivalent to the maximum negative duty is added across the intervals as utility duty to correct the deficit duty for each interval.

3.2.2.1 Illustration Example

Table 3-2 is an illustration example to further explain the method of problem table algorithm described in Section 3.2.2 above, using a minimum temperature difference, $\Delta T_{min} = 10$ ^{0}C.

Table 3-2 Shifted temperature for data from Table 3-1

Stream	Type	$\boldsymbol{T_S}$ [℃]	$\boldsymbol{T_T}$ [℃]	CP[kW/℃]	$\boldsymbol{T_S^*}$ [℃]	$\boldsymbol{T_T^*}$ [℃]
1	Hot	190	30	1.0	185	25
2	Cold	80	160	1.5	85	165
3	Cold	20	130	0.5	25	135

The supply and target temperatures are shifted to T_S^* and T_T^* as indicated by the entries of the last two column of Table 3-2. The intervals temperatures are plot for each streams and a heat balance is carried out within each shifted temperature interval using Equation 3-1. The procedure and results are shown in Figure 3-4. For each interval, the deficit and surplus heat are tabulated accordingly.

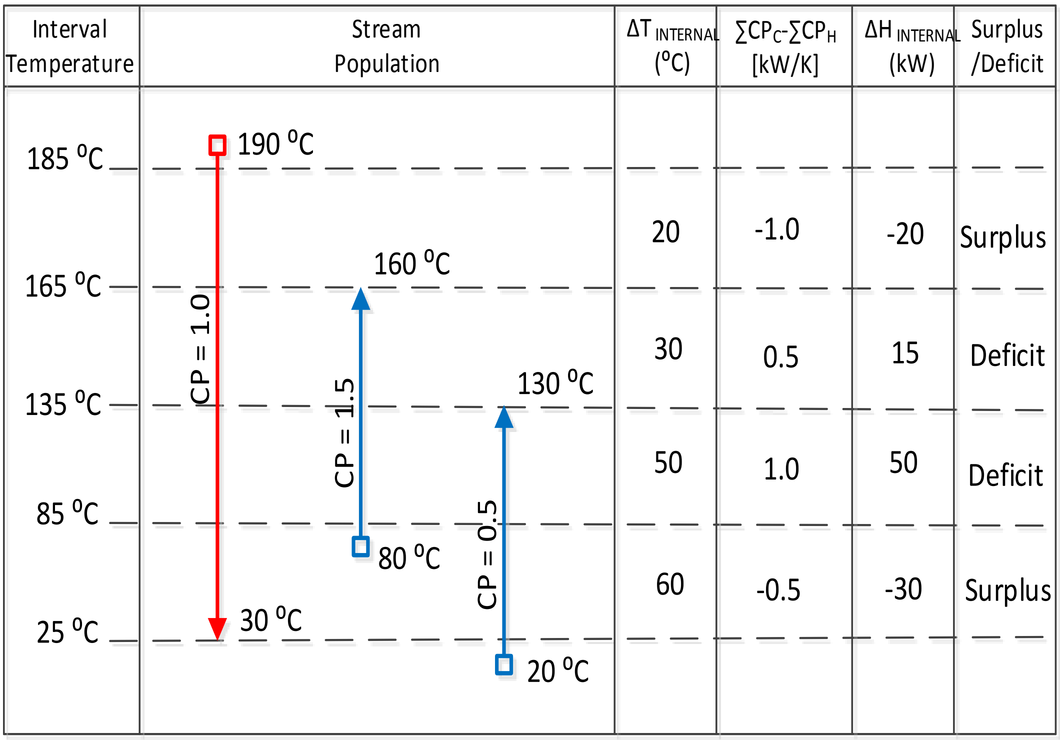

Figure 3-4 Temperature interval heat balances

Figure 3-5 (a) shows the cascade plot for all the temperature intervals. The surplus heat down the interval is cascaded as shown in Figure 3-5 (b). This is necessary because heat flows from the hot utility level downward into the intervals and finally to the cooling utility level. We first assume zero heat supply at the hot utility level, the first interval has surplus of 20 kW which is cascaded down to the level below it. The second level has deficit of 15 kW when cascaded to the level below it make the interval to be -5 kW. The same step applies to the third interval. The fourth interval is surplus by 30 kW and cascading left the interval with -15 kW.

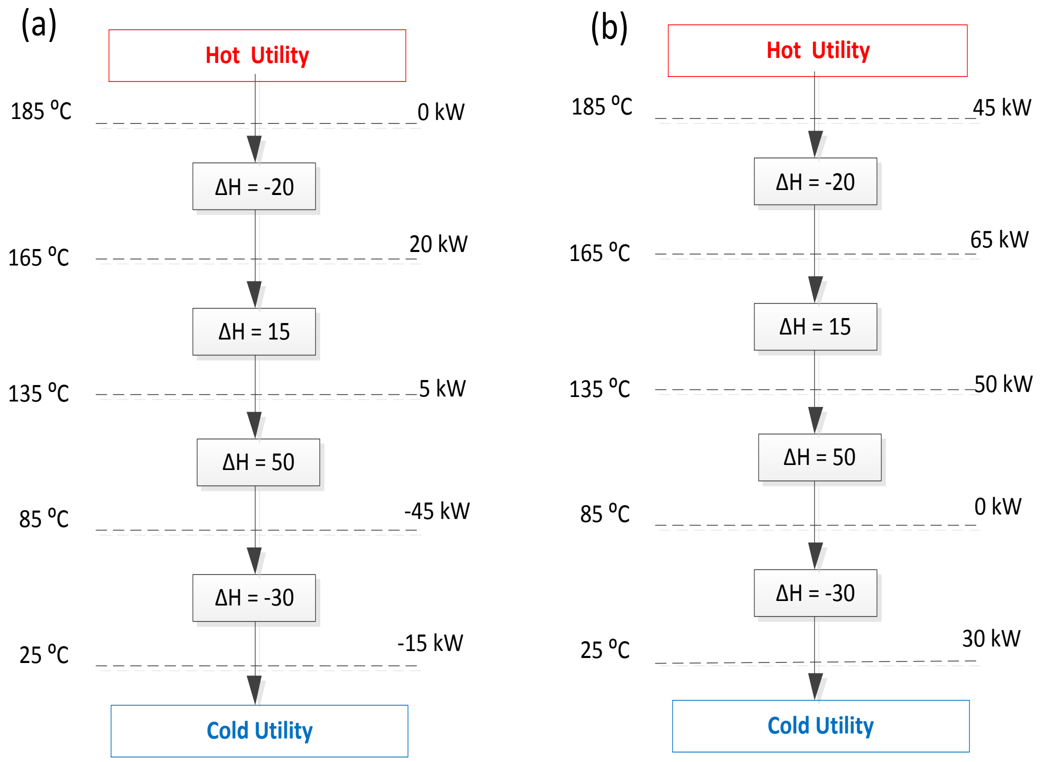

Figure 3-5: **(a) Cascade with surplus heat; (b) Normalized cascade with satisfied stream heat flow**

Thermodynamically, heat cannot be transferred from low temperature to higher temperature, however when this happens, the HEN design may be infeasible. This is indicated by the negative heat flow on the last two intervals in Figure 3-5 (a). To solve this infeasibility problem, sufficient heating utility is needed to be added to make the cascade feasible. The smallest amount of heat flow need to be added, in this case, -45 kW is the least heat flow, the value is added to solve the negative heat flow as shown in Figure 3-5 (b). Therefore the energy targeted for this problem is Q_{Hmin} = 45 kW and Q_{Cmin} = 30 kW which corresponds to the minimum heating and cooling utility requirements obtained in illustration example 1 using composite curves method. The interval where the heat flow is 0 kW is known as the pinch points temperatures which are equals to 90 °C and 80 °C for hot pinch point temperature and cold pinch point temperature respectively.

3.2.3 Heat Recovery Pinch

The pinch point divides the problem into above the pinch (heat sink) and below the pinch (heat source) as indicated by the constricted point on the composite curve Figure 3-6. The value $of\ \Delta T_{min}$ at the pinch points gives the minimum temperature difference between the hot and cold composite curves corresponding to the economically balanced heat recovery pinch. Linnhoff, (1998), Hohman (1971) and (Linnhoff and lower (1978).

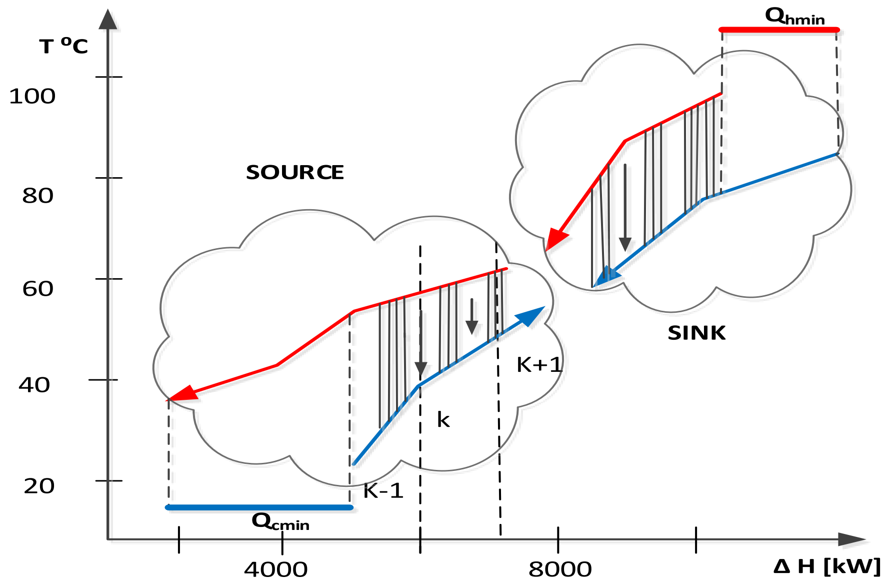

Figure 3-6 Pinch point temperatures

Three basic rules are necessary for effective pinch design with satisfied energy targets. These basic rules prevent enthalpy imbalance both above the pinch and below the pinch. These rules are:

1. Heat must not be transferred across the pinch
2. There must be no external cooling above the pinch
3. There must be no external heating below the pinch

As stated in Section 3.2.2, violating these rules lead to cross pinch problem and increase in energy requirement beyond the targets.

3.2.4 Utility selection in pinch design

Utility targeting is achieved with the use of grand composite curves. It gives the idea on the amount of external heating or cooling requirement in a given plant. The grand composite curve is obtained by plotting the cascade table in Figure 3-5 (b). The most common utility is steam, usually in the form of high pressure steam (HP), low pressure steam (LP) and medium pressure steam (MP). Furnaces and Hot Oil are also used for high temperature heating purposes. The grand composite curves for problem in Table 3-1 is shown.

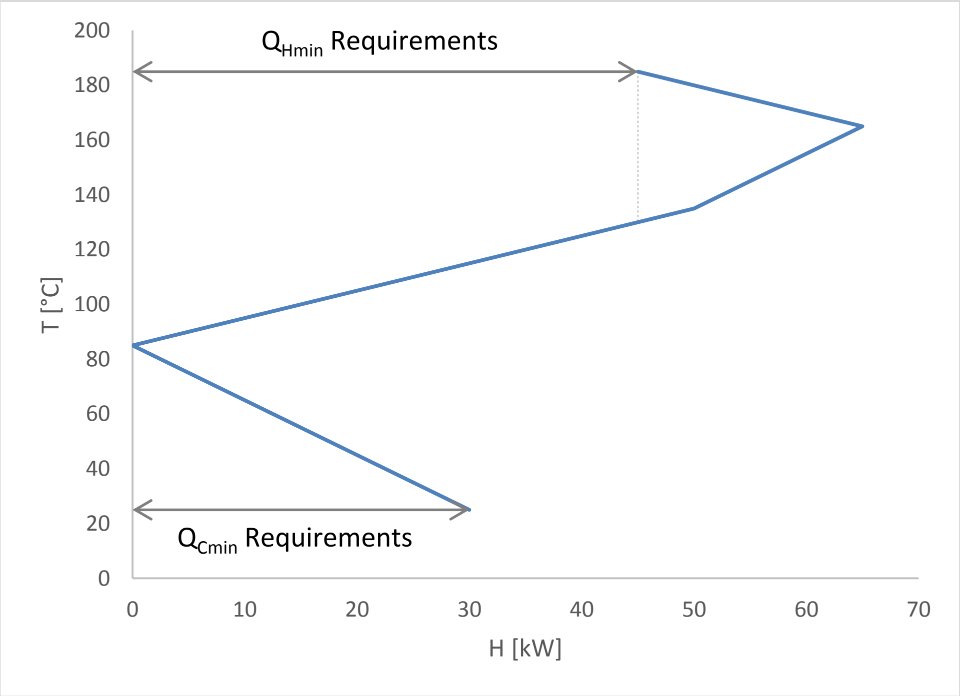

Figure 3-7 Grand composite curves

From Figure 3-7, different utility level can be selected from the grand composite curves depending on the nature of the curves and size of problem with pockets on the curves indicating the heat recovery area.

3.3 Capital-Total Cost Target

According to TEMA Standard (2007), the capital cost of HE is a measure of number of shell, heat exchanger type, heat exchanger area, and pressure rating. These factors can be extended to design of HEN with additional requirement such as number of units of HEs within a given network.

The number units defined by independent loops (L) is, according to Hohman (1971) given by:

$$N_{units} = S + L + C \qquad \textbf{(3-2)}$$

where N_{Units} is the number of matches or units, S number of streams including utilities and C is the number of components. Assume loop free network with single components, Equation 3-2 becomes:

$$N_{units} = S - 1 \qquad \textbf{(3-3)}$$

Equation 3-3 can be applied to either side of the pinch point in the form below;

$$N_{units} = [S_{ABOVE\ THE\ PINCH} - 1] + \ [S_{BELOW\ THE\ PINCH} - 1] \qquad \textbf{(3-4)}$$

In general, a HEN capital cost is minimized when the total number of HE units in the plant is kept at minimum number.

3.3.1 Heat exchanger area target

The most common industrial heat exchangers used in process engineering are the counter-current shell and tube HE (Smith, 2005). The area target requirement for enthalpy interval k (Figure 3-6) from hot to cold streams is

$$A_{Network} = \frac{\Delta H_k}{U \Delta T_{LMk}} \qquad \textbf{(3-5)}$$

where $A_{Network}$ is the heat exchange area for interval k, ΔH_k enthalpy change over k, ΔT_{LMk} log mean temperature difference for k and U overall heat transfer coefficient. For HEN with nth enthalpy interval, the network area taking into consideration of individual stream film heat transfer coefficient is given as:

$$A_{Network} = \sum_{k}^{Interval\ k} \frac{1}{\Delta T_{LMk}} \left[\sum_{i}^{Hot\ stream\ i} \frac{q_{i,k}}{h_i} + \sum_{j}^{Cold\ stream\ j} \frac{q_{j,k}}{h_j} \right] \qquad \textbf{(3-6)}$$

where $q_{i,k}$ and $q_{j,k}$ are stream duty at interval k for hot stream i and cold stream j respectively, h_i and h_j are film heat transfer coefficients. The derivation of the above equation is presented in Smith (2005)

3.3.2 Capital cost target

The capital cost for a single HE is defined by the relationship below,

$$Installed\ Exchanger\ Capital\ Cost = a + bA^{c} \qquad \textbf{(3-7)}$$

where a, b, c are constants depending on material of constructions, rating and exchanger type respectively. For the purpose of this thesis, all standard for materials of construction is assumed to be mild-steel except were stated. For the overall network, the exchanger capital cost becomes:

$$Network\ Capital\ Cost = N[a + b(A_{Network}/N)^{c}] \qquad \textbf{(3-8)}$$

here N represents the number of units of exchangers or sometimes refer to the number of shell in a unit as reported in Kemp (1994) as well as (Smith, 2005).

3.4 Economic trade-off optimization

Economics of trade-off is necessary to determine the optimum value of ΔT_{min} needed to achieve feasible HEN design. The smaller the value of ΔT_{min}, the higher the amount of energy recovery and the higher the area of the heat exchanger and vice versa. Because designing an infinitely large HE is practically impossible, recovering all unused heat energy cannot be achieved in practice. Therefore there is a need to balance between capital and operating cost when during HEN design. An optimum design with feasible trade-off between capital cost and operating cost which include cost of utility usage is necessary. Figure 3-7 describe the trade-off to determine for the minimum value of ΔT_{min} that is required for cost effective HEN design. From the graph, the decrease in ΔT_{min} increased in capital cost and decreased the cost of utilities. A trade-off exists where the value of ΔT_{min} for both energy and capital is at their minimum point; this point is regarded as the desirable ΔT_{min} for HEN design. In Figure 3-7, the desirable $\Delta T_{min} = 25\ ℃$ correspond to the point of interstation between the line describing the cost of energy and that of the capital cost.

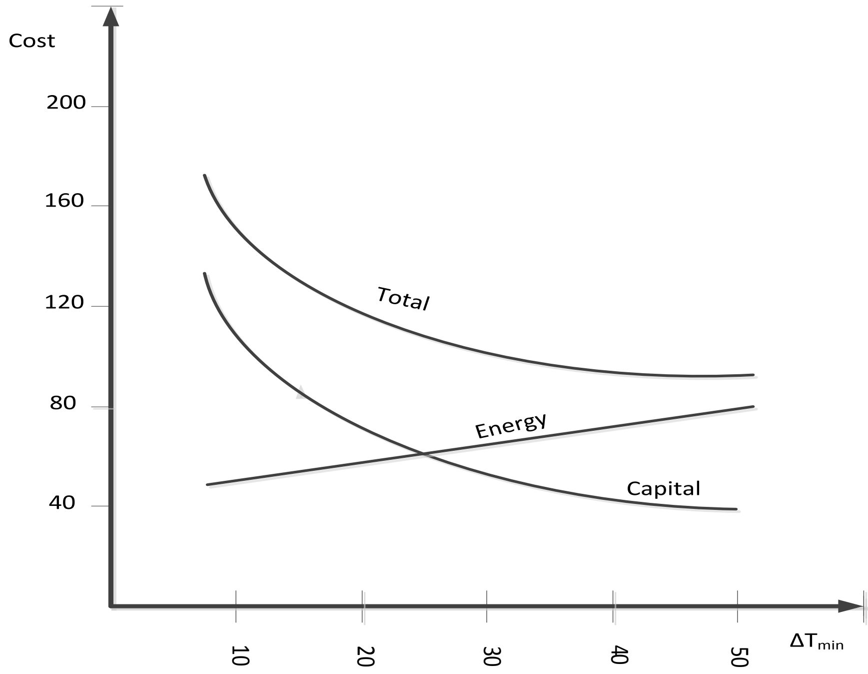

Figure 3-8 Optimization of capital energy trade-off (Smith, 2005)

3.5 Design of Heat exchanger network

Following trade-off optimization to identify the minimum temperature difference required for the design of cost effective HEN, all is now set for the network design using ΔT_{min} which correspond to the minimum optimum temperature difference between the hot and cold composite curves as shown in Figure 3-3 of section 3.2.1 above. A step by step illustration of HEN is shown in illustration example 3.5.1

3.5.1 Illustration Example

The stream data in Table 3-1 are arranged such that the hot stream runs from the left-to-right and the cold streams runs from right-to-left as shown in the grid diagram of Figure 3-9 below. The stream coloured in red represents the hot stream while the blue coloured stream represents the cold stream.

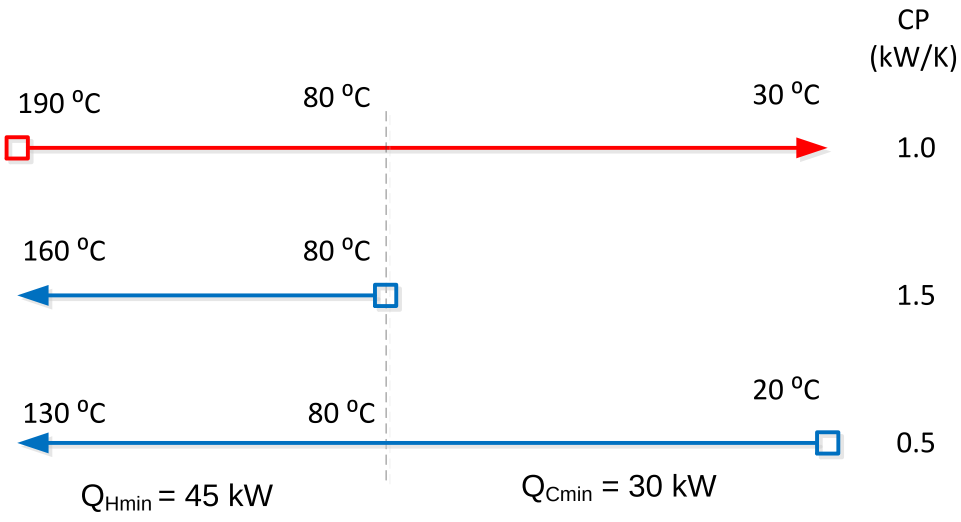

Figure 3-9: Grid diagram for the data from Table 3-1

The streams are divided at pinch temperature of 80 ºC (Figure 3-8) according composite curve Figure 3-4 or the problem table algorithm in Figure 3-6 (b). This division is necessary to avoid transferring heat across the pinch which violate pinch rule discussed in Section 3.2.3. Usually the design is started from the pinch which is the most constrained region either above the pinch or below the pinch due to restriction of the number of feasible matches by pinch point temperatures. When matching the streams to design a HE, the heat capacity flowrates CP inequality rules must be adhered to for above the pinch as well as below the pinch. For above the pinch,

$$CP_H \leq CP_C \tag{3-9}$$

This ensures that the temperature difference between hot and cold stream on the composite curves increases as the design moved away from the pinch point. Similarly, for below the pinch design,

$$CP_H \geq CP_C \tag{3-10}$$

In the case of below the pinch, the CP matching equation is a reverse of what is obtainable at the above the pinch design. What this means is that matching is done when CP_C is less than or equals to CP_H.

Adhering to the inequality rules in equations (3-9) and (3-10) is necessary for feasible network. Figure (3-6), moving away from the pinch point either below or above the pinch increases the temperature difference, which means for this condition to be true, the matching above the pinch should follow Equation (3-9) and below the pinch Equation (3-10) for feasible design.

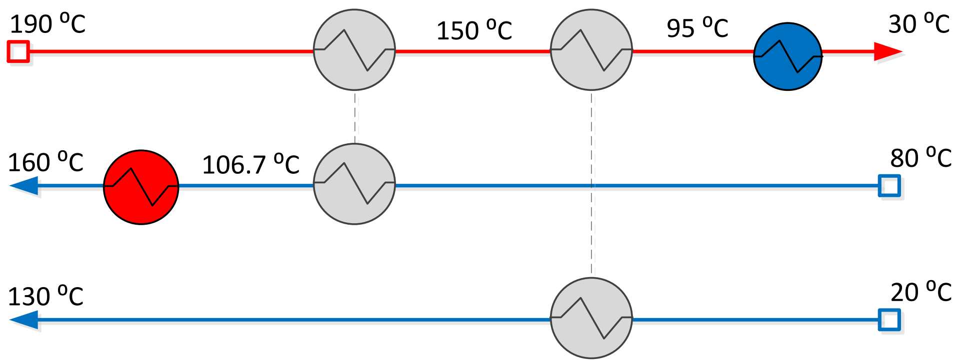

Figure 3-10: Complete HEN at $\Delta T_{min} = 10$ ℃

Figure 3-10 shows a complete HEN design with $\Delta T_{min} = 10$ ℃ for the 3 streams heat recovery problem in Table 3-1. There are a total of four exchangers: Two process-to-process exchangers and one hot and cold utility-to-process exchangers respectively.

3.6 Summary

A step by step procedure for pinch technology approach which has been described introduced briefly in Chapter Two is described in detailed with illustrative example using a simple 3-streams heat exchanger network problem. The methodology for pinch technology beginning with utility and energy targeting to HEN design and optimization is presented and discussed using the illustrative example to enhance implementation to a larger size problem involving HEN for coal-fired power plant retrofitted with CO_2 capture in the next chapter.

Once the thermal data are extracted from process plant and grouped into streams that needed to be cold and streams that needed to be heated, each group can be plotted into hot composite streams population and cold composited streams population on separate graph. The two streams population are then combined to formed composite curves defined by pinch point temperatures. Based on the composite curves, the amount of energy recovery, hot and cold utility demand is evaluated.

The grand composite is an important tool is defined the types of utilities needed to supplement the deficiency in heating and cooling requirements for the design of HEN. Capital cost targeting is used to target the area requirement of HEN design and for trade-off to estimate the true minimum temperature difference. The HEN design is begin from the pinch point, which is either from above the pinch or below the pinch base of some certain pinch rules.

4 HEAT EXCHANGER NETWORK FOR COAL-FIRED POWER PLANT RETROFITTED WITH CO_2 CAPTURE

4.1 Introduction

Integration of Post-combustion Capture (PCC) plant into coal-fired power stations presents significant technical and operational challenges which must be overcome for economic and efficient power generation. The plant fuel requirement increases, the net electrical energy output decreases in the range of 10-40% (Mertz et al., 2005). These challenges affect the design specifications of the base case power plants.

In several literatures (Lawal et al., 2012; Herkin et al., 2010; Harun et al, 2012), integration of power plant with capture unit is carried out through linking (a) the flue gas stream to the feed of capture plant and (b) the bleed stream extracted from the crossover between intermediate pressure turbine (IPT) and low pressure turbine (LPT) for the reboiler in the stripper of the capture plant. Through this connection, the capture plant uses heat from the steam turbine to release CO_2 and to regenerate the solvent. The large quantity of steam needed for the stripper or desorber of CO_2 capture plant overstretched the steam turbine's design and operation and thus other units in the plant.

Proper design of heat exchanger networks (HEN) presents an important opportunity for reducing these energy penalties. HEN design using pinch technology has applications in petro-chemical industries for decades. However, only few studies consider its application in power plant integrated with PCC unit despite its potential in reducing the energy penalty of the power station. The pinch technology minimizes energy consumption through thermodynamically feasible energy targeting processes in order to regain any unutilized heat energy from the process streams. Any make-up demand for energy is supplied by either heating or cooling utilities. The HEN design involves linking of the coal-fired power plant plus PCC process flowsheet with utilities systems to significantly reduce the energy consumption and utility consumptions and hence overall plant running cost. The key challenge associated with the method is to identify the best pair of matching between hot and cold process streams so as to minimize utility consumption in a more economical way.

This Chapter uses pinch approach to design a HEN for coal-fired power plant retrofitted with PCC unit. The stream data is taken from Khalilpour and Abbas (2011), to evaluate the trade-offs between energy, capital and utility costs, and to redesign the HEN network with reduced energy penalty. The novel contributions compared to Khalilpour and Abbas (2011) include: (a) the use of cost and economic data to evaluate achievable trade-offs between energy, capital and utility cost, (b) determination of the optimal minimum temperature difference, (c) redesigning of a cost-effective HEN with fewer number of units

4.2 Process Description

A block diagram representation of the 300MWe coal-fired power plant integrated with PCC plant adopted from Khalilpour and Abbas (2011) is shown in Figure 4-1. Pulverized black coal is combusted at 1480 ^{0}C to produce subcritical steam. The steam leaves the boiler to high pressure turbine (HPT) at 565 ^{0}C where part of it is bled to heat up the feed water before entering the boiler and another part of the bleed is used to run the boiler feed pump turbine. The steam exiting the HPT is returned to the reheater before moving to the next turbine, the IP turbine at 542 ^{0}C. In the IPT, a bleed is channeled to the deaerator while the exit stream from the turbine supplies heat to the next turbine, the LPT. The LPT is fitted with different bleeds for primary heating of feed water and the exiting stream from the LPT condensed and treated to feed the deaerator. The main streams connecting the power plant with capture unit are the flue gas stream which is fed to the absorber column and the steam extracted from IPT/LPT crossover to the reboiler in the stripper or desorber.

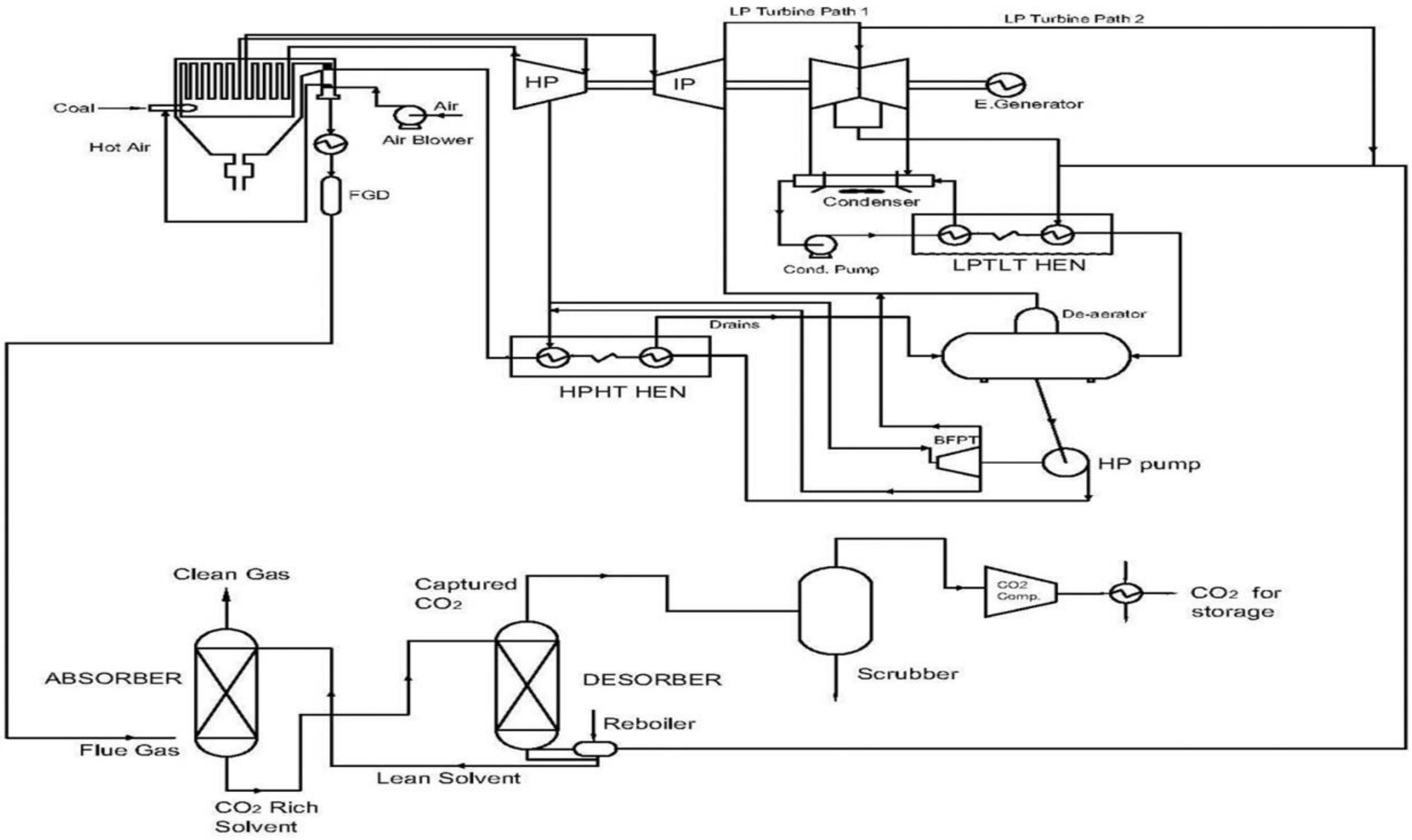

Figure 4-1 PFD for coal-fired power plant with CO_2 capture

4.3 Data Extraction

The data extraction involves selection of the relevant hot and cold streams from the coal-fired power plant retrofitted with CO_2 capture plant process flowsheet. This requires close attention to obtain proper data for pinch analysis and not to be prejudiced by the existing design configuration (Khalilpour and Abbas, 2011). In this study, the base case coal-fired power plant with PCC was simulated by using Aspen HYSYS 7.1 from Aspentech, USA. The simulation file was exported to ASPEN Energy Analyzer V 7.3 to extract the required process data as shown in Table 4-1.

Table 4-1 Extracted Stream Data from Coal-fired Power Plant with CO_2 Capture

Stream Name	Temp, in (^{0}C)	Temp, out (^{0}C)	Heat Capacity Flowrate (kJ/h^{0}C)	Duty (kJ/h)
Flue gas	155.2	49	1442060	153146735
HP turbine bleed	362.6	110	418959	105829214
LP turbine bleed	245	42	142114	28849156
Turbine intercool 1	102	35	222751	14924331
Turbine intercool 2	113	35	222985	17392845
Turbine intercool 3	126.4	35	259252	23695675
To condenser reflux	91.4	30	1076439	66093348
LPLT feedwater	35	110	1830627	137296991
HPHT feedwater	112.6	252	4167000	580879800

4.4 Utility Cost Data

Table 4-2 presents the average annualized cost of utilities which includes: Fuel gas, intermediate and low pressure steam (as the heating utilities), and cooling water (as the cold utility). The total annualized cost for HEN design is necessary to evaluate the annual saving and the time required for paying back the initial investment. The economic data will be evaluated based on the standard assumptions of operating 8150 hours per year, 40 years of plant life, and interest rate of 10%.

Table 4-2 Extracted Stream Data from Coal-fired Power Plant with CO_2 Capture

HUtilities	Average cost	Annualized cost
HEATING UTILITY		
Fuel gas	81.59 US$/1000Nmc	71.23 $/kW
IP Steam	20 US$/ton	278.14 $/kW
LP Steam	17.2 US$/ton	224.4 $/kW
COOLING UTILITY		
Cooling Water	0.031 US$/$m^3$	21.04 $/kW

4.5 Energy Targeting

The first step in performing pinch analysis is to draw the composite curves for cold and hot streams. From the combined composite curves, the minimum heating and cooling requirements for the HEN can be determined once a minimum temperature difference (ΔT_{min}) is given. Figure 4-2 (a) shows the hot and cold composite curves for the seven hot streams and two cold streams from the coal-fired power plant with PCC at minimum temperature difference (ΔT_{min}) of 10 ^{0}C. About 83 MW of heat recovery is achieved at minimum heating and cooling requirement of 115.3 MW and 29.64 MW which corresponds to 122.6 ^{0}C and 112.6 ^{0}C pinch points on the hot and cold composite curves respectively.

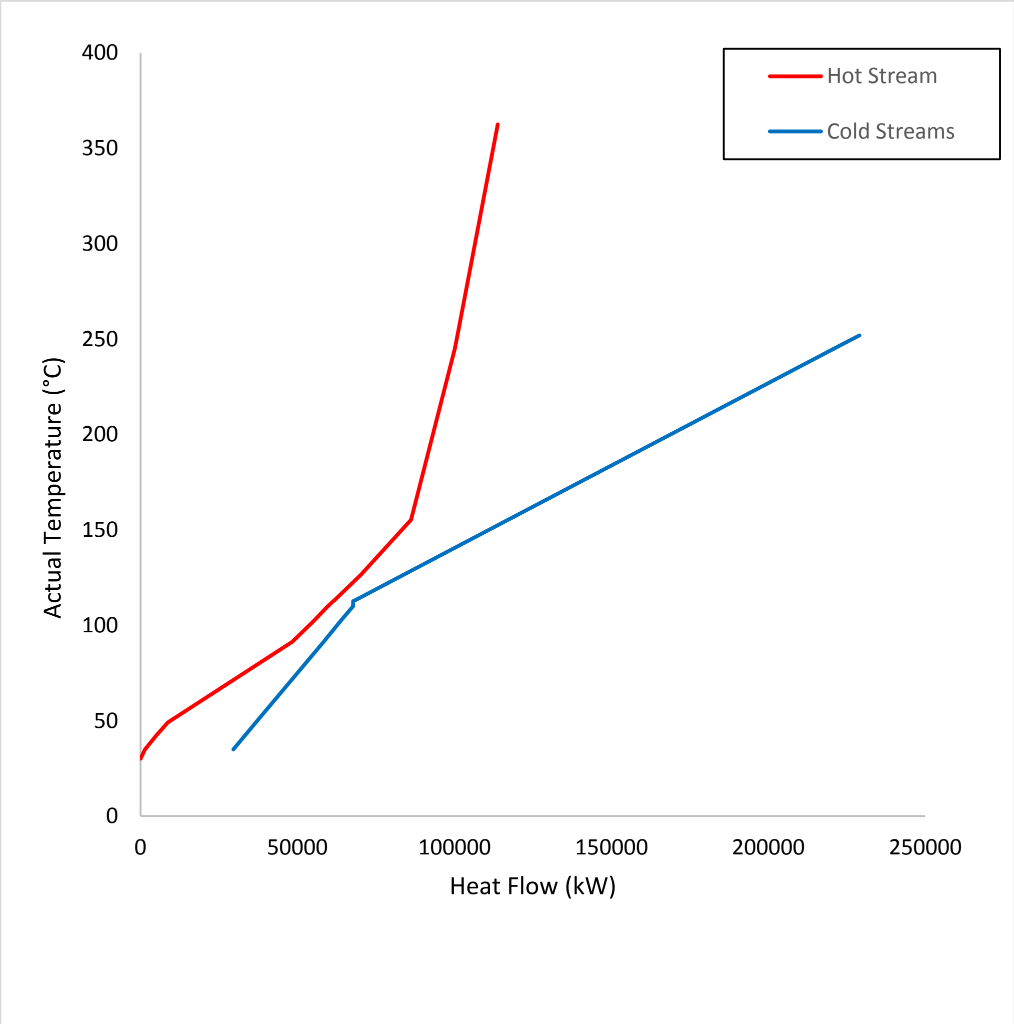

Figure 4-2 Hot and Cold composite Curves at ΔT_{min} = 10^{0}C

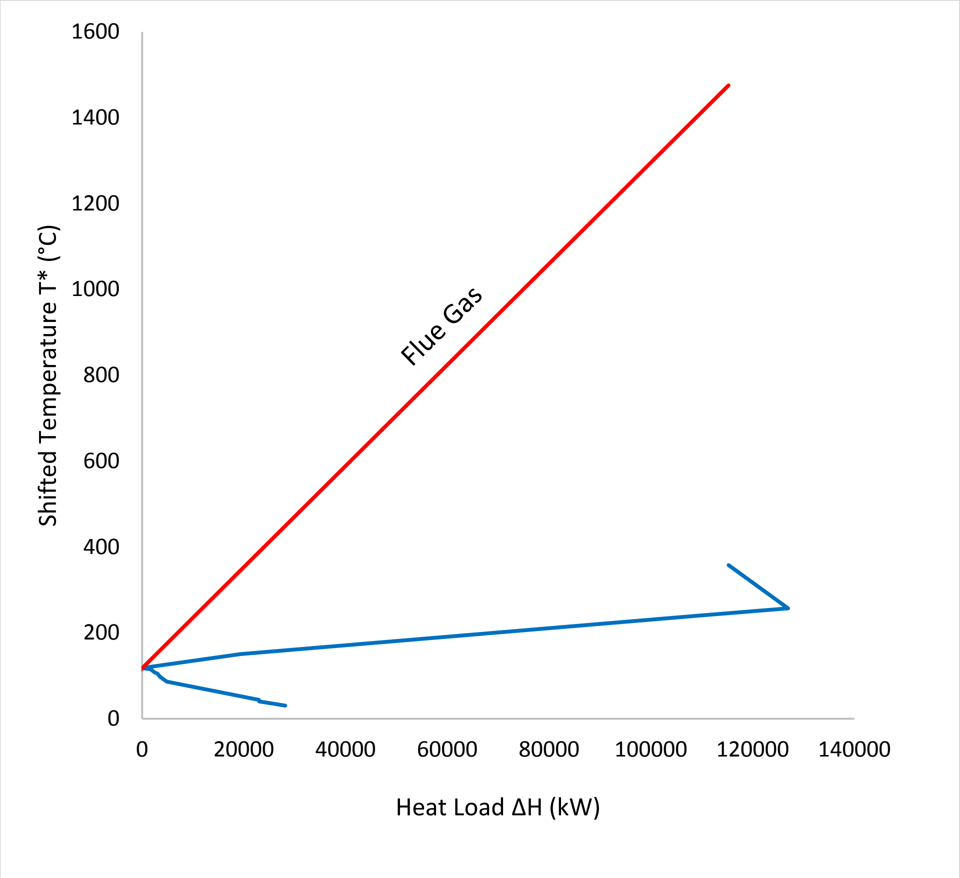

Figure 4-3 Grand composite curve with Flue gas matching

Figure 4-3 shows the flue gas matched against the grand composite curve of the power plant integrated with CO_2 capture. The flue gas starts at its theoretical flame temperature shifted for ΔT_{min} on the grand composite curve and present a sloping profile because it is giving up sensible heat (Smith, 2005). The shifted temperature of 1475 ^{0}C equivalent to the furnace theoretical temperature of 1480 ^{0}C at ΔT_{min} = 10 ^{0}C provides a total fuel requirement of 127.12 MW. In some cases, flue gas exit at process pinch temperature, however, in this case, a restriction imposed by the furnace exit gas temperature of 155.2 ^{0}C which prevents the flue gas being cooled to a shifted pinch value of 117.5 ^{0}C on the grand composite curve. The furnace efficiency in Figure 4-3 was found to be 90 % which corresponds with the value obtained in HYSYS based on assumption of complete combustion. In addition, Kemp (1994), also showed that furnace efficiency of 90 % or more results in flue gas exit temperature greater than or equals to 140 ^{0}C.

4.6 Capital-Energy Trade-off Targeting

For economic design of HEN, the minimum ΔT_{min} target is determined through optimum trade-off between capital and energy cost. From Figure 4-4, when the ΔT_{min} is set at 20 ^{0}C, the desired economic trade-off between the capital and the energy cost is achieved. A further increase in ΔT_{min} would lead to decrease in capital cost due to decrease in heat transfer surface area required (Matijaseviae and Otmaeiae, 2002). On the other hand, decreasing the value of ΔT_{min} from 20 ^{0}C would cause an increase in capital cost whereas the energy cost decreases. Therefore, to achieve economic energy recovery, a 20 ^{0}C minimum temperature difference is determined for this HEN design. At this temperature difference, the overall annualized total cost of the HEN is 3.804351 million USD which can be returned within a maximum payback period of 2.8 years

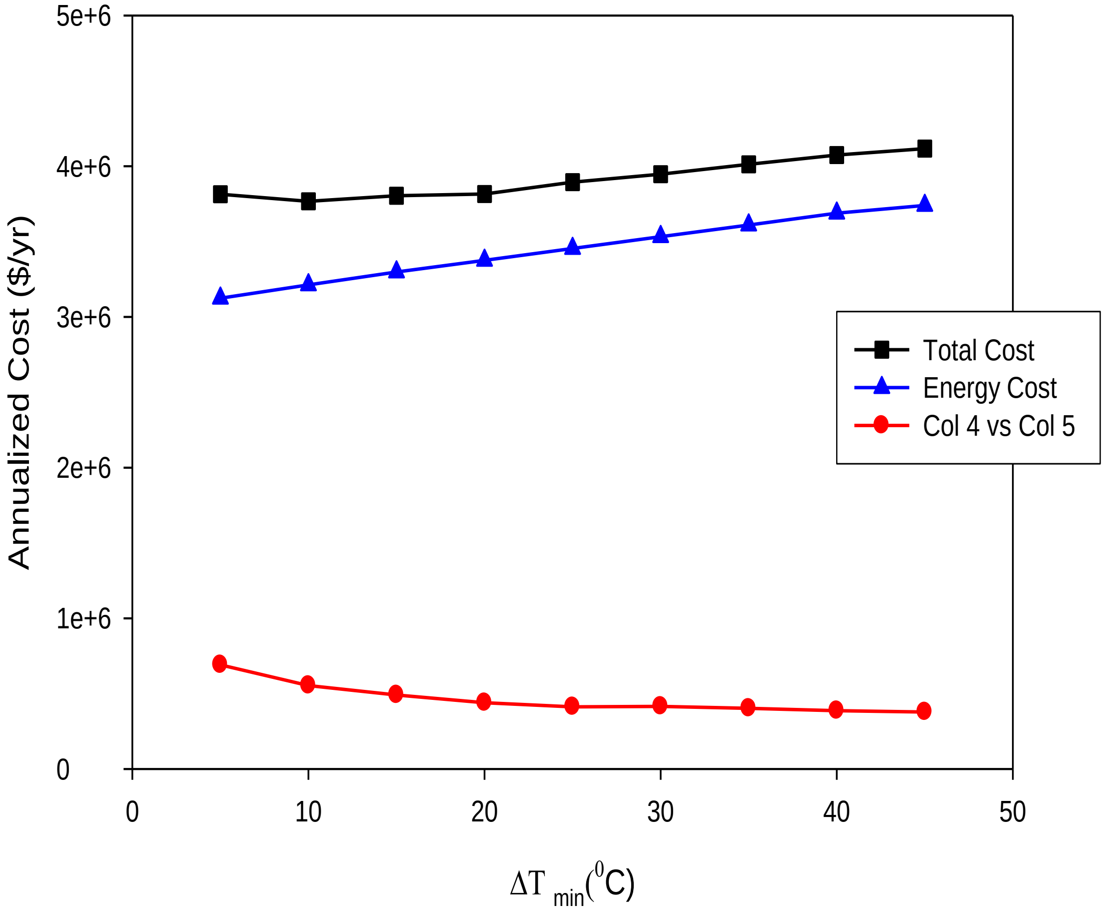

Figure 4-4 The Capital-Energy Trade-off

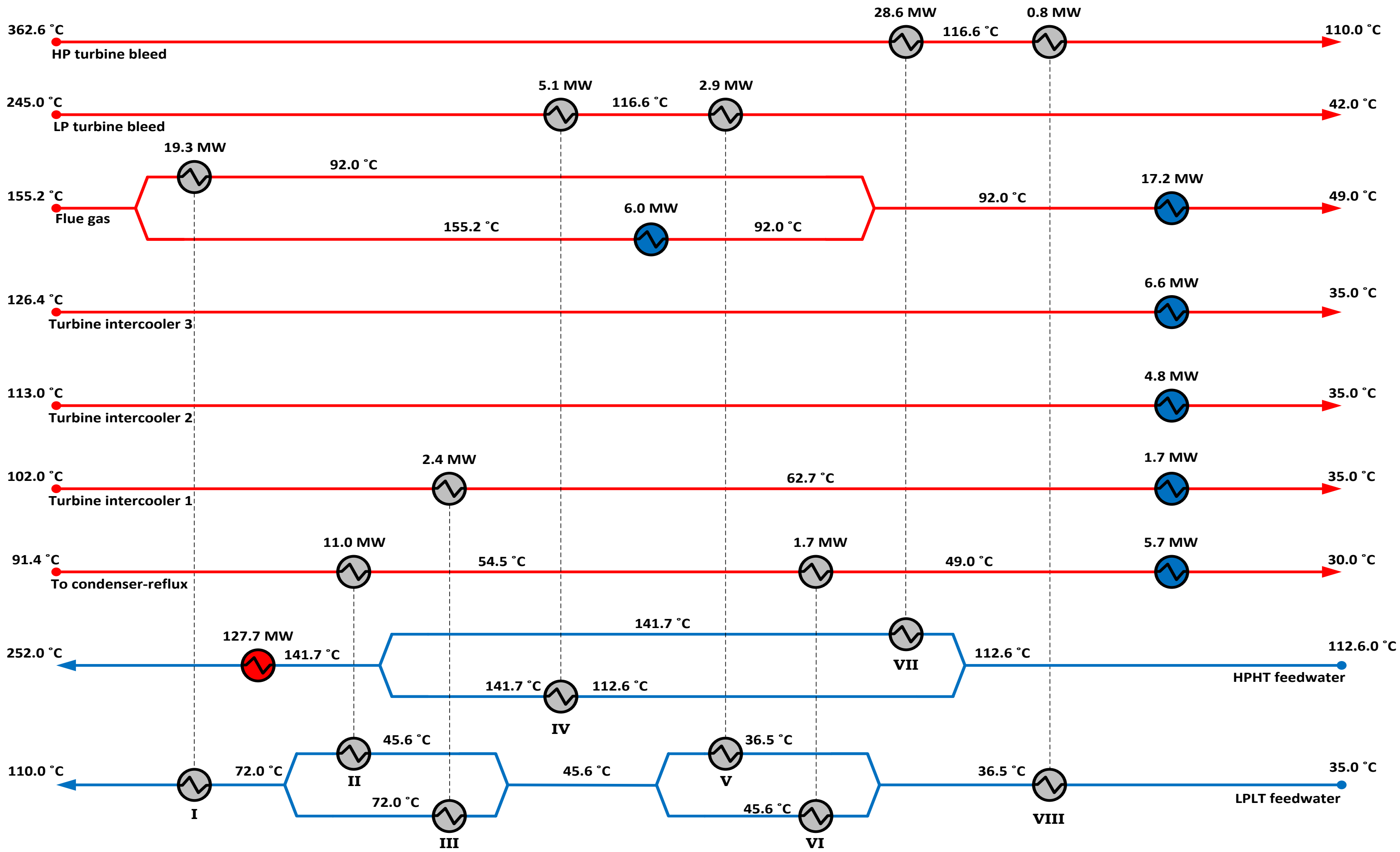

Figure 4-5 HEN design with ΔT_{min} = 20 °C

The optimal HEN design representing ΔT_{min} = 20 ^{0}C is shown in Figure 4-5. Although Khalilpour and Abbas (2011) suggested that there could multiple configurations of the same HEN problem, giving minimum utilities consumptions, a total of 8 Heat exchangers, 6 Coolers and 1 Heater is obtained in this HEN design. This is an improvement in the design cost when compared to 9 heat exchangers, 7 Coolers and 3 Heaters as reported in (Khalilpour and Abbas, 2011). Moreover, Khalilpour and Abbas (2011) did not indicate the minimum temperature difference used in their study, our study found that ΔT_{min} of 20 ^{0}C recovers about 78MW of heat energy from the coal-fired power plant with CO_2 capture unit. For conventional coal-fired power plant with CO_2 capture, the net efficiency can be assumed to be 35 %. This value, when compared to total heat recovery of 78 MW, is equivalent to saving of about 27.3 MWe. This signified that only about 10.6 MWe of electricity is lost due to addition of CO_2 capture unit corresponding to energy penalty of 9.82 %. In Khalilpour and Abbas, (2011) the capacity reduction is about 27.9 MWe with energy penalty of 15.9 %.

4.7 Conclusion

HEN design and economic analysis of coal-fired power plant retrofitted with CO_2 capture have been carried out. The benchmark used for this analysis is extracted from the publication of Khalilpour and Abbas (2011), which has 7 hot streams and 2 cold streams with each stream having a specified supply and target temperature, heat duty and heat capacity flowrates. The study achieved energy savings of 78 MW equivalents to 27.3MWe at a total investment cost of 3.804351 million USD and a payback period of 2.8 years. An optimal HEN with 8 heat exchangers, 1 heater and 6 coolers with a total capacity reduction of 10.6MWe was obtained compared to 27.9MWe as reported in (Khalilpour and Abbas, 2011). This value correspond to energy penalty of 9.82 % compared to the original work in which about 15.9 % energy penalty was achieved through a network containing 9 heat exchangers, 3 heaters and 7 coolers.

5 PROCESS OPERATION AND OPTIMIZATION

5.1 Introduction

A general idea and example of plantwide operation of a typical HEN and the formulation of a steady state optimization problem for HEN is developed in this chapter. Two types of approach to HEN optimization problem, i.e. the LP and NLP formulations are presented. The number of transfer unit (NTU) formulation for evaluating HE outlet temperatures, various logarithmic mean temperature difference (LMTD) approximations and errors associated with each approximations are also presented. The last part of this chapter present degree of freedom (DOF) analysis for heat exchanger network.

5.2 Plantwide Operation and Control

Plantwide control encompasses the design of control systems for overall process plant operations while considering the interactions and changes that may likely arise to affect the safety and optimum operating condition of the entire plant as a whole. During HEN design, integration of different units of process plant to form a network of HEs increased the plant complexity and interactions between the individual units which hitherto are simple and operates independently. For example, Figure 5-1 demonstrates how heat integration of various process units to improve the energy efficiency of the plant could leads to complex plant structure that is difficult to control. The flowsheet consists of two reactors, one separator, two cold streams (streams that are required to be heated or sinks) and two hot streams (streams that are required to be cooled or source) that are to be integrated. These streams are integrated to form a network of HEs for improvement of the plantwide energy recovery process.

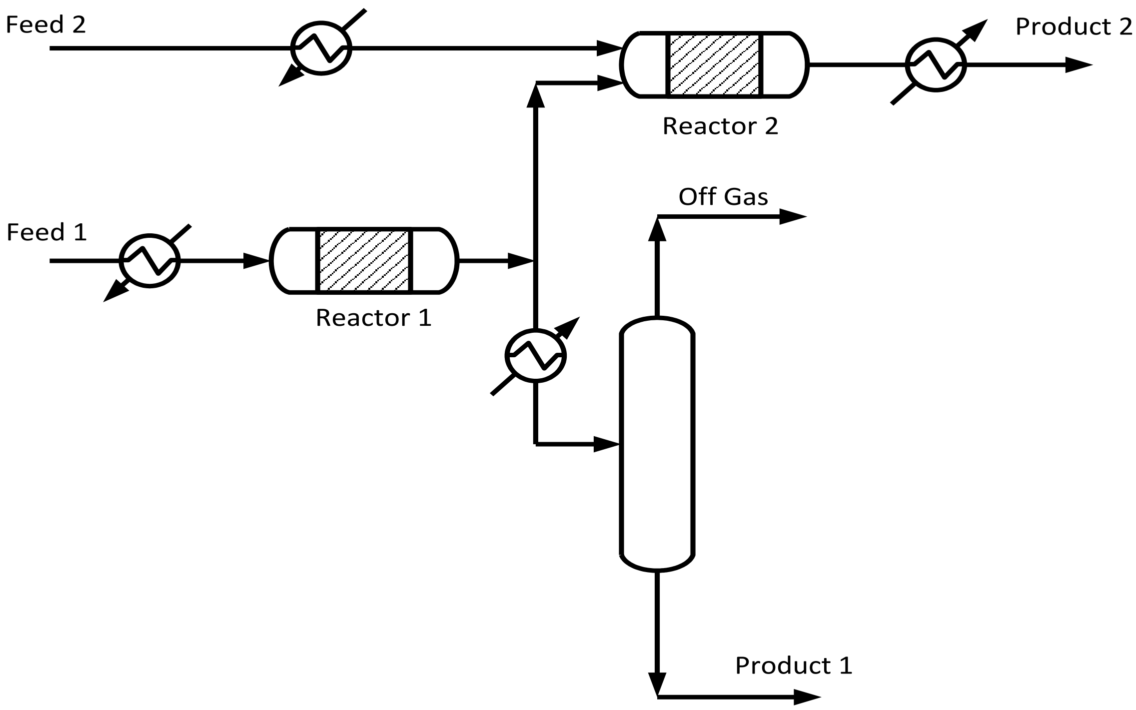

Figure 5-1 Simple unit process flowsheet

Assuming all the pinch HEN design rules are satisfied, the design methodology requires linking the hot and cold streams into process-to-process exchangers and with the utility-process exchangers complementing any deficiency in heating or cooling requirement to form a grid diagram, (Figure 5-2).

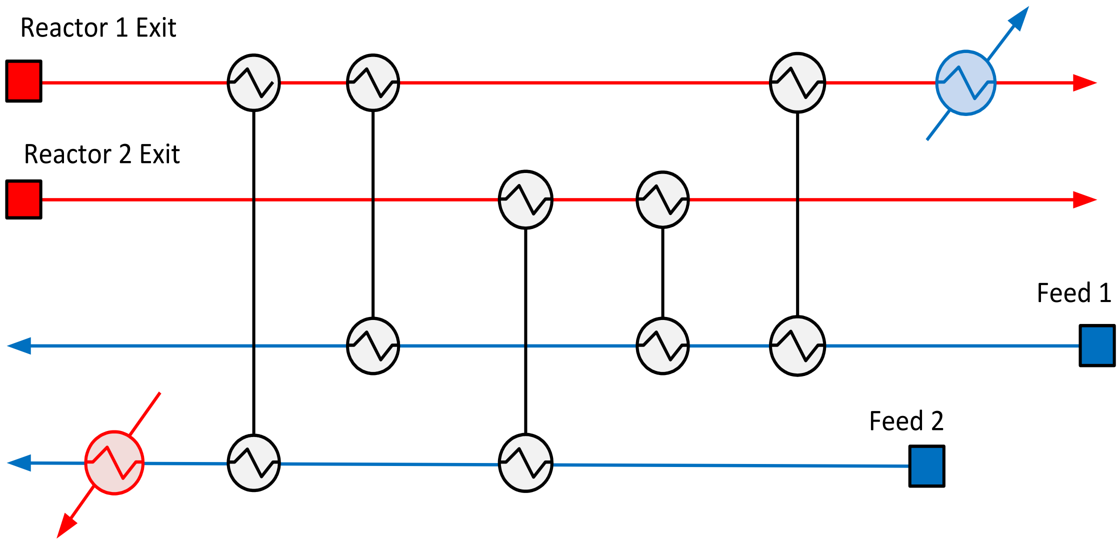

Figure 5-2 HEN grid diagram

Although the grid diagram in Figure 5-2 may look simple, it is however, a collection of coupled inlet or/and outlet streams from individual process vessels such as Reactors, Distillation columns, Reboilers, Condensers etc., depending on whether that stream is a source or a sink. The integrated process flow diagram (PFD) representing the final process unit is shown in Figure 5-3. The outlet temperature of Reactor-2 is integrated with Feed-2 stream to preheat the feed stream while at the same time providing cooling for Reactor-2 exit stream. A further cooling of Reactor-2 stream is achieved through preheating of Feed-1 stream. Similarly, Reactor-1 exit stream is integrated with Feed-2 inlet temperature and twice with Feed-1 inlet stream as indicated in Figure 5-3; the integrated process flowsheet.

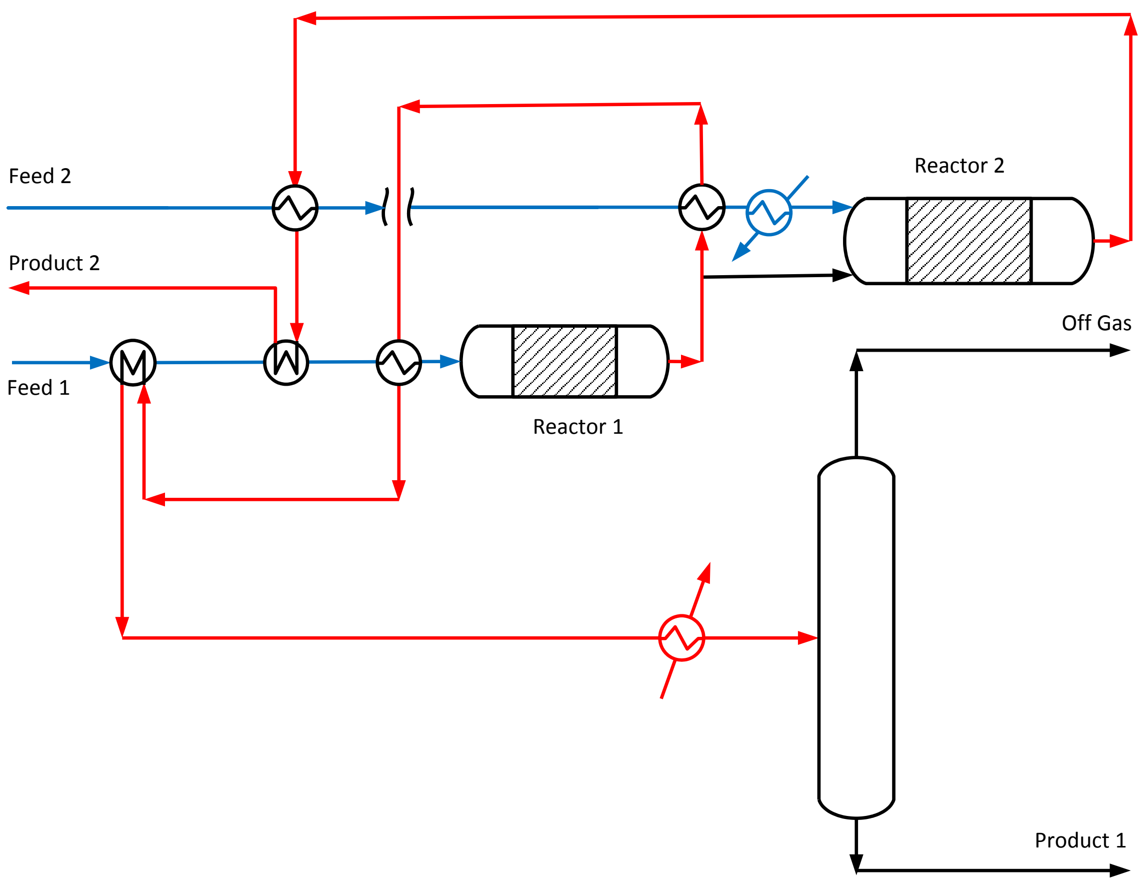

Figure 5-3 Flowsheets of integrated process units HEN

This procedure considerably altered the original plant design and operation schemes, and may lead to suboptimal plantwide operation and control challenges. Any small changes in manipulative inputs or disturbances may not only give rise to a local effect in operation of the individual units that formed part of the HEN grid design, but the disturbance may propagate downstream to greater part of the entire network and subsequently altering setpoints, stream target temperatures and hence the need for plantwide optimum operation of the HEN grid becomes imperative**.**

5.3 Heat Exchanger Network Optimization

The overall goal for optimization of HEN is to maintain target temperatures at their setpoints while achieving maximum energy recovery at a reduced cost of heating and cooling utilities. The profit cost function of heat exchangers depends on effectiveness of the heat transfer during matching of the different hot and cold streams. This cost function J otherwise known as the objective cost function for optimization of HEN represents the total annualized cost of the entire network comprising of the annualized operating cost and capital cost of the exchangers:

$$\min_{u}(J_{operation} + J_{capital}) \qquad \textbf{(5-1)}$$

$$subjected\ to: g(u, d) \leq 0$$

where u is the manipulated variable or degree of freedom consisting of equipment data and operating variables and d is the disturbances, and g is the equality or inequality constraints describing the process model.

For the purpose of this study, only the operational objective term $J_{Operation}$ in Equation (5-1) will be considered. The annualized capital costs term $J_{Capital}$ of exchanger is usually of importance during design which has been discussed in the first part of this thesis. The challenge in solving such an optimization problem is the presence of unknown disturbances d and the difficulties associated with deciding what to control with the available degree of freedom u.

5.4 Steady State Optimization model

Figure 5-4 is a unit HE with a bypass split ϕ_i bypassing the hot stream $T_i^{h,in}$ of the process-to-process exchanger E-101, and mixing with the exchanger hot exit stream $T_i^{*,out}$ at point m as shown in the figure. The main objective is to control matching between the cold and hot streams $T_i^{c,in}$ and $T_i^{h,in}$ to achieve optimal operation. The optimal condition can be determined using linear programming (LP) or nonlinear programming (NLP) formulation depending on whether the bypass split fraction ϕ_i is considered explicitly in the model equation during the HE operation or the bypass fraction is assigned arbitrarily.

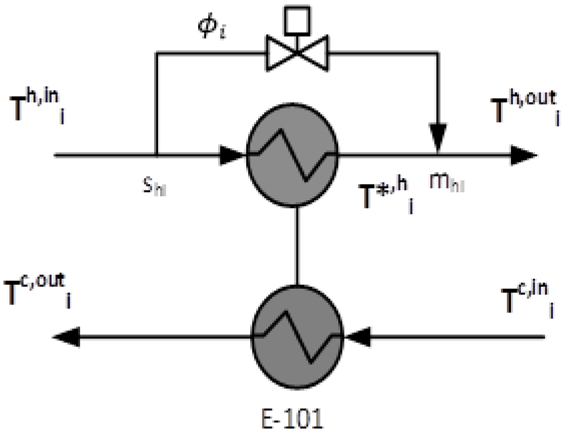

Figure 5-4 Simple heat exchanger with bypass

The model is based on heat balances around heat exchanger where the stream bypass fraction ϕ_i and the heat exchanger stream exit temperatures $T_i^{*,out}$ prior to mixing with the bypass stream are explicitly defined on the model.

$$Q_i = UA\Delta\mathrm{T}_m(T_i^{h,in}, T_i^{c,in}, T_i^{*,out}, T_1^{c,out}) \quad \textbf{(5-2)}$$

$$T_i^{h,out} = \phi_i \, T_i^{h,in} + (1 - \phi_i) \, T_i^{*,out} \quad \textbf{(5-3)}$$

$$Q_i \leq UA\Delta T_m(T_i^{h,in}, T_i^{c,in}, T_i^{h,out}, T_i^{c,out}) \quad \textbf{(5-4)}$$

where A is the heat exchanger area, U is the heat transfer coefficient, $T_i^{h,in}$ and $T_{h,1}^{*}$, and $T_i^{c,in}$ and $T_i^{c,out}$ are the hot and cold streams inlet and outlet to the exchanger respectively. The term $\Delta T_m(\cdot)$ is the logarithmic mean temperature difference (LMTD) or some form of approximation to minimize computational difficulties as described in Underwood (1933), Paterson (1984), Chen (1987) or Average Mean Temperature Difference (AMTD) described in Section 5.5.

Equations (5-2) –(5-4) are the possible model equations that can be obtained from the HE. If the bypass fraction ϕ_i is considered explicitly in the model, the HEN model becomes an NLP problem. Equations (5-2) and (5-3) described the unit whereas if ϕ_i is assigned arbitrarily, it is considered as an LP problem, thus Equation (5-4) is used.

It is important to note that the mixer heat balance Equation (5-3) is the major source of bilinearity in the heat exchanger model. Several authors including Aguilera and Marchetti (1998), Lersbamrungsuk et al. (2008), and Glemmestad et al, (1997; 1999) among others considered formulating a HEN problem as an LP problem by not incorporating the bypass fraction ϕ_i into their HEN models, instead, the bypass fraction ϕ_i is determined after the elapse of optimization process through the use of Equation (5-4). Their formulation has advantage of being linear, however, they do not have control over the bypass fraction due to the fact that it is assigned arbitrarily at the onset of optimization and it is only evaluated after the optimum split heat load is obtained.

In general, the objective operating a HEN is to keep the stream outlet temperature within it specified range while at the same time maintaining a minimum cost of cooling $J_{cooling}$ and heating $J_{heating}$ utilities.

The optimization problem is formulated as an NLP problem shown in Equations (5-2) –(5-4) by imposing the necessary operational and safety constraints

$$\min_u J = \sum_{i \in CU} C_i Qcu_i + \sum_{j \in HU} C_j Qhu_j \qquad \textbf{(5-5)}$$

$$subject\ to\ g = 0$$

where C_i and C_j denotes cost of cooling utility i and heating utility j associated with cooler duty Qcu_i and heater duty Qhu_j respectively, u represents the available degree of freedom and g is the steady state HEN model equation. The general steady state model equation or the constraints g which defines the HEN problem is described in the systems of equations shown below;

Process-to-process exchanger equation:

$$Q_i - (1-\phi_i)wh_i\left(T_i^{h,in} - T_i^*\right) = 0 \tag{5-6}$$

$$Q_i - wc_i\left(T_i^{c,out} - T_i^{c,in}\right) = 0 \tag{5-7}$$

$$Q_i - \mathrm{UA_i}\Delta T_m(T_i^{h,in}, T_i^{c,in}, T_i^{*,out}, T_1^{c,out}) = 0 \tag{5-8}$$

where Q_i is the heat exchanger duty, i is a subset of process-to-process heat exchanger, wh_i and wc_i are the the heat capacity flowrate of hot and cold streams respectively. Equations (5-6) –(5-8) are the performance equation of a single unit HE whether the bypass fraction ϕ_i exist explicitly or arbitrarily assigned. The correlation between equations based on the principle of conservation of energy and mass balance is:

$$Q_i = (1-\phi_i)wh_i\left(T_i^{h,in} - T_i^{*,out}\right) = wc_i\left(T_i^{c,out} - T_i^{c,in}\right) \\ = UA_i\Delta T_m(T_i^{h,in}, T_i^{c,out}, T_i^{*,out}, T_i^{c,in}) \tag{5-9}$$

Bypass mixer equation:

$$T_i - (1-\phi_i)T_i^* - \phi_i T_i^{h,in} = 0 \tag{5-10}$$

Cooling utility-to-process

$$Qcu_i - wc_i\left(T_i^{h,out} - T_i^{h,\mathrm{t}}\right) = 0 \tag{5-11}$$

Heating utility-to-process:

$$Qhu_i - wh_i\left(T_i^{c,out} - T_i^{c,t}\right) = 0 \tag{5-12}$$

Cold and Hot stream target temperatures:

$$T_i^{h,\mathrm{t}} - T_{h,t} = 0 \tag{5-13}$$

$$T_i^{c,out} - T_{c,t} = 0 \tag{5-14}$$

Note: unlike the case of process-to-process heat exchangers where i is a subset of number of process heat exchangers available, for the utility-to-process exchangers, i. is a subset of cooling utilities for the cold utility exchanger and heating utilities for hot utility exchangers respectively.

5.5 The LMTD Approximation

The LMTD term $\Delta T_m(\cdot)$ in Equations (5-8) and (5-9) often results to serious singularity issues during operations, on the event, the minimum temperature difference between the hot side inlet stream $(T_i^{h,in} - T_i^{c,out})$ and the hot side outlet stream $(T_i^{*,out} - T_i^{c,in})$ are the same. For these reasons, several approximations mentioned in Section 5.4 above were devised to avoid numerical computational difficulties that are usually encountered using LMTD as results of division by zero. Some of these approximations include

Average Mean Temperature Difference AMTD

$$\text{AMTD} = \frac{(T_i^{h,in} - T_i^{c,out}) + (T_i^{*,out} - T_i^{c,in})}{2} \quad \textbf{(5-15)}$$

Underwood Approximation

$$LMTD = [\frac{\left[\left(T_i^{h,in} - T_i^{c,out}\right)\right]^{\frac{1}{3}} + \left[\left(T_i^{*,out} - T_i^{c,in}\right)\right]^{\frac{1}{3}}}{2}]^3 \quad \textbf{(5-16)}$$

Chen Approximation

$$LMTD = [\left(T_i^{h,in} - T_i^{c,out}\right)\left(T_i^{*,out} - T_i^{c,in}\right)\frac{\left(T_i^{h,in} - T_i^{c,out}\right) + \left(T_i^{*,out} - T_i^{c,in}\right)}{2}]^{1/3} \quad \textbf{(5-17)}$$

Paterson Approximation

$$LMTD = \frac{2}{3}\left[\left(T_i^{h,in} - T_i^{c,out}\right)\left(T_i^{*,out} - T_i^{c,in}\right)\right]^{0.5} + \frac{1}{6}[\left(T_i^{h,in} - T_i^{c,out}\right) + \left(T_i^{*,out} - T_i^{c,in}\right)] \quad \textbf{(5-18)}$$

The approximation used by Paterson slightly overestimates the true LMTD value whereas the Chen approximation underestimates the LMTD (Verheyen and Zhang, 2006). The AMTD is a rough estimate with large errors especially when temperature difference on both sides of the exchanger are dissimilar, Cramer (2007) shows that about 5 % error is introduced by ATMD if $(T_i^{h,in} - T_1^{c,out})$ and $(T_i^{*,out} - T_i^{c,in})$ defers by a factor of 2. Edvardsen D. G. (2011) reported that, Skogestad (2003) noted that if $\frac{1}{1.4} < \frac{\left(T_i^{c,in} - \mathrm{T_i^{C,out}}\right)}{\left(\mathrm{T_i^{H,out}} - \mathrm{T_i^{C,in}}\right)} < 1.4$ the error is less than 1%. The percentage errors associated with various approximations can be evaluated

$$Error = \frac{\Delta T - \Delta T_{LMTD}}{\Delta T_{LMTD}} \times 100$$

where ΔT is the approximation type, ΔT_{LMTD} is the LMTD. Appendix B shows plot of percentage error for these approximations. The order of accuracy ranges from Underwood, Paterson, Chen and finally the AMTD. In this work, ATMD approximation is used to calculate LMTDs for all the process-to-process heat exchangers. This formulation tends to be slightly easier to solve with less numerical difficulties when compared with LMTD and other approximations.

5.6 Heat Exchanger NTU model

The NTU method is important in tracking down exchanger steady state exit temperatures given the heat capacity flowrates and the exchanger inlet temperatures of both heating and heated streams. The NTU calculates the effectiveness of HEN where there is no sufficient information to evaluate the LMTDs.

The NTU given in Incopera and Dewith (2007) is

$$NTU = \frac{UA}{C_{min}} \qquad \textbf{(5-19)}$$

where U is the overall heat transfer coefficient, A is the heat transfer area/heat exchanger area, C_{min} and C_{min} are the lower and higher of the two fluids heat capacity flowrate ratios respectively. In process engineering, a typical HE used in the design of HEN is the counter-current shell and tube heat exchangers (Smith, 2005). Therefore the effectiveness ε of a counter-current shell-tube exchanger is given as

$$\varepsilon = \frac{1 - \exp[-NTU(1 - C_r)]}{1 - C_r \exp[-NTU(1 - C_r)]} \qquad \textbf{(5-20)}$$

where $C_r = C_{min}/C_{max}$. In most cases, $C_r < 1$ for counter-current exchangers, however, if $C_r = 1,$ or $C_r = 0$ effectiveness ε becomes Equation (5-21) and Equation (5-22) respectively.

$$\varepsilon = \frac{NTU}{1+NTU} \quad \textbf{(5-21)}$$

$$\varepsilon = 1 - \exp(-NTU) \quad \textbf{(5-22)}$$

Therefore, using NTU approach, the stream target for heat exchanger can be evaluated easily as:

$$T_i^{H,out} = (1 - C_r\varepsilon)T_i^{H,in} + C_r\varepsilon\, T_i^{C,in} \quad \textbf{(5-23)}$$

$$T_i^{C,out} = (1 - \varepsilon)T_i^{C,in} + \varepsilon\, T_i^{H,in} \quad \textbf{(5-24)}$$

5.7 Degree of Freedom Analysis

The degrees of freedom in HEN operation are either used for maintaining the outlet target temperatures, i.e. utility optimization or they are used to shift duties internally within the HEN (without affecting the utility cost), in form of stream bypasses. The Kwauk (1952) method of finding degree of freedom which was later modified by Smith (1963) as shown in Equation (5-25) is somewhat very tedious with high chances of making erroneous analysis especially for large, complex and highly nonlinear systems

$$N_{DOF} = N_{Unknowns} - N_{Equations} \quad \textbf{(5-25)}$$

Marselle (1982) proposed a new definition for DOF for HEN

$$N_{DOF} = N_{Units} - N_{targets} \quad \textbf{(5-26)}$$

where $N_{targets}$ is the number of target streams to satisfy at their setpoints and N_{units} is the total number of process-to-process HEs in the network and the utility-to-process HEs. Equation (5-26) is applicable to a limited number of HEN structures. A HEN design with threshold pinch does not satisfied DOF proposed by (Marselle, 1982); HEN with threshold pinch points or simply HEN with 1-heater or 1-cooler are known to violate this rule. This led to Glemmestad and Gundersen (1998) to modify the DOF equation for HEN systems.

Glemmestad and Gundersen (1998) provide a more accurate definition of DOF for utility cost optimization which can be used to check structural feasibility of HEN and any possible opportunity for optimization.

$$N_{DOF,U} = R + N_U - N_{targets} \quad \textbf{(5-27)}$$

Where $N_{DOF,U}$ denotes the number of remaining DOF, R dimensional space spanned by the manipulations in the inner HEN to the outer HEN and N_U the number of utility types.

The following three different cases of DOF were identified by Glemmested and Gundersen (1998):

I. $N_{DOF,U} < 0$: The operation of HEN is not feasible because all target temperatures cannot be controlled independently using the available manipulations

II. $N_{DOF,U} = 0$: The operation of HEN is structurally feasible because all target temperatures can be controlled independently using the available manipulations, however, there is no DOF availed for utility cost optimization

III. $N_{DOF,U} > 0$: The operation of the HEN is structurally feasible because all target temperatures can be controlled independently using available manipulations and there are some degree of freedom for utility cost optimization.

One important role for DOF in HEN operation is to exploit the installed heat exchanger areas as efficiently as possible (minimized energy cost) while maintaining the targets.

5.8 Summary

The importance of plantwide operation to safety and optimum operation of HEN is presented in this Chapter. Because HEN increased the complexity of process plant, it is obvious disturbance from one part of the process may transmits themselves to the entire network thereby affecting the smooth operation of the overall plant.

The goals of optimization of HEN in achieving optimum operation with minimum utility requirements at constant targets temperature are highlighted. Although optimization is to minimize capital and operating cost of HEN, this section only considers the operating cost as the capital cost optimization has been presented in Chapter Three and Four. Most literature consider HEN operation formulations as an LP problem by not explicitly considering the bypass fraction the HEN models, they instead evaluate the bypass fraction arbitrarily after optimization, in this thesis, the HENs problem is NLP problem with the bypass explicitly considered in the model equations.

In avoiding singularity issues during operation of HEN, several LMTD approximation proposed in literatures have been presented and discussed, errors emanating from using each approximation are evaluated in each case. The choice of AMTD over approximations such as Patterson, Chen and Underwood is because of its numerical and computational advantages

The DOF in HEN are used for maintaining constant target temperatures or for manipulating duties of HE using bypasses. DOF analysis are by Kwauk (1952) is difficult to implement on a complex model; DOF proposed by Marselle (1982) is not applicable where the network is a threshold problem. The DOF by Glemmestad and Gundersen (1998) is generic and applicable to all networks including HEN with not utility exchangers.

6 SELF-OPTIMIZING CONTROL

6.1 Introduction

This chapter presents a theoretical framework of self-optimizing control (SOC) for CVs selection and an overview of some of the existing SOCs procedure available in the open literatures. The different approximations of cost functions proposed overtime in the quest for candidate-CVs that minimizes losses as well as returned a better self-optimizing ability are presented and discussed. Our newly developed CV selection based on process data 'data-driven SOC' is detailed. The idea of this presentation is to equip the reader with information on the uniqueness of our new data-driven SOC technique in the whole idea of CV evaluation using SOC and to identify where our research fit-in in the plantwide control schemes.

6.2 Self-optimizing control methods

Self-optimizing control (SOC) presents a systematic procedure for evaluating process control variables (CVs) to achieve plantwide operational and control objectives with constant setpoints despite existence of uncertainties and disturbances that may upset the steady state operation of the entire process plant. Skogestad (2000) described the method in one sentence as, "*when acceptable (close to optimal) operation is achieved with constant setpoints for the controlled variables*".

The concept of SOC is a harbinger of an idea that was introduced previously during the early 1980s by Manfred Morari and his co-workers. In their study, Morari et al. (1980) made a generalized assertion that, "*we want to find a function $\boldsymbol{c}$ of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables and with it, the optimal operating conditions*." That function $\boldsymbol{c}$ is what Skogestad (2000) accordingly termed as self-optimizing CV that satisfies both plant economic and operational objects.

Consider a generalized steady state optimization problem defining process plant operations formulated to minimize a certain objective function subject to some constraints:

$$minimize\ J(x, u_0, d) \qquad \textbf{(6-1)}$$

$$subject\ to\ g_1(x, u_0, d) = 0,$$

$$g_2(x, u_0, d)\ <\ 0$$

where J denotes the scalar cost function to be minimized (i.e. production cost, impurities etc.) or a negative value of the profit function to be maximized (i.e. yield, selectivity etc.), the state variables, steady state degree of freedom and disturbances are represented as $x \in \mathbb{R}^{n_x}$, $u \in \mathbb{R}^{n_u}$ and $d \in \mathbb{R}^{n_d}$ respectively. The equality constraints $g_1(x, u_0\ , d)$ includes the model equations which linked the independent variables u and disturbances d with x, the states. The inequality constraints $g_2(x, u_0, d)$ represents the operating conditions defining the system boundary condition which must be satisfied for all feasible processes, for example, a positive inlet-outlet temperatures of HE as well as positive bypass fractions and stream flowrates. At steady state condition the entire process operation does not change with time. This implies that equality constraints $g_1(x, u_0, d)$ approaches zero leading to elimination of $g_1(x, u_0, d)$ from the optimization problem for all continuous processes operating at steady state condition. This led to the general steady state optimization problem reduced to

$$minimize\ J(\ u_0, d) \qquad \textbf{(6-2)}$$

$$g(\ u_0, d)\ \leq\ 0$$

Now when disturbances d are introduced into the process to upset the steady state operating condition, the process operation becomes suboptimal. In this mode, the inequality constraints part of g are active and should be controlled with equal number of degree of freedom (DOF). The main challenge however is the decision on what to control with the remaining unconstrained DOF in the equality constrained part of the model g

The usual thing to do in order to ensure optimal plant operation in the presence of disturbances d is to solve Equation (6-2) online for optimal values of u_0 for every value of d propagating through the plant giving rise to u_0 becoming u_{opt}. Thus we have

$$\min_{u} J(u,d) = J(u_{opt}(d),d)\ def \stackrel{\text{def}}{=} J_{opt}(d) \qquad \textbf{(6-3)}$$

where $u_{\text{opt}}(d)$ is the true optimal to be found and $J_{\text{opt}}(d)$ is the optimal value of the cost function. In practice, the assumed solution is unattainable because it requires a perfect model and prior knowledge of all measurements and disturbances.

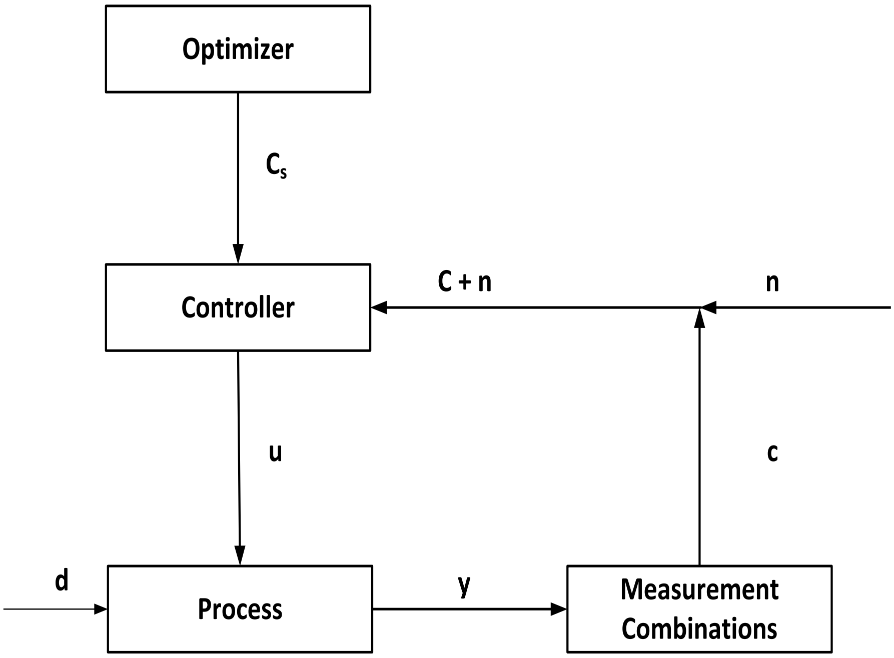

Figure 6-1 Feedback-based operational policy (Halvorsen et al., 2003)

An alternative route to achieving optimal operation is through implementation of feedback control method as shown in Figure (6-1). The optimizer in the diagram can be any of either real time optimization (RTO), (Forbes and Marlin, 1996), the necessary conditions of optimality (NCO) tracking (Srinivasan et al. 2003, Kadam 2007) or the SOC method (Skogestad, 2000).

During process operation, assuming the optimizer in Figure (6-1) is operating RTO, any disturbance d or change in manipulative inputs which propagates into the process block will encounter a controller which tries to keep the controlled variables $c + n$ at their setpoints C_s values. These disturbance changes the output measurements y. The optimizer estimate and provides a new optimal setpoint C_s to be implemented online.

On the other hand, if the optimizer is operating SOC scheme, the SOC method avoids requirement for updating setpoints C_s and obtaining online solution. The SOC maintains the operation at constant setpoint C_s even though disturbances propagate downstream into the process during operation. The CVs achieve close to optimal solution offline with setpoint values insensitive to disturbances, i.e. the setpoints does not change with change in manipulative input.

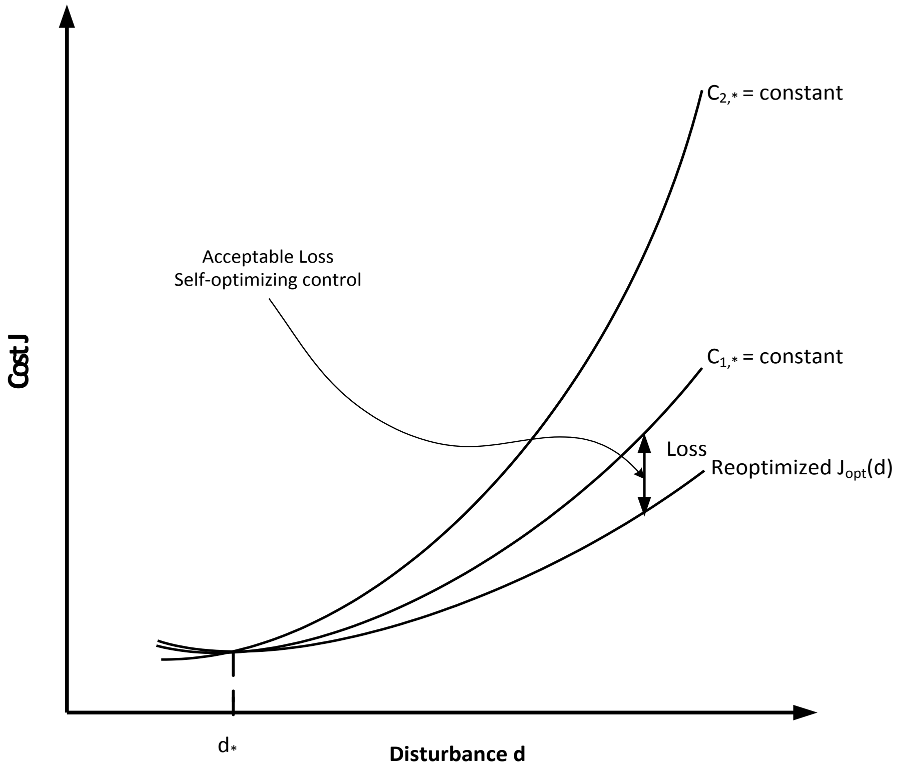

Figure 6-2 Loss incurred keeping Constant setpoint for Controlled Variable (Skogestad, 2000)

Figure (6-2) explains the meaning of the term ‘acceptable loss’ and ‘constant setpoints’ for disturbances which becomes the hub of controller design based on SOC procedure. If the term c_{1*} and c_{2*} are two different CVs evaluated for a particular process model, the loss between keeping the two CVs are measured by the distance of operating line of either of the CVs to the operating line obtained for the optimal (Re-optimized $J_{(opt)}$) solution. From the Figure, it is obvious that c_{1*} incurred smaller loss when compared to the second c_{2*} selected for the same process model. It therefore follows that the $c_{1*}$is more acceptable as a CV than c_{2*}.

The loss is evaluated mathematically as

$$L(u,d) = J(u,d) - Jopt(d) \quad \textbf{(6-4)}$$

A guideline for selecting controlled variable is reported in Skogestad (2000) is given below:

• c_{opt} should be insensitive to disturbances

• c should be easy to measure and control accurately

• c should be sensitive to change in the manipulated variables (degrees of freedom)

• where more than one unconstrained DOF available, c should be independent of one another

Halvorsen and Skogestad (1997) proposed that CVs should be defined as gradient of the objective function J:

$$c_{ideal} = \frac{\partial J}{\partial u} \quad \textbf{(6-5)}$$

The goal of achieving optimal operation is to maintain the gradient at zero for all type of disturbances. However, this approach is somewhat impossible, hence several approximations were proposed overtime to approximate the gradient cost function and achieve self-optimizing CVs. These approximations are classified as local and global SOCs depending on whether or not the CVs are achieved through linear combination of measurements around nominal operating points or they are derived from gradient of cost function.

6.3 Brief Review of SOC methods

Since the introduction of the concept of SOC method by Skogestad (2000), several modifications and methods of selecting CVs based of SOC methodology has been proposed. The main Idea is that when these CVs are kept at their nominal constant set-points through feedback control, the plant operation is optimal or near optimal (Ye et al., 2013). Generally, literatures on SOC methods are grouped into local and global SOC method depending on whether linearization is involve in achieving the self-optimizing CVs. A brief highlight of some of the local and global SOC methods is presented in the following sections. A detailed review of SOC methods can be found in Skogestad (2000) and (Umar et al., 2012).

6.3.1 Local SOCs methods

Local SOCs witnessed the development of CVs with emphasis on finding linear combination of measurements as the self-optimizing CV through linearization of process model around their nominal operating points (Ye et al, 2013). Local self-optimizing CVs are usually suboptimal and as their name implies, they offer local solution (Umar et al., 2012). In linear form, the models are described in terms of measurements y manipulative variable u and disturbances d as shown in Equation (6-6)

$$y = G^y u + G_d^y W_d d + W_n e \qquad \textbf{(6-6)}$$

where G^y, G_d^y, W_d and W_n are respectively defined as the steady state gain matrix of input, steady state gain matrix of disturbances, magnitude of diagonal matrices for normalization of disturbances and implementation errors. The CVs are selected as a linear combination of all available measurements y

$$c = Hy \qquad \textbf{(6-7)}$$

Where H is the combination matrix with full row rank n_u which is to be determined.

Skogestad and Postlethwaite (1996) developed CVs to maximise the minimum singular value rule (MSV) of a scale gain matrix (Umar et al, 2012), however, the MSV often than not identified wrong CVs (Hori and Skogestad, 2008). An improvement to MSV is the Exact method proposed by Halvorsen et al., (2003) based on the assumption that linearization around setpoints results to approximate model that is optimal. CVs are in this case selected as subset of measurements.

The Branch and bound methods proposed by Cao and Kariwala (2008), Kariwala and Cao, (2009) and Kariwala and Cao, (2010) also selects CVs as subset of measurements or their combination in what is regarded as combinatorial optimization problems.

The worst case and the average case losses resulting from the given control structure represented by H are respectively derived in Halvorsen et al. (2003) and Kariwala et al. (2008) as

$$L_{worst} = \frac{1}{2}\sigma_{max}^{2}(M) \tag{6-8}$$

$$L_{average} = \frac{1}{6(n_d + n_y)}\|M\|_F^2 \tag{6-9}$$

The matrix M is defined as $\mathrm{M} = \left[J_{uu}^{\frac{1}{2}}(J_{uu}^{-1}J_{ud} - G^{-1}G_d)W_d \quad J_{uu}^{\frac{1}{2}}G^{-1}HW_n\right]$, where $G = HG_y$, $G_d = HG_{yd}$, $J_{uu} = \frac{\partial J^2}{\partial u^2}$ and $J_{ud} = \frac{\partial J^2}{\partial u \partial d}$ are the steady state gain and disturbance matrices, the second order partial derivatives with respect to manipulated variables u and disturbances d, respectively. A recent review on available different expressions for H, is available in Umar et al. (2012).

Local SOCs methods including the exact method, the Brute-force, the Null space method and are briefly introduced in next sections. A detailed description of some of these methods and many other Local SOCs can be found in Umar et al (2012) and (Skogestad and Postlethwaite, 2005).

6.3.1.1 Brute Force Method

Previously, SOC framework witnessed the use of brute-force optimization techniques to select measurements as CVs and directly calculate and compare losses associated with each of these CVs. The worst-case $L_{c,worst}(d,e)$ and average-case $L_{c,average}(d,e)$ loss are evaluated for various $d \in \mathcal{D}$ and $e \in \mathcal{E}$ with d and e regarded as random variables. These allow for evaluation of all possible alternative CVs and the CVs that resulted in small worst-case loss and average case loss are adopted as the true self-optimizing CVs that return optimal solution

$$L_{c,worst}(d,e) = \max_{d \in \mathcal{D}, e \in \mathcal{E}} L_c(d,e) \quad \textbf{(6-10)}$$

$$L_{c,average}(d,e) = \mathbb{E}[L_c(d,e)] \; ; \; d \in \mathcal{D}, e \in \mathcal{E}$$

where $\mathbb{E}[\cdot]$ is expectation operator, $\mathcal{D}$ and $\mathcal{E}$ represent allowable sets of d and e respectively. It is important to note that the active constraints changes during brute-force optimization approach.

6.3.1.2 The Null space Method

The Null space method has advantage of selecting CVs as combination of measurements unlike the previously discussed methods which consider CVs as subsets of available measurements. Because the implementation error are not considered in the CVs evaluation, the Null space method remain suboptimal, however its significance cannot be overlooked because the idea can successfully applied to somewhat more difficult and complex problems. Thus $c = c_s$ because c_{opt} is independent of disturbances (i.e. $c_{opt} = 0.d$). We therefore have

$$\Delta c_{opt} = Hy_{opt} = HFW_d d' \quad \textbf{(6-11)}$$

where F is the locally optimal sensitivity matrix. If H is selected such that the loss due to setpoint error is zero, we have

$$HF = 0 \quad \textbf{(6-12)}$$

The above equation denotes that H is a Null space of F provided enough measurements are available. $n_y \geq n_u + n_d$. where n_y is the number of measurements, n_u the number of manipulated variables and n_d the number of disturbances.

6.3.1.3 The Exact Method

The exact local method is another example of local SOCs which finds linear combination of measurements as CVs. Based on second-order approximation around optimal point, Halvorsen et al., (2003) developed the exact local method. If W_d and W_e are diagonal matrix of disturbances and implementation error, the worst-case loss is given as

$$\max_{\|f\|_2 \leq 1} L = \frac{1}{2}\bar{\sigma}(M_d M_e)^2, \tag{6-13}$$

where $\|f\|_2 = 1$ and $f = [d \quad e]^T$, $M_d = J_{uu}^{1/2}(J_{uu}^{-1}J_{ud} - G^{-1}G_d)W_d$ and $M_e = J_{uu}^{1/2}G^{-1}W_e$ and $\bar{\sigma}$ is the upper singular value, J is the cost function, G and G_d are the steady state gain matrix and disturbance model respectively, and u degree of freedom. With this theory, the step by step procedure for exact local method were highlighted by Halvorsen et al., (2003) as follows

i. Specify the cost function J
ii. Solve the nominal optimization, find J_{uu} and J_{ud}
iii. For each c, find the linear model $\Delta G = G\Delta u + G_d\Delta d$
iv. Find W_d and W_e
v. Compute the singular value $\bar{\sigma}([M_d \quad M_e])$ for each c
vi. The set c with the lowest singular value minimizes the loss

6.3.2 Global SOCs Methods

Generally, local SOCs methods are associated with CVs derived from linearization of nonlinear models around their nominal operating points. They are known to suffer losses due to linearization, hence, suboptimal in some cases. Cao (2003; 2005) suggest global approach based on the use of gradient function as CVs for global optimal solution. A look into some of these global approach based on how the gradient function is attained are briefly highlighted in the preceding sections.

6.3.2.1 Analytical Method

Analytical method finds the CVs analytically given any systems' performance equations. The gradient function are determined and used directly as CVs for global optimal solution (Cao, 2003; 2005). However, some models are complex and highly nonlinear, thus using gradient method to obtain the CVs is challenging and somewhat impossible in some cases. This makes analytical solution unsuitable for obtaining CVs. The idea of CVs selection from gradient function was also extended to include the use of sensitivities of gradient function to disturbances and implementation error. Cao (2004) proposed explicitly expressing the systems Jacobian via chain rule differentiation. Constrained optimization problem was used to demonstrate the approach and on the event of active constraints, cascade control structure was proposed.

6.3.2.2 The Necessary Condition of Optimality Method

Suppose the solution to Equation (6-2) is $u_{opt}(\mathrm{d})$, then the following Karush-Kuhn-Tucker (KKT) conditions from Cao (2005) and Edgar et al., (2012) otherwise referred to as first-order NCO is true:

$$g(u_{opt}, \mathbf{d}) \leq 0 \qquad \textbf{(6-14)}$$

$$\mu^T g(u_{opt}, \mathbf{d}) = 0 \quad \mu_k \geq 0, \; k = 1, \dots n_g$$

$$\frac{\partial J}{\partial u}(u_{opt}, \mathbf{d}) + \mu^T \frac{\partial g}{\partial u}(u_{opt}, \mathbf{d}) = 0$$

where μ $(n_g \times 1)$ is the vector of Langrange multiplier. Once the active constraints g_a, which corresponds to nonzero Lagrange multipliers is known, μ can be eliminated from above equations and the NCO can be represented as two parts: First part, the active constraints g_a and second part, the reduced gradient $\nabla_r J$. Chachuat et al., (2008) as show below:

$$\begin{cases} g_a = 0 \\ \nabla_r J = \dfrac{\partial J}{\partial u}\left[I - \left(\dfrac{\partial g_a}{\partial u}\right)^+ \left(\dfrac{\partial g_a}{\partial u}\right)\right] = 0 \end{cases} \qquad \textbf{(6-15)}$$

Note, the matrix inside the square brackets is a null space projection matrix of $\frac{\partial g_a}{\partial u}$. The reduced gradient $\nabla_r J$ has n_u components which are to be compressed to $n_u - n_a$ dimension using singular value decomposition. Now, let $\frac{\partial g_a}{\partial u} = USV^T$

and $V = [V_1\, V_2\,]$, where V_2 are $n_u - n_a$ right singular vectors corresponding to $n_u - n_a$ zero singular values. Therefore, the NCO compressed reduced gradient is thus:

$$g_a = 0, g_a \in \mathbb{R}^{n_a} \tag{6-16}$$

$$\nabla_{cr} J = \frac{\partial J}{\partial u} V_2 = 0, \qquad \nabla_{cr} J \in \mathbb{R}^{n_u - n_a}$$

Equation (6-16) indicates that the optimal inputs $u_{opt}(\mathrm{d})$ can be achieved through satisfying set of NCO with exactly n_u components. However, from Equation (6-16) the NCO will vary depending on whether the subsets of constraints are inactive or active due to disturbances. For simplicity, Kariwala et al., (2008) assumed that active set does not change with disturbances.

The main difficulty associated with the NCO approach is the immeasurability of the compressed reduced gradient $\nabla_{cr} J$. Cao (2005), suggested selecting CVs by indirectly controlling their gradients to reduce their sensitivity to disturbances. This approach is nevertheless local because the sensitivity measure was derived following linearization around nominal operating points.

6.4 The Main Idea and Thesis Contributions in Self-optimizing Control Framework

The main idea of data-driven SOC method in this thesis is to improve on the two step regression method presented by Ye et al., (2012). In their work, they presented a two-steps regression data-driven SOC method which processed measurements to evaluate the CVs in a two regression steps. In the first step, they derived a regression model for the economic cost as a function of independent variables using operational data and then determine the CVs by incorporating the NCO in the second steps. The method was implemented on exothermic reactor and reported to be superior to model-based SOC of Kariwala et al., (2008) which minimizes average local loss and those of Alstad et al., (2009) extended null space method.

In spite of better self-optimizing performance under uncertainties as demonstrated by the exothermic reactor case study, large regression errors arising in both regression steps are a limitation of this approach. To improve on the disadvantage, this thesis presented a one-step regression procedure for data-driven SOC based on finite difference method to determine the CVs as a function of measurements without evaluating the gradient function.

The main advantage of this method is that CVs can be evaluated without incurring large regression errors as it is the case with the Ye et al., (2012) method. However, this method does not deal with constraints directly, instead constraints are implicitly satisfied with data generated for regression. This makes data collection time consuming and sometimes difficult. And for a system with a large number of constraints and wide disturbance range, converging to every points in the entire operation range is numerically or operationally challenging. Moreover, for dynamic systems, this method requires all data point to wait until a steady-state is reached.

To circumvent this challenges, this thesis further extended the data-driven method to include the use of equality constraints. CVs as a function of measurement in SOC problems with equality constraints. This method has advantage of tightening the optimization problem towards a right and feasible solution which required satisfying all the equality constraints especially in the event of large range of uncertainties and disturbances affecting the system.

6.4.1 Data-driven SOC method without Constraints

In Section 6.2, the general steady state optimization problem is by represented in Equation (6-2). When considering unconstrained systems, Equation (6-2) reduced to the form

$$\min_{u} J(u, d) \quad \textbf{(6-17)}$$

where J is the objective function (or cost function), u and d are the manipulative variables and disturbances respectively. Our main goal is to find a set of measurements function as CVs such that if they are maintained at constant setpoints, the overall process operation is optimal or near optimal. Now, assumed that the required CVs to be measurement functions $C = C(y, \boldsymbol{\theta})$ with parameters, $\boldsymbol{\theta}$ to be determined through regression. Recall that, the optimum operation is realized through maintaining $dJ/du = 0$ in the presence of disturbances. Accordingly, we can find $\boldsymbol{\theta}$ such that

$$\frac{dJ}{du} = C(y, \boldsymbol{\theta}) \tag{6-18}$$

This is equivalent to

$$dJ = C(y, \boldsymbol{\theta})du \tag{6-19}$$

Equation (6-18) is the derivative of the objective function and can be replaced with a difference formula which can be either forward, backward or central difference formulas. For forward difference

$$J_{k+1} - J_k = C(y_k, \boldsymbol{\theta})(u_{k+1} - u_k) \tag{6-20}$$

where the subscript k indicates a reference point. The above equations can be applicable to a system with one degree of freedom (DOF). For problems with DOF>1, Equation (6-20) remain the same with the term $C(y_k, \boldsymbol{\theta})$ taking a vector form as $C^T(y_k, \boldsymbol{\theta})$ in all the three equations. It can therefore be inferred that for a set of data u_i, y_i, J_i, and d_i (unknown), $i = 1, \ldots, N$, the regression problem can be expressed as follows:

$$\min_{\theta} \sum_{i=1}^{N} \sum_{j=i_1}^{i_k} J_j - J_i - C^T(y_i, \boldsymbol{\theta})(u_j - u_i)^2 \tag{6-21}$$

where, $i_1, \ldots, i_k$ are k neighbourhood points of point i and k may depend on i. Note that with Equation (6-18), depending on the complex nature of the problem at hand, different system such as polynomials and neural networks can be used to approximate measurement function C as the CV. In this work, only first- and second-order polynomials are considered for approximating the CVs as shown in Equation (6-22) and Equation (6-23) below.

First order polynomial model

$$C_1(y_0, \boldsymbol{\theta}) = \boldsymbol{\theta}_0 + \sum_{j=1}^{m} \boldsymbol{\theta}_j y_{j0} \tag{6-22}$$

Second order polynomial

$$C_1(y_0, \boldsymbol{\theta}) = \boldsymbol{\theta}_0 + \sum_{j=1}^{m} \boldsymbol{\theta}_j y_{j0} + \sum_{j=1}^{m} \boldsymbol{\theta}_{jj} {y_{j0}}^2 + \sum_{i=1}^{j-1} \sum_{j=2}^{m} \boldsymbol{\theta}_{ij} y_{i0} y_{j0} \tag{6-23}$$

The coefficients $\boldsymbol{\theta}$s are unknown parameters that must be estimated from experimental data and m is interaction factor representing the total number of measurements. The finite difference is evaluated as shown in Fig. 6-3. The solid squares represent the location of known manipulative variables u (reference points), u_{k-1} as the backward neighbourhood points and u_{k+1} as the forward neighbourhood points. The open square represents the known disturbances d_u and the open circles indicates the position of interior points where the finite difference approximation is computed. Between any two solid squares lies in the neighbourhood points.

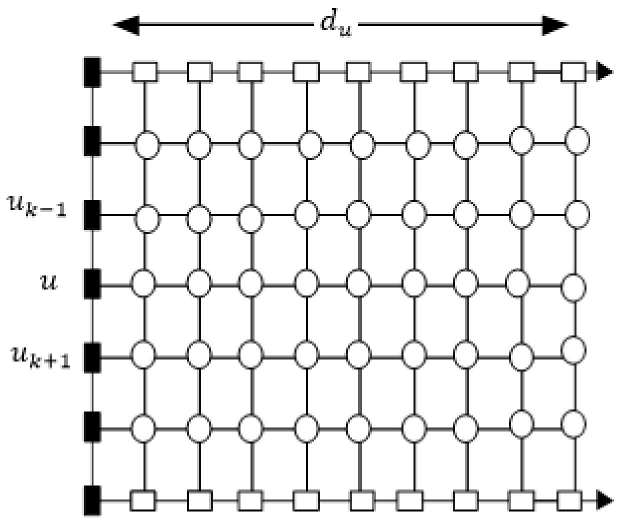

Figure 6-3 Finite difference mesh

6.4.2 Data-driven SOC method with Equality Constraints.

In contrast to Section 6.5.1, most problems of engineering optimization are constrained problems. The approach presented does not deal with constraints directly; instead, constraints are implicitly satisfied with data generated for regression. This makes data collection time consuming and sometimes difficult especially for a system with a large number of constraints and wide disturbance range. It is numerically or operationally challenging for such system to converge to every point in the entire operation range and for dynamic system, this method requires all data points to wait until a steady-state is attained. For constrained optimization problem as given:

$$\min_{\mathrm{u}} J(u, d) \tag{6-24}$$

$$s.t.\, \mathrm{g}(u, d) = 0$$

Lagrange function $L(u, d, \lambda)$ can be applied here to transform the problem into unconstrained optimization and to evaluate the first order NCO as shown in Equation (6-25)

$$\min_{u} L(u, d, \lambda) = J(u, d) + \lambda^T \mathrm{g}(u, d) \tag{6-25}$$

The NCO in this case is given

$$\frac{\partial L}{\partial u} \tag{6-26}$$

Now, let the CV regression function equals

$$C(y, \boldsymbol{\theta}) \approx \frac{\partial L}{\partial u} = \frac{\partial J}{\partial u} + \lambda^T \frac{\partial g}{\partial u} \tag{6-27}$$

Similarly like the case of unconstrained data-driven SOCs, finite difference approximation maybe applied to Equation (6-28) to evaluate the CVs. If forward difference formula is substituted, the equation takes the form

$$C(y_k, \boldsymbol{\theta}) = \frac{J_{k+1} - J_k}{u_{k+1} - u_k} + \lambda^T \frac{g_{k+1} - g_k}{u_{k+1} - u_k} \tag{6-28}$$

The Lagrange multiplier λ is eliminated as discussed in Section 6.4.2 using compressed reduced gradient to obtain a final expression of CV as

$$C(y_k, \boldsymbol{\theta}) = \nabla_{Cr} J|_k \tag{6-29}$$

The model coefficient θ is to be determined for both first- and second-order polynomials through least-square regression as shown in Equation (6-22) and Equation (6-23) respectively.

The following steps are followed to determine the CV parameters θ, through linear regression:

1. A set of process data is collected for all measurements, target temperatures and manipulative variables is collected for the whole range of disturbances during process operations.
2. Each manipulative variable is used as a reference points and the finite difference is computed for the objective function based on Equation (6-20) as shown in the finite difference mesh Figure 6-3.
3. Least-square regression is performed for both first order polynomial and second order polynomials Equations (6-22) and (6-23) expressed in Equation (6-21) by minimizing the value of squared 2-norm of the residual through adjustment of the regression parameter θ in either of Equation (6-22) and (6-23).
4. For SOC problem with equality constraints, the compressed reduced gradient instead is computed as in Equation (6-29).

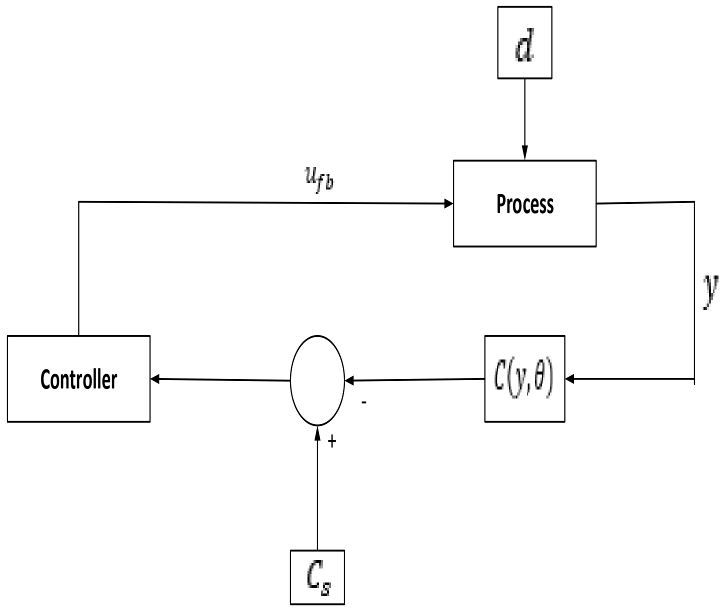

Figure 6-4: CV Implementation

The CV is implemented as shown in Figure 6-4 for evaluating its performance. The CV is represented by $C(y,\theta)$ with y denoting the process measurements. A controller with integral action is used to update the feedback control u_{fb} and keep the CV constant at constant setpoints C_s for all sets of disturbances range d upsetting the processes.

6.5 Summary

An offline-optimization approach which does not update setpoints to keep the HEN operation optimal in the presences of disturbances is considered. This offline approach is referred to as self-optimizing control procedure and it is the hub of this thesis.

Plantwide operation based on self-optimizing control for control variable (CV) selections was introduced by Skogestad (2002). It is capable of achieving optimal or near optimal operation with reasonable loss in cost function at constant setpoints for control variables, in the presence of uncertainties and disturbances. The method use model offline and maintain gradient of cost function at zero for all types of disturbances.

Several approximations and methods of keeping gradient of cost function zero are devised overtime. These methods are categorized into local and global SOCs. The local SOC is when it involves linearization of nonlinear models around their nominal operating points and quadratic approximation of loss functions. On the other hand, the global method uses directly as CVs the gradient of cost function. Some of the local methods includes: the Exact Method (Halvorsen et al., 2003), the Null Space Method (Alstad and Skogestad, 2007). Example of global methods is the NCO approximations (Ye et al., 2012).

The last part presented the main contribution of this thesis which is the data-driven SOC technique for control variable selection. This method drives CVs from process data obtained during operation, in a single regression step. Two theories of data-driven method have been presented: (i) data-driven method without constraint requirement, and (ii) data-driven with equality constraints. In both cases, gradient of objective function are obtained using finite difference and fitted to polynomial function through least-square regression technique. The steady state loss function is finally determined using the CVs to evaluate the losses in cost function.

7 DATA-DRIVEN SELF-OPTIMIZING CONTROL FOR HEAT EXCHANGER NETWORK

7.1 Introduction

In part one of this thesis, i.e. in Chapter Three and Chapter Four, an optimal HEN design was presented. Such design may be optimal in both capital expenditure (CAPEX) and operational expenditure (OPEX) which is usually achieved through trade-off optimization to obtain the total annualized cost at a particular minimum temperature difference. However, during operation, chances are that the operation may be suboptimal. The tendencies that disturbances and uncertainties, such as changes in stream temperatures, flowrates and heat transfer properties due to leakages or fouling in HE may occurred in the HEN during operation, when these happened, the HEN becomes suboptimal and operates outside the optimal design specifications.

The most common engineering practice is to make the network flexible; to be able to accommodate changes in the nominal design parameters. Kotjabasakis and Linnhoff (1986) suggested the idea of increasing the area of the affected HEs in a given network and then equip them with bypasses and controllers in order to achieve controllability. Alternatively, increasing the coolers or heaters duties by supplying more cooling and heating utilities to compensate for any increase or decrease in temperature of the stream target in question was suggested in (Glemmestad et al. 1999). Both strategies are found to increase the capital and operating cost of the HEN and hence economically undesirable solution.

In Mathisen et al., (1992) bypassing of HEN was considered for control purposes without regards to the amount of utility consumed; the fact that bypass opening and closing has direct effect on the overall amount of utility supply in the networks is not given prominence. Later, Mathisen et al., (1994) proposed a method for operation of HENs that minimized utility consumption. A method based on repeated steady state optimization without emphasis on closed loop control implementation was proposed by (Boyaci et al. 1996). Glemmestad et al (1997) proposed online optimization of HEN with emphasis on choice of optimization variable for the control of HEN. Aguilera and Marchetti (1998) proposed DOF for HENs during operation and also on-line optimization and control of same. Jaschke and Skogestad (2012) considered developing control structure which maximized mixed-end temperature of a split and mixed streams. They investigated different SOCs procedure such as the Null space, the Exact local method and a method based on selecting subsets of measurements as CVs. A shared similarity in all these methods is that they depend heavily on process models, the ability to solve the optimization problem offline and linearization of nonlinear process model which results in local solutions. These factors render the SOC method somewhat inapplicable for practical situations, where a model is not available.

A different but complementary approach to SOC strategy is CV selection based on the concept of necessary condition of optimality (NCO) approximation as reported in (Ye et. al, 2013). The NCO technique can be used to overcome the localness associated with linearization required by existing approaches. Instead, CVs are selected to approximate unmeasured NCO over entire operation region with zero setpoint to achieve near optimal operation globally. Furthermore, Ye et al. (2012) proposed a two-step data-driven CV selection approach using regression to approximate the NCO or reduced gradient using measurement function. These two steps approach is entirely data-driven and is able to achieve near optimal control in a much wider operational range. However, a large regression error cumulate in both regression steps is a limitation of the approach.

In this Chapter, the novel data-driven SOC procedure proposed in Section 6.5 and which is reported in Girei et al. (2014a; 2014b) is presented. The first part (Girei et al. 2014a) is the unconstrained data-driven method presented in Section 6.5.21 while the second part (Girei et al., 2014b) is the constrained data-driven SOC presented in Section 6.5.2. Both approaches have been successfully applied to a 3-streams heat exchange network (HEN), which has been used as a benchmark by several researchers, such as Glemmestad et al. (1996) and Lersbamrunsuk et al. (2008) to validate their HEN operation procedures. The case study shows that the proposed methodology is capable of achieving near optimal operation of the HEN with uncertainties in operation parameters.

The last section (Section 7.4) demonstrates the effectiveness of the proposed method on a more complex HEN with several process-to-process and utility-to-process exchangers, and loops. The HEN is for a coal-fired power plant retrofitted with CO_2 capture with all measurement-data directly extracted from ASPEN HYSYS through steady state simulation. CVs are derived from the process data and compared with CV derived analytically using local SOC method. It is observed that data-driven SOC shows better optimal operation under uncertainties when compared to the Local SOC technique.

7.2 Brief account of the Heat Exchanger Network Case Studies

The HEN case studies used in implementing the newly developed Data-driven methodology presented in this thesis has been discussed in detailed, in Section 3.5 and Chapter 4. Case study one (Case 1) is the simple 3-streams HEN structure with two process-to-process heat exchangers and two utility-to-process exchangers. The second case study, Case 2, is the HEN design to reduce the energy penalty in coal-fired power plant retrofitted with CO_2 capture systems.

The simple case study is first used to demonstrate the effectiveness of the Data-driven SOC on a simple HEN operation problem before extending the demonstration to the second case study (Case 2) which is a complex HEN structure with several process-to-process and utility-to-process exchangers, and looping.

7.3 Case 1: Data-driven Self-optimizing control for Heat Exchanger Network.

The simple 3-streams HEN used as a case study to implement our new data-driven SOC procedure for CV selection is a famous motivating HEN example used in several studies such as: Glemmestad et al., (1996), Aguilera and Marchetti (1998), Glemmestad et al., (1999) and Lersbamrunsuk et al. (2008) among others. The network consists of 1-hot stream (H1), 2-cold streams (C1 and C2), 2-process-to-process HEs, 1-Cooler and 1-Heater satisfying a target temperature of 30 ºC on the hot stream H1 and, 160 ºC and 130 ºC on the cold streams C1 and C2 respectively, as shown in Figure 3-10, Section 3.5, Heat exchanger network design.

The same HEN is presented for operation but with bypasses fitted on each process-to-process HEs for manipulation of heat duty during process operation as shown in Figure 7-1. Bypass ϕ_1 is placed on hot stream H1 and ϕ_2 is fitted on cold stream C2 as indicated in the figure.

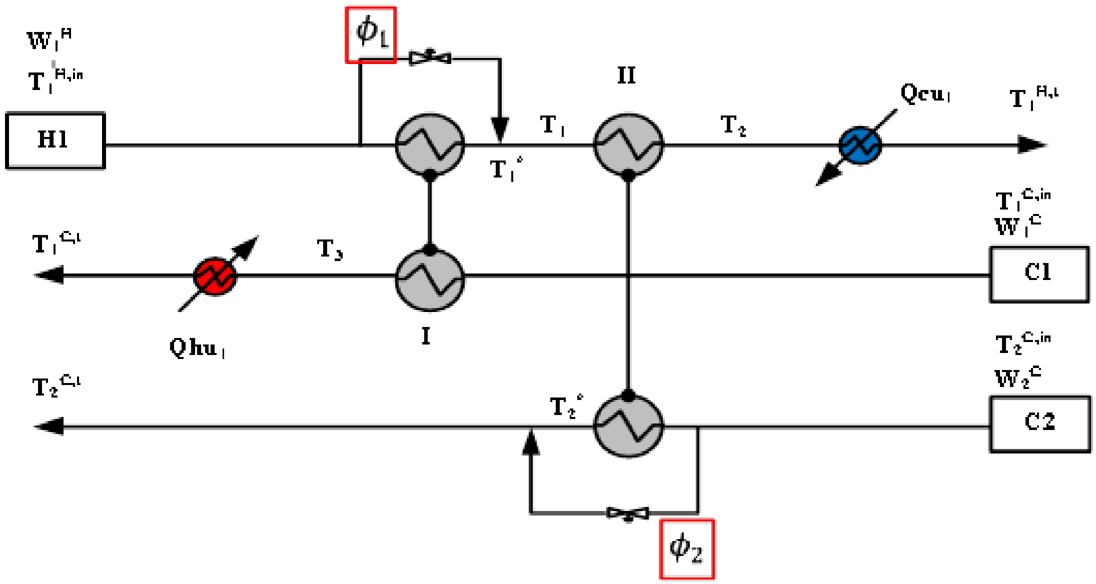

Figure 7-1 Stream Heat exchanger network model

7.3.1 Problem Description

The degree of freedom (DOF) analysis is required to ascertain whether or not the network is capable of achieving optimal operation. From Equation (5-27), the number of utility HE $N_u = 2$, number of target streams to be kept at setpoints $N_{targets} = 3$, and the dimensional space spanned by manipulated variables in the inner HEN to the outer is $R = 2$, therefore number of degree of freedom for utility cost optimization $N_{DOF,U} = 2 + 2 - 3 = 1$. This shows that there is 1 DOF for utility cost optimization.

There are a total of three target streams T_{H1}^{t}, T_{C1}^{t} and T_{C2}^{t}, that are needed to be kept at their constant setpoint values of 30 °C, 160 °C and 130 °C respectively. From the HEN in Figure 7-1, two utility-to-process exchangers Q_{cu}^{1} and Q_{Hu}^{1} are located right at the end of stream H1 and stream C1. These streams are referred to as utility controlled target streams. The third stream, stream C2 is controlled by bypass fraction ϕ_2 on exchanger HX2 and thus referred to as bypass controlled stream. With a total of four manipulative variables, three are identified to control the target temperatures. Therefore the remaining one manipulative variables available for utility cost optimization as defined by the DOF analysis is ϕ_1, the bypass fraction on exchanger HX1. According to Kotjabasakis and Linhoff (1986), the network interconnection temperatures T_1, T_2 and T_3 are the available measurements.

The classification of manipulative variables, available measured variables and disturbances are given as

$$u = [\phi_1] \tag{7-1}$$

$$y = [\phi_1, T_1, T_2, T_3,]^T \tag{7-2}$$

$$d = [T_1^{H,t}, w_2^c]^T \tag{7-3}$$

Although there are four manipulative variables ($\mathrm{Qcu}_1, \mathrm{Qhu}_1$, ϕ_1 and ϕ_2) in the network, $\mathrm{Qcu}_1, \mathrm{Qhu}_1$, ϕ_2 are used for maintaining the target temperatures at their setpoint values, hence only ϕ_1 is available for SOC.

The objective is to minimize utility cost while satisfying the target temperatures.

$$\min_u J = \sum_{i \in CU} C_i Qcu_i + \sum_{j \in HU} C_j Qhu_j \tag{7-4}$$

where i and j, are indexes representing cooling and heating utilities, Q_{CU} represent cold utility and Q_{CU} hot utility, and u the available degree of freedom.

NOTE: Since our method is solely data-driven, process model are used only to generate data for experiment which is used to obtain the self-optimizing CVs. The steady state equality constraint g is not important here because data are generated within feasible operation region for all combination of disturbances.

Table 7-1 Nominal Utility Cost Optimization (Zero disturbances)

$\boldsymbol{Q_{cu}^1}$(kW)	$\boldsymbol{Q_{Hu}^1}$(kW)	$\boldsymbol{\phi_1}$	$\boldsymbol{\phi_2}$	$\boldsymbol{J_{opt}}$
65	80	0	0	145

The nominal HEN design with ENERGY ANALYZER operates at maximum cooling and heating requirements of $\boldsymbol{Q_{cu}^1}$ and $\boldsymbol{Q_{Hu}^1}$ and zero bypasses as shown in Table 7-1.

7.3.2 Simulation and Data Sampling

Assume disturbances with magnitude $190 \pm 5\,°C$ in temperature T_{H1}^{in} of the inlet supply stream H1 and $0.5 \pm 0.05\ kW/°C$ in heat capacity flowrate w_{c2} of stream C2 as shown in Table 7-1. Factorial design was used in MATLAB to divide the disturbances into 10 equal parts to generate a total of $11^2 = 121$ pairs of disturbances. Exchanger I & II design parameters UA_1 and UA_2 are given as 0.523 kW/^{0}C and 1.322 kW/^{0}C, respectively.

Table 7-2 Disturbances and Process Stream Data

Stream Number	TS (^{0}C)	TT (^{0}C)	CP (kW/^{0}C)
H1	$\mathbf{190 \pm 10}$	30	1.0
C1	80	160	1.5
C2	20	130	$\mathbf{0.5 \pm 0.5}$

Suppose that the HEN model equations are not readily available for control structure selection and only process data was collected from the plant. The network interconnection temperatures T_1, T_2, T_3 are the available measurements as suggested in Kotjabasakis and Linnhoff (1986). In Figure 7-1, data samples were collected by manipulating the bypass fraction ϕ_1 over the specified range of disturbances in hot stream H1 inlet temperature $T_1^{H,t}$ and cold stream C2 heat capacity flowrate w_2^c as shown in Table 7-2. It is assumed that utility exchangers Qcu_1, and Qhu_1 have sufficient duties to maintain the stream targets $T_1^{H,t}$ and $\mathrm{T}_1^{\mathrm{C,t}}$ for all ranges of bypass fractions. For each manipulation ϕ_1, the utility duties and the bypass split ϕ_2 satisfy the stream outlet temperatures $T_1^{H,t}$, $T_1^{C,t}$ and $T_2^{C,t}$ at their respective target values. Data samples are generated for measurements T_1, T_2 and T_3 by operating the HEN as indicated above. The primary manipulated variable ϕ_1 is used as the reference point for 100 samples with each sampling point considered as a neighborhood point, Equation (6-21). Regression was carried out by using finite difference method in Equation (6-24) to obtain two measurement combination CVs through a linear and a second-order polynomial regressions in Equation (6-25) and (6-26) respectively. A Monte Carlo experiment of 100 sets of randomly generated disturbances was conducted to evaluate the CVs with no consideration for implementation errors.

Results

The CVs using linear (CV_1) and second-order (CV_2) polynomial regressions are respectively given in Equation (7-5) and Equation (7-6) as follows

$$CV_1 = -30.58 - 29.331\phi_1 - 0.5736T_1 - 0.0881T_2 - 1.0890T_3 \qquad \textbf{(7-5)}$$

$$\begin{aligned} CV_2 \; - 20.1311 - 40.3810\phi_1 - 0.6067T_1 + 0.0460T_2 + 1.0565T_3 \qquad \textbf{(7-6)} \\ + +0.0778\phi_1 T_1 + 0.0182\phi_1 T_2 + 0.2108\phi_1 T_3 \\ + 0.0015T_1T_2 - 0.0172T_1T_3 - 0.0016T_2T_3 - 11.5729{\phi_1}^2 \\ + 0.0075{T_1}^2 - 4.240\ x\ 10^{-11}{T_2}^2 + 0.0091{T_3}^2 \end{aligned}$$

The R^2 indices for the two CVs are 0.9746 and 0.9999 which denotes the acceptability of both the first and second-order regressions with the later indicating that no higher than second-order polynomial regression is required.

Table 7-3 Average economic loss with measurement as CV

CV	Average loss	Maximum loss	Standard deviation
CV_1	6.2174	11.1077	3.8000
CV_2	2.5261	8.6073	3.0916

Table 7-3 shows different losses obtained from Monte Carlo experiment. The results indicate that measurement data can be used as self-optimizing CV of HEN with minimum losses. The average loss for the second-order CV gives better loss with less deviation when compared to the first-order polynomials which has an average loss of 3.6913 high and a maximum loss and standard deviation of 11.1077 and 3.8000 respectively

7.3.3 Conclusion

This method presented in this Section is the newly developed data-driven self-optimizing control procedure for CV selection with no requirement for process model. The procedure is applicable to any unconstrained systems. The method uses finite difference method to evaluate the CV from measurement data in a single regression step. It was tested on a HEN for first- and second-order CVs obtained through regression with the first-order CV giving the best economic loss. The advantage of this new approach over all existing SOC methods is that the CV can be achieved without evaluating the derivative function. With this new approach, selecting CVs for complex industrial processes can be achieved directly through simulations using commercially available simulators such as HYSYS and UniSim.

7.4 Case 2: Data-driven Self-optimizing control with equality constraints for Heat Exchanger Network

An improvement to our work in Girei et al., (2014a) which was presented in the preceding section is presented in this Section and was reported in (Girei et al., 2014b). Although both method are a single regression step, approximate NCO directly by CVs from measurement data, and does not require evaluation of derivatives so that process models associated with commercial simulators can be used directly for CV selection, a disadvantage to Girei et al., (2014b) is that the method does not deal with constraints directly. Instead, constraints are implicitly satisfied with data generated for regression. This makes data collection time consuming and sometimes difficult. For a system with a large number of constraints and wide disturbance range, to converging to every points in the entire operation range is numerically or operationally challenging and for a dynamic system, this method requires all data points to wait until a steady-state is reached.

The approach proposed in this section evaluates CVs as a function of measurement in SOC problem with equality constraints. The new method also relies on measurements to derive CVs that gives optimal control with minimum economic loss in the presence of disturbances. The new approach is again demonstrated on the same 3-stream heat exchanger network (HEN) problem and compared with the approach presented in 7.3 to show the effectiveness of the constrained data-driven method.

7.4.1 Problem Description

The DOF analysis, simulation and data collection methods discussed in Section 7.3.1 and 7.3.2 respectively are the same for both constrained and unconstrained data-driven SOC techniques. However, the problem formulation for the constrained data-driven SOC is different from the unconstrained method. In the previous discussion, only the objective function is important for the optimization problem. The reason mentioned earlier was that the constraints have to be satisfied during data collection. However, this may be time consuming and sometimes difficult for large scale problem to come to their steady state before data collation.

The optimization problem is formulated as an NLP problem shown in (16) by imposition of necessary operational and safety constraints:

$$\min_{u} J = \sum_{i \in CU} C_i Qcu_i + \sum_{j \in HU} C_j Qhu_j \tag{7-7}$$

$$subject\ to\ g(u,d) = 0 \tag{7-8}$$

where u represents the available degree of freedom, i and j are indexes representing cooler on hot stream i and heater on cold stream j respectively, and g is the steady state HEN model equation. The Equality constraint equations $g(u,d)$ arising from the physical model describe in Equation (5-6) – (5-14) are for general HEN problem formulation. For this particular network with 3 streams, 2-exhangers, 1-heater and 1-cooler, thus the constraints equation $g(u,d)$ are

$$g_a = \left\{ \begin{array}{c} qcu_1 - w_1^h\left(T_2 - T_1^{h,out}\right) \\ qhu_1 - w_1^c\left(T_1^{c,out} - T_3\right) \\ T_1^{h,out} - T_1^{h,t} \\ T_1^{c,out} - T_1^{c,t} \\ T_2^{c,out} - T_2^{c,t} \\ Q_1 - w_1^c\left(T_3 - T_1^{c,in}\right) \\ Q_1 - w_1^h(1-\phi_1)\left(T_1^{h,in} - T_1^{*,out}\right) \\ Q_1 - UA_1\left(\Delta T_{m_1}\right) \\ T_1 - (1-\phi_1)T_1^{*,out} - \phi_1 T_1^{h,in} \\ Q_2 - w_1^c(T_1 - T_2) \\ Q_2 - w_2^c(1-\phi_2)\left(-T_2^{*,out} - T_2^{c,in}\right) \\ Q_2 - UA_2\left(\Delta T_{m_2}\right) \\ T_2^{c,out} - (1-\phi_2)T_2^{*,out} - \phi_2 T_2^{c,in} \end{array} \right\} \tag{7-9}$$

where T_1, T_2, T_3 are network interconnection temperatures, UA_1 and UA_2 are exchanger I & II design parameters, ΔT_{m_1}, and ΔT_{m_2} are the log mean temperature difference.

Note that, because our approach is data-driven, the equality constraint equations above are only necessary to generate data for experiment which could have been done with ASPEN ENERGY ANALYZER or any other software for HEN design. These constraints depend on the states in addition to n_u of manipulative variables and n_d of disturbances.

The classification of manipulative variables u, available measured variables y and disturbances d is given as

$$u = [\phi_1, X] \tag{7-10}$$

$$y = [\phi_1, T_1, T_2, T_3,]^T \tag{7-11}$$

$$d = [T_1^{H,t}, w_2^c]^T \tag{7-12}$$

where Φ_1 is the only manipulative variable available for SOC as shown in (Girei et al., 2014a). X is a vector of states variables which in the case of this network includes $T_1^{h,out}$, $T_1^{c,out}$, $T_2^{c,out}$, $T_1^{*,out}$, T_1, $T_2^{*,out}$, T_2, T_3, Q_1, Q_2, qcu_1, qhu_1, ϕ_2. The network interconnection temperatures T_1, T_2, T_3 and ϕ_1 are the available measurements as suggested in Kotjabasakis and Linnhoff (1986) and (Glemmestad et al. 1999).

There are two disturbances with magnitude ± 10 ^{0}C in the supply stream H1 and ± 0.05 kW/^{0}C in the heat capacity flowrate (CP) of stream C2 as show in Table 1. Using factorial design method, the disturbances are divided into 10 equal parts and 11^2 = 121 pairs of disturbances were generated. Exchanger I & II design parameters UA_1 and UA_2 are given as 0.523 kW/^{0}C and 1.322 kW/^{0}C, respectively.

Results

The CVs obtained using linear first (CV_{LR}) and second-order (CV_{PR}) least-square regression for the data-driven SOC with equality constrained method are given in Equation (7-13) and Equation (7-14) respectively as follows:

$$CV_{LR} = 5.6 \times 10^{-2}\phi_1 + 1.90 \times 10^{-3}T_2 - 2.98 \times 10^{-3}T_3 \qquad \textbf{(7-13)}$$

$$CV_{PR} = 4.59 \times 10^{-2}\phi_1 T_1 + 2.98 \times 10^{-3}T_1 T_3 + 1.78 \times 10^{-3}\phi_1^2 - 2.3 \times 10^{-5}T_1^2 - 2.79 \times 10^{-3}T_3^2 \qquad \textbf{(7-14)}$$

The fitted values of R^2 for the two CVs are 0.9973 and 1.0 indicating that the regression line in the CV evaluation satisfactorily approximates the real data points for both the first and second order CVs where the R^2 regression indices for the second order CV confirming no further requirement for the CVs to be evaluated beyond second-order least-square regression

The CVs evaluated based on SOC with equality constraints approach in Equation (7-13) and Equation (7-14) are compared with those shown in Equation (7-15) and Equation (7-16) calculated using our earlier data-driven method discussed in Girei et al., (2014b) without explicit considerations of constraints, and those shown in Equation (7-17) and Equation (7-18) using the NCO approximation approach of (Ye et al., 2013).

1. First and second order CVs based on Data-driven SOC without explicit constraints (Girei et al., 2014a)

$$CV_{LR} = 329.614 + 0.3992\phi_1 + 1.9624T_1 + 2.6831 \times 10^{-14}T_2 - 6.2250T_3 \qquad \textbf{(7-15)}$$

$$CV_{PR} = 33.2570\phi_1 - 2.4359T_1 - 1.1578 \times 10^{-11}T_2 - 0.0318T_3 + 4.7768\phi_1T_1 + 8.2580 \times 10^{-13}\phi_1T_2 - 8.9310\phi_1T_3 + 6.8302 \times 10^{-14}T_1T_2 + 0.0095T_1T_3 + 5.6829 \times 10^{-14}T_2T_3 + 0.0021{\phi_1}^2 - 0.0014{T_1}^2 - 2.6222 \times 10^{-14}{T_2}^2 + 0.0238{T_3}^2 \quad \textbf{(7-16)}$$

2. First and second order CVs based on NCO approximation method (Ye et al., 2013).

$$CV_{LR} = 1.29 \times 10^{-4}\phi_1 + 4.28 \times 10^{-3}T_1 + 8.27 \times 10^{-4}T_2 - 7.40 \times 10^{-3}T_3 \quad \textbf{(7-17)}$$

$$CV_{PR} = 4.49 \times 10^{-9}\phi_1T_3 + 11.36 \times 10^{-4}T_1T_2 - 1.95 \times 10^{-8}T_1T_3 - 1.915\phi_1^2 + 6.72 \times 10^{-9}T_1^2 - 1.50 \times 10^{-4}T_2^2 \quad \textbf{(7-18)}$$

The R^2 indexes for first and second order CVs in Equation (7-15) and Equation (7-16) based on data-driven SOC presented in Section 7.3 are 0.9999 and 1.0 respectively, while the NCO approximation method in Ye et al, (2013) results in R^2 indexes of 0.9993 and 1.0 for the first and second order CVs respectively. In all cases, the second order least-square regressions fit the actual data points very well.

The CVs equations for both the first and second order are dissimilar for all the three different SOC methods. Note that the CVs in Equation (7-15) and Equation (7-16) differ from those presented in Section 7.3 for the same example. The CVs obtained in Section 7.3 was evaluated from data obtained using number of transfer unit method (NTU-method) while in the paper, we use ordinary energy balance Equation (5-6) – (5-24). The first order CV_{LR} in the data-driven SOC with equality constraints Equation (7-13) and the NCO approximation method Equation (7-17) have only three measurement combinations in the CV equation while the data-driven SOC without constraint requires all the measurement combinations. In Equation (7-14) and Equation (7-18), not all the unknown coefficients θ appeared in the second order polynomial CV_{PR} equations whereas the unconstraint data-driven SOC Equation (7-18) is evaluated with all the measurements coefficients θ. Kariwala (2007) showed that it is not always necessary to consider all measurement combination in CV selection as a similar or superior economic performance could be achieve using fewer measurements.

The economic performance of the CVs are evaluated over the entire range of d using equation

$$L = J(u_{fb}, d) - J_{opt}(d) \tag{7-19}$$

where $J(u_{fb}, d)$ is the objective function J correspond to implementation of feedback control to maintain the CVs at zero and $J_{opt}(d)$ is the true optimal J.

Table 7-4 shows the utility requirement for the three SOC approaches resulting from implementing feedback control $J(u_{fb}, d)$ compared with optimum objective function $J_{opt}(d)$. The J_{opt} for the specified range of uniformly distributed disturbances in hot stream H1 inlet temperature, and cold stream C2 heat capacity flowrate is 145.0040 kW.

Table 7-4 Values of J_{reg} for different CVs

Cost function	Constrained Data-driven	Data-driven	NCO approximation
$J_{reg}(CV_{LR})$	152.295	157.998	159.462
$J_{reg}(CV_{PR})$	148.605	152.883	152.386

Similar value of J_{opt} was reported in Glemmestad et al., (1997) and Glemmestad et al., (1999) using model Equation (5-4) which considers HEN problem as an LP problem by not incorporating exchanger bypasses. It is apparent from Table 7-4 that $J_{reg}(CV_{PR})$ from second order data-driven SOC with equality constraints Equation (7-14) gives the best result with minimum utility usage followed by first order CV Equation (7-13) from the same. This is obvious because each state variable is defined within its minimum and maximum interior points for the range of disturbance as shown on the finite difference mesh Figure 6-3. Moreover, the SOC with equality constraints method is capable of eliminating the effect of disturbances in each variable within the constraints equations as opposed to the unconstrained data-driven method. There is no significant difference between utility consumption for second-order NCO approximation 152.3857 kW and that of data-driven SOC without constraints 152.8828 kW. However, the first order CV in the NCO approximation is higher than the unconstraint data-driven SOC by a value of 1.4637 kW in which the latter has a total utility requirement of 157.9982 kW.

Monte Carlo experiment is conducted for 100 set of uniformly distributed disturbances to evaluate the steady state losses for all the SOCs method tabulated in Table 7-5. The result indicates that the data-driven SOC method with equality constraints has good performance in both first and second order compared to the NCO approximation and the unconstrained data-driven method. The average losses are 2.2951 and 5.9488 for second- and first-order data-driven SOC with equality constraints, equivalent to 1.58 % and 4.10 %. The NCO approximation and the unconstrained data-driven SOC method on the other hand has 12.9244 and 11.8641 average losses in first order CVs and 6.2188 and 6.6456 average losses in second order CVs respectively. In all cases, the standard deviations are similar for CVs obtained using NCO approximation method and the CVs from data-driven SOC with equality constraints. A large deviation obtained in data-driven SOC without constraint is obvious due to the likelihood of having unbound solution hence large disturbance propagation.

Table 7-5: Comparison of economic losses for different CVs

CV	Average Loss	Maximum Loss	Standard Deviation
$\boldsymbol{CV_{LR_{NCO}}}$	12.9244	15.8865	3.1923
$\boldsymbol{CV_{PR_{NCO}}}$	6.2188	8.7596	3.7364
$\boldsymbol{CV_{LR_{DD}}}$	11.8641	13.9790	4.1643
$\boldsymbol{CV_{PR_{DD}}}$	6.6456	8.8617	2.5557
$\boldsymbol{CV_{LR_{CDD}}}$	5.9488	7.7587	3.6687
$\boldsymbol{CV_{PR_{CDD}}}$	2.2951	4.7681	2.2206

7.4.2 Conclusion

A data-driven SOC method with equality constraints have been presented and applied to a HEN problem. The method is a sequel to the work in Section 7.3 on data-driven SOC method with no considerations for constraints equations in the CVs selection. As in the previous method, this approach also uses finite difference to evaluate CVs from measurement data in a single regression step. The method was compared with the unconstrained data-driven approach and the NCO approximation method for first and second-order CVs obtained through least-square regressions. Both the first and second-order CVs for data-driven SOC with equality constraints gives minimum economic losses in comparison to CVs obtained through NCO approximation and data-driven SOC method without constraints. The advantage of the equality constraint method is that large disturbance range can be controlled from measurements without evaluating the derivative function as opposed to existing SOC method which are model based.

7.5 Case 3: Data-driven self-optimizing control for Heat Exchanger Network for coal-fired power plant with CO_2 capture

7.5.1 Introduction

Integration through heat exchanger network (HEN) design plays a major role in reducing energy burden on power plants with post combustion capture (PCC) systems as well as in mitigating the global CO_2 emissions Girei et al., (2013) to the atmosphere by approximately 80-90% compared to plants without the PCC systems (IPCC, 2005). In spite of these advantages, HEN design impedes the ability of power plants to respond to load changes, reboiler heat duty (Biliyok et al., 2012), flue gas flowrates and temperatures due to changes in coal feedstock (Harun et al., 2012) or some other perturbations from the furnaces. In general, HEN design in power plant with PCC can lead to increased interactions between hitherto separate plant units resulting into changes in characteristics and behaviours of the overall plant operations whenever the nominal operating conditions are altered due to disturbances or changes in the manipulative inputs. These disturbances may propagates into the downstream paths (Kotjabasakis and Linnhoff, 1986) of the HEN and to the whole-length of the network causing changes in stream target temperatures and setpoints thereby resulting into suboptimal plant operation.

A variety of studies have been completed that covers design of HEN on power plant with PCC systems. Some of these studies investigated the basic HEN design, the energy penalty on power plant with CO_2 capture and capital cost, integration of power plant with PCC through linking of (a) the flue gas stream to the feed of PCC systems and (b) the bleed stream extracted from the crossover between intermediate pressure turbine (IPT) and low pressure turbine (LPT) turbine to the reboiler on the stripper of the PCC systems in order to use the heat from the steam turbine to release CO_2 and regenerate the solvent (Khalilpour and Abbas 2011; Girei et al, 2013). The studies also include the large quantity of steam needed for the stripper or desorber of the PCC and how these overstretched the steam turbine design and operation and thus other units in the plant. In short, the operations and control of the HEN for coal-fired power plant with PCC system is limited in comparison to numerous literatures that investigated HEN design for same systems.

The key to operation and control of process systems including HEN for Power plant with capture systems is the design of control structure through selection of control variables. Mathisen et al. (1992), Mathisen et al. (1994), Boyaci et al. (1996), Aguilera and Marchetti (1998), Glemmestad et al. (1996), Glemmestad et al. (1999), Lersbamrungsuk et al. (2008), and most recently, Jaschke and Skogestad (2012) have all presented different ideas for achieving optimal HEN operation and control. Their methods proposed different control variables (CVs) selection procedure for achieving economically optimal operation in the presence of uncertainties and disturbances. CVs usually are selected for performance monitoring online or for real time optimization (RTO) using model based approaches to reduce the frequency at which setpoints updates itself whenever disturbances occurred, therefore making traditional RTO relatively expensive and difficult to implement (Jaschke and Skogestad, 2012a).

7.5.2 Process Description

The process flowsheet of the 300 MWe coal-fired power plant with PCC and the base case HEN grid diagram are presented in Figure (4-1) and Table (4-1) in Chapter Four. The HEN is a 9-streams network comprising of 7-hot streams and 2-cold streams with each stream having a specified supply and target temperatures, heat duty and heat capacity flowrates extracted from the plant. The hot streams are: HP turbine bleed, LP turbine bleed, Flue gas and Compressor intercool streams. The cold streams are: LPLT feedwater and HPHT feedwater as shown in Table (4-1), Chapter Four.

The nominal HEN designed using ENERGY ANALYZER is incapable of handling operational mode changes due to disturbances or uncertainties.

Table 7-6: HEN network temperature profile

Exchanger Name	Heat Capacity Flowrates ($MW/^0C$)		UA ($W/^0C$)	Duty (MW)	Hot stream Flow (^0C)		Cold stream Flow (^0C)	
	Cold	Hot			$T_i^{h,in}$	$T_i^{h,out}$	$T_i^{c,in}$	$T_i^{c,out}$
E-101	0.98272	0.11638	0.2546	28.630	362.6	116.6	112.6	141.7
E-102	0.50851	0.11638	0.0100	0.7681	116.6	110.0	35.0	36.5
E-201	0.17478	0.03948	0.0985	5.069	245.0	116.6	112.6	141.7
E-202	0.31782	0.03948	0.0772	2.945	116.6	42.0	36.5	45.6
E-301	0.11638	0.30566	0.5927	19.320	155.2	92.0	72.0	110
E-601	0.09306	0.06189	0.1008	2.432	102.0	62.7	45.6	72.0
E-701	0.41545	0.29901	0.7937	11.030	91.4	54.5	45.6	72.0
E-702	0.19069	0.29901	0.1728	1.681	54.5	49.0	36.5	45.6

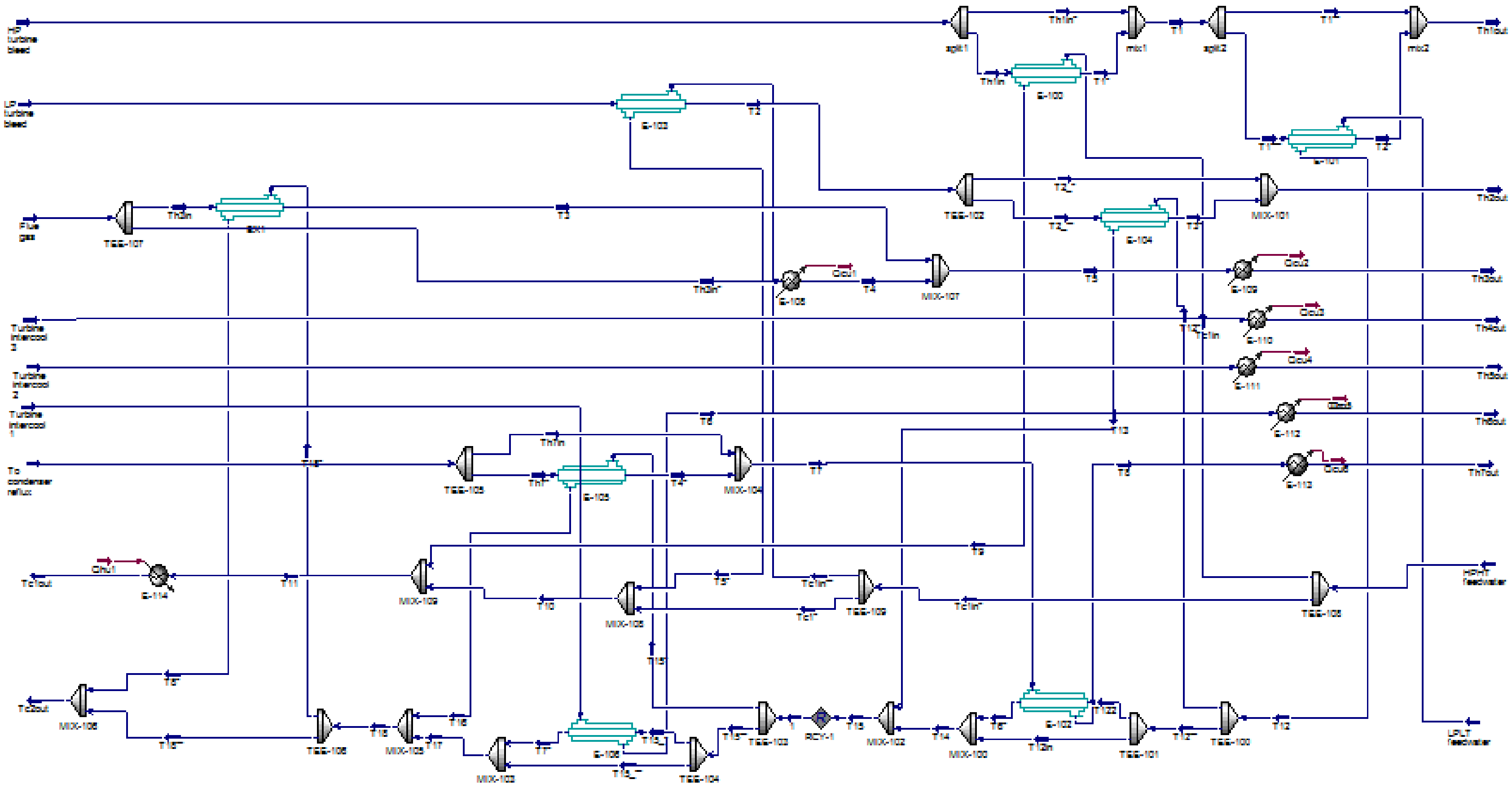

Figure 7-2: HEN process flowsheet with bypasses modelled in HYSYS

The Design data extracted from ENERGY ANALYZER is shown in Table 7-6. The network is reproduced with Aspen HYSYS 8.3 to make it flexible and by addition of bypasses on each of the process-to-process HE for manipulation of duty and accommodating changes in flowrates, temperatures as shown in Figure 7-2. Peng-Robinson equation of state is used as the thermodynamic fluid package to model the material stream containing H_2O only as the working fluid in both the hot and the cold supply streams. The process-to-process HEs in this case unlike the original HE design with the ENERGY ANALYZER presented are fitted with splitter that bypasses the HEs to allow flow into the HE (main stream) or into the bypass stream depending of the bypass fractions ϕ_i's during manipulation. At the onset of the simulation, the bypass streams are fully closed i.e $\phi_i = 0$, (where subscript 'i' denote number of exchangers) making the HEN parameters in both simulators to be the same.

7.5.3 Disturbances in Power Plant with CO_2 Capture Systems

In power plant integrated with PCC, apart from changes in load and energy demand, disturbances may also results from changes in input parameters like flue gas or lean solvent flowrate or any disturbance such as fluctuating CO_2 concentration in the flue gas (Biliyok et al., 2012). In MEA PCC for example, adjusting reboiler heat duty to control the amount of CO_2 removals from the plant may also affect the performance of capture unit. This affects heat supply from the power plant or from any external auxiliary units operating in parallel with the reboiler. Harun et al., (2012) suggested keeping the lean under closed loop control, because disturbance propagating to the boiler could lead to creation of injurious deviations in the nominal design specifications.

Three disturbances with potential of propagating into the downstream path of the HEN to destabilize the optimal operation of HEN leading to increase in utility consumption and changes in stream target setpoints are: (i) flue gas temperature, (ii) flue gas heat capacity flowrates, and (iii) LPLT feedwater flowrates. The simple explanation behind the choice of these disturbances is that, because the flue gas stream is connected to the absorber, any small changes in flue gas temperature and heat capacity flowrate due to change in coal feedstock or furnace condition may propagate into the network and affect the target streams. Moreover, LPLT feedwater stream is reported as one of the main bottlenecks and causes of production losses. These three disturbances are adapted for a feasible range of operating conditions given in Equation (7-20) – (7-22)

$$T_{h,3}^{in} = 155.2 \pm 10℃ \quad \textbf{(7-20)}$$

$$wh_3 = 0.400600 \pm 0.1 \text{ MW/℃} \quad \textbf{(7-21)}$$

$$wc_2 = 0.5085400600 \pm 0.1 \text{ MW/℃} \quad \textbf{(7-22)}$$

where $T_{h,3}^{in}$, represent the flue gas inlet temperature, wh_3 and wc_2 are the flue gas and LPLT feedwater heat capacity flowrates respectively. Factorial design was applied to divide the disturbances magnitude into 4 equal parts to generate a total of $5^3 = 125$ pair disturbances for use in ASPEN HYSYS to operate the HEN and extract operational data for the CV evaluation.

7.5.4 Heat Exchanger Network Operation and Data Collection

The steady state operation is limited to the HEN operation only for the full range of disturbances –this means that each pairs of disturbances is fed into the network's inlet streams and the simulator is activated. There are a total of eight process-to-process exchanger units that are to be bypassed to enable manipulation of the heat duty of each unit. It is however important to note that while all bypasses on process-to-process exchangers are regarded as manipulations, not all bypasses are used for achieving optimal operations depending on whether or not the bypass is located mid- or end- streams.

Disturbances in flue gas stream $T_{h,3}^{in}$ and wh_3 propagate downstream HE E-301 to upset the LPLT feedwater target temperature $T_{c,2}^{t}$ shown in Figure 7-3. At this point, the bypass stream ϕ_8 is either opened or closed to keep the stream target temperature $T_{c,2}^{t}$ at its setpoints value of 110 ℃ depending on the nature of the disturbance. Similarly, as disturbance wc_2 propagates into the HEN, the bypass fractions of HEs on its path are manipulated to maintain all the setpoints and streams target temperatures at their required setpoints.

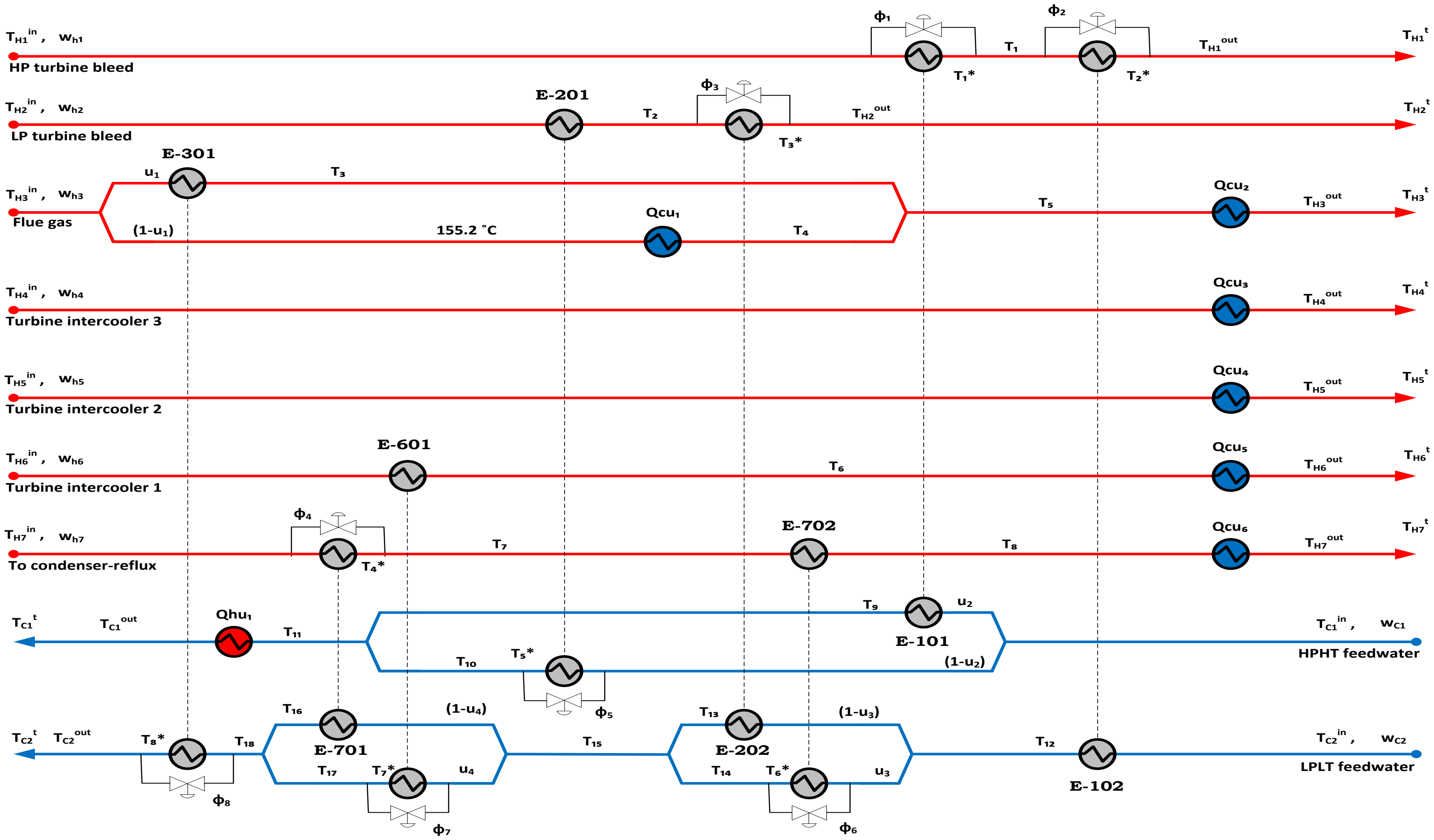

Figure 7-3: HEN process flowsheet with bypasses

The utility-to-process exchangers $Qcu_1, \ldots, Qcu_6$ and Qhu_1 are used in keeping streams target temperatures $T^t_{h,3,}, \ldots, T^t_{h,7}$ and $T^t_{c,1}$ at their setpoints values of 49, 35, 35, 35, 30 and 252 ℃ respectively. And where there is no utility-to-process HEs as the last unit of the stream, the bypasses ϕ's are employed to achieved the same objective control objective; bypasses on E-102, E-202 and E-301 are opened or closed to keep the exit temperature of the remaining three streams $T^t_{h,1,}$, $T^t_{h,2,}$ and $T^t_{c,3}$ at their target temperatures. Bypasses on process-to-process HEs E-101, E-201, E-601, E-701 and E-702 are free bypasses which are used as free DOF to reject disturbance load by adjusting them to provide the desired HE stream exit temperature.

After manipulating the bypasses and ensuring that each setpoints and target temperature are adjusted to their desired setpoint values, the process data are collected and recorded and new set of disturbance is introduced.

The entire procedure is repeated for all combinations of disturbances and for each run the measurements are collected and recorded. It is interesting to note that not all the combinations of disturbance results into feasible operations. When this happens, the bypass ϕ_2, ϕ_3 and ϕ_8 failed to satisfy the requirements for stream target temperatures $T^t_{h,1}$, $T^t_{h,2}$ and $T^t_{c,2}$ respectviely. Such combination are outside the feasible operating points as described by Lersbamrunsug (2008) and by operational flexibility index of Swaney and Grossmann (1985) which describe theoretical framework for process formulation within operable region. The measurements pair is discarded due to infeasibility and the next pair is selected for operation. This allows all the measurement to be collected while satisfying the constraint requirement for the network.

7.5.5 Self-optimizing Control and Control Variable Selection

The control objective for the HEN is to minimize the cost of utilities while maintaining the network target temperatures within values specified by the setpoints.

For this HEN, the objective is mathematically represented as follow

$$\min_u J = \sum_{i \in CU} C_i Qcu_i + \sum_{j \in HU} C_j Qhu_j \quad \textbf{(7-23)}$$

where C_i and C_j represents utilities cost associated with each coolers Qcu_i and heaters Qhu_j respectively. Indexes i and j, denotes cooling and heating utilities and u is the available degree of freedom. Since the process measurements data for all feasible operations are extracted from ASPEN HYSYS the equality constraints describing the steady state models equations are unknown and the data satisfied the model requirement for all possible combinations.

The manipulative variables u, available measured variables y and the disturbancces d are classified as follows

$$u = [\phi_1, \phi_4, \phi_5, \phi_6, \phi_7] \quad \textbf{(7-24)}$$

$$y = [T_1,\ T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9, T_{10}, T_{11}, T_{12}, T_{13}, T_{14}, T_{15}, T_{16}, T_{17}, T_{18}]^T \quad \textbf{(7-25)}$$

$$d = \left[T_{h,3}^{in}, wh_3, w_{C2}\right]^T \quad \textbf{(7-26)}$$

From Equation (7-24), 5 DOF are available for manipulating the HEN, however from the process data generated in ASPEN HYSYS, bypasses ϕ_1 and ϕ_5 on HE E-101 and E-201 are saturated at zero. This means that the bypass has no effect on process running. Although Boyaci et al., (1996) and Mathisen et al., (1992) have shown bypass placements are necessary to satisfy the DOF required to achieve control objective, bypass placement on E-101 and E-201 are not necessary due to simple fact that the streams where the bypasses are located are not affected by disturbances. Moreover, either of the disturbances does not propagate the downstream paths leading to the inlets of exchanger E-101 and E-201 in the network (Kotjabasakis and Linnhoff, 1986) Thus 3 DOF are available for selecting CVs from the process data via self-optimizing control methodology

7.5.6 Data-Driven Self-optimizing Control Variables

The data extracted from HYSYS simulation comprises of 18 measurements and 3 DOF as the primary manipulative variables for control. The primary manipulated variables ϕ_4, $\phi_6$and ϕ_7 are used as the reference point for 72 samples with each sampling point considered as a neighborhood point as indicated in Equation (6-21).

Regression is carried out by using finite difference method in Equation (6-24) to obtain measurement combination as CVs via first-order polynomial regressions Equation (6-25). A Monte Carlo experiment is conducted for 100 sets of uniformly distributed disturbances to evaluate the steady state losses with no consideration for the implementation errors.

1. Data-driven SOC method

$$CV_{\phi_4} = -4.7048T_8 + 0.3922T_{11} - 0.3077\phi_4 \tag{7-27}$$

$$CV_{\phi_6} = 0.1188T_4 + 0.0206T_7 + 0.07590T_8 - 0.1147T_{11} - 0.0356T_{15} - 0.5531\phi_6 \tag{7-28}$$

$$CV_{\phi_7} = 2.2117T_4 + 1.3855T_7 + 1.14164T_8 - 2.1678T_{11} - 0.6641T_{15} - 0.7697\phi_7 \tag{7-29}$$

A total of three CVs are derived from the HYSYS data as shown in Equation (7-27) - (7-29). Each CVs represents one free manipulative variables ϕ_4, ϕ_6 and ϕ_7 excluding ϕ_1 and ϕ_5 which saturates at zero. The regression index $R^2 = 0.9076$, indicates that the least-square regression line in the CV evaluation satisfactorily approximates the real data points. It is interesting to note that whileϕ_4, $\phi_6$and ϕ_7 are all associated with measurements T_8 and T_{11}, bypasses ϕ_6 and ϕ_7 have additional measurements T_4 , T_7 and T_{15} reflecting in their CV Equation (7-28) and (7-28) respectively. Kariwala (2007) have made known that it is not always necessary to consider all measurement combination in CV selection as a similar or superior economic performance could be achieved using fewer measurements.

7.5.7 Local Self-optimizing Control Variables

As described in the preceding sections, there are a total of 5 DOF which corresponds to the five bypasses ϕ_1, ϕ_4, ϕ_5, ϕ_6 and ϕ_7 required for control. Five

CVs equations describing the steady state mode operation of the HEN are needed for classical control.

From Equation (5-6)-(5-8) each HE equipped with bypass stream is described by model equations and has 1 DOF for control. The requirement for CVs Cao (2003; 2005) is that CVs are selected analytically and used directly as gradient of cost function. This guaranteed optimum operation if the gradient of cost function is maintained at zero $dJ/du = 0$. Where J the objective is function and u is the manipulations. In this case

$$J = [Q_{cu1} + Q_{cu2} + Q_{cu3} + Q_{cu4} + Q_{cu5} + Q_{cu6} + Q_{hu1}] \quad \textbf{(7-30)}$$

$$u = [\phi_1 \, \phi_4 \, \phi_5 \, \phi_6 \, \phi_7] \quad \textbf{(7-31)}$$

During HE operation, the desire is to control HE exit temperatures $T_i^{*,out}$ such that any excess heating or cooling is bypassed. In this way, the HE duty is maintained within the design requirement. The cost function J in this network cannot be explicitly expressed in terms of u, therefore substituting the setpoint values of HE exit temperatures $T_i^{*,out}$, Table 7 - 7, in Equation (5 -6) - (5 - 6) and solving for the bypasses ϕ's satisfied the requirement of $dJ/du = 0$ at steady state.

Table 7-7: Steady state HE exit stream temperatures

Setpoints	$\boldsymbol{T_1^{*,out}}$ °C	$\boldsymbol{T_4^{*,out}}$ °C	$\boldsymbol{T_5^{*,out}}$ °C	$\boldsymbol{T_6^{*,out}}$ °C	$\boldsymbol{T_7^{*,out}}$ °C
	114.9	56.27	41.86	114.9	59.72

Therefore, the expression for the CV's at steady state such that each $CV = f(\phi' s\,, T' s)$, independent of disturbances (Skogestad, 2000) is thus given in Equation (7-32) –(7-33)

1. Local SOC method

$$CV_{\phi_1} = -T_1 + 114.9(1 - \phi_1) + 362.6\phi_1 \quad \textbf{(7-32)}$$

$$CV_{\phi_4} = -T_7 + 56.27(1 - \phi_4) + 91.4\phi_4 \quad \textbf{(7-33)}$$

$$CV_{\phi_5} = -T_{10} + 41.8597(1 - \phi_5) + 112.6\phi_5 \quad \textbf{(7-34)}$$

$$CV_{\phi_6} = -T_{14} + 46.9285(1 - \phi_6) + T_{12}\phi_6 \quad \textbf{(7-35)}$$

$$CV_{\phi_7} = -T_{17} + 59.7192(1 - \phi_7) + T_{15}\phi_7 \quad \textbf{(7-36)}$$

Equation (7-32)-(7-36) represent the local self-optimizing CVs derived from the HEN process model equations. Recall that the HP turbine bleed and HPHT feedwater streams has no disturbances –a simple explanation as to why the bypasses ϕ_1 and ϕ_5 extracted from the HYSYS data are saturated at zero. Substituting the steady states nominal temperatures T_1 and T_{10} into Equation (7-32) and (7-34) of the local SOC gives the values of bypasses ϕ_1 and ϕ_5 to be 9.9343×10^{-5} and 2.0474×10^{-5} almost equals to zero as recorded in HYSYS measurements for the data-driven SOC.

The economic performance of the CVs are evaluated over the entire range of d using Equation (6-4) in Monte Carlo simulation for 100 set of uniformly distributed disturbances $T_{H,3}^{in}$, wh_3, wc_2 and the steady state loss is evaluated and presented in Table (7 - 8).

Table 7-8: Average losses with measurement combination as CV

CV	Min loss	Ave loss	Max loss	STD
$\boldsymbol{CV_{L-SOC}}$	4.2462	5.7016	8.0917	1.1282
$\boldsymbol{CV_{DD-SOC}}$	2.3818	3.4296	5.6714	0.9562

The results in Table 7-8 indicate that the data-driven SOC method has better performance compared to the Local SOC method. The minimum loss, the average loss and the maximum loss are all superior using data-driven SOC. The average loss is 2.9878 for the data-driven SOC equivalent to 2.02 % and 5.5308 corresponding to 3.35 % loss for the local SOC method. The standard deviation for local SOC is small compared to deviation in data-driven SOC method.

The average annualized cost of utilities is presented in Table 4-2, Section 4.4 which includes; Fuel gas, IP and LP steams and cooling water. The total annualized cost of each SOC methods can be evaluated from Table 7-9 by substituting utility cost in Table 4-2 into cost function in Table 7-9.

Table 7-9: Cost function

Cost function	Data-driven SOC	Local-SOC	Optimum
Cooling Utility (J_{Qcu}) $	43.0338($/MW)	41.1359($/MW)	40.4594($/MW)
Heating Utility (J_{Qhu})$	129.8127($/MW)	133.8441($/MW)	129.4937($/MW)
Total Utility ($J_{Qcu+Qhu}$)$	172.8465($/MW)	174.9801($/MW)	169.9531($/MW)

For optimum operation for example, the total utility consumption is 169.9531 MW with 40.4594 MW of cooling and 129.4937 MW of heating. Assuming IP steam to be used for heating and water for cooling, the total cost function per annum of optimum operation is $36.869 \times 10^6\ \$ \cdot y^{-1}$ while the annualized cost function for data-driven SOC and Local SOC will respectively becomes 37.012×10^6 and $38.093 \times 10^6\ \$ \cdot y^{-1}$ respectively. This indicates that the data-driven SOC was able to save $1.08146\ \times 10^6\ \$ \cdot y^{-1}$ cost of utilities compared to Local self-optimizing control.

7.5.8 Conclusions

This Section presented a novel data-driven self-optimizing control procedure CV selection and its successful implementation on a HEN for coal-fired power plant retrofitted with CO_2 capture systems. This procedure select CVs from process measurement collected using ASPEN HYSYS during plant operations contrasting the existing SOCs procedure which requires process model and model linearization –a causation of unaccounted losses in CV evaluation. The method uses finite difference method to evaluate the CV from measurement data in a single regression step. The method was tested on a HEN for first and second-order CVs obtained through regression with the first-order CV giving the best economic loss. The advantage of the new approach over all existing SOC methods is that the CV can be achieved without evaluating the derivative function.

With the new approach, for complex industrial processes, CVs can be selected directly through simulation using commercial simulators such as HYSYS and UniSim.

7.6 Summary

The effectiveness of the proposed Data-driven SOC methodology proposed in this thesis has been tested on different HEN case studies. The first case study is the simple HEN example while the second case study is the HEN for coal-fired power plant retrofitted with CO2 capture unit. Two different data-driven SOC methodology has been implemented; i.e. (i) Data-driven SOC without constraints and (ii) Data-driven SOC with equality constraints.

In the first case study, the HEN example has 1 DOF for utility cost optimization, the remaining DOF are used for satisfying the network stream target temperatures at their setpoint values. Disturbances of $\pm\ 10\ ℃$ and $\pm\ 0.05\ kW/℃$ is introduced into the hot stream inlet and cold stream heat capacity flowrate during process operation to generate data for CV evaluation.

From the process data generated during operation, CVs are evaluated using finite difference for first and second order in a single regression. The results of losses in cost function for the Data-driven SOC without constraints and the Data-driven SOC with equality constraints developed in this thesis are compared with losses obtained with CVs derived using NCO method in a Monte Carlos experiments. The results indicates that the data-driven SOC method without and –with equality constraints has good performance compared to the NCO approximation method.

Following successful implementation of the data-driven method on a simple HEN, a more complex network with several loops and HEs is considered. The data-driven method is applied to control the operation of HEN for coal-fired power plant retrofitted with CO2 capture unit.

Three disturbances; (i) flue gas inlet temperature, (ii) flue gas heat capacity flowrate and (iii) LPLT feedwater heat capacity flowrates are considered. The framework has 5 DOF for manipulation of the HEN, however, the network data generated in ASPEN HYSYS during operation saturates the two HE bypasses at zero, reducing the number of DOF for CVs selection to three instead of 5 DOF. The results of losses obtained with CVs generated using data-driven method are compared and found to be superior to losses obtained using local SOC method.

The advantage of this new approach over all existing SOC methods is that the CV can be achieved without evaluating the derivative function. With this new approach, selecting CVs for complex industrial processes can be achieved directly through simulations using commercially available simulators such as HYSYS and UniSim.

8 CONCLUSION AND RECOMMENDATION

8.1 Conclusion

This thesis presented a detailed procedure for achieving economically optimal design and operation of HENs. The thesis is divided into two parts and in each part, the methodology developed is first tested on a 3-streams simple HEN case study before extending to a more complex case involving HEN for coal-fired power plant retrofitted with CO_2 capture systems.

The first part covers the design and economic analysis of HEN for coal-fired power plant retrofitted with CO_2 capture system. The design approach adopted to develop the network, given stream parameters, is the famous pinch technology procedure. The stream data was lifted from the work of Khallilpour and Abbas (2011) to evaluate the trade-offs between energy, capital and utility costs, and to redesign the HEN network with reduced energy penalty. The novel contributions include: (a) the use of cost and economic data to evaluate achievable trade-offs between energy, capital and utility cost, (b) determination of the optimal minimum temperature difference, (c) redesigning of a cost-effective HEN with fewer number of units. The study achieved energy savings of 78 MW equivalents to 27.3MWe at a total investment cost of 3.804351 million USD and a payback period of 2.8 years. An optimal HEN with 8 heat exchangers, 1 heater and 6 coolers with a total capacity reduction of 10.6 MWe was obtained compared to 27.9 MWe reported in Khallilpour and Abbass (2011). This value correspond to energy penalty of 9.82 % compared to the original work in which about 15.9 % energy penalty was achieved through a network containing 9 heat exchangers, 3 heaters and 7 coolers.

The second part of this thesis developed a new methodology for the selection of control variables for plantwide operations based on self-optimizing control method. Contrary to the existing SOCs CV selection methods which are model based and required linearization of process models around their nominal operating point if its involved rigorous nonlinear process model –a reason for large losses and difficult practical application, the newly developed method does not require process model to obtain the CVs as gradient of objective function, instead, CVs are computed from process data using finite difference method fitted to polynomial function by regression method. Like in the design part, the new data-driven SOC is first implemented on the 3-stream HEN before extending to a more complex HEN structure for coal-fired power plant retrofitted with CO_2 capture. The data-driven HEN was later modified to select CVs for a system with equality constraints and compared with the unconstrained method as well as the method of NCO approximation proposed by Ye et al., (2012). Although a HEN model equation for the 3-streams HEN was used to generate data for the CVs selection in both the equality constrained and the unconstrained methods, the data generated and collected for the operation of HEN for coal-fired power plant with CO_2 capture is directly form ASPEN HYSYS simulation. In all cases, the data-driven SOCs have proven to be promising in rejecting disturbances and uncertainties with minimum economic losses during process operation in comparison to the NCO approximations, in the case of 3-streams HEN and classical control, in the case of HEN for coal-fired power plant with CO2 capture. A major advantage of this method is that, apart from selecting CVs from process measurements, it can be applied to any process systems not necessarily HEN case studies.

8.2 Recommendations

The following recommendations are made for further investigation and implementation of the procedure developed in this thesis.

The HEN designed in this thesis is a pinch based network in which the driving force limits the amount of energy recovery right from the beginning of the design. A network design based on mathematical programming does not have such restriction and recent studies have shown that it is capable of handling both isothermal and non-isothermal phase changes in heat exchanger network. It will be interesting if such approach is explored to study the extent of energy penalty in the design of HEN for power plant with PCC system.

Although this work investigates the effect of two types of disturbances, that is, temperature and heat capacity flowrates, it is recommended that phase changes be considered in evaluating the performances of this method to enable its applicability in all types of exchangers. This recommendation if considered may be difficult to implement even for a small size HEN especially in simultaneous design approaches considering the fact that HEN design problem is NP-hard and finding even local optimum solution is difficult, since assuming Isothermal mixing may according to Yee and Grossmann (1990), restrict the area trade-offs between the exchangers and overestimate the cost, incorporating non-isothermal mixing may offers superior HENs.

The HYSYS design network uses H_2O as working fluids. Further studies should be carried out with streams composition representing the realities in power plant and capture plant as different fluids have different thermal properties.

Finally further studies on data-driven SOC technique should include the CV selection for dynamic systems in order to control process operation during startup and shutdown.

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APPENDICES

Appendix A Typical ΔT_{min} Values

A.1 ΔT_{min} For various types of processes (Linnhoff M., 1998)

No	Industrial Sector	Experience ΔT_{min} values	Comments
1	Oil Refining	20-40 °C	Relatively low heat transfer coefficients, parallel composite curves in many applications, fouling of heat exchangers
2	Petrochemical	10-20 °C	Reboiling and condensing duties provide better heat transfer coefficients, low fouling
3	Chemical	10-20 °C	As for petrochemicals
4	Low Temperature Processes	3-5 °C	Power requirement for refrigeration systems is very expensive. ΔT_{min} decreases with low refrigeration temperatures

A.2 ΔT_{min} For matching against Process streams (Linnhoff M., 1998)

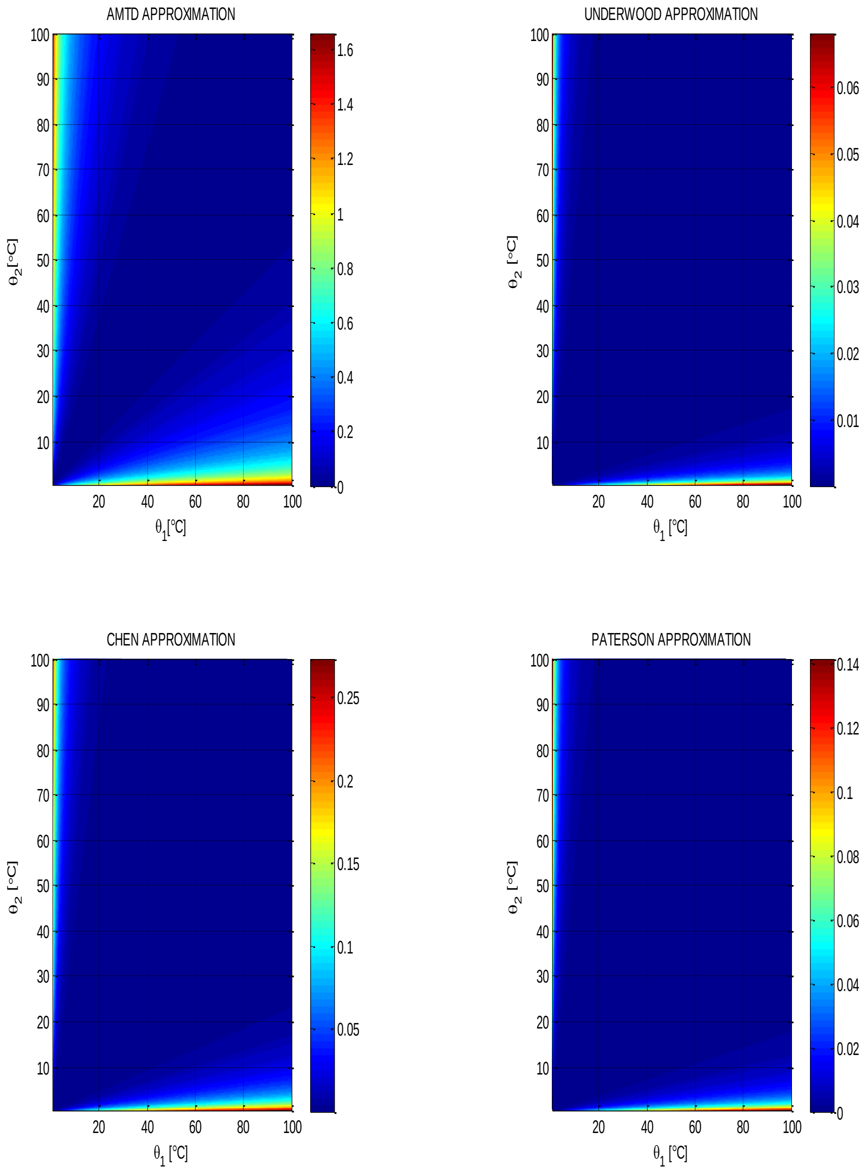
Match	ΔT_{min}	Comments
Steam against Process stream	10-20 °C	Good heat transfer coefficient for steam condensing or evaporating
Refrigeration against Process stream	3-5 °C	Refrigeration is expensive
Flue gas against process stream	40 °C	Low heat transfer coefficient for flue gas
Flue gas against steam generation	25-40 °C	Good heat transfer coefficient for steam
Flue gas against air	50 °C	Air on both sides. Depends on acid dew point temperature
CW against process stream	15-20 °C	Depends on whether or not the CW is competing against refrigeration. Summer/Winter operations should be considered

A.3 ΔT_{min} Retrofit targeting of refinery processes (Linnhoff M., 1998)

Process		ΔT_{min}	Comments
CDU		30-40 °C	Parallel (tight) composites
VDU		20-30 °C	Relatively wider composites (compared to CDU) but lower heat transfer coefficient
Naphtha Reformer/Hydrotreater		30-40 °C	HEN dominates by feed effluent exchanger with $\Delta \boldsymbol{P}$ limitations and parallel temperature driving force. Can get closer $\Delta \boldsymbol{T_{min}}$ with packinox exchangers (upto-20 °C
FCC		30-40 °C	Similar to CDU and VDU
Gas Oil Hydrotreater/Hydrotreater		30-40 °C	Feed-effluent exchanger dominant. Expensive high pressure exchangers required. Need to target separately for high pressure section (40 °C) and low pressure section (30 °C)
Residue Hydrotreating		40 °C	As above for Gas Oil Hydrotreater/Hydrotreater
Hydrogen Production Unit		20-30 °C	Reformer furnace requires high $\Delta \boldsymbol{P}$ (30-50 °C). rest of process 10-20 °C

Appendix B LMTD Approximation plots

B.1 LMTD Approximations



Appendix C Heat capacity of liquid water (Vaxa Software, 2015)

Heat capacity of liquid water from 0 °C to 100 °C www.vaxasoftware.com

Temp.	Heat capacity		Temp.	Heat capacity		Temp.	Heat capacity	
°C	$\frac{kJ}{K \cdot kg}$	$\frac{kcal}{K \cdot kg}$	°C	$\frac{kJ}{K \cdot kg}$	$\frac{kcal}{K \cdot kg}$	°C	$\frac{kJ}{K \cdot kg}$	$\frac{kcal}{K \cdot kg}$
0 (ice)	1.960	0.468	**34**	4.178	0.999	**68**	4.189	1.001
0	4.217	1.008	**35**	4.178	0.999	**69**	4.189	1.001
1	4.213	1.007	**36**	4.178	0.999	**70**	4.190	1.001
2	4.210	1.006	**37**	4.178	0.999	**71**	4.190	1.001
3	4.207	1.005	**38**	4.178	0.999	**72**	4.191	1.002
4	4.205	1.005	**39**	4.179	0.999	**73**	4.192	1.002
5	4.202	1.004	**40**	4.179	0.999	**74**	4.192	1.002
6	4.200	1.004	**41**	4.179	0.999	**75**	4.193	1.002
7	4.198	1.003	**42**	4.179	0.999	**76**	4.194	1.002
8	4.196	1.003	**43**	4.179	0.999	**77**	4.194	1.002
9	4.194	1.002	**44**	4.179	0.999	**78**	4.195	1.003
10	4.192	1.002	**45**	4.180	0.999	**79**	4.196	1.003
11	4.191	1.002	**46**	4.180	0.999	**80**	4.196	1.003
12	4.189	1.001	**47**	4.180	0.999	**81**	4.197	1.003
13	4.188	1.001	**48**	4.180	0.999	**82**	4.198	1.003
14	4.187	1.001	**49**	4.181	0.999	**83**	4.199	1.004
15	4.186	1.000	**50**	4.181	0.999	**84**	4.200	1.004
16	4.185	1.000	**51**	4.181	0.999	**85**	4.200	1.004
17	4.184	1.000	**52**	4.182	1.000	**86**	4.201	1.004
18	4.183	1.000	**53**	4.182	1.000	**87**	4.202	1.004
19	4.182	1.000	**54**	4.182	1.000	**88**	4.203	1.005
20	4.182	1.000	**55**	4.183	1.000	**89**	4.204	1.005
21	4.181	0.999	**56**	4.183	1.000	**90**	4.205	1.005
22	4.181	0.999	**57**	4.183	1.000	**91**	4.206	1.005
23	4.180	0.999	**58**	4.184	1.000	**92**	4.207	1.005
24	4.180	0.999	**59**	4.184	1.000	**93**	4.208	1.006
25	4.180	0.999	**60**	4.185	1.000	**94**	4.209	1.006
26	4.179	0.999	**61**	4.185	1.000	**95**	4.210	1.006
27	4.179	0.999	**62**	4.186	1.000	**96**	4.211	1.006
28	4.179	0.999	**63**	4.186	1.000	**97**	4.212	1.007
29	4.179	0.999	**64**	4.187	1.001	**98**	4.213	1.007
30	4.178	0.999	**65**	4.187	1.001	**99**	4.214	1.007
31	4.178	0.999	**66**	4.188	1.001	**100**	4.216	1.008
32	4.178	0.999	**67**	4.188	1.001	**100** (gas)	2.080	0.497
33	4.178	0.999						

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