

Steam System Network Analysis, Synthesis and Optimisation

Sheldon Grant Beangstrom

Steam System Network Analysis, Synthesis and Optimisation

by

Sheldon Grant Beangstrom

A dissertation submitted in partial fulfilment of the requirements for the degree

**Master of Engineering
(Chemical Engineering)**

in the

Department of Chemical Engineering

Faculty of Engineering, the Built Environment and Information Technology

Prepared under the supervision of

Prof Thokozani Majozi

University of Pretoria

March 2013

Synopsis

Steam is a commonplace utility in chemical processing plants across the globe. The many benefits of steam ensure its continued use, but concerns about the cost of energy and of the equipment associated with steam systems has led to the development of a number of techniques to reduce energy and capital costs. One such topic is the reduction of boiler purchase cost, brought about by a reduction in steam flowrate. Recent publications have shown that the flowrate of steam required for heating purposes can be minimised by employing hot liquid reuse, with systematic methods developed for targeting the minimum flowrate, and synthesising the heat exchanger network.

In this work, a mathematical analysis has been performed to gain insight on how choosing different steam levels affects the minimum total steam flowrate. The analysis covered both the traditional practice of only utilising latent heat, as well as the new practice of hot liquid reuse. It was found that the lowest flowrate obtainable occurs in the case of hot liquid reuse, when only a single high pressure steam level is considered.

Since the need to provide shaft work or generate electricity necessitates the presence of steam turbines on plants, the inclusion of additional steam levels is unavoidable. For this reason, a novel MINLP formulation was developed to provide a holistic coverage of the heat exchanger network and the power block. The purpose of the new formulation is to target the minimum total steam flowrate, whilst simultaneously selecting the optimum saturation temperatures for the additional steam levels, designing the turbines to meet shaft work requirements and synthesizing the heat exchanger network. Application of this new method to a case study yielded a 28.6% reduction in total steam flowrate, compared to common design practice.

I, Sheldon Grant Beangstrom, with student number 27069771, declare that:

- I understand what plagiarism entails and am aware of the University of Pretoria's policy in this regard.
- This dissertation is my own, original work. Where the work of another has been used (whether from a printed source, the internet or otherwise) due acknowledgement has been given and reference made in accordance with the departmental guidelines.
- I have not made use of another student's previous work in an attempt to submit it as my own.
- I have not allowed, nor will I allow another person to copy this work with the intention of presenting it as his or her own work.
- The material presented in this dissertation has not been submitted to another institution in partial or whole fulfilment of another degree.

S.G. Beangstrom

Acknowledgements

First, I would like to thank my supervisor, Prof Thoko Majozi. Our conversation in 2009 altered history, and you have moulded me ever since. Thank you for your guidance, and for your patience during the times when I simply couldn't express clearly the ideas in my head.

I would like to thank my parents and my darling sister for their love and support, even though they thought I wouldn't survive a month away from home. Also to my mom, I greatly appreciate the regular shipment of chocolate chip biscuits.

On a high note, I would like to thank George King, Will Viljoen, and the rest of the choir at Christ Church, Arcadia. Thank you for giving me a song in my heart and for ensuring that Thursday evenings were never boring. Also to St. Wilfrid's Church, for giving me the post of parish organist even though many would have advised against it. And to the parishioners of both churches, especially Carol Steyn, Peter & Isabel Beukes, Pam Ryans, Allan & Cathy Cordes and Heidi Kohn, thank you for your constant interest in my progress.

A special thanks must go to all my colleagues, especially Bola Adekola, Jane Stamp, Tim Price and Vincent Gololo. Thank you for many insightful discussions and good laughs.

Lastly, to all my friends past and present, thanks for all the great times.

A.M.D.G.

Contents

1	Introduction.....	1
1.1	Background.....	1
1.2	Motivation	3
1.3	Objective of Investigation	4
1.4	Structure	6
1.5	References	7
2	Literature Survey.....	9
2.1	Pinch Analysis	9
2.1.1	Heat Integration	9
2.1.2	Batch Process Heat Integration.....	21
2.1.3	Mass Integration.....	24
2.1.4	Combined Heat and Mass Integration	29
2.2	Mathematical Programming and Pinch Analysis.....	32
2.2.1	Models for Utility System Synthesis	32
2.2.2	Decomposition Methods	40
2.2.3	Mathematical Transformations	44
2.3	Utilities	48
2.3.1	Cold Utilities.....	48
2.3.2	Hot Utilities.....	52
2.4	Pressure Drop Considerations	56
2.5	Exergy Analysis	59
2.6	References	62
3	Background	72

3.1	System Description.....	72
3.2	Steam Levels	76
3.3	Flowrate Minimisation	77
3.3.1	Single Level – Graphical Targeting.....	77
3.3.2	Single Level – Network Synthesis.....	80
3.3.3	Single Level – Simultaneous Targeting and Synthesis	84
3.3.4	Multiple Steam Levels	88
3.4	Shaft Work Estimation	92
3.5	Heat Exchanger Layout.....	96
3.6	References	99
4	Mathematical Analysis.....	101
4.1	Latent Heat Only	102
4.2	Latent and Sensible Heat (Hot Liquid Reuse).....	110
4.3	Discussion.....	114
4.3.1	Example	114
4.3.2	Nonlinear Composite Curves.....	119
4.3.3	Solving Equation 4.17.....	122
4.4	References	124
5	Model Development.....	125
5.1	Problem Statement	126
5.2	Superstructure.....	127
5.3	Constraints.....	128
5.4	Solution Procedure	136
5.5	References	138

6	Case Study.....	139
6.1	Problem Description.....	139
6.2	Mathematical Analysis	141
6.3	MINLP Model Results	146
6.4	References	151
7	Conclusions and Recommendations	152
	Appendix A	156
	Appendix B	159
	Appendix C	163
	Appendix D	164

List of Figures

Figure 1.1: Different regions for the application of heat integration.....	2
Figure 1.2: Steam boiler purchase cost as a function of required flowrate.	3
Figure 2.1: Onion diagram for the above mentioned design steps, with a focus on heat integration.....	10
Figure 2.2: Heat availability diagram. The shaded region represents lost available energy	12
Figure 2.3: Grand Composite Curve showing the proper placement of multiple utilities.....	15
Figure 2.4: Use of the grid diagram in designing HENs.	18
Figure 2.5: Removing a heat exchanger.	20
Figure 2.6: Feasible and infeasible heat transfer	22
Figure 2.7: Formation of a pinch on a heat transferred vs. time diagram	23
Figure 2.8: Targeting the minimum water flowrate.....	26
Figure 2.9: Two-dimensional grid diagram	32
Figure 2.10: The three sections of a total processing plant	35
Figure 2.11: Superstructure used to synthesize the utility system.....	36
Figure 2.12: Flowchart for the Genetic Algorithm.....	39
Figure 2.13: Composite curves showing division into stages at arbitrary locations	42
Figure 2.14: Composite curves showing the use of nodes to obtain temperature intervals, and the grouping of intervals to form a block with physical meaning	43
Figure 2.15: Superstructure for two hot streams and three cold streams	43
Figure 2.16: Efficiency of a cooling tower as a function of flowrate and return temperature.....	49
Figure 2.17: Targeting the minimum cooling water flowrate.....	50
Figure 2.18: Two methods of preserving boiler efficiency	55
Figure 2.19: Superstructure for minimising pressure drop over a HEN.....	57

Figure 2.20: Example illustrating the Critical Path Algorithm.....	58
Figure 3.1: A typical chemical plant steam system.	73
Figure 3.2: Modified steam system for maintained boiler efficiency.....	75
Figure 3.3: Latent heat of steam and heat capacity of water as a function of saturation temperature.....	77
Figure 3.4: The importance of ΔT_{\min} in determining feasible and infeasible hot utilities.....	78
Figure 3.5: Using the limiting temperature composite curve to target the minimum flowrate.....	79
Figure 3.6: Superstructure for the synthesis of the sensible heat region HEN..	81
Figure 3.7: Superstructure for simultaneously targeting flowrate and synthesizing the HEN.....	84
Figure 3.8: Superstructure for steam flowrate minimisation in the presence of multiple steam levels.....	88
Figure 3.9: The Willans line for a simple turbine.....	93
Figure 3.10: Nonlinear variation of turbine efficiency with operating conditions	94
Figure 3.11: The division between latent and sensible heat.	97
Figure 3.12: T-H diagram and heat exchanger layout.....	98
Figure 4.1: An arbitrary process stream heated using latent heat from two steam levels.	102
Figure 4.2: An arbitrary process heated only with latent heat from multiple steam levels.	107
Figure 4.3: An arbitrary process heated using latent and sensible heat from two steam levels.	110
Figure 4.4: Minimum total steam flowrate as a function of IP steam saturation temperature, using only latent heat from two steam levels.	115
Figure 4.5: Minimum total steam flowrate as a function of MP and LP steam saturation temperatures, using only latent heat from three steam levels	116

Figure 4.6: Minimum total steam flowrate as a function of IP steam saturation temperature, using latent and sensible heat from two steam levels..... 117

Figure 4.7: Minimum total steam flowrate as a function of MP and LP steam saturation temperatures, using latent and sensible heat from three steam levels. 118

Figure 4.8: Use of a linear approximation to the GCC for the placement of intermediate steam levels 119

Figure 4.9: Adjusting a steam level in the middle of a pocket 120

Figure 4.10: Placing steam levels when utilising latent and sensible heat 122

Figure 5.1: Superstructure for the present model. 127

Figure 5.2: The ability of steam from different levels to provide latent heat... 133

Figure 6.1: Limiting hot utility composite curve..... 140

Figure 6.2: Minimum steam flowrate for the case study problem as a function of MP and LP steam level saturation temperatures using latent heat only. 142

Figure 6.3: Placement of steam levels according to the new heuristic..... 144

Figure 6.4: Minimum steam flowrate for the case study problem as a function of MP and LP steam level saturation temperatures using latent heat only 145

Figure 6.5: Base case HEN. 147

Figure 6.6: HEN obtained using new model..... 148

Figure 6.7: Placement of the utilities above the limiting hot utility composite curve..... 149

List of Tables

Table 3.1: Typical steam levels	76
Table 3.2: Turbine model coefficients	96
Table 6.1: Cold process stream data	139
Table 6.2: Limiting hot utility data	140
Table 6.3: Minimum steam flowrate based on the number of allowed heat exchanger splits	150

Nomenclature

Sets

I	Set of all heat exchangers
J	Set of all heat exchangers (alias)
L	Set of all steam levels

Parameters

c_p	Heat capacity of water	[kJ/kg·K]
FRR_i^U	Upper limit on reuse in i	[kg/s]
Q_i	Duty required by stream i	[kW]
$SS_{i,l}^U$	Upper limit on steam of level l in i	[kg/s]
$T_i^{in,L}$	Limiting utility inlet temperature for i	[°C]
$T_i^{out,L}$	Limiting utility outlet temperature for i	[°C]

Continuous Variables

A_l	Regression parameter for level l	[-]
B_l	Regression parameter for level l	[-]
F_i^{in}	Inlet flow to i	[kg/s]
F_i^{out}	Outlet flow from i	[kg/s]
$FRR_{i,j,l}$	Liquid reuse to i from j of level l	[kg/s]
FR_i	Boiler return from i	[kg/s]
FS_l	Total steam supply of level l	[kg/s]
$\overline{\Delta H}_l^{is}$	Specific isentropic enthalpy change between levels	[MWh/t]
$HL_{i,j,l}$	Hot liquid to i from j of level l	[kg/s]
m	Additional heat exchanger splits permitted	[-]
q^{in}	Heat load of steam	[MWh/t]
Q_i^{SS}	Heat supplied to i from saturated steam	[kW]
Q_i^{HL}	Heat supplied to i from liquid	[kW]
$SL_{i,j,l}$	Saturated liquid to i from j of level l	
$SS_{i,l}$	Saturated steam supplied to i from level l	[kg/s]
T_l^{sat}	Saturation temperature of level l	[°C]
TR	Total return to boiler	[kg/s]
TS	Total steam supply	[kg/s]
TUS_l	Steam supplied to turbine of level l	[kg/s]
W^s_i	Shaft work produced by turbine l	[MW]

Binary Variables

x_i	Binary variable for use of liquid in i	[-]
$y_{i,l}$	Binary variable for use of steam in i of level l	[-]

Greek

Γ	Linearization substitution variable	[-]
λ_l	Latent heat of level l	[kJ/kg]

Chapter 1

Introduction

1.1 Background

The primary objective of process integration is to optimise the performance of a chemical plant by means of intelligent consideration of the interactions between various unit operations. Through process integration, a number of economic and environmental advantages can be achieved. Utility minimisation, steam system optimisation, cooling water system optimisation and wastewater minimisation improve the profitability of a plant through reduced total costs, efficient plant operation, and reduced environmental legislation charges stemming from reduced carbon emissions and effluent discharges. The defining feature of process integration is the unified view of the process, consisting of many individual unit operations, and the effects each unit has on other units. Process integration therefore uses a holistic approach to optimise large sections of a chemical plant.

The field of process integration came to the fore during the 1970's energy crisis, when AOPEC (Arab Organisation of Petroleum Exporting Countries) placed embargos on the exportation of oil. Energy costs rose rapidly, and plants began to seriously consider the energy efficiency of their processes, whereas previously energy costs had been considered negligible compared to capital costs. Arguably the first work of this nature was by Hohmann (1971), in which

the trade-off between utility costs and heat exchanger area was considered. This was followed by the works of Linnhoff and Flower (1978), Umeda, Harada and Shiroko (1979), Linnhoff, Mason and Wardle (1979), and Townsend and Linnhoff (1983), all of which culminated in the work of Linnhoff and Hindmarsh (1983), in which a systematic graphical method was presented for the minimisation of utilities.

The method presented by Linnhoff and Hindmarsh (1983) demonstrated the power of process integration by providing a clear, systematic and accessible method of minimising utility costs, which still remains seminal 30 years later. The method, which is graphical in nature, exploits the ability to transfer heat from hot process streams to cold process streams in order to simultaneously reduce the need for external heating and cooling. Following this work, other regions of heat integration have now been investigated. Figure 1.1 shows the three regions of heat integration, along with the defining works of each region from the perspective of steam system synthesis.

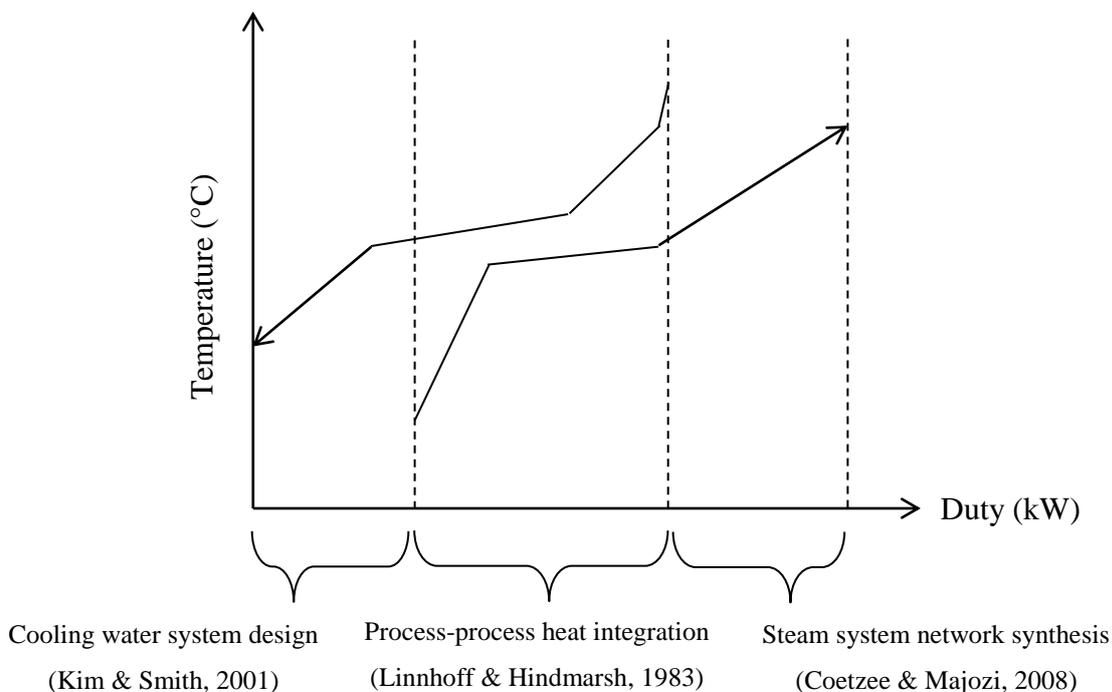


Figure 1.1: Different regions for the application of heat integration.

1 Introduction

In this work, only the region to the right of Figure 1.1 is considered, with emphasis on the steam system. This follows on the work of Coetzee and Majozi (2008), and Price and Majozi (2010). These methods treat the boiler, the associated set of heat exchangers and the steam turbines as an entity, instead of discrete unit operations.

1.2 Motivation

The motivation behind process integration is to yield economically viable chemical plants operating at an optimum point, whilst taking into account environmental concerns. In this work, the saving is achieved through capital cost reduction, stemming from reduced boiler purchase costs. The motivation behind this investigation can be seen in Figure 1.2. Here, it is clearly seen that the purchase cost of a boiler rises dramatically with an increase in the required flowrate of steam. Minimising the flowrate of steam required for the heat exchanger network requires a smaller, hence cheaper, boiler. In the case of a retrofit design, minimising the flowrate of steam results in debottlenecking of the boiler, making more steam available for expansion projects and eliminating the need for investing in additional boilers.

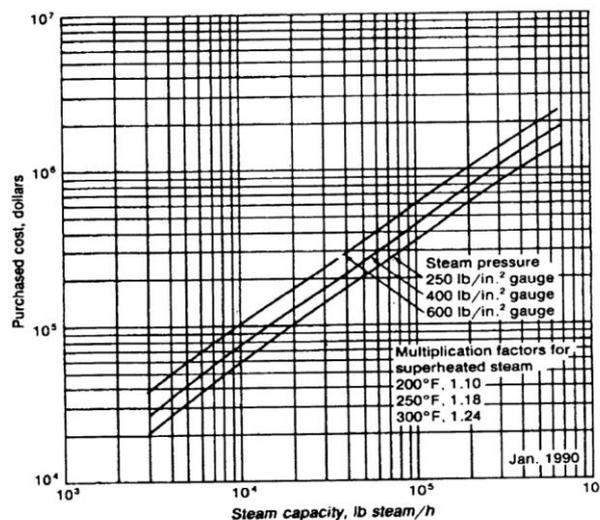


Figure 1.2: Steam boiler purchase cost as a function of required flowrate (Peters & Timmerhaus, 1991).

Further motivation behind this work arises from the need to address a number of serious shortcomings in previous works of this nature, specifically those by Coetzee and Majozi (2008), and Price and Majozi (2010). The two most important shortcomings are the need to properly design for multiple steam levels, and to include the steam turbines in the design process. These shortcomings can be addressed through a more detailed understanding of the steam system. Consequently, a novel model was developed which covers the steam system in greater detail. It is demonstrated in this thesis that the comprehensive model can then be used to obtain better designs than previously possible.

1.3 Objective of Investigation

The previous works by Coetzee and Majozi (2008) and Price and Majozi (2010) did not consider a number of critical factors surrounding steam systems. More specifically, the work by Coetzee and Majozi (2008) considers the situation of only using a single steam level, whilst the work by Price and Majozi (2010) attempts to redress this by including multiple steam levels and steam turbines, but assumes that the available steam levels and the steam turbine operational parameters are fixed *a priori*. By making these assumptions, the work by Price and Majozi (2010) fails to consider that in reality, the boiler, the steam levels, the heat exchanger network and the steam turbines are inherently interdependent and should be optimised in unison. The aim of this work was therefore to address these shortcomings, and to build upon the contributions made by Coetzee and Majozi (2008) and Price and Majozi (2010).

The first goal of this work was to understand what effect the choice of steam levels has on the minimum steam flowrate. This is important, since hitherto, steam levels have been selected from best practice tables or heuristics. Since the steam levels are so closely linked to the heat exchanger network and the steam

turbines, it is crucial to understand how the steam levels produced by the turbines can affect the heat exchanger network, and how an optimum operating point can be obtained.

Since steam turbines are linked to the production of the lower steam levels, and therefore linked to the heat exchanger network, the second goal was to develop a model that incorporates the power block with the heat exchanger network. Various combinations of flowrate and pressure drop can be employed in a steam turbine to achieve the same quantity of shaft work, which suggests that the power block should be included with optimisation of the steam system and not designed beforehand. For this reason, a novel model was developed that optimises the entire steam system holistically. The aims of the model can be summed up in the following problem description.

Given:

- a set of cold process streams,
- the fixed duties required by each cold process stream,
- the supply and target temperatures for each cold process stream,
- the minimum temperature difference for heat exchange,
- a shaft work target.

Determine:

- the minimum total steam flowrate,
- the saturation temperatures of the intermediate steam levels required to satisfy the energy demands of the heat exchangers and shaft work requirements and
- the network of heat exchangers that will fulfil this target.

1.4 Structure

Chapter 2 gives a survey of the literature connected with this study. The literature is not only limited to heat integration, but also to other related fields that are of benefit to this topic. Chapter 3 gives an in-depth background to specific techniques used in this work. These topics provide the information that is vital to understanding the current work. In Chapter 4, a mathematical analysis of steam systems is presented. A short discussion is given at the end of Chapter 4 to highlight the results and implications of the analysis. In Chapter 5, the new model is presented. A case study is presented in Chapter 6, in which the mathematical analysis is applied to an industrial problem, and the new model used to synthesize a heat exchanger network. Chapter 7 contains the conclusions and recommendations drawn from this study.

1.5 References

- Coetzee, W. A., & Majozi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Hohmann, E. C. (1971). Optimum networks for heat exchange. PhD Thesis: University of Southern California.
- Kim, J. K., & Smith, R. (2001). Cooling water system design. *Chem. Eng. Sci.*, 56, 3641-3658.
- Linnhoff, B., & Flower, J. R. (1978a). Synthesis of heat exchanger networks: I. systematic generation of energy optimal networks. *AICHE J.*, 24(4), 633-642.
- Linnhoff, B., & Flower, J. R. (1978b). Synthesis of heat exchanger networks: II. evolutionary generation of networks with various criteria of optimality. *AICHE J.*, 24(4), 642-654.
- Linnhoff, B., & Hindmarsh, E. (1983). The pinch design method for heat exchanger networks. *Chem. Eng. Sci.*, 38(5), 745-763.
- Linnhoff, B., Mason, D. R., & Wardle, I. (1979). Understanding heat exchanger networks. *Comp. Chem. Eng.*, 3, 295-302.
- Peters, M. S., & Timmerhaus, K. D. (1991). Plant Design and Economics for Chemical Engineers. USA: McGraw-Hill.
- Price, T., & Majozi, T. (2010). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Townsend, D. W., & Linnhoff, B. (1983a). Heat and power networks in process design. I. Criteria for placement of heat engines and heat pumps in process networks. *AICHE J.*, 29, 742-748.

Townsend, D. W., & Linnhoff, B. (1983b). Heat and power networks in process design. II. Design procedure for equipment selection and process matching. *AIChE J.*, 29, 748-771.

Umeda, T., Harada, T., & Shiroko, K. (1979). A thermodynamic approach to the synthesis of heat integration systems in chemical processes. *Comp. Chem. Eng.*, 3, 273-282.

Chapter 2

Literature Survey

This section gives an overview of the various contributions that have led up to this present work. Although primarily on the topic of heat integration, a number of related topics are also discussed. It is important that one is familiar with works outside the immediate topic of interest, as a technique developed for one situation can often be used in another situation in a modified form.

2.1 Pinch Analysis

The concepts of pinch analysis were first introduced in the field of process-process heat integration. This concept has subsequently grown to be included in many other fields of process integration as well. For example, due to the similarities between the governing equations of heat and mass transfer, the concept of pinch analysis has also been successfully applied to mass integration. Therefore, it is important to analyse these fields.

2.1.1 Heat Integration

When designing chemical processes, there are a number of sequential steps to be followed in the design process. The following list (adapted from Seider *et al*, 2004) illustrates very briefly the steps to be followed:

- 1) Eliminate differences in molecular types (decide on what reactions to perform)

2 Literature Survey

- 2) Eliminate differences in composition (decide on the type and proper placement of separation units)
- 3) Eliminate differences in temperature, pressure and phase (add heat exchangers, pumps, valves, etc.)
- 4) Integrate the tasks

The order of the last two steps in the above list is very important; it shows that one should first identify where heating and cooling are needed before trying to integrate the processes. Although it is not explicitly stated in the list, after integrating the tasks one must then assign the various external utilities.

One way to visualise the dependencies of these process design steps is to consider what is commonly called an “Onion diagram” (Figure 2.1). Any layer in the onion is only affected by changes to layers inside of it, and any changes to a layer only affects layers outside of it. The heat integration step is thus ideally placed, as it gives one the freedom to alter the design of the heat exchanger network (HEN) without disrupting the energy requirements of the core processes.

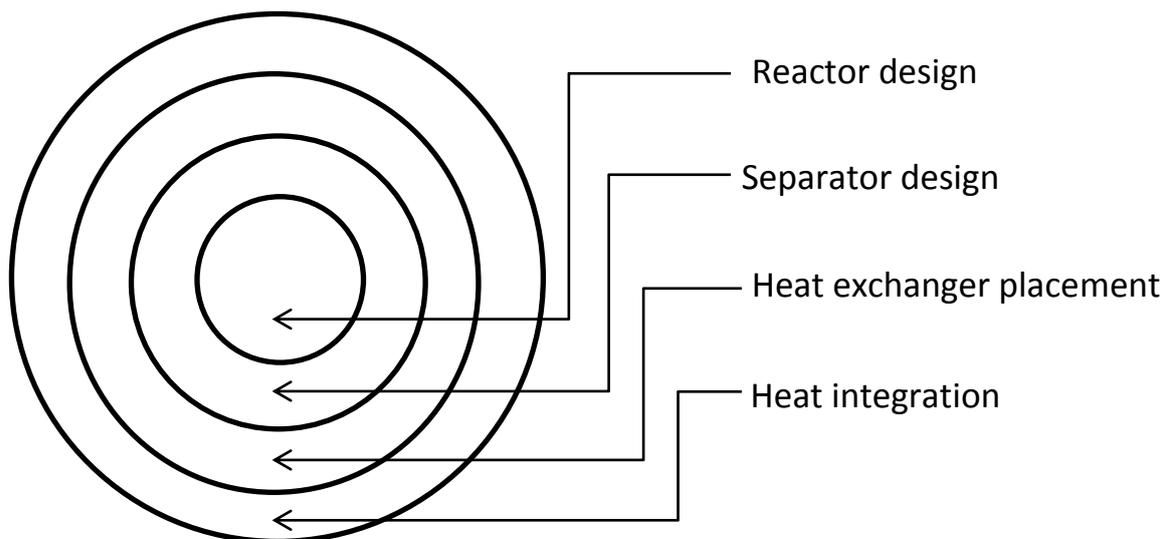


Figure 2.1: Onion diagram for the above mentioned design steps, with a focus on heat integration. (Kemp, 2007)

2 Literature Survey

Most handbooks on process design recommend that the design should be optimised after each step in the process design sequence. By the time one reaches the heat integration step, one can assume that the process and its energy requirements are fixed, with no scope to improve them. The only task remaining is to optimise the energy efficiency of the heat exchanger network.

The earliest works on process integration are graphical methods, using the designer's knowledge of the system to guide the process towards the optimal solution. Hohmann (1971) looks at the trade-off between the cost of utilities and the heat exchange area (a commonly used indicator of the capital cost of the HEN). This graphical technique is carried out on a diagram of temperature versus enthalpy (or duty), and seeks to reduce the quantity of utilities required. Hohmann shows how the minimum temperature difference for heat exchange (ΔT_{\min}) affects the quantity of utilities required, and also develops the N-1 rule to predict the smallest number of heat exchanger units that satisfy the problem.

Umeda *et al* (1979) use the concept of thermodynamically available energy in order to minimise the quantity of utilities required. The aim is to minimise the required utilities by reducing the quantity of "available energy" that is lost. The quantity of energy available for heating purposes is a function of the two thermodynamic states of the stream (initial state and final state). These energy states are a function of temperature and pressure. By knowing the temperature and pressures at both ends of a stream, the quantity of energy available for transfer to lower temperature streams can be calculated. With the Carnot efficiency as a basis, Umeda *et al* (1979) plot the hot and cold streams on a diagram of $\frac{T-T_0}{T}$ versus Q (Figure 2.2). Using the concept of composite curves, first developed by Huang and Elshout (1976), Umeda *et al* (1979) express all the stream data as a single pair of hot and cold composite curves. It should be noted that even if the heat capacity of a stream is constant, the line representing

2 Literature Survey

the stream will not be straight due to the unusual scale of the y axis, resulting in curved composite curves.

Using this definition for the axes of the graph, Umeda *et al* (1979) show that the area under a composite curve represents the energy of the constituent process streams available for transfer to cooler streams. Therefore, when considering both the hot and cold composite curves, the area between these two graphs (and between the utilities at the extremities) represents the quantity of useful energy that is lost. Figure 2.2 shows a pair of composite curves on a heat availability diagram, where the area representing the lost available energy is shaded. It can be seen that the quantity of lost energy, the shaded portion, can be minimised by shifting the two curves until they meet. Although Umeda *et al* do not give details concerning the construction of their composite curves, one must remember to compensate for the minimum temperature difference for heat exchange if a visual pinch, as in Figure 2.2, is to be feasible.

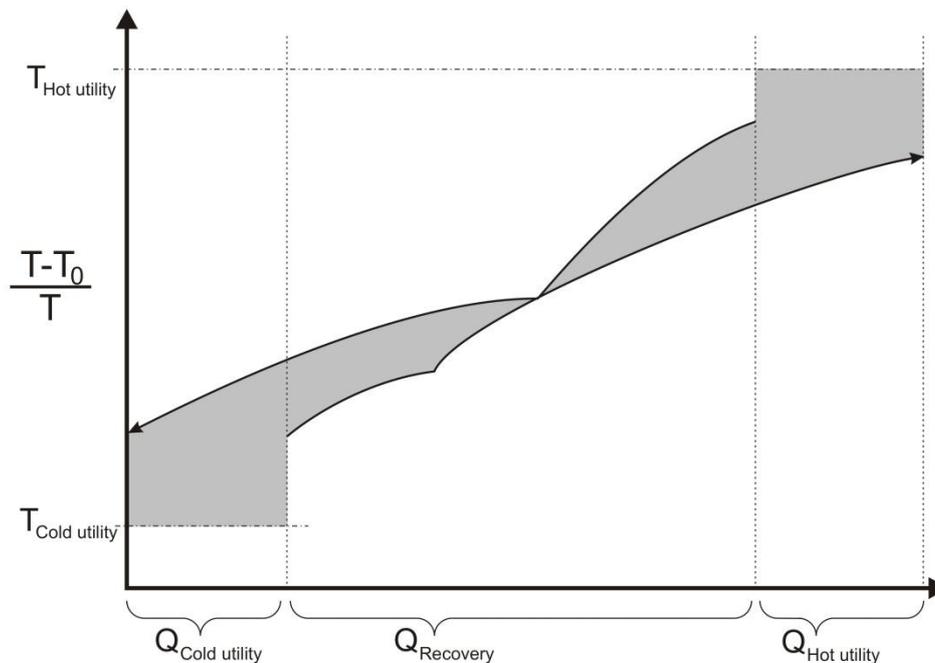


Figure 2.2: Heat availability diagram. The shaded region represents lost available energy (Umeda et al, 1979)

2 Literature Survey

Umeda *et al* (1979) call the point at which the two composite curves meet the ‘pinch point’ and explain that it represents a bottleneck in the process. They discuss how it is this point that prevents further energy savings, and that if changes could be made that would smooth the composite curves, a better energy target could be realised. They briefly discuss some of the possible changes, such as changing the operating temperature or pressure of process streams.

One distinguishing feature of the work by Umeda *et al* (1979) is their use of computer aided calculations. They mention two programmes used in applying the method. The first programme targets the maximum quantity of energy recovery using the concepts illustrated in Figure 2.2. The second synthesises the network while minimising the total heat exchange area. The authors give little information as to how the programmes perform these tasks.

Linnhoff and Flower (1978a,b) develop a mathematical method of locating the pinch temperature, rather than obtaining it by manually shifting graphs. First, what is now known as the problem table algorithm is developed. A set of temperature intervals is first created, based on the supply and target temperatures of the streams, taking into consideration the minimum temperature difference for heat exchange. The duty of each hot stream present in a particular temperature interval is summed, and the same is done for the cold streams. Since the total duty of the hot streams represents energy that must be removed, and the total duty of the cold streams represents a demand for energy, the difference of these two sums represents the total energy surplus or deficit of that temperature interval. Any surplus energy from a higher temperature interval can be cascaded down to a lower temperature interval, but no interval is permitted to have negative energy, or a nett deficit. The quantity of hot utility must thus be adjusted until the largest negative energy vanishes and becomes zero, that is, when no interval has an energy deficit. The temperature at which this zero

2 Literature Survey

surplus energy is located is the pinch temperature. Additionally, the quantity of hot and cold utility indicated in the problem table represents the minimum utility requirements.

Linnhoff and Flower (1978a,b) also develop a graphical method for designing the layout of heat exchangers inside a HEN. Previously, designers would identify matches on the existing process flow diagram (PFD). The PFD of a plant is quite complicated, and identifying heat integration matches on the PFD is awkward and impractical. Linnhoff and Flower (1978a,b) make use of a grid diagram, in which all the process streams are represented by horizontal lines, with high temperatures on the left and low temperatures on the right. Streams are matched by linking them with vertical lines connected at the relevant temperatures. This produces a clean and uncluttered diagram on which one can easily keep track of the energy being transferred and the resulting temperatures of the streams.

Townsend and Linnhoff (1983b) developed what is now known as the Grand Composite Curve (although originally called it a cascade diagram) by using the data from the problem table algorithm. The Grand Composite Curve (GCC) shows the energy surpluses and deficiencies on a plot of temperature versus enthalpy or duty, as in Figure 2.3. An advantage of the GCC lies in its ability to show at which temperature energy must be supplied to or removed from the process. This aids in the proper placement of multiple utilities, and the determination of the duty required of each utility. Furthermore, regions of pure process-process integration are easily identified as pockets in the GCC (shaded in Figure 2.3).

2 Literature Survey

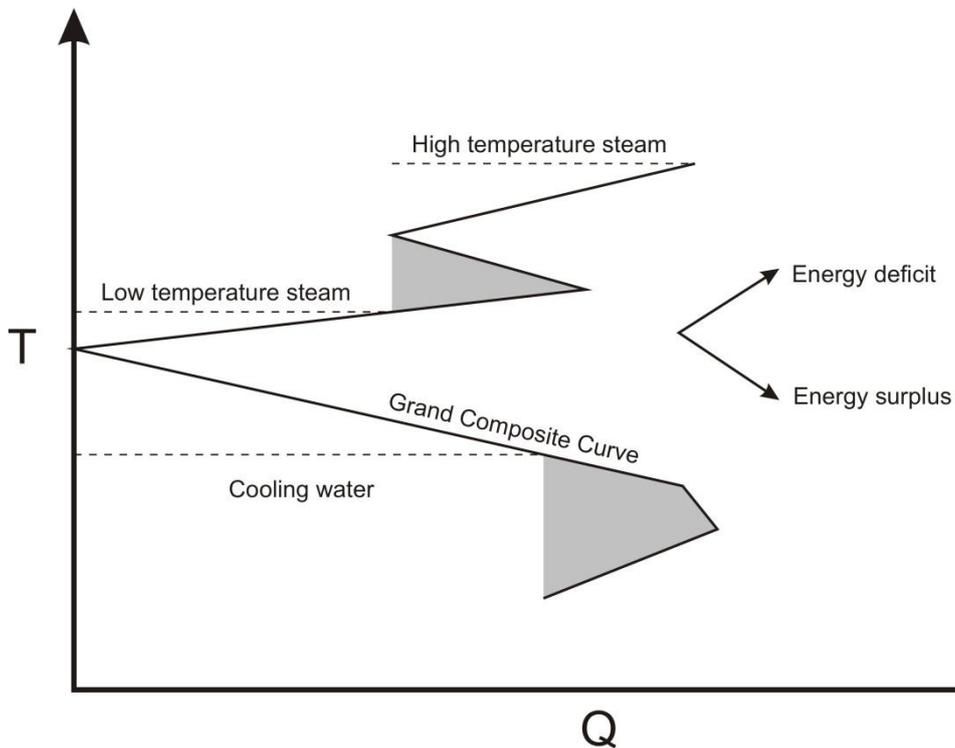


Figure 2.3: Grand Composite Curve showing the proper placement of multiple utilities. (Kemp, 2007)

The ability to use the composite curve in allocating multiple utilities is of great benefit to industry. When targeting the minimum utilities using any method that requires two composite curves to be shifted together to form a pinch, such as the method used in Figure 2.2, the resulting diagram shows that the hot and cold utilities have to be at very high and low temperatures. By using the GCC, one can see that not all of the heating or cooling duty has to be supplied at the highest or lowest temperature. The GCC tells one exactly how much expensive utility is required, and how much utility can be supplied at temperatures with lower costs.

Linnhoff, Mason and Wardle (1979), in response to the explosion in research on synthesising optimal heat exchanger networks, outline some fundamental facts that must be considered in the design of heat exchanger networks. They criticise the work of others as being too rigid, and express their belief that “synthesis methods designed to ‘replace’ the user have little chance of practical

2 Literature Survey

application”. They explain how a method that is flexible and “helps the user think” rather than “think for the user” is more desirable in industry. While giving important considerations in the design of HENs, the authors show how the minimum approach temperature, ΔT_{\min} , has a large influence on the solution to the problem, as well as the significance of the threshold temperature. Multiple utilities are considered, and Hohmann’s N-1 rule (Hohmann, 1971) for the case of multiple utilities is extended using graph theory. Stream splitting and multiple matches are also considered, as well as the influences of constraints upon the network and the uncertainty in the data. The authors further show how the topology of the network has an effect on the quantity of energy recovered. Using their formula for predicting the minimum number of units, it is proposed that all synthesis methods should first attempt to design for the minimum number of units at maximum energy recovery. Only if the designer is unsuccessful, may the minimum number of units be relaxed in order to meet maximum energy recovery. Linnhoff, Mason and Wardle (1979) conclude by solving a number of problems from literature, including one that was previously deemed unsolvable.

The work by Linnhoff, Mason and Wardle (1979) was intended to take HEN design methods out of the realm of small scale academic problems, and to start applying them in large industrial scale problems. The authors stress many times that a good design method must rely on the engineering insight of the designer, and must challenge the designer to use his own knowledge to come up with a design that would uniquely fit the needs of the plant.

Linnhoff and Hindmarsh (1983) combine the best aspects of the above methods into a clear, systematic and accessible design procedure. The use of process-process heat integration is popularised as a means of saving energy and capital by creating one clear and simple procedure out of all the available knowledge.

2 Literature Survey

From the observation by Grimes (1980) that minimum utilities is mutually incompatible with minimum number of units in problems featuring a pinch, Linnhoff and Hindmarsh (1983) centred their method around designing for minimum total cost. This is accomplished by first designing for minimum utility usage, and then breaking “heat loops” to reduce the number of units at the expense of increasing the utilities.

The method proposed by Linnhoff and Hindmarsh (1983) begins by targeting the minimum utility duties and the process pinch temperature using the problem table algorithm developed by Linnhoff and Flower (1978). This target is determined before any design is synthesised. Linnhoff and Hindmarsh (1983) furthermore stipulate three rules regarding the pinch, that are necessary for maintaining the minimum utility target:

1. Do not transfer energy across the pinch,
2. Do not apply cooling above the pinch, and
3. Do not apply heating below the pinch.

Having obtained the minimum utility targets, Linnhoff and Hindmarsh (1983) move on to synthesising the layout of the heat exchanger network. This is accomplished on the grid diagram, introduced by Linnhoff and Flower (1978). Linnhoff and Hindmarsh (1983) explain that the pinch represents the most constrained region inside the processes, and as such, the design should begin at the pinch. Previously, the process of matching streams for heat integration began at one extremity and progressed towards the other end, giving suboptimal results. Linnhoff and Hindmarsh (1983) propose that since the pinch is the most constrained point, the design procedure should begin at the pinch and move outwards towards the hot and cold ends. Because of the three rules regarding the pinch, the design of the HEN can be broken into two independent sub-networks

2 Literature Survey

that are connected at the pinch. Each one is designed separately and then combined to give the final network. Figure 2.4 shows this concept of designing away from the pinch, and then combining the two independent designs into one.

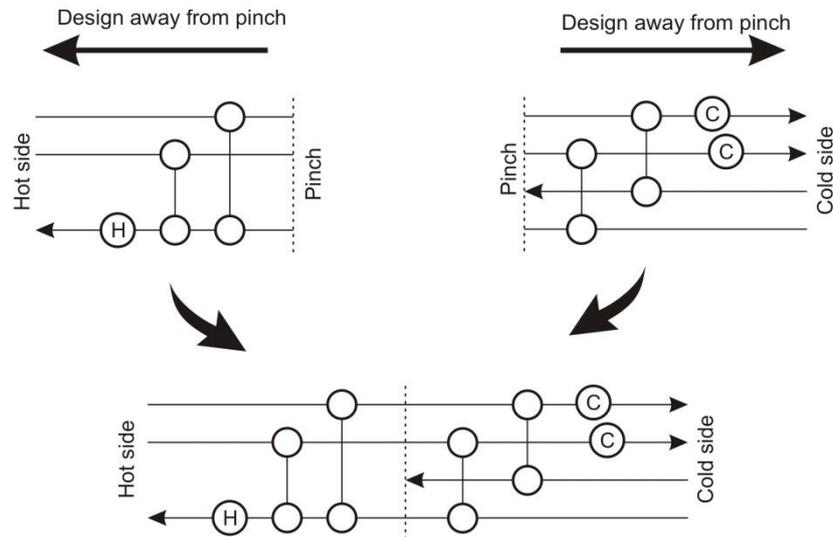


Figure 2.4: Use of the grid diagram in designing HENs.

Although Figure 2.4 looks relatively simple, it is not always easy to identify which streams to match. Linnhoff and Hindmarsh give a set of rules to aid in identifying matching streams to ensure feasible solutions. This involves considering the heat capacity flowrate (CP) of the streams. The heat capacity flowrate is the product of the heat capacity of the fluid in each stream and the flowrate of the respective streams, having units of kW/K or similar. At the pinch, the streams are already separated by the minimum approach temperature, ΔT_{\min} . Any match that causes the temperature difference to decrease as one moves away from the pinch is infeasible, since ΔT_{\min} will be breached immediately as one moves away from the pinch. For this reason, Linnhoff and Hindmarsh state that when designing against the pinch, the heat capacity flowrate of the hot stream (CP_H) must be less than the heat capacity flowrate of the cold stream (CP_C) on the hot side, and vice versa on the cold side. This rule allows one to identify feasible matches adjacent to the pinch. This rule does not

2 Literature Survey

hold when identifying matches away from the pinch, but the designer must be aware that matching streams that break this rule will cause their temperatures to converge, and one must be careful not to breach the ΔT_{\min} constraint. In addition to this rule, Linnhoff and Hindmarsh (1983) also provide several rules based on the CP of the streams that allow the designer to identify when streams must be split.

Having designed the HEN, the last step is to relax the energy targets in order to reduce the number of heat exchanger units. Linnhoff and Hindmarsh (1983) do not explicitly state how far the targets should be relaxed to give an optimal network, rather leaving it to the designer to choose the relative importance of energy savings versus capital savings. The ability to reduce the number of units stems from the observation that when the two halves of the HEN are combined, a number of heat loops are formed. A heat loop occurs when one can begin at a particular heat exchanger and, following a closed path, arrive back to that heat exchanger. This is illustrated in Figure 2.5(a) by a bold, dashed line. Having identified a heat loop, one of the heat exchangers can be removed and its load redistributed amongst the remaining heat exchangers. By doing this, one will cause the temperature differences at certain points to become infeasible. A heat path must then be identified, running from a hot utility to a cold utility, such that raising the duty of both the heater and the cooler will eliminate the infeasibility. A bold, dashed line Figure 2.5(b) shows an example of a heat path after one of the heat exchangers is removed.

It must be noted that all of the methods described above are graphical methods. Such methods are desirable from the perspective of allowing the engineer to gain insight and apply knowledge to the problem. There are also drawbacks to using graphical methods, such as limited accuracy and the need to express all

2 Literature Survey

the information on a two dimensional plot. These drawbacks have led to the development of mathematical programming methods for synthesising HENs.

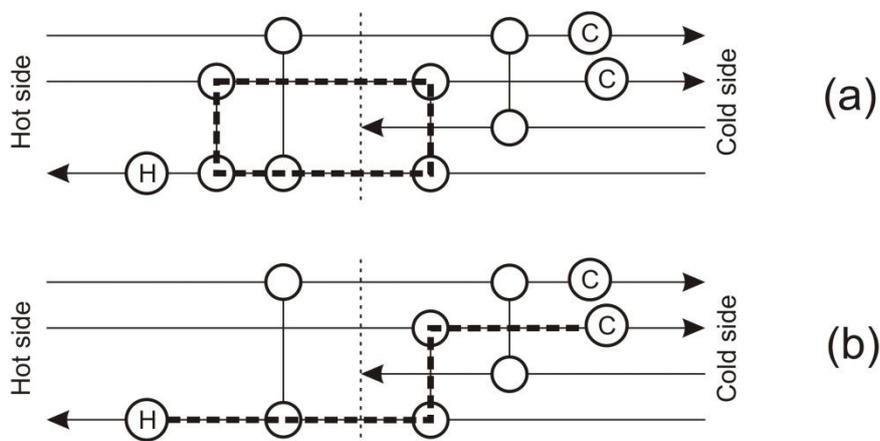


Figure 2.5: Removing a heat exchanger. (a) identifying a heat loop (b) correcting for temperature infeasibilities.

Using the techniques of heat integration discussed above, Ahmad and Polley (1990) discuss how pinch can be applied to debottleneck existing processes. Particular attention is paid to the capital implications of retrofitting a plant, and other negative effects such as the increased pressure drop for the new network. A plot of heat exchanger area versus energy is used to determine whether it is better to install new pumps to overcome the additional pressure drop, or to replace the heat exchangers with ones with larger area to reduce the pressure drop.

On large chemical plants, the total site is usually divided into a number of separate processing regions. Typically, heat integration is only applied within the individual regions, since performing heat integration on the entire plant using the methods already discussed would result in a network with impractical matches and costly lengths of additional piping. Hui and Ahmad (1994) propose that heat available in one region can be transported to another region using the existing steam headers. Here, surplus energy in one region is used to raise steam

in a waste heat boiler, which can then be supplied to the steam header and be used to provide heat elsewhere on the plant. Hui and Ahmad (1994) use the GCCs of the individual regions to target how much low and intermediate level steam can be raised, and how much is in demand. Since steam is being raised using waste heat in certain operations, there is a simultaneous reduction in both boiler and cooling water demands. This brings about further reductions in utilities compared to applying heat integration to the individual regions only.

2.1.2 Batch Process Heat Integration

The methods of heat integration given above are for use in continuous processes. Since not all chemical processes are continuous, it is important to consider how heat integration can be applied to batch processes. The necessity to treat time as a variable in batch processes adds considerable complexity in applying heat integration to batch processes. In continuous processes, it is sufficient to ensure that heat is transferred from a hot stream to a cold stream. In batch processing, one must ensure that temperature differences allow for heat transfer as well as ensuring that this occurs at the correct time. This additional dimension to the problem is illustrated in Figure 2.6.

The concept of batch process heat integration was first introduced by Vaselenak, Grossmann and Westerberg (1986). This work considers three different configurations in which batch process heat integration can be applied. In the first, both the hot and the cold liquids remain in their original tanks, and are circulated through the two sides of a heat exchanger. As the hot tank cools, the temperature in the cold tank rises, with the temperature in both tanks approaching some common average, similar to a co-current heat exchanger. In the second configuration, both fluids are pumped to new vessels while passing through a heat exchanger. The temperature of the hot fluid can be reduced to a much lower temperature, and the temperature of the cold fluid raised much

2 Literature Survey

higher than in the previous case, similar to a counter-current heat exchanger. The third configuration involves one of the fluids remaining in its original vessel, while the second fluid moves to a new vessel, reported as being somewhat of a combination of a co-current and a counter-current heat exchanger.

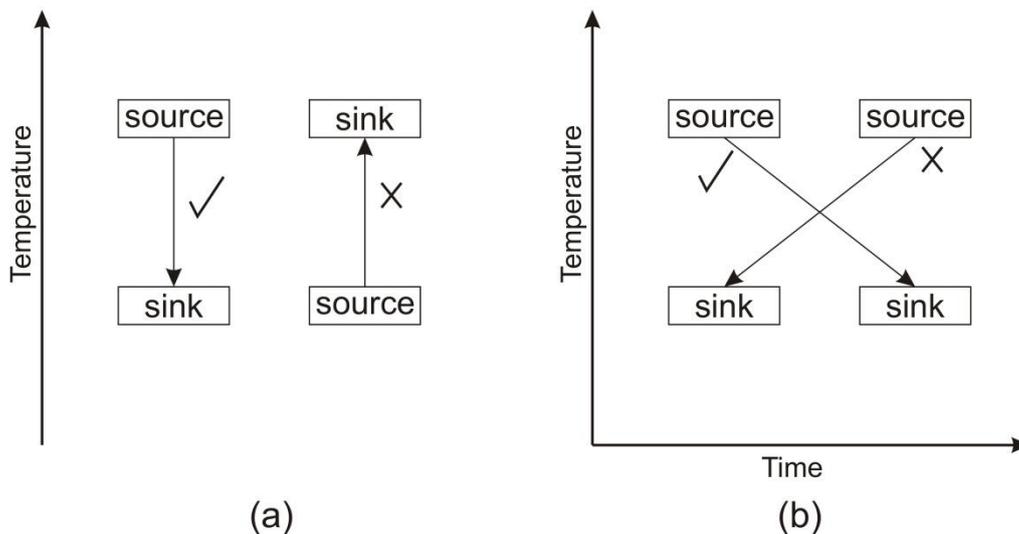


Figure 2.6: Feasible and infeasible heat transfer in (a) a continuous process (b) a batch process. (Wang & Smith, 1995)

The introduction of the concept of time pinch analysis by Wang and Smith (1995) represents a great advancement in the application of heat integration to batch plants. To apply process integration adequately to batch processes, one must include time as a variable, and recognise the constraints that it places on the system, as demonstrated in Figure 2.6. Wang and Smith (1995) plot the processes on a graph of heat transferred versus time, an analogy of the temperature versus duty plot used in continuous processes. Using a series of time intervals, the total quantity of heat transferred from the hot processes and the total heat transferred to the cold processes is plotted for each time interval. This results in two curves, one representing hot processes and the other cold processes, similar to the composite curves in continuous processes.

2 Literature Survey

To target the minimum utilities, Wang and Smith (1995) state that the hot composite curve must be shifted down until a pinch forms. The quantity of heating, cooling and energy recovered is then read off (Figure 2.7). This diagram does not, however, indicate whether the temperature differences are feasible or not. For this, Wang and Smith modify the problem table algorithm to have temperature intervals going downwards, and time intervals going to the right. From this, a plot similar to the GCC is obtained.

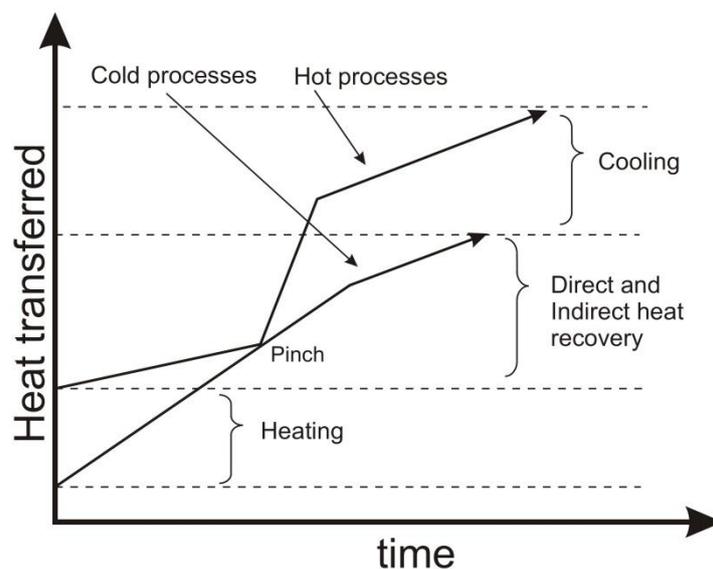


Figure 2.7: Formation of a pinch on a heat transferred vs. time diagram. (Wang & Smith, 1995)

An important aspect in batch processing, whether considering heat integration or not, is the scheduling of the processes. Adonyi *et al* (2003) introduce the concept of developing the schedule and the heat integration plan at the same time. Before, either the schedule was fixed and then heat integration applied, or heat integration was optimised before planning the schedule. Adonyi *et al* (2003) show that improved results are obtained when performing the two tasks simultaneously. Combinatorial algorithms and branch-and-bound procedures are used to perform these tasks, based on the application of the “S-graph”.

Given the flexible nature of batch processing, it is logical that numerous techniques have been developed to handle different scenarios. Papageorgiou, Shah and Pantelides (1994) develop a method for optimising both the schedule and the heat integration of a multipurpose batch plant, with capabilities to handle both direct and indirect heat transfer. Majozi (2006) presents a model for performing heat integration in multipurpose and multiproduct batch plants using a continuous time frame work, for the case when direct heat transfer opportunities exist. This method results in smaller problems and produces significant savings. Stamp and Majozi (2011), based on work by Majozi (2009) on multiproduct batch plants, consider both direct and indirect heat transfer in a multipurpose batch plant. By treating time as a variable, a Mixed Integer Non-Linear Program (MINLP) is obtained that produces substantial reductions in the required utilities. Provisions for optimising the size of the heat storage unit and allowances for heat losses are made, which gives a more realistic model.

2.1.3 Mass Integration

In heat transfer, it is Fourier's law that governs the transfer of heat from a hot object to a cold object. Similarly, in mass transfer, it is Fick's law of diffusion that describes how a substance can diffuse from a rich medium to a lean medium. The equations for both these laws are in most respects the same, both having the form of

$$\left(\begin{array}{c} \text{amount} \\ \text{transferred} \end{array} \right) = \left(\begin{array}{c} \text{proportionality} \\ \text{constant} \end{array} \right) \times \left(\begin{array}{c} \text{driving} \\ \text{force} \end{array} \right)$$

In heat transfer, the substance being transferred is heat, the constant is the conductivity of the heat exchanger and the driving force is the temperature difference. When the substance being transferred is mass, the constant

2 Literature Survey

represents the movement of the specific species through the specific medium, and the driving force is the concentration difference. Since heat and mass transfer share these characteristics, one can also use the tools developed for heat integration to perform mass integration and vice versa.

El-Halwagi and Manousiouthakis (1990) develop a model to automatically synthesize a Mass Exchanger Network (MEN) for a single component. The model considers the transfer of a single component from a set of rich streams to a set of lean streams. The model uses a variety of mass separating agents (MSAs) as the lean streams, and using mathematical optimisation, seeks to design the MEN and allocate the correct MSAs to minimise the annual cost of the system while still performing the required separation. If the minimum permissible concentration is specified globally, the model results in a Linear Programming (LP) problem, but if the minimum permissible concentration differences are specified per match, then the model results in a Mixed-Integer Linear Programming (MILP) problem.

The method of El-Halwagi and Manousiouthakis (1990) is a complicated method and works on the assumption that the designer is prepared to consider various mass separating agents. In many cases, water is the only MSA considered, since water is a safe, cheap and readily available solvent. Once the contaminants have been transferred out of the rich process streams and into the lean water stream, the water must be treated. The problem becomes one of minimising the quantity of wastewater produced, both for economic and environmental reasons. By only having one lean stream, the cost scaling factors required in El-Halwagi and Manousiouthakis's (1990) method become redundant, and the solution procedure is much simplified.

2 Literature Survey

Wang and Smith (1994) develop a graphical method of minimising the quantity of wastewater produced when water is the only lean stream. The method is best suited to single contaminant cases, but can be used for multi-contaminant problems. The method works on the grounds that not all water using processes require absolutely clean water, and can tolerate a certain maximum level of contamination. The method begins with a composite curve composed of the limiting concentration profiles of each process on a plot of concentration versus mass load (Figure 2.8). A water utility line is also drawn, its gradient being inversely proportional to the flowrate. Figure 2.8 shows how the flowrate is then reduced until a pinch forms, representing the minimum feasible flowrate of wastewater.

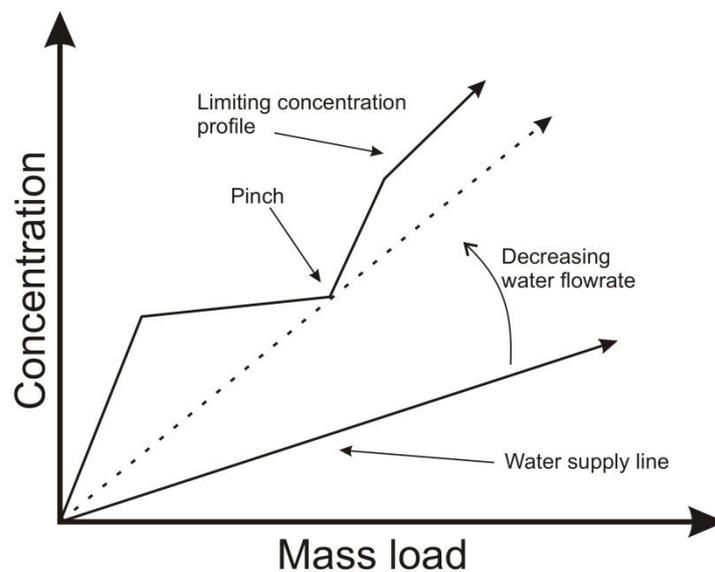


Figure 2.8: Targeting the minimum water flowrate. (Wang & Smith, 1994)

An advantage of using this method is that it does not require any knowledge of the method or mechanics of mass transfer, or the equipment performance. All it requires is a limiting maximum concentration profile for each process. In addition, Wang and Smith (1994) consider the possibility of regenerating the water, while distinguishing between reuse and recycling this regenerated water. Wang and Smith (1994) go on to expand their graphical method further to

incorporate multiple contaminants, but the method is complicated and not well suited to large industrial scale problems.

Olesen and Polley (1997) observe that in cases of regeneration-reuse, there are instances where the method of Wang and Smith (1994) requires some operations to be split in two. A simplified procedure is proposed for targeting and designing wastewater networks using a “load table”, which expresses the contaminant load above and below the pinch for each process. The design procedure is based on inspection and intuition, and the authors themselves state that the method can become complex and is best suited to small problems. The incorporation of water draw-off and multiple sources is also considered, albeit a very short discussion.

Doyle and Smith (1997) develop a mathematical method for targeting the maximum water reuse in a system, based on the concepts of Wang and Smith (1994). They look at two cases, the first based on a fixed mass load and the second based on a fixed outlet concentration. In the first case, the problem results in an NLP, while in the second case the problem results in an LP problem. Since many processes require that a fixed mass load be exchanged, Doyle and Smith propose a combined method wherein the LP problem is solved first, and the solution used as the starting point of the NLP problem. This reduces some of the difficulties associated with NLP problems.

Kuo and Smith (1998a) develop a conceptual and graphical method for designing for minimum water use while keeping in mind the interaction between water use and the effluent treatment system. Their justification is that some effluent treatment systems might work better if, say, the concentration of the contaminant is higher. In this method, instead of using the water supply line as in Figure 2.8, they use a “composite effluent curve” to represent the

interaction between effluent treatment and mass transfer. Kuo and Smith (1998a) also develop the “water mains” method for use in determining the layout of the network that will achieve these targets. This graphical method can be used to design the network by hand in mass integration problems, but can also be used in heat integration problems if modified. Kuo and Smith (1998b) expand upon these developments to include regeneration reuse and regeneration recycling.

Savelski and Bagajewicz (2000a) present and prove a number of necessary conditions for the optimality of water using systems. This stems from their belief that the mathematical methods in existence up until that point are over-complicated and usually result in Non-Linear Programming (NLP) models. These necessary conditions are intended to help linearize the models. Savelski and Bagajewicz (2000b) use these necessary conditions in an algorithmic method for designing the water network for minimum flowrate.

Savelski and Bagajewicz (2001a) further refine this method into a non-iterative algorithmic method. Through the use of necessary and sufficient conditions, it is claimed that the method provides a globally optimal design without the need to target the minimum water flowrate first. The authors also claim that the procedure is sufficiently simple to be carried out by hand for problems of any size. Savelski and Bagajewicz (2001b) propose some linear models for the optimum design of water utilisation systems. These models are either LP or MILP, depending on the choice of objective function

The several works by Savelski and Bagajewicz mentioned above focus on the design of water utilizing systems with only one contaminant. Savelski and Bagajewicz (2003) provide a number of necessary conditions for optimality in the presence of multiple contaminants, similar to those of the single

contaminant case (Savelski & Bagajewicz, 2000a). These new conditions allow the old algorithms to be used in multi-contaminant problems.

Gunaratnam *et al* (2005) develop a solution strategy for minimising multi-contaminant wastewater using LP, MILP and MINLP models. The LP and MILP models are solved iteratively until convergence, and the solution then used as the starting point of the MINLP model. In order to reduce network complexity, the authors include the ability to specify the minimum permissible flowrate in a connection and the maximum number of streams allowed at a mixing point.

2.1.4 Combined Heat and Mass Integration

It seldom happens that water and heat are mutually exclusive on a chemical processing plant. There exist processes in which both heat and water must be considered together. It is widely known that soapy water washes best when it is hot. So too, on a chemical plant one finds processes in which the efficiency and operating characteristics of a water using unit are affected by the temperature. Thus, one can see that there exists a trade-off between water use and energy use.

Srinivas and El-Halwagi (1994) consider the problem of combining heat integration and reactive mass transfer. The economic objectives of minimum heat and minimum water resulted in conflicting designs, and as such should be considered simultaneously in order to obtain the most economic design. Srinivas and El-Halwagi (1994) propose a method that starts by defining sets of rich and lean streams with specified flowrates and supply and target temperatures. Similar to the mass integration model of El-Halwagi and Manousiouthakis (1990), the work by Srinivas and El-Halwagi (1994) considers different solvents as MSAs. Each lean stream, representing a different MSA, is

2 Literature Survey

divided into a number of lean sub-streams, each characterised by a variable composition and temperature. Srinivas and El-Halwagi (1994) make use of an MINLP formulation to solve the problem for minimum operating cost. A simplified LP formulation is also given which may be used to generate a starting point for the MINLP. Srinivas and El-Halwagi (1994) show how the solution for minimum operating cost decomposes the original problem into two sub-problems that may be solved to find the minimum number of heat exchangers required.

Savulescu, Kim and Smith (2005a,b) develop a graphical method for simultaneous integration of heat and mass, with consideration for single contaminant systems. First, Savulescu *et al* (2005a), develop the framework for the procedure while looking at systems with no water reuse. A number of simplifying assumptions are used, some of which are relaxed in the second part.

In Savulescu *et al* (2005a) the focus is on developing the methods of designing the heat exchanger network for the system. By stipulating that there is no water reuse, each process must be supplied with fresh water. Minimising the flowrate of water simply becomes a matter of maximising the outlet concentration of each operation. In order to ensure that the feed water to each operation is heated to the required temperature, and that the effluent is cooled back down to acceptable levels, Savulescu *et al* (2005a) develop a graphical method of designing the heat exchanger network to meet these energy demands. This is based largely on the grid diagram method of Linnhoff and Flower (1978) used in process-process heat integration. The major difference is that in the grid method of Linnhoff and Flower, only sub streams that resulted from the splitting of the same process stream are allowed to be mixed, whereas the method of Savulescu allows the mixing of unrelated water streams, but not processes streams.

Savulescu *et al* (2005b) introduces the option for the reuse of water from one operation to another. Savulescu *et al* (2005b) look at two important aspects of the reuse problem: multiple designs attaining the same minimum target, and the trade-off between direct and indirect heat transfer. The first aspect stems from the observation that different reuse connections can result in the same water target, but different energy targets. The second aspect looks at the trade-off between direct heat transfer, which requires fewer heat exchangers, and indirect heat transfer, which can recover more energy at the expense of additional heat exchangers. To do this, Savulescu *et al* develop a two-dimensional grid diagram.

The two-dimensional grid diagram is similar to the water mains method of Kuo and Smith (1998a), but includes a temperature scale on the vertical axis in addition to the concentration scale on the horizontal axis (Figure 2.9). Here, the operations are positioned between the water mains corresponding to the inlet and outlet concentrations of the operation, and also at the correct vertical height to represent the required temperature. Water streams moving upwards inside the water mains represent cold streams that require heating and water streams moving downwards represent hot stream requiring cooling. This allows matches between the hot and cold streams to be made while exploring the different reuse connections. Again, this method is limited to single contaminant problems, and being a graphical method, it becomes tedious for large problems.

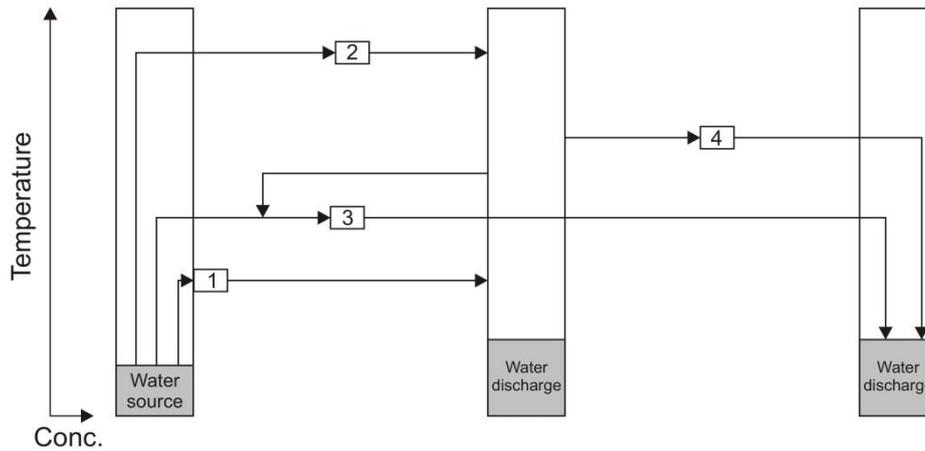


Figure 2.9: Two-dimensional grid diagram. (Kuo & Smith, 1998a)

2.2 Mathematical Programming and Pinch Analysis

The computer is an indispensable tool when applying pinch analysis. In contrast to the graphical methods, methods performed on computers using mathematical programming give accurate results with minimal effort from the user. In this section, some of the models used are presented. Attention is also given to some of the decomposition methods and transformation methods that are used to solve large problems more easily.

2.2.1 Models for Utility System Synthesis

Many of the above methods are graphical, intuitive or algorithmic in nature. This can be desirable in a solution method as it keeps the design engineer involved with the design process. At any stage in the design, the engineer is fully aware of what is happening, and can use his or her knowledge to guide the problem towards the best solution, or to relax the design where potential problems would occur. These methods also have their drawbacks: many methods use simplifying assumptions to begin with, and even then, the

2 Literature Survey

procedures are not accurate and become complicated for large problems. Due to the limitations of a two-dimensional graph, many graphical methods are limited to simple systems, such as single contaminant problems in wastewater minimisation.

An advantage to using mathematical optimisation techniques lies in the ability to handle multiple dimensions. To use optimisation techniques, one must be able to express that which must be optimised as an objective function. The various equations that govern the operation and limit the interactions of the system must then be posed as constraints. This mathematical programming problem can then be solved using an appropriate optimisation routine to give the desired solution. Depending on the structure of the model, a globally optimal solution can either be guaranteed or not.

The advantage to using mathematical models is that commercial optimisation routines are programmed to find the best possible solution quickly and efficiently. By using computers to perform the calculations, one can solve very large problems in a comparatively short time. Furthermore, the accuracy of the obtained solution is only limited by the processing power of the computer, and will usually be much greater than would be needed for any engineering application. The drawback is that the solution method becomes a black-box design. Once the data is supplied, the computer performs its calculations and provides an output without further human involvement.

A mathematical model is only as powerful as the computing technology supporting it. As such, one can observe how the complexity of the various models has grown over the years as the available power of computers has increased. Some of the earliest models for synthesising system designs use heuristic and thermodynamic insights to simplify the models. In a series of three

2 Literature Survey

papers under the direction of Rudd (Rudd, 1968; Musso & Rudd, 1969; Sirola, Powers & Rudd, 1971), knowledge and insight are used to decompose the problem into sub-problems of small enough size to “suite the available technology”. The methods do not make use of any initial structure, but instead attempt to use artificial intelligence along with the heuristics. Similar to this is the method of Nishio *et al* (1980) which uses thermodynamic techniques to develop an LP formulation for the minimisation of energy losses in steam-power systems. The drawback of using heuristic techniques to simplify the problem is that it might preclude the true optimum, leading the optimisation routine to a suboptimal solution.

Grossmann and Santibanez (1980) demonstrate the power of binary variables when they develop an MILP formulation for the synthesis of steam generation systems. Binary variables assume the value of 0 or 1 only, and as such act as a mathematical switch on the various aspects of a design. They assume a value of 1 if the unit, stream or operating condition exists and a value of 0 if it does not exist. This way, several options can be included in the mathematical formulation, and the optimisation routine can select the best option.

As has been mentioned, binary variables can be used to select between available options. This, however, can only be done if these options are present in the problem formulation. For this, a superstructure can be developed which encompasses many options, as demonstrated by Papoulias and Grossmann (1983a, 1983b, 1983c). However, this technique is only as good as the options included in the superstructure.

Papoulias and Grossmann (1983a) develop a technique for finding the optimal structure of the utility section of a chemical process plant. First, an entire process plant is divided into three sections: the chemical plant, the heat recovery

2 Literature Survey

network and the utility systems, with the relation between these sections shown in Figure 2.10. The design of a chemical plant is optimised to meet the production objectives; to produce the required products at the required rate and quality. After the chemical plant has been specified, one can then design and optimise the supporting systems.

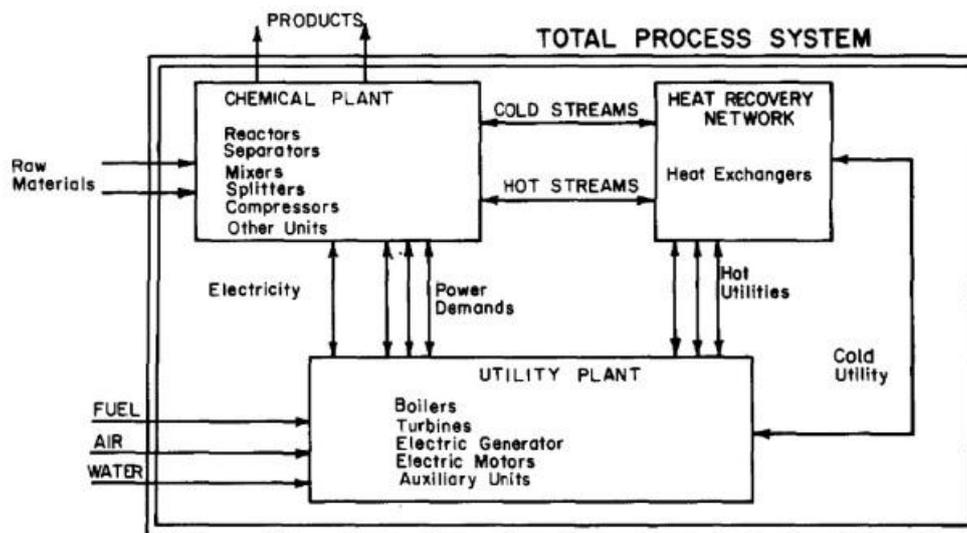


Figure 2.10: The three sections of a total processing plant. (Papoulias & Grossmann, 1983c)

In the first of three papers, Papoulias and Grossmann (1983a) consider the synthesis of the utility plant. A superstructure (Figure 2.11) that includes most of the possible units one would find in a utility plant is developed. Using this, an MILP model of the process is developed, with the objective to minimise the cost of the plant while ensuring that the required utilities are provided. Papoulias and Grossmann (1983a) note that the cost of process equipment is usually a non-linear concave function of the unit's capacity. In order to keep the objective function linear, linear approximations between two bounds are used, or piece-wise linear approximations where needs be. A number of constraints to ensure that each utility demand is met are then established. Where more than one option is available for supplying a utility, binary variables are used to select between options. Binary variables are also used to choose between various

2 Literature Survey

discreet operating conditions for a particular unit. In the formulation, Papoulias and Grossmann (1983a) include constraints that ensure that if two operations are dependent on one another, the existence of one operation forces the existence of the other.

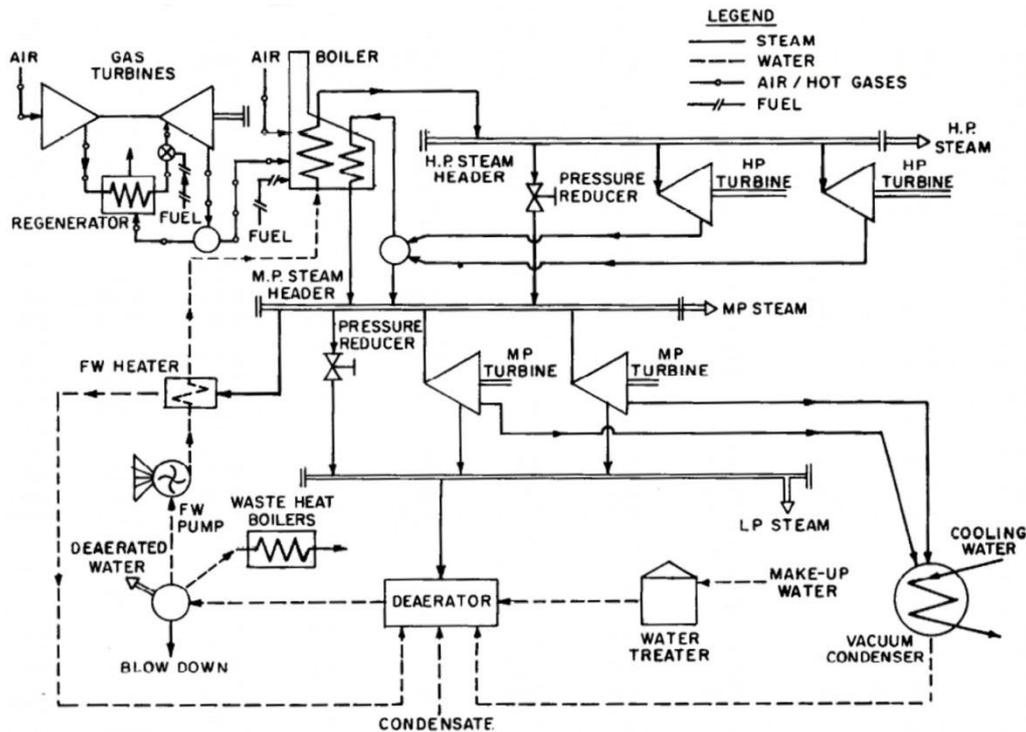


Figure 2.11: Superstructure used to synthesize the utility system. (Papoulias & Grossmann, 1983a)

In the second of three papers, Papoulias and Grossmann (1983b) look at the synthesis of the heat recovery network. An LP formulation is first developed to target the minimum utility costs for the case where there are no forbidden matches. For this, a transshipment model is used to ensure thermodynamic feasibility. In operations research, a transshipment model is a type of problem in which one attempts to minimise the cost of transporting a particular commodity from a set of factories, each with its own production limits, to a set of consumers, each with their own demands, via a number of storage warehouses (Winston & Venkataramanan, 2002). In terms of a heat recovery network, the commodity is heat, the factories are the hot streams, the consumers the cold

streams, and the warehouses are the temperature intervals in which heat transfer occurs. These temperature intervals are important in maintaining the thermodynamic feasibility of heat transfer in the model. The problem table algorithm of Linnhoff and Flower (1978) may be used to obtain these intervals, but Papoulias and Grossmann (1983b) claim that intervals obtained using the methods of Grimes (1980), Cerda *et al* (1981) and Cerda *et al* (1983) yield smaller and faster transshipment models.

Papoulias and Grossmann (1983b) go on further to develop two more MILP formulations: one to target the minimum utility cost for the case where there are forbidden matches, and one to synthesize the network layout. Papoulias and Grossmann (1983c) then provide a number of steps in which all the above mentioned models are linked together and used to synthesize the optimal total utility system.

Floudas and Grossmann (1986) consider the synthesis of heat exchanger networks in multiperiod operation. This type of operation is characterised by changes in the stream flowrates and temperatures over a sequence of time periods. Floudas and Grossmann (1986) use multiperiod adaptations of the LP and MILP transshipment models given by Papoulias and Grossmann (1983) to synthesize their networks. Pintaric and Kravanja (2004) develop an MINLP problem to design flexible and operable networks for multiperiod operation following a two-step process.

Papalexandri and Pistikopoulos (1994a,b) use a multiperiod hyperstructure representation of a heat recovery network to automatically synthesise the network for new or retrofit cases. An iterative framework for the design is developed, based on a multiperiod MINLP model. A total annualised cost is used as the objective function, but the model incorporates a number of very

2 Literature Survey

important additional constraints. Given that the operation is multiperiod, the resulting network must be capable of handling changes in the flow and temperatures of the streams. Papalexandri and Pistikopoulos (1994) emphasise the controllability of the resulting network, considering process disturbances and heat exchanger fouling. Papalexandri and Pistikopoulos (1994) explicitly state that a modified generalised Benders decomposition algorithm was used in the solution procedure.

The optimisation routines used in classical non-linear programming suffer a common problem; all use gradient based information to move towards a minimum or maximum solution. If the objective function surface is not convex, or if the initial solution is poorly chosen, then the routine might converge to a local minimum or fail to converge at all. One of the more recent classes of optimisation techniques being applied to process integration is Genetic Algorithms (GA). These techniques have shown themselves to be less susceptible to local minima and better at finding the global minimum of an NLP model (Rao, 2009).

Genetic Algorithms are based on the evolution theory of animals, using the concept of survival of the fittest. In nature, any particular specimen that exhibits a beneficial genetic mutation will have a better chance at survival, and an increased chance of passing its genetic material on to future generations. So too, in GA optimisation, solution vectors showing low objective values (in minimisation problems) have a better chance of surviving to the next iteration.

The GA procedure begins by randomly generating a number of solution vectors, the initial population. These initial solution vectors are then converted into long continuous binary coded strings. It is these binary strings that will represent the DNA sequence of the “animals”. Once the initial population has been

2 Literature Survey

established, the “fitness” of each specimen is determined by evaluating the objective function; the lower the objective function value, the fitter the specimen is to breed. A number of methods have been proposed to simulate the breeding of the fittest solutions. These all, however, include some way of crossing the genetic material of two parent specimens and adding random mutations (Rao, 2009). This cycle, illustrated in Figure 2.12, is repeated until some convergence criterion is achieved. It is the inclusion of the random mutations that gives GAs their power; a random mutation will cause a specimen to jump away from a local minimum and potentially closer to the global optimum. Since slightly inferior specimens are also allowed to breed, further protection from falling into a local minimum trap is obtained.

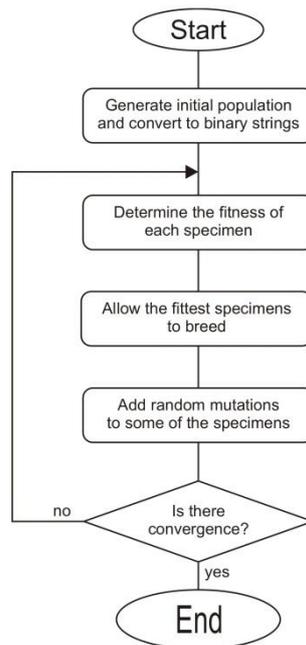


Figure 2.12: Flowchart for the Genetic Algorithm. (Rao, 2009)

The use of a binary string to represent the solution vector is beneficial to process synthesis as many binary variables are used in process synthesis, which are easily handled by GAs. GAs are not very good at handling constraints though; the most common method being to include the constraint in the objective function as penalties (Rao, 2009).

One of the earliest published works on the application of Genetic Algorithms to process synthesis was that of Androulakis and Venkatasubramanian (1991). GAs are used to optimise the structure of the process, whilst simultaneously using a simpler routine to optimise the continuous variables. Lewin, Wang and Shalev (1998) use a similar procedure, but focus on the synthesis of HENs for maximum energy recovery. Firstly, HENs with no stream splitting are analysed, resulting in an MILP. A GA is used to determine the structure of the network, and the Simplex method is used to maximise the resulting LP problem of determining the maximum energy recovery possible for the fixed structures. The maximum of each LP problem is used to determine the fitness of each structure for the next iteration of the GA routine. Secondly, Lewin *et al* (1998) adapt the procedure to take into account stream splitting, which results in an MINLP problem. A GA is still used to fix the network structure, but a new step is added to optimise the stream splits. This decomposes the problem into an LP, which is then treated as above.

Ma *et al* (2008) use a combination of genetic algorithms and simulated annealing algorithms in a formulation for the synthesis of multi-stream heat exchanger networks. As with Papalexandri and Pistikopoulos (1994), these networks are for multiperiod operation. The formulation works in two steps: first one model is solved that over-synthesises the network, and then a second model is used to refine the solution.

2.2.2 Decomposition Methods

The use of mathematical programmes has proven itself to be a very attractive method in the synthesis of heat recovery networks. These methods are readily programmed into software packages for use in a wide variety of problems. Modern mathematical models, however, are making use of an ever increasing

number of variables. These models work well for small problems, but large industrial scale problems generate such overwhelmingly large numbers of variables that it becomes nearly impossible to solve the problem, especially when the problem is non-linear.

One method of combating this problem is to decompose the original problem into a number of sub-problems that are smaller and easier to solve. These methods attempt to use the features of process-process heat integration to provide natural divisions in the system, such as dividing the network synthesis into above pinch and below pinch sections.

Yee *et al* (1990a, b, c) propose a “stage” decomposition method for reducing the size of the problem. In this method, the hot and cold composite curves are divided into a number of stages, as in Figure 2.13. The total number of stages is decided by the user, although Yee *et al* (1990a, b, c) recommend using either the number of hot streams or the number of cold streams as a guide, whichever is larger. The temperatures at which the stages change are not fixed, but rather are treated as variables that will be optimised along with the rest of the system. Yee *et al* (1990a, b, c) then develop an NLP to target simultaneously the minimum utility usage and the minimum exchanger area within these stages. By making the assumption of isothermal mixing, Yee *et al* (1990a, b, c) manage to remove all non-linear terms from the constraints of the formulation. This leaves a non-linear objective function with linear constraints, or alternatively a linear feasible region. Yee *et al* (1990a, b, c) also provide a method of initialising the NLP search, which is claimed to lead to quick solutions with a high probability of being globally optimal. The stage decomposition method has been widely criticised for creating divisions in arbitrary locations, and creating stages that have no physical meaning

2 Literature Survey

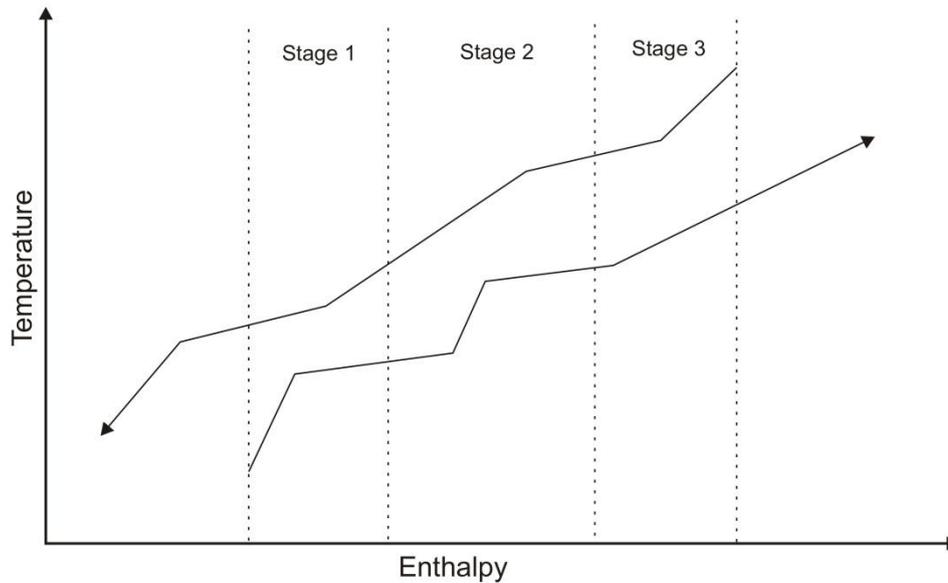


Figure 2.13: Composite curves showing division into stages at arbitrary locations. (Yee et al, 1990)

Zhu *et al* (1995a, b, c) develop the “block” decomposition technique. Like the stage technique, the block technique also uses the composite curves to divide the problem into smaller sections. First, the composite curve is divided at every node, giving the same temperature intervals as the problem table algorithm, following which a number of adjacent temperature intervals are combined in a logical fashion to create a block (Figure 2.14). These blocks begin and end at fixed temperatures and have physical meaning: the boundaries of each block are characterised by the beginning or ending of streams. The design procedure can then be applied individually to each block. Since the blocks have physical meaning, it is easier to obtain a physically significant initial point.

Zhu *et al* (1995a, b, c) develop a MILP problem for area minimisation, and a simple MINLP problem for cost minimisation, both methods using the block decomposed intervals. Either one is solved to provide the initial point for a much more rigorous MINLP in each block. The authors make use of an elegant superstructure for their model, shown in Figure 2.15. It can be seen that this structure allows for most matches between hot and cold streams, as well as for

2 Literature Survey

stream splitting. Additional features can be added to the superstructure to include every possible combination, but these result in very difficult non-linear equations. The simple version in Figure 2.15 is sufficiently accurate when applied to individual blocks, and for obtaining initial solutions. Zhu (1997) uses the same approach, but includes heuristic rules to aid in match selection.

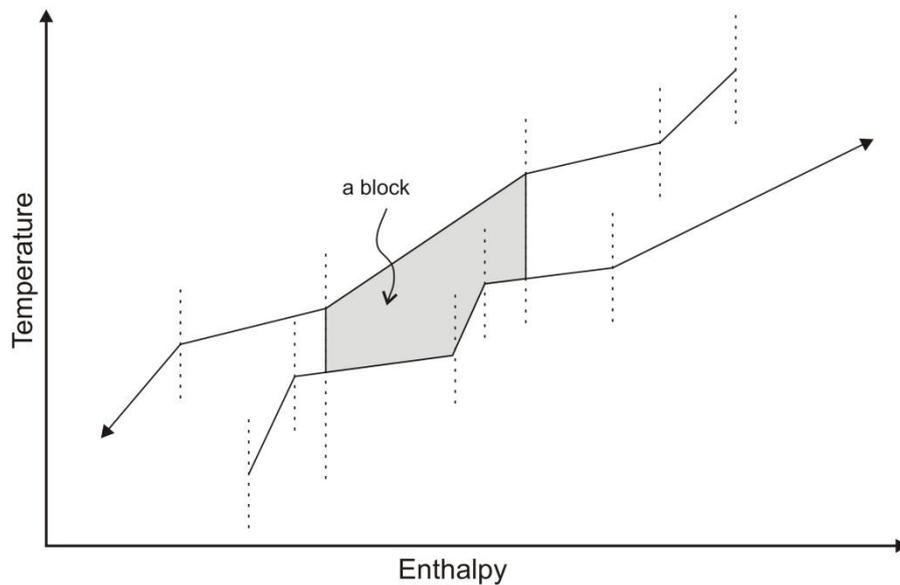


Figure 2.14: Composite curves showing the use of nodes to obtain temperature intervals, and the grouping of intervals to form a block with physical meaning. (Zhu et al, 1995)

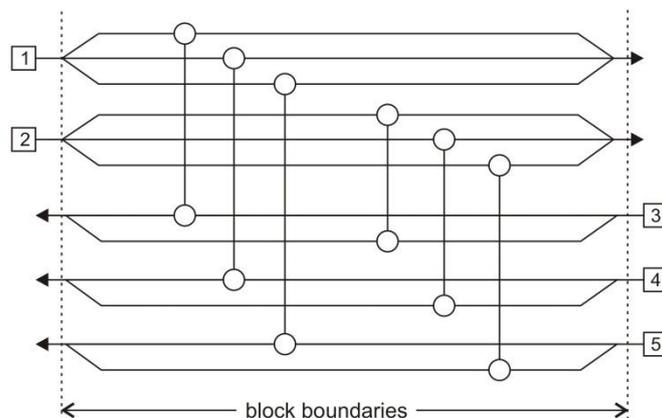


Figure 2.15: Superstructure for two hot streams and three cold streams. (Zhu et al, 1995)

Isafiade and Fraser (2008) use the same superstructure proposed by Zhu *et al* (1995a, b, c) to develop an interval based approach, but an assumption of isothermal mixing is used to remove the non-linear mixing terms. The authors claim that the MINLP model is formulated in such a way that no specialised initialisation technique is required for the first guess in order to obtain the optimal solutions. A distinguishing feature of this model is that it incorporates the option of multiple utilities into its formulation.

2.2.3 Mathematical Transformations

It is well known that LP optimisation problems are significantly easier to solve than their NLP counterparts. A linear problem is guaranteed to converge to a globally optimal solution in a finite number of iterations (Rao, 2009). A convex non-linear problem will still have one global optimum, but will require many more iterations to attain. Difficulties arise in non-convex non-linear problems since local minima exist that could potentially trap an optimisation routine.

Given this insight, one would want to attempt to develop linear models. Physical insights or heuristic rules can be used to remove non-linear terms from the model, but this is not always best, as the use of such techniques might preclude the true global optimum from the design space. A better method is to substitute one of the constraints into the non-linear term. Where this is possible, a linear constraint may be formed that retains all the original information of the system.

It is not always possible to get away from a non-linear problem. In these cases, the best one can do is to ensure that a good initial point is obtained, from which the non-linear solution technique may begin. One way to obtain a good initial

2 Literature Survey

guess is to solve a relaxed form of the original problem. If the original problem can be relaxed to a linear problem, then the new LP model can be solved without the need for an initial guess. The solution to the relaxed model may then be used as the initial guess for whatever NLP solver is to be used.

Glover (1975) introduces a novel method of removing non-linearities occurring due to the product of a binary variable and a continuous variable. Let x be a continuous variable and y a binary variable, both defined as

$$x \in \mathbb{R}, y \in [0,1] \quad (2.1)$$

The product of x and y is now replaced with a new continuous variable

$$xy \equiv \Gamma \quad (2.2)$$

We now see that Γ assumes a value of 0 when y is 0, and a value of x when y is equal to 1. Furthermore, if we know that x has upper and lower bounds

$$X^L \leq x \leq X^U \quad (2.3)$$

then the original non-linear term xy can be replaced with Γ , and the following constraints are added to the formulation:

$$X^L \cdot y \leq \Gamma \leq X^U \cdot y \quad (2.4)$$

$$x - X^U(1 - y) \leq \Gamma \leq x + X^L(1 - y) \quad (2.5)$$

It can be seen that Equations (2.4) and (2.5) are linear in terms of x and y . Using Equation (2.2) to remove non-linear terms and adding Equations (2.4) and (2.5) to the existing constraints is an effective method of removing non-linear terms

2 Literature Survey

arising from the multiplication of a binary and continuous variable. This is an exact transformation technique (Glover, 1975), and as such, will not interfere with finding a globally optimal solution provided the remainder of the formulation is linear.

Another useful linearization technique is that of Quesada and Grossmann (1995) for bilinear terms. A bilinear term arises from the product of two continuous variables, defined as

$$x \in \mathbb{R}, \quad y \in \mathbb{R} \quad (2.6)$$

Again the following substitution is made, keeping in mind that now we are dealing with two continuous variables.

$$xy \equiv \Gamma \quad (2.7)$$

If both of these variables have lower and upper bounds, defined as

$$X^L \leq x \leq X^U \quad (2.8)$$

$$Y^L \leq y \leq Y^U \quad (2.9)$$

then the following constraints arise

$$x - X^L \geq 0 \text{ and } X^U - x \geq 0 \quad (2.10)$$

$$y - Y^L \geq 0 \text{ and } Y^U - y \geq 0 \quad (2.11)$$

Taking the product of the first constraint in both Equations (2.10) and (2.11) one gets

$$X^U Y^U - x Y^U - X^U y + xy \geq 0 \quad (2.12)$$

2 Literature Survey

which is a valid constraint since the product of two positive constraints must be positive itself. Rearranging the terms, the following constraint is obtained.

$$\Gamma \geq xY^U + X^U y - X^U Y^U \quad (2.13)$$

A further three constraints can be derived in a similar fashion using different combinations of Equations (2.10) and (2.11). These are given below.

$$\Gamma \leq xY^U + X^L y - X^L Y^U \quad (2.14)$$

$$\Gamma \leq xY^L + X^U y - X^U Y^L \quad (2.15)$$

$$\Gamma \geq xY^L + X^L y - X^L Y^L \quad (2.16)$$

The bilinear term can thus be removed by making the substituting the term xy for Γ , and adding the four additional constraints to the existing constraints.

This technique is not an exact linearization technique, but it does create a convex solution space (Quesada & Grossmann, 1995). In essence, this technique creates an over-estimating and an under-estimating envelope around the non-linearity. Furthermore, it can be seen that the additional constraints imposed on the linearized systems are all linear in terms of x and y . As stated, this linearization technique is not exact, but the resulting system is easy to solve without an initial starting point. The result of the linear optimisation routine is then used as the initial starting point for the non-linear optimisation routine to get a solution to the original model. Quesada and Grossmann (1995) show that if the solution to both the linear and non-linear models match exactly, then the solution is globally optimal. If the solutions do not match, there is no guarantee that the local optimum found is also globally optimal.

2.3 Utilities

So far, only process-process heat integration has been covered. From Figure 1.1 it is seen that this is the most intuitive form of heat integration; there are both hot streams and cold streams which can be used to reduce the total utility demand of a plant. But there are also the regions of hot and cold utilities in which heat integration might be employed. Although the energy demanded from the utilities is fixed, applying heat integration might improve the efficiency of a piece of equipment, or reduce the purchase cost. Below are discussed both the cold utility and the hot utility.

2.3.1 Cold Utilities

With the exception of a few specialised cases, the dominant cold utility on the typical plant is typically cooling water. Cold water is used to remove heat from a hot stream, and pass it on to the surrounding environment. Most commonly, this is achieved inside of a cooling tower, but where water consumption is restricted, costly dry-cooling radiators can be used.

Bernier (1994) found that there are two very important factors that influence the efficiency of a cooling tower during operation: the flowrate of the water, and the return temperature of the water to the cooling tower. Bernier (1994) found that as the flowrate is decreased or the return temperature increased, the cooling tower effectiveness improves (Figure 2.16). This is convenient, since for a fixed heat load, if the flowrate is decreased the return temperature will rise simultaneously. Kim and Smith (2001) constructed a mathematical model of the performance of a cooling tower and confirmed these observations.

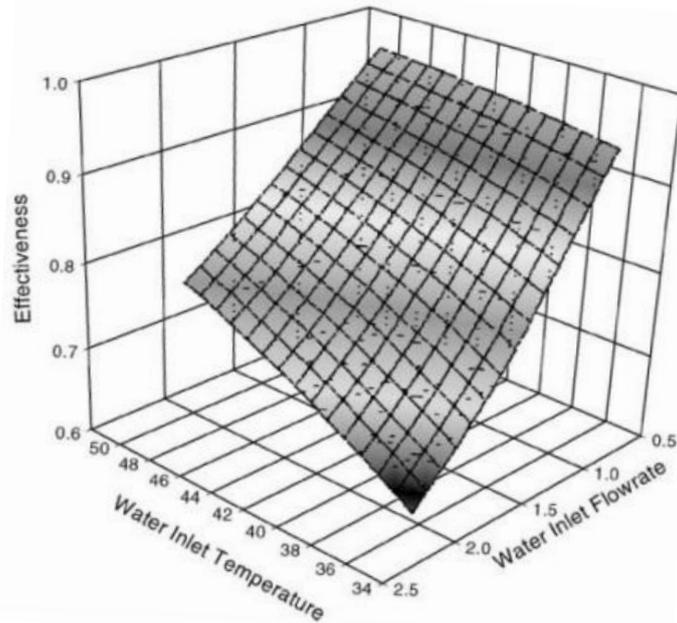


Figure 2.16: Efficiency of a cooling tower as a function of flowrate and return temperature. (Kim & Smith, 2001)

Using the findings of Bernier (1994), Kim and Smith (2001) show how the concepts of pinch may be used to reduce the flowrate of cooling water through the cold utility system, with the objective of optimising the cooling tower performance. Before this, all heat exchangers were placed in parallel and supplied with cold water from the cooling tower. Kim and Smith (2001) adapt the graphical wastewater minimisation method by Wang and Smith (1994), gradually increasing the outlet temperature until a pinch has formed. Kim and Smith (2001) also adapt the water mains method of Kuo and Smith (1998) to design the heat exchanger network that will accomplish this target.

The method of Kim and Smith (2001) is a graphical method that systematically targets the minimum flowrate of cooling water. The procedure begins with a temperature versus enthalpy plot, showing the composite curve comprised of the limiting temperature profiles of the hot streams that must be cooled using cooling water. As shown in Figure 2.17, the cooling water supply line begins at

2 Literature Survey

the temperature supplied by the cooling tower. Since the change in temperature can be represented by

$$\Delta T = \frac{1}{\dot{m}c_p} Q \quad (2.17)$$

it is seen that a reduction in the flowrate will result in an increase in the gradient. The flowrate is reduced by increasing the gradient of the cooling water supply line until a pinch is formed. From this, both the minimum feasible flowrate of cooling water is targeted, as well as the return temperature to the cooling tower. As mentioned, the HEN is then designed using the water mains method.

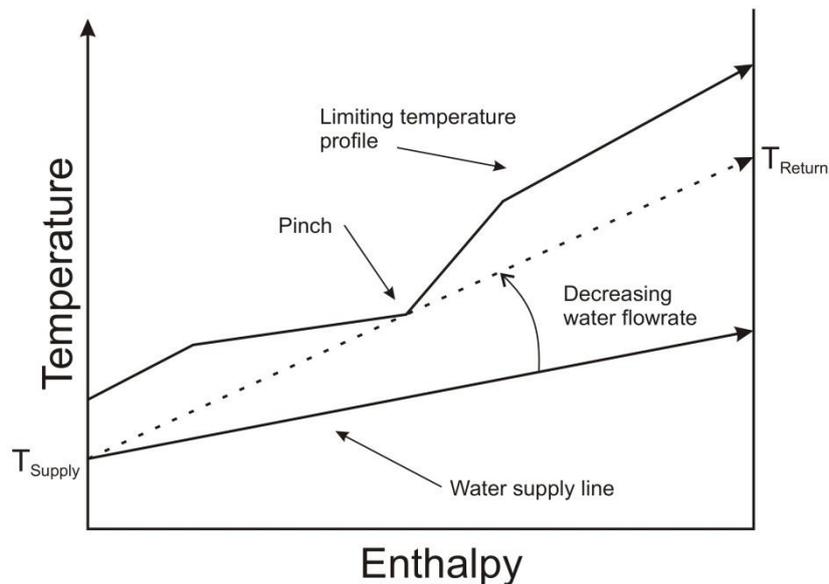


Figure 2.17: Targeting the minimum cooling water flowrate. (Kim & Smith, 2001)

The work by Kim and Smith (2001) represents a holistic approach to the design of a cold utility system. Instead of treating the cooling tower and the HEN as two separate systems, this method treats the whole cold utility system as one operation. By doing this, the effects of the cooling tower on the HEN and vice versa are taken into account. This allows one to manage simultaneously both the energy and water aspects of the cooling system, a point emphasised by Zhelev

(2005). Kim and Smith (2001) also consider the side effects of reduced flowrate and increased temperature, such as fouling.

Kim and Smith (2003) convert the graphical method of Kim and Smith (2001) into a mathematical formulation. Kim and Smith (2003) present a MINLP formulation for the automatic synthesis of cooling water systems in retrofit projects. Of special interest in this work is the inclusion of pressure drop correlations. Kim and Smith (2003) use the Critical Path Algorithm, commonly used in project management, to minimise the total pressure drop of the system. This will be explained in more detail in a later section.

The method of Kim and Smith (2001) assumes that there is only one cooling tower supplying the cold utility. This makes it possible to use a graphical procedure. Majozi and Moodley (2008) consider the use of multiple cooling water sources, and as such resort to mathematical programming. Majozi and Moodley (2008) developed a rigorous superstructure that looks holistically at the cold utility. Through the superstructure, it is possible to include many possible design options. The use of the superstructure also makes it possible for the designer to add custom constraints, based on individual needs.

Majozi and Moodley (2008) identify four cases. In the first, slightly unrealistic case, there are no limitations on either the return temperature or the network topology. Since fouling is likely to occur at elevated temperatures and large plants seldom do not have topology limitations, this case is more of academic interest. In the second case, no limitations are placed on the return temperature of the water, but each water-using process has a specified source and sink. In the third case, there are no topology limitations, but limits are placed on the return temperature to each cooling tower. The fourth and most realistic case imposes limitations on both the return temperature and the topology.

Four models are developed, one for each case. Case 1 results in an LP problem, case 2 in an MILP problem, while cases 3 and 4 both result in MINLP problems. One of the conditions proven by Savelski and Bagajewicz (2000a) is used to remove some non-linear terms. Some non-linear terms still remained in cases 3 and 4, so the authors used the linearization technique of Quesada and Grossmann (1995) to linearize the problems. These linearized forms are then used to obtain an initial point for the non-linear optimization routine.

Gololo and Majozi (2011) also develop a model for the heat integration of cooling water systems supplied by multiple cooling towers. Most importantly, this formulation includes a model of the cooling tower thermal performance. This allows the efficiency of the entire cold utility to be optimised holistically. Gololo and Majozi (2011) consider two cases. In the first case, there are no restrictions on the source and sink of each water using operation, and in the second case the water using operations have a dedicated source and sink. The first case results in an NLP formulation while the second case results in an MINLP formulation. Since the model includes differential equations, Gololo and Majozi (2011) provide a solution algorithm, including the use of a fourth order Runge-Kutta method for approximating the solution of differential equations.

2.3.2 Hot Utilities

As with the cold utility, it is possible to apply heat integration to the hot utility. The type of utility used depends on the process, and can vary from hot oil to steam to furnaces. The most common form of hot utility in use is steam. In practice, steam is raised in a boiler and then supplied to a number of heat exchangers where it is allowed to condense, providing latent heat to the process

stream. When dealing with the design of steam systems, there are two important aspects: selecting the best levels of steam, and designing the HEN.

As was discussed in section 2.2.1, Papoulias and Grossmann (1983) developed a superstructure that contains a wide variety of utilities. Included in the superstructure are three levels of steam. The mathematical model selects, amongst other things, whether the steam should be supplied by a boiler, by turbine exhaust or by letting down higher level steam.

Marechal and Kalitventzeff (1998) discuss the use of an MILP formulation to integrate the hot utility on a site scale. Using the same concept as Hui and Ahmad (1994), steam headers are used as a means to transport energy from one process on the site to another. As such, the levels of the utility must be optimised to perform the necessary tasks required, and to provide the best process-process heat integration between the various regions of the site.

Mavromatis and Kokossis (1998a,b) consider the interactions between the various levels of steam and the turbines used to provide mechanical power. A number of models are developed; both to select between steam levels and to synthesize the network of turbines and their connection to the steam levels. A model of turbine efficiency is also developed which is subsequently used by Shang and Kokossis (2004).

Shang and Kokossis (2004) develop an MILP formulation to optimise the steam levels of a total site utility for multiperiod operation. A transshipment model is used as the basis of the formulation. To this constraints are added for the efficiency of the boiler and turbines, and to ensure that the turbines provide the required power. The turbine hardware model (THM) from Mavromatis and Kokossis (1998) is used, and a new boiler hardware model (BHM) is developed.

Abdallah & Ismail (2001) further explain how proper consideration for the efficiency of a boiler and the correct insulation is essential to the optimum operation of a utility system.

Coetzee and Majozi (2008), following the work of Kim and Smith (2001) and Moodley and Majozi (2008), develop a method of minimising the flowrate of steam through the HEN by utilising hot liquid condensate and reuse streams. The motivation for this comes from the observation that the cost of a boiler increases rapidly with required flowrate. Minimising the flowrate of steam will thus minimise the cost of the boiler. Coetzee and Majozi (2008) develop both a graphical method and mathematical model for targeting the minimum steam flowrate for single level problems. In the case of the graphical method, a separate LP model is used to synthesize the HEN after the minimum steam flowrate is targeted. In the second MILP model, the targeting and synthesis are performed simultaneously.

Price and Majozi (2010a) continue the work of Coetzee and Majozi (2008) by focusing on sustained boiler efficiency. It is shown that in order to maintain a constant efficiency, the return temperature to the boiler must be increased as the flowrate of steam is decreased. Since in the model by Coetzee and Majozi (2008), both the flowrate and the return temperature are reduced simultaneously, the efficiency of the boiler is reduced and more energy is required to provide the required hot utility.

Price and Majozi (2010a) include the boiler efficiency model developed by Shang and Kokossis (2004) in their formulation to minimise the loss in boiler efficiency. In order to raise the return temperature to the boiler, two possibilities are considered: sensible heat from the superheated steam supplied to the processes can be used (Figure 2.18a), or a dedicated preheater can be employed

2 Literature Survey

(Figure 2.18b). In both cases, the model allows the designer to choose whether to minimise the flowrate while relaxing the boiler efficiency, or to keep the efficiency constant while relaxing the minimum flowrate.

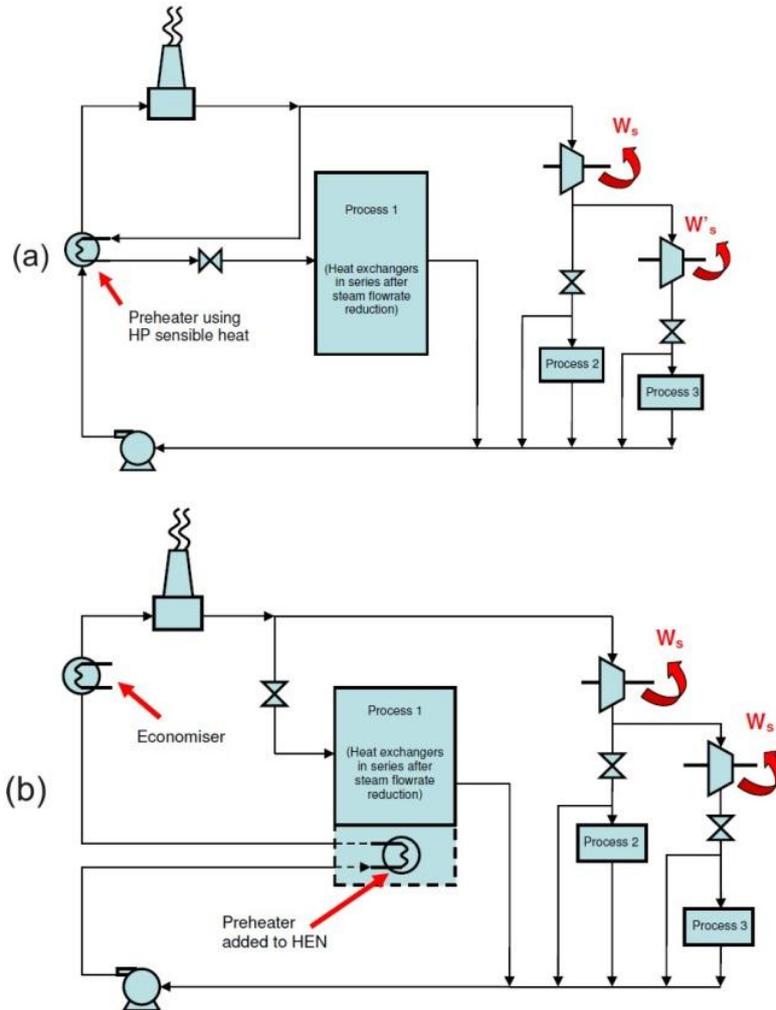


Figure 2.18: Two methods of preserving boiler efficiency: (a) using sensible heat (b) using a dedicated preheater. (Price & Majozi, 2010a)

Price and Majozi (2010b) include the possibility of multiple steam levels to the above model. An adapted version of the superstructure developed by Coetzee and Majozi (2008) is used to minimise the total flowrate of steam across the multiple levels while maintaining boiler efficiency.

Price and Majozi (2010c) further consider the pressure drop of the HEN. Coetzee and Majozi (2008) noted that in some instances, multiple network

configurations exist that are capable of attaining the minimum flowrate. After targeting the minimum steam flowrate, Price and Majozi (2010c) use the Critical Path Algorithm to synthesize the network for minimum pressure drop while keeping the flowrate fixed at the target, similar to Kim and Smith (2003). They use pressure drop correlations developed by Nie (1998), Nie and Zhu (1999) and Zhu and Nie (2002)

2.4 Pressure Drop Considerations

The following is a brief description of the method used by Price and Majozi (2010c) for pressure drop calculations. The correlation for the pressure drop over the tube side of a heat exchanger was derived by Nie (1998) and is written in terms of mass flowrate by Price and Majozi (2010c):

$$\Delta P_t = N_{t1} \dot{m}_t^{1.8} + N_{t2} \dot{m}_t^2 \quad (2.18)$$

$$N_{t1} = \frac{1.115567}{\pi^{2.8}} \frac{\mu^{0.8} n_{tp}^{2.8} A}{\rho N_t^{2.8} d_o d_i^{4.8}} \quad (2.19)$$

$$N_{t2} = \frac{20}{\pi^2} \frac{n_{tp}^3}{\rho N_t^2 d_i^4} \quad (2.20)$$

These correlations are for a homogenous liquid phase on the tube side of a heat exchanger. For the case of a vapour (steam), condensing to form a liquid, Kern (1950) suggests using 50% of the pressure drop predicted for the homogenous liquid case.

2 Literature Survey

Kim and Smith (2003) provide the following correlation for the pressure drop in a pipe. Again, it is rewritten to be a function of mass flowrate (Price & Majozi, 2010c).

$$\Delta P_p = N_p \frac{1}{\dot{m}_p^{0.36}} \quad (2.21)$$

$$N_p = \frac{188.318}{\pi^{1.8}} \rho^{0.536} \mu^{0.2} L \quad (2.22)$$

Price and Majozi (2010c) adapt the model developed by Kim and Smith (2003) for minimising the pressure drop over the HEN. The method makes use of the Critical Path Algorithm, widely used in the field of project management to locate the path of tasks that is most constrained, and hence the path determining the minimum duration of the project. The pressure drop model uses the “activity on arc” model (Winston & Venkataramanan, 2002), where the nodes represent mixing and splitting points, and the arcs represent pressure drops, either due to a heat exchanger, or due to process piping. Price and Majozi (2010c) use a new superstructure (Figure 2.19) that accommodates the phase change experienced in steam flowrate minimisation.

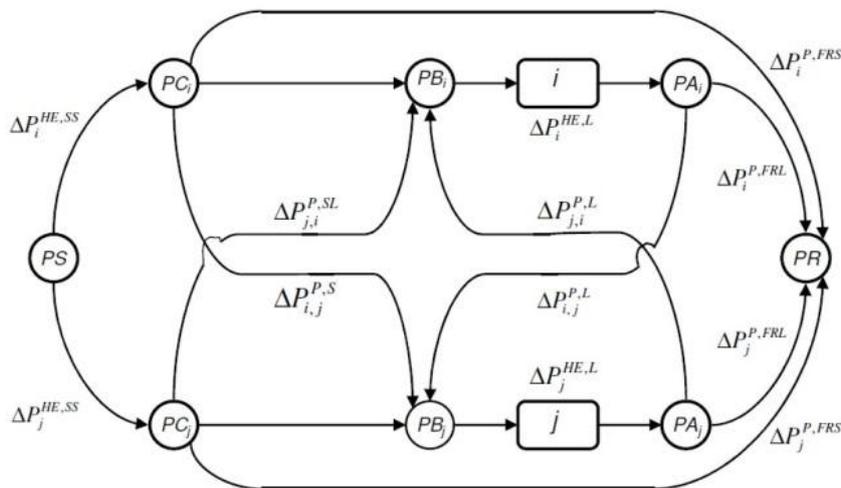


Figure 2.19: Superstructure for minimising pressure drop over a HEN. (Price & Majozi, 2010c)

2 Literature Survey

The foundation of the Critical Path Algorithm, as applied to HENs, is that the difference between the pressures of two nodes must be equal to or greater than the pressure drop of the arc connecting the two nodes directly. Consider the hypothetical network shown in Figure 2.20. The pressure drop in the pipe connecting nodes A and B is 7 kPa. However, this does not mean that the difference in pressure between A and B is 7 kPa. If one follows the path ACB then one will find that the pressure drop from A to B is now 19 kPa. Thus the constraint for the arc AB is

$$P_A - P_B \geq \Delta P_{A,B} \quad (2.23)$$

Similar constraints must be developed for each arc in the network.

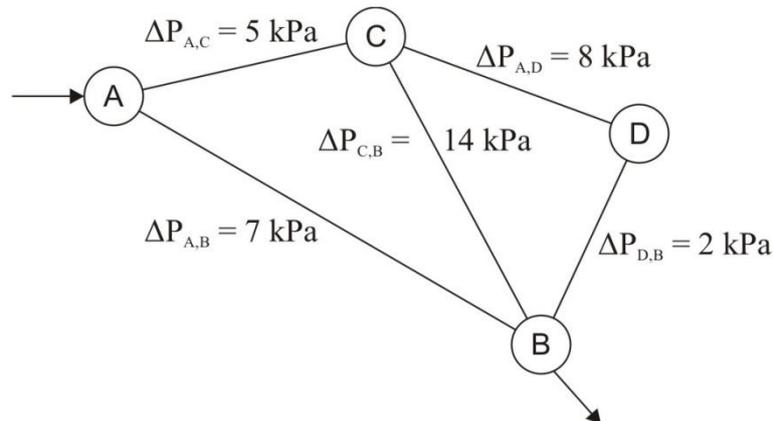


Figure 2.20: Example illustrating the Critical Path Algorithm.

If the topology of the final network is known, then finding the critical path results in an LP problem. The superstructure used by Price and Majozi (2010c) is a general representation containing all possible connections. Since many of these connections will not feature in the final topology, Price and Majozi (2010c) modify Equation 2.23 to include a binary variable indicating whether or not the stream exists:

$$P_A - P_B + M(1 - y_{A,B}) \geq \Delta P_{A,B} \quad (2.24)$$

Here, M is a sufficiently large value and $y_{A,B}$ is a binary variable indicating the existence of a stream connecting nodes A and B. If the stream does not exist, the large number M dominates the constraint and the constraint is automatically satisfied. If the stream does exist, the last term on the left hand side becomes zero and the constraint becomes active. Price and Majozi (2010c) use this constraint, along with others, to synthesize the HEN for minimum pressure drop once the minimum flowrate had been targeted and fixed.

2.5 Exergy Analysis

All of the methods discussed up until this point, with the exception of Umeda *et al* (1979) have made use of only the first law of thermodynamics: the conservation of energy. In pinch analysis, the focus is on the quantity of heat and not the quality. The only use of the second law of thermodynamics lies in the constraint that heat cannot be transferred from a cold stream to a hot stream. Here, the second law is not being used to add value to the design method but to exclude infeasible designs.

Like pinch analysis, there exist methods of providing heat integration using “second law analysis” or “exergy analysis”. Here, the available energy or “exergy” is the central focus, and methods are sought that provide feasible designs that are not wasteful of this exergy. As Tsatsaronis (1999) states, the trouble with exergy analysis is that it lacks a formal method of execution. Whereas pinch analysis has clear and easily followed procedures, exergy analysis uses intuitive methods and relies on the “artistry of the engineer”. The strength of exergy analysis lies in its ability to point out gross inefficiencies in a

process. Exergy analysis does not provide a way of correcting these problems, experience and knowledge is used to propose better solutions.

In a series of two papers, pinch analysis and exergy analysis are pitted against each other in a response to a challenge posed by Bodo Linnhoff. Both papers look at the integration of a new nitric acid production unit into an existing site. The challenge is to provide as much saving as possible through the application of the respective techniques. Linnhoff and Alanis (1991), the advocates for pinch technology, use the principles of pinch to bring about the energy savings common to this method. Gaglioli *et al* (1991), the advocates for exergy analysis, use the concepts of exergy to bring about similar savings. Although it is reported that exergy analysis resulted in savings roughly four times that of pinch analysis, these results are inconclusive since the authors of both papers accuse each other of cheating and making unjustifiable assumptions where information was lacking.

Sama (1995a) gives a brief introduction to the use of exergy analysis in process design. It is shown how exergy analysis can be used to point out “second law errors” and provide ways of correcting these errors to bring about energy savings. A list of 13 “common-sense second law guidelines” is provided to aid engineers in designing energy efficient processes. Sama (1995a) also emphasises greatly the dangers of putting too much faith in a globally optimal solution. Sama (1995a) argues that when so many uncertainties exist in the pricing and operating data, the global optimum given by pinch analysis has no significant meaning. Rather, it is proposed that the designer should be flexible and explore other options in the region of the global optimum.

Sama (1995b) compares, once again, the differences between pinch and exergy analysis. A small problem first solved by Linnhoff (1989) is used. The problem

2 Literature Survey

considers an existing industrial process with two hot streams and two cold streams. Linnhoff (1989) uses pinch analysis to reduce the energy consumption of the HEN by 56.6 %, meeting the Maximum Energy Recovery (MER) target. Sama (1995b) uses the common-sense law given by Sama (1995a) to design an intuitive HEN that reduced the energy consumption by 43.5%. Although this does not meet the MER target, it represents a significant saving for a network designed using nothing more than a few heuristics. Sama (1995b) goes further to explain how a deeper exergy analysis of the system can design a HEN to meet MER targets, although this network has one extra heat exchanger compared to the design of Linnhoff (1989).

Although pinch analysis has gained a wider following in the engineering world, exergy analysis should not simply be ignored. There is much that can be gained from exergy analysis. Concepts from exergy analysis can be used to guide pinch analysis towards better solutions. For example, one of the common-sense rules given by Sama (1995a) states that the throttling of superheated steam to form saturated steam should be avoided. In the case where Price and Majozi (2010a) look at two options for preheating the boiler return, using sensible superheat or using a dedicated preheater, the common-sense law indicates the former option to be superior to the latter. Indeed, this is the conclusion Price and Majozi (2010a) came to. Here, exergy analysis could have been used to choose the better option before testing both models. Exergy analysis should not be forgotten, but rather used as a tool to help pinch analysis.

2.6 References

- Abdallah, A. M., & Ismail, A. L. (2001). Saving energy lost from steam boiler vessels. *Renewable Energy*, 23, 537–550.
- Adonyi, R., Romero, J., Puigjaner, L., & Friedler, F. (2003). Incorporating heat integration in batch process scheduling. *App. Therm. Eng.*, 23, 1743-1762.
- Ahmad, S., & Polley, G. T. (1990). Debottlenecking of heat exchanger networks. *Heat Recovery Systems & CHP*, 10(4), 369-385.
- Androulakis, I. P., & Venkatasubramanian, V. (1991). A genetic algorithmic framework for process design and optimisation. *Comp. Chem. Eng.*, 15, 217-228.
- Bernier, M. A. (1994). Colling tower performance: Theory and experiments. *ASHRAE Trans. Res.*, 100, 114-121.
- Cerda, J., Westerberg, A. W., Mason, D., & Linnhoff, B. (1981). Minimum utility usage in heat exchanger network synthesis- a transportation problem. Tech. Rep. DRC-06-25-81. Pittsburgh: Carnegie-Mellon University.
- Cerda, J., Westerberg, A. W., Mason, D., & Linnhoff, B. (1983). Minimum utility usage in heat exchanger network synthesis: a transportation problem. *Chem. Eng. Sci.*, 38(3), 373-387.
- Coetzee, W. A., & Majozi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Doyle, S. J., & Smith, R. (1997). Targeting water reuse with multiple contaminants. *Trans IChemE*, 78(B3), 181-189.

- El-Hawagi, M. M., & Manousiouthakis, V. (1990). Automatic synthesis of mass-exchange networks with single-component targets. *Chem. Eng. Sci.*, 45(9), 2813-2831.
- Floudas, C. A., & Grossmann, I. E. (1986). Synthesis of flexible heat exchanger networks for multiperiod operation. *Comp. Chem. Eng.*, 10(2), 153-168.
- Gaggioli, R. A., Sama, D. A., Qian, S., & El-Sayed, Y. M. (1991). Integration of a new process into an existing site: A case study in the application of exergy analysis. *Journal of Engineering for Gas Turbines and Power*, 113, 170-183.
- Glover, F. (1975). Improved linear integer programming formulaions of nonlinear integer problems. *Management Science*, 22(4), 455-460.
- Gololo, K. V., & Majozi, T. (2011). On synthesis and optimization of cooling water systems with multiple cooling towers. *Ind. Eng. Chem. Res.*, 50, 3775-3787.
- Grimes, L. E. (1980). The synthesis and evaluation of networks of heat exchangers that feature the minimum number of units. MSc Thesis: Carnegie-Mellon University.
- Grossmann, I. E., & Santibanez, J. (1980). Applications of mixed integer linear programming in process synthesis. *Comp. Chem. Eng.*, 4, 205-214.
- Gunaratnam, M., Alva-Argaez, A., Kokossis, A., Kim, J. K., & Smith, R. (2005). Automated design of total water systems. *Ind. Eng. Chem. Res.*, 44, 588-599.
- Hohmann, E. C. (1971). Optimum networks for heat exchange. PhD Thesis: University of Southern California.

- Huang, F., & Elshout, R. V. (1976). Optimizing the heat recovery of crude units. *Chem. Eng. Progr.*, 72, 68-74.
- Hui, C. W., & Ahmad, S. (1994). Total site heat integration using the utility system. *Comp. Chem. Eng.*, 18(8), 729-742.
- Isafiade, A. J., & Fraser, D. M. (2008). Interval-based MINLP superstructure synthesis of heat exchange networks. *Chem. Eng. Res. & Design*, 86, 245-257.
- Kemp, I. C. (2007). *Pinch Analysis and Process Integration: a User Guide on Process Integration for the Efficient Use of Energy*. Great Britain: Butterworth-Heinemann.
- Kim, J. K., & Smith, R. (2001). Cooling water system design. *Chem. Eng. Sci.*, 56, 3641-3658.
- Kim, J. K., & Smith, R. (2003). Automated retrofit Design of cooling-water systems. *AIChE J.*, 49(7), 1712-1730.
- Kuo, W. C., & Smith, R. (1998a). Designing for the interactions between water-use and effluent treatment. *Trans IChemE*, 76(Part A), 287-301.
- Kuo, W. C., & Smith, R. (1998b). Design of water-using systems involving regeneration. *Trans IChemE*, 76(Part B), 94-114.
- Lewin, D. R. (1998). A generalized method for HEN synthesis using stochastic optimization - II The synthesis of cost-optimal networks. *Comp. Chem. Eng.*, 22(10), 1387-1405.
- Lewin, D. R., Wang, H., & Shalev, O. (1998). A generalized method for HEN synthesis using stochastic optimization - I General framework and MER optimal synthesis. *Comp. Chem. Eng.*, 22(10), 1503-1513.

- Linnhoff, B., (1989). Pinch technology for the synthesis of optimal heat and power systems. *ASME Journal of Energy Resources Technology*, 111, 137-147.
- Linnhoff, B., & Alanis, F. J. (1991). Integration of a new process into an existing site: A case study in the application of pinch technology. *Journal of Engineering for Gas Turbines and Power*, 113, 159-169.
- Linnhoff, B., & Flower, J. R. (1978a). Synthesis of heat exchanger networks: I. systematic generation of energy optimal networks. *AICHE J.*, 24(4), 633-642.
- Linnhoff, B., & Flower, J. R. (1978b). Synthesis of heat exchanger networks: II. evolutionary generation of networks with various criteria of optimality. *AICHE J.*, 24(4), 642-654.
- Linnhoff, B., & Hindmarsh, E. (1983). The pinch design method for heat exchanger networks. *Chem. Eng. Sci.*, 38(5), 745-763.
- Linnhoff, B., Mason, D. R., & Wardle, I. (1979). Understanding heat exchanger networks. *Comp. & Chem. Eng.*, 3, 295-302.
- Ma, X., Yao, J., Luo, X., & Roetzel, W. (2008). Synthesis of multi-stream heat exchanger network for multi-period operation with genetic/simulated annealing algorithms. *App. Therm. Eng.*, 28, 809-823.
- Majozi, T. (2009). Heat integration of multipurpose batch plants using a continuous-time framework. *App. Therm. Eng.* 26, 1369-1377.
- Majozi, T. (2009). Minimization of energy use in multipurpose batch plants using heat. *Journal of Cleaner Production*, 17, 945-950.

- Majozi, T., & Moodley, A. (2008). Simultaneous targeting and design for cooling water systems with multiple cooling water supplies. *Comp. Chem. Eng.*, 32, 540-551.
- Marechal, F., & Kalitventzeff, B. (1998). Energy integration of industrial sites: tools, methodology and application. *App. Therm. Eng.*, 18, 921-933.
- Mavromatis, S. P., & Kokossis, A. C. (1998a). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Mavromatis, S. P., & Kokossis, A. C. (1998b). Conceptual optimisation of utility networks for operational variations -II. Network development and optimisation. *Chem. Eng. Sci.*, 53(8), 1609-1630.
- Musso, A. H., & Rudd, D. F. (1969). The synthesis of system designs: II Heuristic Structuring. *AIChE J.*, 15, 10-17.
- Nie, X. (1998). Heat exchanger network retrofit considering pressure drop and heat transfer enhancement. PhD Thesis: UMIST, Manchester.
- Nie, X., & Zhu, X. X. (1999). Heat exchanger retrofit considering pressure drop and heat transfer enhancement. *AIChE J.*, 5, 1239-1254.
- Nishio, M., Itoh, J., Shiroko, K., & Umeda, T. (1980). Thermodynamic approach to steam and power systems design. *Ind. Eng. Chem.*, 19, 306-312.
- Olesen, S. G., & Polley, G. T. (1997). A simple methodology for the design of water networks handling single contaminants. *Trans. IChemE* , 75(Part A), 420-426.

- Papageorgiou, L.G., Shah, N., & Pantelides, C.C. (1994). Optimal scheduling of heat-integrated multipurpose plants. *Ind. Eng. Chem. Res.*, 33, 3168-3186.
- Papalexandri, K. P., & Pistikopoulos, E. N. (1994a). Synthesis and retrofit of operable heat exchanger networks.1. Flexibility and structural controllability aspects. *Ind. Eng. Chem. Res.*, 33, 1718-1737.
- Papalexandri, K. P., & Pistikopoulos, E. N. (1994b). Synthesis and retrofit of operable heat exchanger networks.2. Dynamics and control structure considerations. *Ind. Eng. Chem. Res.*, 33, 1738-1755.
- Papoulias, S. A., & Grossmann, I. E. (1983a). A structural optimization approach in process synthesis - I Utility systems. *Comp. Chem. Eng.*, 7(6), 695-706.
- Papoulias, S. A., & Grossmann, I. E. (1983b). A structural optimization approach in process synthesis - II Heat recovery networks. *Comp. Chem. Eng.*, 7(6), 707-721.
- Papoulias, S. A., & Grossmann, I. E. (1983c). A structural optimization approach in process synthesis - III Total processing systems. *Comp. Chem. Eng.*, 7(6), 723-734.
- Pintaric, Z. N., & Kravanja, Z. (2004). A strategy for MINLP synthesis of flexible and operable processes. *Comp. Chem. Eng.*, 28, 1105-1119.
- Price, T., & Majozi, T. (2010a). On Synthesis and Optimization of Steam System Networks. 1. Sustained Boiler Efficiency. *Ind. Eng. Chem. Res.*, 49, 9143-9153.
- Price, T., & Majozi, T. (2010b). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.

- Price, T., & Majazi, T. (2010c). On Synthesis and Optimization of Steam System Networks. 3. Pressure Drop Consideration. *Ind. Eng. Chem. Res.*, 49, 9165-9174.
- Quesada, I., & Grossmann, I. E. (1995). Global optimisation of bilinear process networks with multi component flows. *Comp. Chem. Eng.*, 19(12), 1219-1242.
- Rao, S. S. (2009). *Engineering Optimization: Theory and Practice*. Hoboken: John Wiley & Sons.
- Rudd, D. F. (1968). The synthesis of system designs: I. Elementary decomposition theory. *AIChE J.*, 14, 343-349.
- Sama, D. A. (1995a). The use of the second law of thermodynamics in process design. *Journal of Energy Resources Technology*, 117, 179-185.
- Sama, D. A. (1995b). Differences between second law analysis and pinch technology. *Journal of Energy Resources Technology*, 117, 186-191.
- Savelski, M. J., & Bagajewicz, M. J. (2000a). On the optimality conditions of water utilization systems in process plants with single contaminants. *Chem. Eng. Sci.*, 55, 5035-5048.
- Savelski, M. J., & Bagajewicz, M. J. (2000b). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.
- Savelski, M. J., & Bagajewicz, M. J. (2001a). Algorithmic procedure to design single component water utilization systems in process plants. *Chem. Eng. Sci.*, 56(5), 1897-1912.

- Savelski, M. J., & Bagajewicz, M. J. (2001b). On the use of linear models for the design of water utilization systems in refineries and process plants. *Chem. Eng. Res. & Design*, 79(A5), 600-610.
- Savelski, M. J., & Bagajewicz, M. J. (2003). On the optimality conditions of water utilization systems in process plants with multiple contaminants. *Chem. Eng. Sci.*, 58, 5349-5362.
- Savulescu, L., Kim, J. K., & Smith, R. (2005a). Studies on simultaneous energy and water minimisation-Part I: Systems with no water reuse. *Chem. Eng. Sci.*, 60, 3279-3290.
- Savulescu, L., Kim, J. K., & Smith, R. (2005b). Studies on simultaneous energy and water minimisation-Part II: Systems with maximum re-use of water. *Chem. Eng. Sci.*, 60, 3291-3308.
- Seider, W. D., Seader, J. D., & Lewin, D. R. (2004). *Product & Process Design Principles*. USA: John Wiley & Sons.
- Shang, Z., & Kokossis, A. (2004). A transshipment model for the optimisation of steam levels of total site utility systems. *Comp. Chem. Eng.*, 28, 1673-1688.
- Siirola, J. J., Powers, G. J., & Rudd, D. F. (1971). The synthesis of system designs: III Toward a process concept generator. *AIChE J.*, 17, 677-682.
- Srinivas, B.K., & El-Halwagi, M.M. (1994). Synthesis of combined heat and reactive mass-exchange networks. *Chem. Eng. Sci.*, 49, 2059-2074.
- Stamp, J. D., & Majози, T. (2011). Optimum heat storage design for heat integrated multipurpose batch plants. *Energy*, 36, 5119-5131.

- Townsend, D. W., & Linnhoff, B. (1983a). Heat and power networks in process design. I. Criteria for placement of heat engines and heat pumps in process networks. *AIChE J.*, 29, 742-748.
- Townsend, D. W., & Linnhoff, B. (1983b). Heat and power networks in process design. II. Design procedure for equipment selection and process matching. *AIChE J.*, 29, 748-771.
- Tsatsaronis, G. (1999). Strengths and limitations of exergy analysis. In A. Bejan, & E. Mamut, *Thermodynamic optimization of complex energy systems* (pp. 93-100). Netherlands: Kluwer Academic Publishers.
- Umeda, T., Harada, T., & Shiroko, K. (1979). A thermodynamic approach to the synthesis of heat integration systems in chemical processes. *Comp. Chem. Eng.*, 3, 273-282.
- Vaselenak, J. A., Grossmann, I. E., & Westerberg, A. W. (1986). Heat integration in batch processing. *Chem. Eng. Sci.*, 25, 357-366.
- Wang, Y. P., & Smith, R. (1994). Wastewater minimisation. *Chem. Eng. Sci.*, 49(7), 981-1006.
- Wang, Y. P., & Smith, R. (1995). Time pinch analysis. *Trans IChemE*, 73, 905-914.
- Winston, W. L., & Venkataramanan, M. (2002). *Introduction to mathematical programming* (4th ed., Vol. 1). Duxbury Press.
- Yee, T. F., Grossmann, I. E., & Kravanja, Z. (1990a). Simultaneous optimization models for heat integration - I. Area and energy targeting and modeling of multi-stream exchangers. *Comp. Chem. Eng.*, 14(10), 1151-1164.

- Yee, T. F., & Grossmann, I. E. (1990b). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comp. Chem. Eng.*, 14(10), 1165-1184.
- Yee, T. F., Grossmann, I. E., & Kravanja, Z. (1990c). Simultaneous optimization models for heat integration - III. Process and heat exchanger network optimization. *Comp. Chem. Eng.*, 14(11), 1185-1200.
- Zhelev, T. K. (2005). Water conservation through energy management. *Journal of Cleaner Production*, 13, 1395-1404.
- Zhu, X. X. (1997). Automated design method for heat exchanger network using block decomposition and heuristic rules. *Comp. Chem. Eng.*, 21(10), 1095-1104.
- Zhu, X. X., & Nie, X. (2002). Pressure drop considerations for heat exchanger network grassroots design. *Comp. Chem. Eng.*, 26, 1661-1676.
- Zhu, X. X., O'Neill, B. K., Roach, J. R., & Wood, R. M. (1995a). A new method for heat exchanger network synthesis using targeting procedures. *Comp. Chem. Eng.*, 19(2), 197-222.
- Zhu, X. X., O'Neill, B. K., Roach, J. R., & Wood, R. M. (1995b). Area-targeting methods for the direct synthesis of heat exchanger networks with unequal film coefficients. *Comp. Chem. Eng.*, 19(2), 223-239.
- Zhu, X. X., O'Neill, B. K., Roach, J. R., & Wood, R. M. (1995c). A method for automated heat exchanger network synthesis using block decomposition and non-linear optimization. *Trans. IChemE*, 73(A), 919-930.

Chapter 3

Background

The purpose of this section is to give background information that is imperative to understanding the work presented in the sections to come. These brief explanations are sufficient to enable one to understand the work in sections to come, but represent condensed versions of the original works. Should one require greater insight into a particular topic, then the referenced work should be consulted.

3.1 System Description

Although steam systems differ from plant to plant, all steam systems will have common elements. One or more boilers must always be present to raise the required steam. There will also be a heat exchanger network which will utilise the steam for heating process streams and equipment. In addition to this, there might be a set of turbines to provide shaft work if needed, and then the process piping and other auxiliary pieces of equipment to ensure the proper functioning of the steam system. Within the context of this investigation, the generalised format of a steam system shown in Figure 3.1 will be used.

3 Background

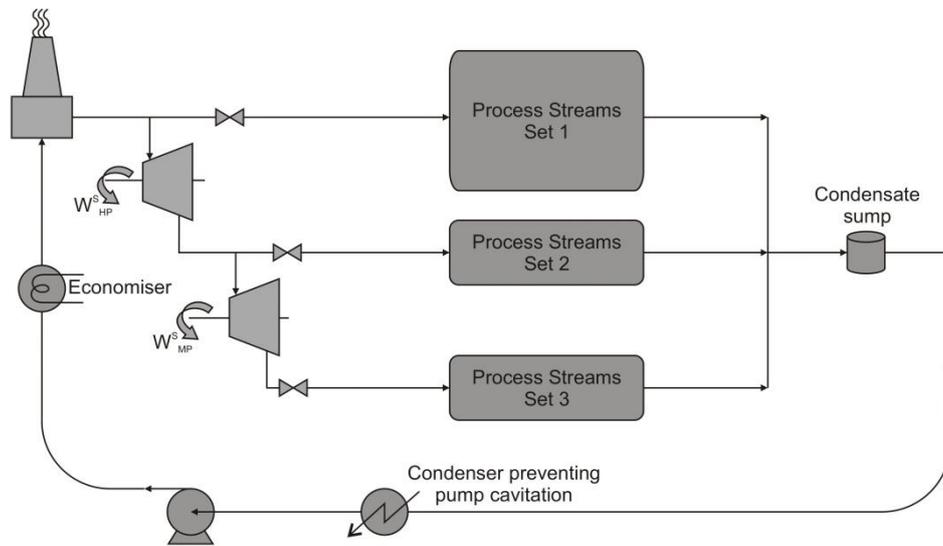


Figure 3.1: A typical chemical plant steam system.

In Figure 3.1, a central boiler raises high pressure (HP) superheated steam. Part of this HP steam is distributed through headers to areas on the plant that require a high temperature heat source. Since in many cases only latent heat is used, the superheated steam must first pass through a let-down valve to bring the steam to saturation conditions. This let-down valve brings about a reduction in the temperature and pressure in the steam in order to achieve saturation conditions. It is vital that the final saturation pressure is correctly determined to ensure that the associated saturation temperature is sufficiently high to fulfil the highest temperature requirements of the system. This saturation pressure is often referred to as “process pressure” steam.

In the heat exchanger network, the heat exchangers are traditionally laid out in a parallel configuration, which is ideal for the use of latent heat. Saturated steam is supplied to the individual heat exchangers, where it condenses as the latent heat is transferred to the process stream, and the condensate collected for return to the boiler. If one were to consult a set of steam tables, it will be seen that steam sources with lower saturation temperatures possess greater latent heat

3 Background

values. It is therefore sensible to have multiple steam levels to supply heat to process streams with differing temperature requirements.

The portion of HP steam that is not used for process heating is passed to a high pressure boiler. Here, the high pressure steam expands inside the turbine to produce shaft work to drive generators, compressors or other equipment. The exhaust steam from the high pressure turbine is at a medium pressure (MP), and is usually kept slightly superheated to prevent condensate droplets from damaging the turbine. A portion of this MP steam is let down to saturation conditions and is used to provide heat to processes that do not require high temperature heat, taking advantage of the higher latent heat of MP steam. Some of the steam from the exhaust of the high pressure turbine can be further expanded in a medium pressure turbine to generate additional shaft work and to provide low pressure (LP) steam. If there is more MP steam available than what is required by the process and the medium pressure turbine combined, then the remainder of the MP steam must be condensed and returned to the boiler (not shown in Figure 3.1), as is conventional in power production.

The LP steam provided by the medium pressure turbine can also be let down to saturation conditions and supplied to a heat exchanger network, or condensed and returned to the boiler. The LP steam could also be sent to yet another turbine, if it is of sufficient temperature or pressure. There is nothing preventing a plant from having more than three steam levels, but in this investigation, only three will be considered.

Once all the steam has been condensed, it is collected and returned to the boiler. Often, a tank is included to aid in smoothing out variations in the flowrate caused by process control equipment. Since the condensate is at saturation conditions, it must be sub cooled to prevent cavitation in the pump which

3 Background

returns the condensate to the boiler. This problem is most commonly associated with centrifugal pumps, which make up the majority of pumps in use. The pump is required to raise the pressure of the condensate before returning it to the boiler. Before entering the boiler, the condensate passes through an economiser which uses waste heat from the boiler to preheat the boiler feed. Not shown in Figure 3.1 is provision for make-up water and blow down. This again is a feature that will vary between plants.

If one were to reduce the flowrate of steam whilst maintaining the quantity of heat supplied to the process, one would find that the boiler return would have both a reduced flowrate and a reduced temperature. Price and Majozi (2010a) showed, through the use of a boiler efficiency model (Shang & Kokossis, 2004), that in order to maintain boiler efficiency, the return temperature should increase as the flowrate decreased. A modification to the conventional steam system was proposed (Figure 3.2) to address this issue.

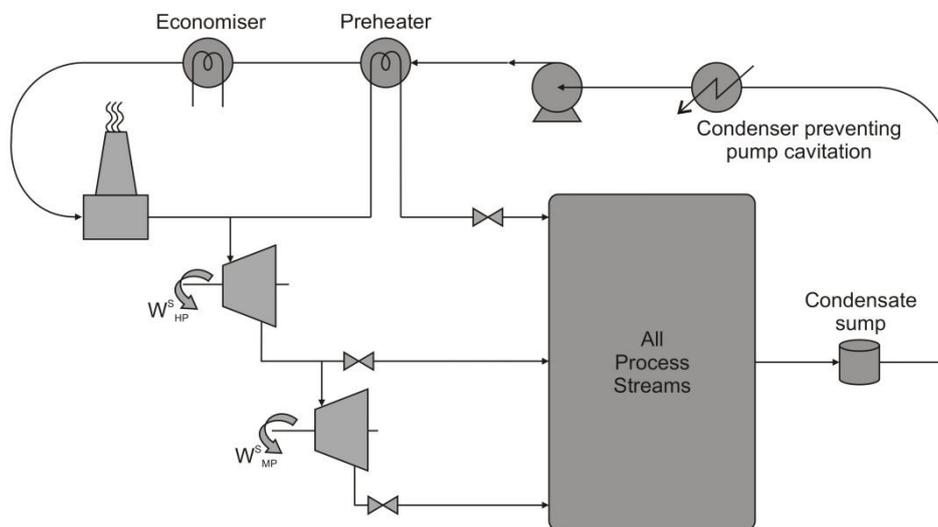


Figure 3.2: Modified steam system for maintained boiler efficiency.

Here, Price and Majozi (2010a) proposed that the superheat of the HP stream, rather than being lost through the use of a let-down valve, should be used to preheat the boiler return stream, providing the required rise in boiler return

temperature. It was also proposed, in the case of multiple steam levels, that the various heat exchanger networks not be kept separate with individual steam sources, but should form one heat exchanger network with multiple steam sources. This allows for better reuse of hot liquid between heat exchangers and can lead to lower total steam flowrates. With the exception of these two modifications, the remainder of the steam system functions as described above.

3.2 Steam Levels

There is no hard and fast method for determining the temperatures of the individual steam levels, but a number of heuristics do exist to aid in this matter. Harrel (1996) performed a survey of various steam systems, and tabulated the temperatures and pressures of typical steam levels (Table 3.1).

Table 3.1: Typical steam levels. (Harrel, 1996)

	T (°C)	P (kPa)	T^{sat} (°C)
High pressure (HP)	399	4238	254
Medium pressure (MP)	327	1480	197
Intermediate pressure (IP)	209	377	141
Low pressure (LP)	221	164	113
Boiler return (after pump)	116	6310	277

The justification for multiple steam levels arises from variations in the latent heat of steam. Figure 3.3 shows how the latent heat of steam increases as the saturation temperature decreases. With this in mind, it makes sense that each heat exchanger should be supplied with steam from the lowest feasible steam level.

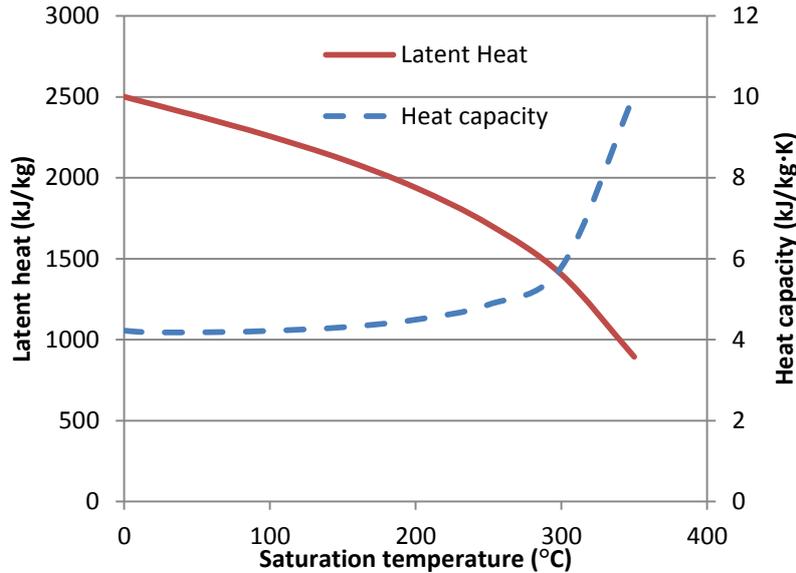


Figure 3.3: Latent heat of steam and heat capacity of water as a function of saturation temperature. (Cooper & Le Fevre, 1969)

A simple correlation between latent heat and saturation temperature is of great use in any model attempting to optimise a steam system. With this in mind, Mavromatis and Kokossis (1998) observed that between 100°C and 300°C, the latent heat of steam varies approximately linearly with saturation temperature. The following linear fit is given with λ in kJ/kg and T^{sat} in °C.

$$\lambda = 2726 - 4.13T^{sat} \quad (3.1)$$

Mavromatis and Kokossis (1998) report that this correlation is accurate over the given range with an average deviation of 2%.

3.3 Flowrate Minimisation

3.3.1 Single Level – Graphical Targeting

The steam flowrate minimisation technique developed by Coetzee and Majozi (2008) forms the core of this investigation. Here, steam flowrate is reduced by reusing the hot condensate from preceding heat exchangers as a heat source in other heat exchangers. Coetzee and Majozi (2008) developed a graphical

3 Background

targeting method with an LP model to synthesize the HEN, as well as an MILP model that both targets and synthesizes. Although this method was developed for single steam levels, the graphical method will be outlined here to give understanding in the method of steam flowrate minimisation.

The method begins by considering the functioning of a heat exchanger. In order for a heat exchanger to provide the necessary heat transfer, there must be sufficient driving force. Depending on the material and construction of the heat exchanger, there will be a minimum temperature difference for heat exchange, commonly referred to as ΔT_{\min} . Figure 3.4 shows a hypothetical cold process stream being heated in a counter current heat exchanger. Located a distance ΔT_{\min} above the process stream line is a limiting temperature line. This line forms a boundary between the feasible region above and the infeasible region below. All hot utilities that lie above or on this boundary are capable of successfully heating the cold process stream, but any hot utility that crosses or lies below this boundary violates the minimum temperature difference for heat exchange, and cannot be used.

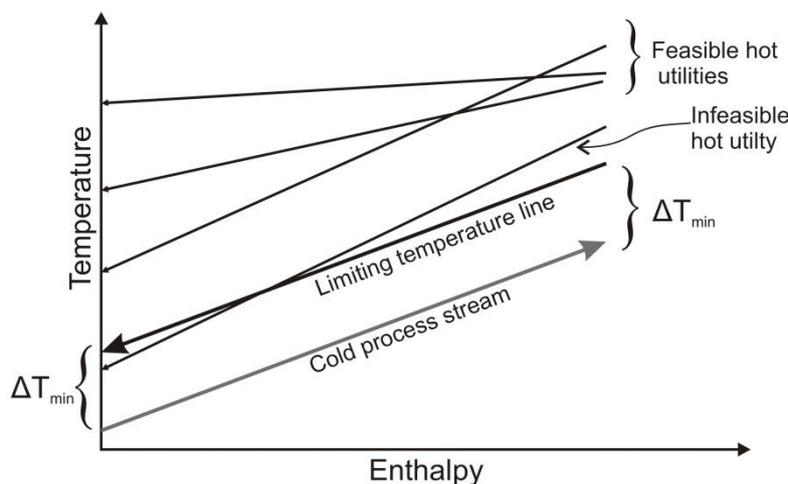


Figure 3.4: The importance of ΔT_{\min} in determining feasible and infeasible hot utilities.

3 Background

Just as a composite curve of the cold process streams can be drawn on a plot of temperature versus enthalpy, so too can a composite curve be drawn of the limiting temperature lines for each heat exchanger, as in Figure 3.5. Again, this limiting temperature composite curve creates a feasibility boundary. Any hot utility that lies above or on the boundary is a feasible hot utility for the entire system. Any hot utility that lies below or crosses the boundary, no matter how briefly, is deemed infeasible for the system as a whole. The beauty of using this limiting temperature composite curve lies in the fact that it does not require complicated models for the heat exchangers. One only needs the limiting data, which in the case of counter current heat exchangers is easily obtained from the process stream data and a ΔT_{\min} value, specified either globally or per heat exchanger.

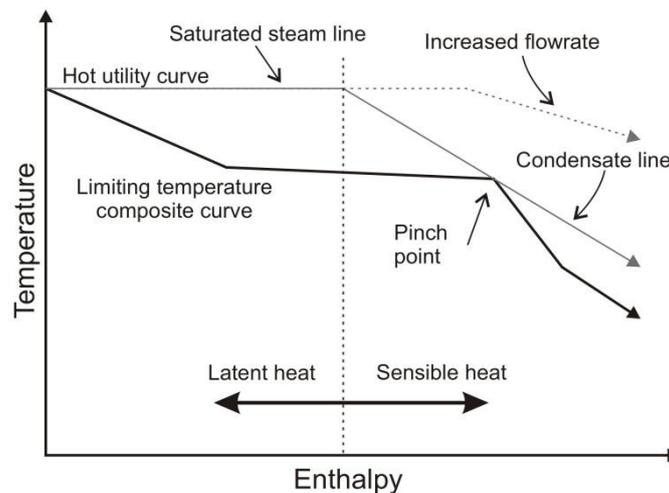


Figure 3.5: Using the limiting temperature composite curve to target the minimum flowrate.

Having constructed a composite curve of the limiting temperature data, one must then construct a curve that is representative of the hot utility. In this case, the hot utility curve will have two visibly distinct regions, one to represent the latent heat provided by the saturated steam, and one to represent the sensible heat provided by the hot condensate. These two regions can be seen in Figure 3.5, along with the division between latent and sensible heat use. Equations 3.2

and 3.3 describe respectively the latent and sensible heat portions of the hot utility curve. By comparing these equations to Figure 3.5, one can see how increasing the steam flowrate will increase the length to the latent steam section, and decrease the slope of the sensible heat section.

$$Q_{latent} = \dot{m}\lambda \quad (3.2)$$

$$Q_{sensible} = \dot{m}c_p(T_{sup} - T) \quad (3.3)$$

Equations 3.2 and 3.3 can be combined and solved in terms of flowrate to give Equation 3.4. With Equation 3.4, one is able to determine the flowrate of steam that is required to provide a total duty of Q while allowing the condensate to cool to a temperature of T . With the calculated flowrate, one can construct the hot utility curve using Equations 3.2 and 3.3, and then test for feasibility by checking that it does not cross the limiting temperature composite curve. Coetzee and Majozi (2008) recommend testing the right hand most node on the limiting temperature composite curve by substituting the duty and temperature at that node into Equation 3.4, and drawing the hot utility curve for the flowrate obtained. This procedure is repeated with each node, moving leftwards, until the first feasible flowrate is obtained, visible by the formation of a pinch. This flowrate is the minimum steam flowrate.

$$\dot{m} = \frac{Q}{\lambda + c_p(T_{sat} - T)} \quad (3.4)$$

3.3.2 Single Level – Network Synthesis

Once the minimum total steam flowrate has been targeted, the heat exchanger network must be synthesized to achieve this flowrate. The portion of the process streams heated with latent heat are laid out in the traditional parallel configuration. For the network utilising sensible heat, a much more complicated

3 Background

network is required, with features such as series connections and reuse streams. In light of this, Coetzee and Majozi (2008) developed an LP formulation to synthesize the heat exchanger network for the sensible heat region.

Coetzee and Majozi (2008) make use of the superstructure shown in Figure 3.6 as the basis to the LP model. Here, all the process streams that are supplied with sensible heat are elements of the set I . In Figure 3.6, i is one of the heat exchangers in I , and j represents all the rest. Here, one can see that heat exchanger i can be supplied with saturated liquid and/or hot liquid reuse from any heat exchanger j . Likewise, heat exchanger i can return its hot liquid to the boiler and/or pass it on for reuse in any other heat exchanger j .

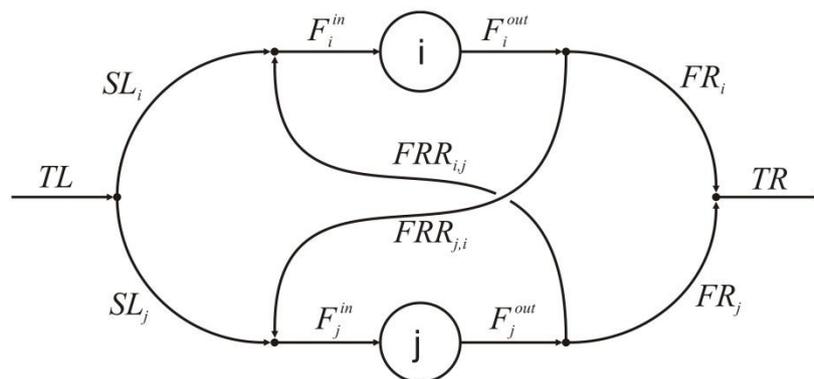


Figure 3.6: Superstructure for the synthesis of the sensible heat region HEN.

The LP model developed by Coetzee and Majozi (2008) is made up of a number of constraints based on mass and energy balances over various components in the superstructure. Equation 3.5 is a mass balance stating that the sum of saturated liquid supplied to all heat exchangers must be equal to the total flowrate of saturated liquid, with slack variables S_1^+ and S_1^- included to allow for undershooting and overshooting in the total steam flowrate target, errors introduced by the graphical nature of the targeting procedure. Equation 3.6 states that the total return to the boiler must equal the sum of the return streams from all the heat exchangers, again with slack variables to compensate for a

3 Background

graphically obtained flowrate target. If leakages are negligible, then the flow into the network must equal the flow out, as is expressed in Equation 3.7. Equation 3.8 is the objective function in which the sum of the four slack variables are minimised, ensuring that the final network has a total flowrate as close as possible to the graphically obtained target.

$$TL + S_1^+ - S_1^- = \sum_{i \in I} SL_i \quad (3.5)$$

$$TR + S_2^+ - S_2^- = \sum_{i \in I} FR_i \quad (3.6)$$

$$TL = TR \quad (3.7)$$

$$Min \left(\sum_{k=1,2} (S_1^+ + S_1^-) \right) \quad (3.8)$$

Just as a mass balance has been performed over the network, so too can a mass balance be performed over each heat exchanger. Equation 3.9 states that the flowrate into heat exchanger i is equal to the sum of the flowrate of saturated liquid supplied to it plus the sum of the reuse streams supplied to i from all heat exchangers j . Likewise, Equation 3.10 states that the flow out of heat exchanger i is made up of the boiler return and the sum of hot liquid supplied to all other heat exchangers j . Equation 3.11 arises from the conservation of mass inside the heat exchanger.

$$F_i^{in} = SL_i + \sum_{j \in J} FRR_{i,j} \quad \forall i \in I \quad (3.9)$$

$$F_i^{out} = FR_i + \sum_{j \in J} FRR_{j,i} \quad \forall i \in I \quad (3.10)$$

$$F_i^{in} = F_i^{out} \quad \forall i \in I \quad (3.11)$$

3 Background

Using the limiting inlet and outlet temperatures for the hot utility, it is possible to calculate an upper bound on the flowrate of hot liquid supplied to heat exchanger i (Equation 3.12). With this, Equation 3.13 stipulates that the actual flowrate of hot liquid supplied to heat exchanger i may not exceed this upper bound. Equation 3.14 is used to ensure that a heat exchanger cannot recycle hot liquid back to itself.

$$F_i^{in,U} = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (3.12)$$

$$F_i^{in} \leq F_i^{in,U} \quad \forall i \in I \quad (3.13)$$

$$FRR_{i,i} = 0 \quad \forall i \in I \quad (3.14)$$

To ensure that the required duty is transferred, energy balances are performed over all of the heat exchangers. Equation 3.15 relates the heat transferred in heat exchanger i to the flowrate of hot liquid and the change in temperature through i . Equation 3.16 calculates the temperature of the stream entering heat exchanger i caused by the blending of feed streams.

$$Q_i = F_i^{in} c_p (T_i^{in} - T_i^{out}) \quad \forall i \in I \quad (3.15)$$

$$T_i^{in} = \frac{\sum_{j \in J} (FRR_{i,j} T_j^{out}) + SL_i T^{sat}}{F_i^{in}} \quad \forall i \in I \quad (3.16)$$

It can be seen that both Equation 3.15 and Equation 3.16 contain the bilinear term $F_i^{in} T_i^{in}$. To linearize this, Coetzee and Majozi (2008) substituted Equation 3.16 into Equation 3.15. Following this, the term T_i^{out} is fixed at its limiting value $T_i^{out,L}$. This second step has been shown to be a necessary condition for optimality by Savelski and Bagajewicz (2000) for the problem of waste water

minimisation. Given the analogies between heat and mass transfer, Coetzee and Majozi (2008) use it as a necessary condition in steam flowrate minimisation. The resulting linearized constraint is given in Equation 3.17.

$$Q_i = c_p \sum_{j \in J} (FRR_{i,j} T_j^{out,L}) + c_p S L_i T^{sat} - F_i^{in} c_p T_i^{out,L} \quad \forall i \in I \quad (3.17)$$

These constraints constitute an LP model for synthesizing the sensible heat region heat exchanger network once a flowrate target has been obtained via graphical means.

3.3.3 Single Level – Simultaneous Targeting and Synthesis

Having developed the LP model to accompany the graphical targeting technique, Coetzee and Majozi (2008) developed an MILP formulation to simultaneously target the minimum steam flowrate and synthesize the entire heat exchanger network. The superstructure used (Figure 3.7) is very similar to that used in the LP formulation previously discussed (Figure 3.6). The difference here is that this superstructure encompasses both the latent heat and the sensible heat regions. The set I is also made up of all the heat exchangers, and not only those utilising sensible heat.

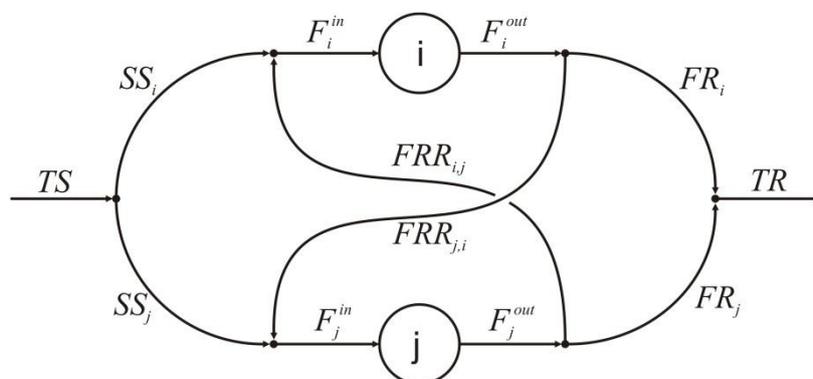


Figure 3.7: Superstructure for simultaneously targeting flowrate and synthesizing the HEN.

3 Background

Coetzee and Majozi (2008) begin by calculating an upper bound on the saturated steam flowrate (Equation 3.18) and the hot liquid flowrate (Equation 3.19) to heat exchanger i .

$$SS_i^U = \frac{Q_i}{\lambda} \quad \forall i \in I \quad (3.18)$$

$$FRR_i^U = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (3.19)$$

As in the previous model, a number of constraints are derived from elementary mass balances. Equation 3.20 states that the sum of the saturated steam supplied to the individual heat exchangers must equal the total steam flowrate. Equation 3.21 states that the sum of the return flowrates from each heat exchanger must be equal to the total boiler return flowrate. If leakages are assumed to be negligible, then the total supply and total return must be equal (Equation 3.22).

$$TS = \sum_{i \in I} SS_i \quad (3.20)$$

$$TR = \sum_{i \in I} FR_i \quad (3.21)$$

$$TS = TR \quad (3.22)$$

Since this model must account for both saturated steam and hot liquid, Equation 3.23 states that the flowrate into a particular heat exchanger is flowrate of the saturated steam supplied to that heat exchanger plus the sum of hot liquid supplied to that heat exchanger from all other heat exchangers. Here, one must remember that the reuse stream is now made up of saturated condensate and hot liquid (Equation 3.24). Equation 3.25 prevents a heat exchanger from recycling hot liquid back to itself.

3 Background

$$F_i^{in} = SS_i + \sum_{j \in J} FRR_{i,j} \quad \forall i \in I \quad (3.23)$$

$$FRR_{i,j} = SL_{i,j} + HL_{i,j} \quad \forall i, j \in I, J \quad (3.24)$$

$$HL_{i,i} = 0 \quad \forall i \in I \quad (3.25)$$

Since saturated liquid is formed through the condensation of steam, Equation 3.26 states that the total flowrate of saturated liquid supplied by heat exchanger i to all other heat exchangers may not exceed the flowrate of saturated steam supplied to heat exchanger i . Likewise, Equation 3.27 states that the flowrate of hot liquid supplied by heat exchanger i to all other heat exchangers may not exceed the total flowrate to reuse liquid that entered heat exchanger i .

$$\sum_{j \in J} SL_{j,i} \leq SS_i \quad \forall i \in I \quad (3.26)$$

$$\sum_{j \in J} HL_{j,i} \leq \sum_{j \in J} FRR_{i,j} \quad \forall i \in I \quad (3.27)$$

In order to control which heat exchangers use steam and which use liquid, Coetzee and Majozi (2008) introduce two binary variables, x_i and y_i . The first takes on a value of 1 if heat exchanger i is supplied with hot liquid, and a value of 0 if it is not. The second performs a similar function, but for the use of saturated steam. These two binary variables are used along with the upper bounds calculated in Equations 3.18 and 3.19 to limit the flowrate of saturated steam (Equation 3.28) and hot liquid reuse (Equation 3.29).

$$SS_i \leq SS_i^U y_i \quad \forall i \in I \quad (3.28)$$

$$\sum_{j \in J} FRR_{i,j} \leq FRR_i^U x_i \quad \forall i \in I \quad (3.29)$$

3 Background

The binary variables give the user control over the splitting of heat exchangers. If Equation 3.30 is implemented, then each heat exchanger is restricted to using either hot liquid or saturated steam, but not both. In this way it is guaranteed that no heat exchanger will be split.

$$x_i + y_i \leq 1 \quad \forall i \in I \quad (3.30)$$

If one were to permit a total of m heat exchangers to be split between hot liquid and saturated steam, then Equations 3.31 and 3.32 must be implemented in place of Equation 3.30. Here, $|i|$ represents the number of elements in set I .

$$\sum_{i \in I} x_i + \sum_{i \in I} y_i \geq |i| \quad (3.31)$$

$$\sum_{i \in I} x_i + \sum_{i \in I} y_i \leq |i| + m \quad (3.32)$$

Equation 3.33 shows how in this model, the duty required of each heat exchanger can be supplied as latent heat and sensible heat. Equation 3.34 models the quantity of heat provided as latent heat, while Equation 3.35 models the quantity of heat provided as sensible heat. Note that Equation 3.35 has already been linearized as discussed previously.

$$Q_i = Q_i^{SS} + Q_i^{HL} \quad \forall i \in I \quad (3.33)$$

$$Q_i^{SS} = SS_i \lambda \quad \forall i \in I \quad (3.34)$$

$$Q_i^{HL} = c_p \sum_{j \in J} (SL_{i,j} T^{sat}) + c_p \sum_{j \in J} (HL_{i,j} T_j^{out,L}) - F_i^{in} c_p T_i^{out,L} \quad \forall i \in I \quad (3.35)$$

3 Background

The above constraints constitute an MILP model for the simultaneous targeting of the minimum steam flowrate and HEN synthesis. Since the minimum steam flowrate is not targeted elsewhere, the object function is to minimise the total steam flowrate (Equation 3.36).

$$\text{minimise}(TS) \quad (3.36)$$

3.3.4 Multiple Steam Levels

The major drawback to the steam flowrate minimisation techniques outlined above is their limitation to a single steam level. In amongst the notable contributions of Price and Majozi (2010a,b,c) is a model that addresses this issue. Price and Majozi (2010b) developed a model for steam flowrate minimisation in the presence of multiple steam levels.

The superstructure used for the model by Price and Majozi (2010b) is shown in Figure 3.8. Here, instead of a single steam source, each heat exchanger can be supplied with steam from three different levels, each belonging to the set L . In the model developed by Price and Majozi (2010b), the flowrate of HP steam is unlimited, while the flowrates of MP and LP steam are limited to fixed values determined by the operation of steam turbines.

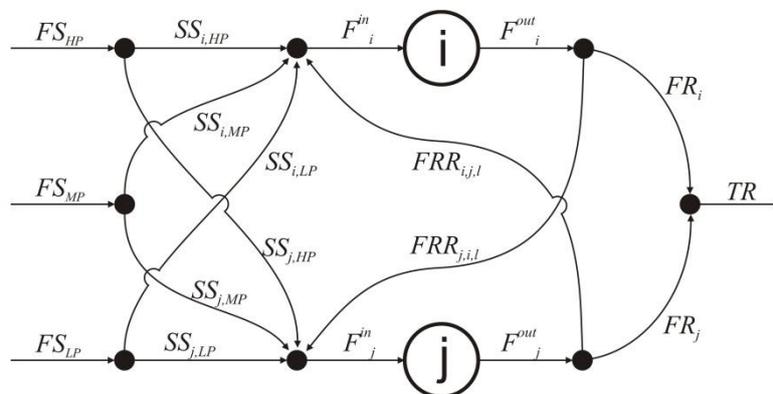


Figure 3.8: Superstructure for steam flowrate minimisation in the presence of multiple steam levels.

3 Background

The constraints of the model are derived from elementary mass balances. Equation 3.37 states that the total flowrate of a particular steam level l must equal the sum of the steam flowrates supplied to heat exchangers at that level. Equation 3.38 states that the total boiler return must equal the sum of the return flowrates from the individual heat exchangers. Ignoring any leakages, Equation 3.39 states that the total boiler return must equal the sum of the total steam flowrates supplied across the various levels.

$$FS_l = \sum_{i \in I} SS_{i,l} \quad \forall l \in L \quad (3.37)$$

$$TR = \sum_{i \in I} FR_i \quad (3.38)$$

$$\sum_{l \in L} FS_l = TR \quad (3.39)$$

Equation 3.40 states that the flow entering heat exchanger i is equal to the sum of saturated steam across the various levels plus the sum of hot liquid streams supplied to heat exchanger i from all other heat exchangers. Equation 3.41 states that the flow exiting heat exchanger i is divided between the boiler return, and reuse streams supplied to all other heat exchangers. Equation 3.42 is a result of conservation of mass inside the heat exchanger.

$$F_i^{in} = \sum_{l \in L} SS_{i,l} + \sum_{j,l \in J,L} FRR_{i,j,l} \quad \forall i \in I \quad (3.40)$$

$$F_i^{out} = FR_i + \sum_{j,l \in J,L} FRR_{j,i,l} \quad \forall i \in I \quad (3.41)$$

$$F_i^{in} = F_i^{out} \quad \forall i \in I \quad (3.42)$$

Price and Majozi (2010b) go on to separate the reuse stream into saturated liquid and hot liquid (Equation 3.43). Equation 3.44 states that the total quantity of saturated liquid leaving a particular heat exchanger may not exceed the quantity of saturated steam that enters the heat exchanger. Equation 3.45 states that the quantity of hot liquid leaving a particular heat exchanger may not exceed that quantity of liquid entering it. Equation 3.46 is implemented to prevent local recycle.

$$FRR_{i,j,l} = SL_{i,j,l} + HL_{i,j,l} \quad \forall i, j, l \in I, J, L \quad (3.43)$$

$$\sum_{j \in J} SL_{j,i,l} \leq SS_{i,l} \quad \forall i, l \in I, L \quad (3.44)$$

$$\sum_{j \in J} HL_{j,i,l} \leq \sum_{j \in J} FRR_{i,j,l} \quad \forall i, l \in I, L \quad (3.45)$$

$$HL_{i,i,l} = 0 \quad \forall i, l \in I, L \quad (3.46)$$

An upper bound to the flowrate of saturated steam and hot liquid passing through each heat exchanger can be calculated using Equations 3.47 and 3.48 respectively. Just as in the model by Coetzee and Majozi (2008), Price and Majozi (2010b) use these upper bound in conjunction with binary variables to control the flow of saturated steam and hot liquid through the heat exchangers (Equations 3.49 and 3.50). It must be noted from the limitation given in Equation 3.47 that Price and Majozi (2010b) do not allow steam of a particular level with a saturation temperature lower than the limiting inlet temperature of a process to be used. In effect, this prohibits lower steam levels from being used to preheat streams.

3 Background

$$SS_{i,l}^U = \frac{Q_i}{\lambda_l} \quad \forall i, l \in I, L \quad T_l^{sat} > T_i^{in,L} \quad (3.47)$$

$$FRR_i^U = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (3.48)$$

$$SS_{i,l} \leq SS_{i,l}^U y_{i,l} \quad \forall i, l \in I, L \quad (3.49)$$

$$\sum_{j,l \in J,L} FRR_{i,j,l} \leq FRR_i^U x_i \quad \forall i \in I \quad (3.50)$$

As in the model by Coetzee and Majozi (2008), these binary variables give the user control over split heat exchangers. If no split heat exchangers are desired, then Equation 3.51 is implemented. If a total of m split heat exchangers are permitted, then Equations 3.52 and 3.53 are implement instead of Equation 3.51

$$x_i + \sum_{l \in L} y_i \leq 1 \quad \forall i \in I \quad (3.51)$$

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_i \geq |i| \quad (3.52)$$

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_i \leq |i| + m \quad (3.53)$$

As was mentioned, the flowrate of the lower steam levels are fixed at the operating conditions of the steam turbine. Equation 3.54 is therefore used to ensure that the demand for lower level steam does not exceed the supply for that level FF_l .

$$FS_l \leq FF_l \quad \forall l \in L, l \neq HP \quad (3.54)$$

Again, the duty required of each heat exchanger can be supplied as latent heat and sensible heat (Equation 3.55). Equation 3.56 models the quantity of heat provided as latent heat, while Equation 3.57 models the quantity of heat provided as sensible heat. Note that Equation 3.57 has already been linearized as discussed previously.

$$Q_i = \sum_{l \in L} Q_{i,l}^{SS} + Q_i^{HL} \quad \forall i \in I \quad (3.55)$$

$$Q_i^{SS} = SS_{i,l} \lambda_l \quad \forall i \in I \quad (3.56)$$

$$Q_i^{HL} = c_p \sum_{j,l \in J,L} (SL_{i,j,l} T_l^{sat}) + c_p \sum_{j,l \in J,L} (HL_{i,j,l} T_j^{out,L}) - F_i^{in} c_p T_i^{out,L} \quad \forall i \in I \quad (3.57)$$

The above constraints constitute an MILP model for the simultaneous targeting of the minimum steam flowrate and HEN synthesis in the presence of multiple steam levels. Since the flowrate of the lower steam levels are fixed by the steam turbines, the object function is to minimise the flowrate of HP steam (Equation 3.58).

$$\text{minimise}(FS_{HP}) \quad (3.58)$$

3.4 Shaft Work Estimation

When developing mathematical formulations for the optimization of a system, it is beneficial to have simple, reasonably accurate and quick-solving models of the process units. This will allow the optimization routine to test many options rapidly and select the best design from amongst them. Once this initial target has been achieved, more rigorous and accurate simulations can be performed to fine-tune the design. Although these detailed simulations are time consuming, only a small number of runs will be required to find the optimum, since the

3 Background

target obtained using the quick model has already placed the design at a very good starting point.

For the purposes of this investigation, a simple model for a steam turbine is used. Mavromatis and Kokossis (1998) provide a model for estimating the shaft work production of a steam turbine that is both simple and founded upon sound principles. Mavromatis and Kokossis (1998) begin by considering the Willans line (Figure 3.9), a common tool for describing simple turbines. From this, it can be seen that the Willans line can be expressed as:

$$E = nM - E^{loss} \quad (3.59)$$

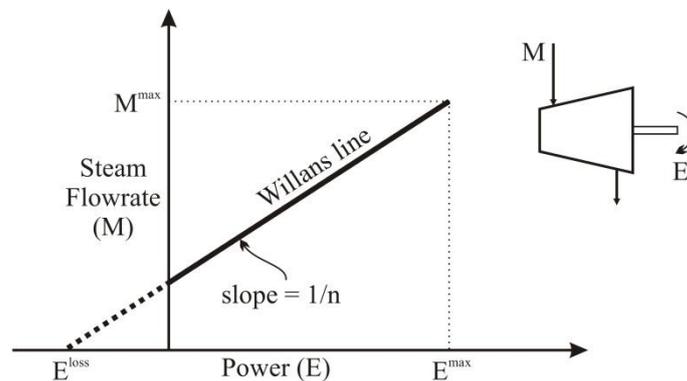


Figure 3.9: The Willans line for a simple turbine. (Mavromatis & Kokossis, 1998a)

Mavromatis and Kokossis (1998) note that the slope of a line from the origin to any operating point on the Willans line (Figure 3.10a) is inversely proportional to the isentropic efficiency of the turbine. This allows a nonlinear locus of the isentropic efficiency to be drawn at different operating loads (Figure 3.10b). The shape obtained in Figure 3.10 agrees well with actual turbine data collected by Peterson and Mann (1985).

3 Background

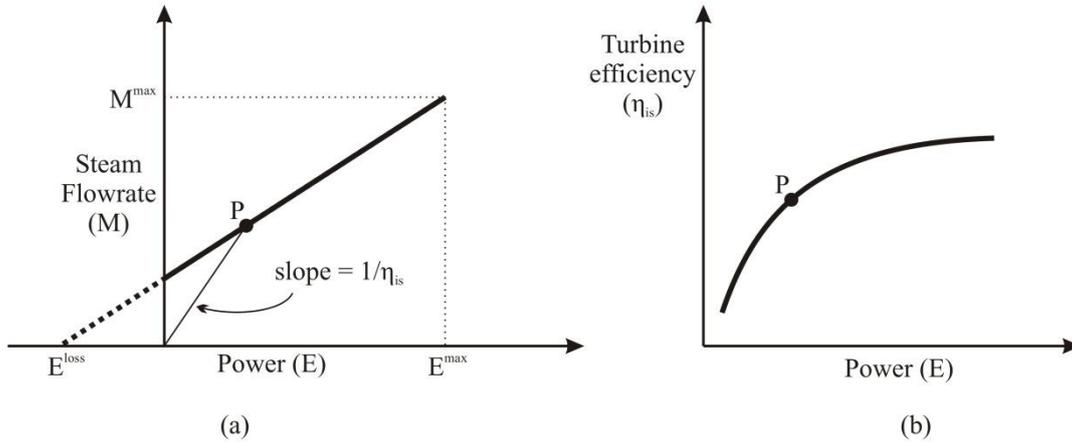


Figure 3.10: Nonlinear variation of turbine efficiency with operating conditions. (Mavromatis & Kokossis, 1998a)

The data in Figure 3.10b, through a change in axes, can be expressed as a linear function (Equation 3.60). Mavromatis and Kokossis (1998) state that the two parameters, A and B , are linear functions of the saturation temperature of the steam entering the turbine (Equations 3.61 and 3.62)

$$\frac{E^{max}}{\eta_{is}^{max}} = A + B E^{max} \quad (3.60)$$

$$A = a_1 + a_2 T_{in}^{sat} \quad (3.61)$$

$$B = b_1 + b_2 T_{in}^{sat} \quad (3.62)$$

Using the definition of isentropic efficiency (Equation 3.63), Equation 3.64 is obtained, which is substituted into Equation 3.60. Also, based on experience, Mavromatis and Kokossis (1998) assume the internal energy losses to be about 20% of the value of the maximum energy output (Equation 3.65).

$$\eta_{is} = \frac{\bar{E}}{\overline{\Delta H_{is}}} = \frac{E}{\overline{\Delta H_{is}} M} \quad (3.63)$$

3 Background

$$\frac{E^{max}}{\eta_{is}^{max}} = \overline{\Delta H}_{is} M^{max} \quad (3.64)$$

$$E^{loss} = 0.2E^{max} \quad (3.65)$$

Using Equations 3.59, 3.60, 3.64 and 3.65, Mavromatis and Kokossis (1998) obtained the following two expressions for the parameters n and E^{loss} in Equation 3.59.

$$n = \frac{5}{6} \frac{1}{B} \left(\overline{\Delta H}_{is} - \frac{A}{M^{max}} \right) \quad (3.66)$$

$$E^{loss} = \frac{1}{5} \frac{1}{B} (\overline{\Delta H}_{is} M^{max} - A) \quad (3.67)$$

By substituting Equations 3.66 and 3.67 into Equation 3.59, Mavromatis and Kokossis (1998) obtain Equation 3.68, an expression for estimating the shaft work production of a steam turbine as a function of the steam flowrate. Table 3.2 gives the coefficients determined by Mavromatis and Kokossis (1998) for Equations 3.61 and 3.62. Mavromatis and Kokossis (1998) claim that this turbine model is accurate to within approximately 3% if the correct values from Table 3.2 are used. If the turbine operates at full load, it can be shown that Equation 3.68 reduces to Equation 3.69.

$$E = \frac{5}{6} \frac{1}{B} \left(\overline{\Delta H}_{is} - \frac{A}{M^{max}} \right) \left(M - \frac{1}{6} M^{max} \right) \quad (3.68)$$

$$E^{max} = \frac{1}{B} (\overline{\Delta H}_{is} M^{max} - A) \quad (3.69)$$

Table 3.2: Turbine model coefficients. (Mavromatis & Kokossis, 1998)

	a_1	a_2	b_1	b_2
General case	-0.538	0.00364	1.112	0.00052
$E < 1.2MW$	-0.131	0.00117	0.989	0.00152
$E > 1.2MW$	-0.928	0.00623	1.12	0.00047

Equation 3.69 requires the term $\overline{\Delta H}_{is}$ to be calculated. Singh (1997) provides a correlation for approximating this isentropic enthalpy change (Equation 3.70). Here q^{in} is the heat load of the steam, that is, the quantity of energy contained in the steam above the energy content of saturated liquid.

$$\overline{\Delta H}^{is} = \frac{\Delta T^{sat}}{1854 - 1931 \cdot q^{in}} \quad (3.70)$$

3.5 Heat Exchanger Layout

The distinctive fingerprint of process integration on the HEN of a steam system is the presence of both serial and parallel connections. The need for this parallel-serial hybrid stems from the various sources of heat. As depicted in Figure 3.11a, reuse of condensate for heating results in two distinct regions within the HEN, namely latent heat and sensible heat regimes. Whilst the latent heat region entails only a parallel configuration of heat exchangers, the sensible heat region involves a complex combination of parallel and series connections. Some heat exchangers may need to be split between latent and sensible heat. The distinction between the simple parallel layout of latent heat using heat exchangers, and the more detailed layout of the sensible heat using heat exchangers is seen in Figure 3.11b.

3 Background

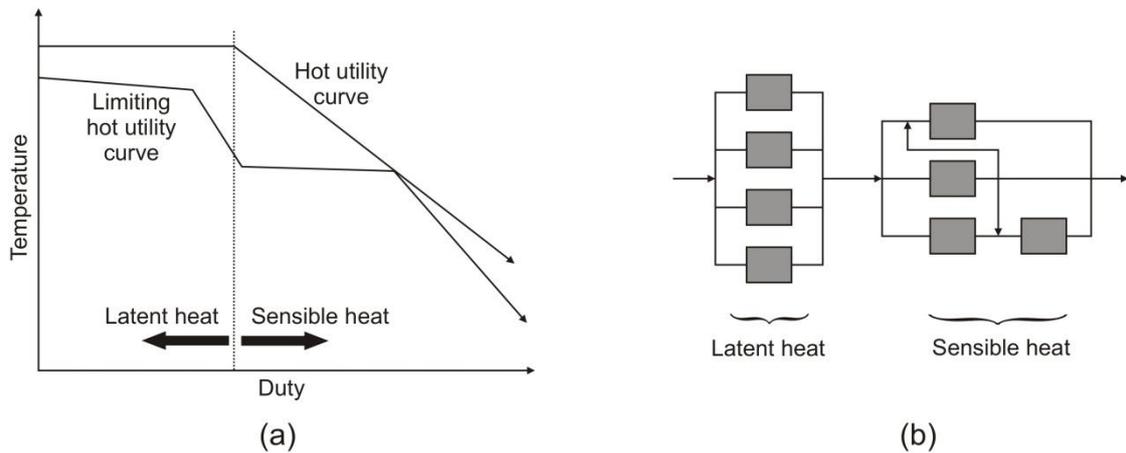


Figure 3.11: The division between latent and sensible heat using processes (a) on a T-H diagram (b) in the HEN.

Split heat exchangers occur whenever a particular process stream requires heat from two or more different heat sources. At this point, it is worth emphasising the distinction between serial and parallel heating since this will feature prominently when using multiple steam levels. Consider the case of a single cold process stream being heated using two levels of saturated steam. Figure 3.12 shows this process, along with the limiting temperature profile that arises due to the minimum temperature difference for heat exchange, ΔT_{\min} . In the first instance (Figure 3.12a) the lower steam level may have sufficient energy to supply the entire process, but is limited by its temperature. In the second instance (Figure 3.12b) both steam levels are hot enough to successfully heat the cold process stream, but the lower steam level may have insufficient energy to supply all the heat demands, necessitating an additional steam level.

3 Background

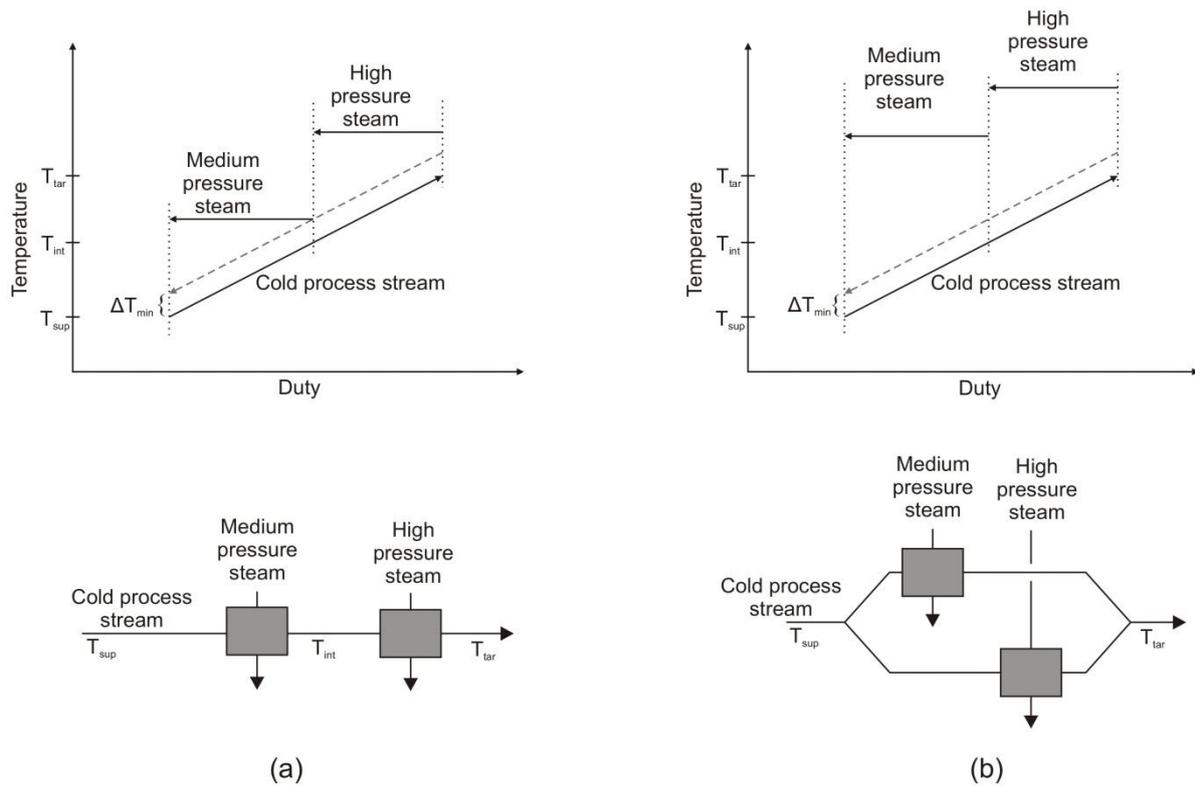


Figure 3.12: T-H diagram and heat exchanger layout for (a) one steam level colder than T_{tar} (b) both steam levels hotter than T_{tar} .

In Figure 3.12a, since the medium pressure steam is not hot enough to heat the cold stream to its target temperature T_{tar} , it can only raise the temperature of the cold stream to T_{int} . The remainder of the duty required is provided by high level steam. In Figure 3.12b, since both steam levels are hot enough to bring the cold stream to its target temperature, but the total heating duty is shared between them, the cold stream can be split in two and heated to T_{tar} in parallel heat exchangers before being recombined. It is also possible to use serial heat exchangers in this case, but heat exchangers in series will cause a higher total pressure drop than heat exchangers in parallel.

3.6 References

- Coetzee, W. A., & Majazi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Cooper, J. R., & Le Fevre, E. J. (1969). Thermophysical properties of water substance. Butterworth-Heinemann, London, UK.
- Harrel, G. (1996). Steam system survey guide. ORNL/TM-2001/263: Oak Ridge National Laboratory.
- Mavromatis, S. P., & Kokossis, A. C. (1998). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Peterson, J. F., & Mann, W. L. (1985). Steam-system design: how it evolves. *Chem. Eng.*, 92(21), 62-74.
- Price, T., & Majazi, T. (2010a). On Synthesis and Optimization of Steam System Networks. 1. Sustained Boiler Efficiency. *Ind. Eng. Chem. Res.*, 49, 9143-9153.
- Price, T., & Majazi, T. (2010b). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Price, T., & Majazi, T. (2010c). On Synthesis and Optimization of Steam System Networks. 3. Pressure Drop Consideration. *Ind. Eng. Chem. Res.*, 49, 9165-9174.
- Savelski, M. J., & Bagajewicz, M. J. (2000). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.

Shang, Z., & Kokossis, A. (2004). A transshipment model for the optimisation of steam levels of total site utility systems. *Comp. Chem. Eng.*, 28, 1673-1688.

Singh, H. (1997). Strategies for emissions minimisation in chemical process industries. Ph.D. thesis, Department of Process Integration, UMIST, Manchester, UK.

Chapter 4

Mathematical Analysis

In the model developed by Price and Majozi (2010) for minimising the total steam flowrate in the presence of multiple steam levels, a set of fixed steam levels is supplied to the solver, and the mathematical programme determines a minimum flowrate required for a particular case study. If a different set of steam levels is provided for the same case study, then a different minimum total steam flowrate will be achieved, either higher or lower than the first minimum achieved with the original set of steam levels. This leads one to believe that the minimum steam flowrate is also a function of the choice of steam levels.

In this section, a mathematical analysis of the minimum total steam flowrate is undertaken for two cases involving multiple steam levels. The first case considers only the use of latent heat, while the second case considers the use of latent heat and sensible heat from hot liquid reuse. The purpose of this analysis is to gain insight into the effects the choice of steam levels has on the minimum steam flowrate achieved. In particular, since the purchase cost of a boiler increases with steam flowrate, it is of benefit to analyse how steam levels can be selected to ensure that the minimum total steam flowrate is indeed as low as it can possibly be made.

4 Mathematical Analysis

It must be noted that all temperatures mentioned in this section are saturation temperatures. As such, for the sake of improving readability the superscript in T^{sat} will not appear in this section.

4.1 Latent Heat Only

In the first case to be analysed, only latent heat from multiple steam levels is used. The analysis begins by considering an arbitrary process stream that requires a heating duty of some positive value Q . Based on the supply and target temperatures of the cold process stream, and the ΔT_{min} value for the heat exchanger, a limiting temperature curve for the hot utility can be plotted on a temperature versus enthalpy plot (Figure 4.1) with minimum inlet and outlet temperatures of T_{in} and T_{out} respectively.

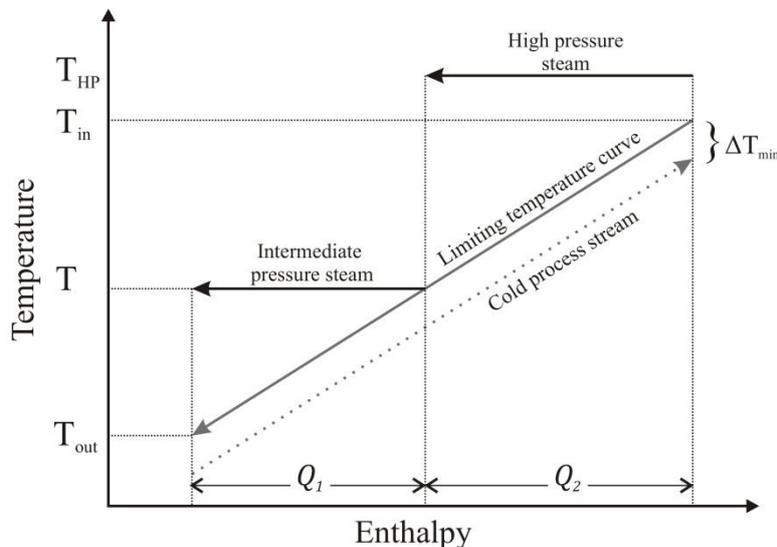


Figure 4.1: An arbitrary process stream heated using latent heat from two steam levels.

In this analysis, only two steam levels will be considered at first for demonstration purposes, with a more general analysis presented after. The first steam level considered is a high pressure steam level supplied directly from the boiler. This steam level has a fixed saturation temperature of T_{HP} , determined

4 Mathematical Analysis

by the boiler operation. Ultimately, this temperature is specified in the early stages of design to ensure that the HP steam level is hot enough to fulfil the highest temperature demands of the plant. In this analysis, T_{HP} can be fixed at any temperature greater than or equal to T_{in} .

The second steam level considered is an intermediate pressure steam level with an arbitrarily chosen saturation temperature T . It is this steam level that will be altered in order to view the effects of steam level selection on the minimum steam flowrate.

Before the analysis begins, it must be shown that the situation as it is depicted in Figure 4.1 indeed represents the minimum steam flowrate for the given selection of steam levels. That is to say, that the intermediate steam level must form a pinch with the limiting temperature to ensure a minimum steam flowrate. To show this, it is noted that the saturation temperature of the IP steam is lower than the saturation temperature of the HP steam (Equation 4.1). Multiplying both sides of Equation 4.1 by -4.13 , and adding 2726 , one arrives at Equation 4.2. Through the use of Equation 3.1, Equation 4.3 states that the latent heat of the IP steam is greater than the latent heat of the HP steam.

$$T < T_{HP} \quad (4.1)$$

$$2726 - 4.31T > 2726 - 4.13T_{HP} \quad (4.2)$$

$$\lambda_{IP} > \lambda_{HP} \quad (4.3)$$

Taking the reciprocal of both sides of Equation 4.3 and multiplying by Q , one obtains Equation 4.4. Since duty divided by latent heat gives the mass flowrate of steam required to provide a given duty, Equation 4.5 is obtained, which states

4 Mathematical Analysis

that the flowrate of IP steam required to provide a particular duty is lower than the flowrate of HP steam required to provide the same duty.

$$\frac{Q}{\lambda_{IP}} < \frac{Q}{\lambda_{HP}} \quad (4.4)$$

$$\dot{m}_{IP} < \dot{m}_{HP} \quad (4.5)$$

Equation 4.5 implies that for a minimum steam flowrate, one should only use IP steam. This, however, is not feasible since the saturation temperature of the IP steam level is not high enough to fulfil the temperature requirements of the cold process stream. The maximum quantity of IP steam that can be used is seen when the utility line for IP steam forms a pinch with the limiting temperature curve. Any more than this, and the minimum temperature difference for heat transfer (ΔT_{\min}) will be violated. The remainder of the duty required by the cold process stream must be supplied from HP steam. Thus the situation depicted in Figure 4.1 represents the minimum steam flowrate for the given set of steam levels.

If the saturation temperature of the intermediate steam level in Figure 4.1 were to be changed, a different minimum total steam flowrate would be achieved. It is this effect that altering the choice of steam levels has on the minimum steam flowrate that is to be analysed. First, The portion of the duty Q that is provided by IP steam and HP must be determined as a function of T . Through the use of similar triangles in Figure 4.1, Equations 4.6 and 4.7 relate the quantity of heat supplied by IP steam and HP steam respectively as a function of T .

$$Q_1 = \frac{(T - T_{out})}{(T_{in} - T_{out})} Q \quad (4.6)$$

4 Mathematical Analysis

$$Q_2 = \frac{(T_{in} - T)}{(T_{in} - T_{out})} Q \quad (4.7)$$

The flowrate of steam required from both levels can be calculated by dividing their individual duties by their respective latent heats. By summing these two flowrates, the minimum total steam flowrate as a function of T is obtained (Equation 4.8). For the sake of generality, λ is expressed as Equation 4.9, and not with numerical coefficients as in Equation 3.1. This allows the present analysis to be adapted for use with different latent heat coefficients derived for different temperature ranges.

$$\dot{m}(T) = \frac{(T - T_{out})}{(T_{in} - T_{out})} \frac{Q}{\lambda} + \frac{(T_{in} - T)}{(T_{in} - T_{out})} \frac{Q}{\lambda_{HP}} \quad (4.8)$$

$$\lambda(T) = a - bT \quad (4.9)$$

To analyse the change in the total steam flowrate as a result of a change in T , the first derivative of Equation 4.8 with respect to T is calculated and given in Equation 4.10. Equation 4.10 is set equal to 0, and solved for in terms of T to obtain the stationary points T^* (Equation 4.11). It is noted here that only the positive root leads to a sensible stationary point in the context of Figure 4.1. The negative root leads to a temperature that is abnormally large and beyond the critical point of steam.

$$\frac{d\dot{m}}{dT} = \frac{Q\lambda + (T - T_{out})Qb}{(T_{in} - T_{out})\lambda^2} - \frac{Q}{(T_{in} - T_{out})\lambda_{HP}} \quad (4.10)$$

$$T^* = -\frac{1}{b} \left(\pm \sqrt{a\lambda_{HP} - bT_{out}\lambda_{HP} - a} \right) \quad (4.11)$$

4 Mathematical Analysis

To test whether the stationary point represented by the positive root in Equation 4.11 is a minimum or a maximum, the sign of the second derivative of Equation 4.8 with respect to T must be checked. Equation 4.12 gives the second derivative of Equation 4.8 with respect to T , evaluated at the stationary point T^* .

$$\left. \frac{d^2 \dot{m}}{dT^2} \right|_{T^*} = \frac{2(T^* - T_{out})Qb^2 + 2Qb\lambda^*}{(T_{in} - T_{out})(\lambda^*)^3} \quad (4.12)$$

In Appendix A it is shown that T^* indeed lies between T_{HP} and T_{out} , implying that T^* is greater than T_{out} . Noting that Q , b and λ^* are all by definition positive quantities, it is observed that the second derivative evaluated at T^* is positive, indicating that the optimum point is a minimum.

In words, this states that the minimum total steam flowrate obtained when the IP steam level has a saturation temperature of T^* is lower than the minimum total steam flowrate obtained using any other saturation temperature. The set of saturation temperatures $[T_{HP}, T^*]$ should therefore be considered to be the optimal set of steam levels.

It is interesting to note that with the aid of Equation 4.9, Equation 4.11 can be rewritten as Equation 4.13. This states that the latent heat of the IP steam level evaluated at the optimal saturation temperature T^* should be the geometric mean of the latent heat of steam evaluated at T_{HP} and T_{out} .

$$\lambda^* = \sqrt{\lambda_{out}\lambda_{HP}} \quad (4.13)$$

To extend this analysis to any number of steam levels, one must once again consider an arbitrary cold process stream requiring a heating duty of Q . In

4 Mathematical Analysis

Figure 4.2, one sees the limiting temperature curve of this arbitrary cold process stream being heated by N intermediate steam levels and an HP steam level directly from the boiler. Again, T_{HP} is fixed at any temperature greater than or equal to T_{in} . The saturation temperatures of the intermediate steam levels are variables, and altering one or more of them will change the minimum total steam flowrate. It is this change in minimum total steam flowrate that is analysed.

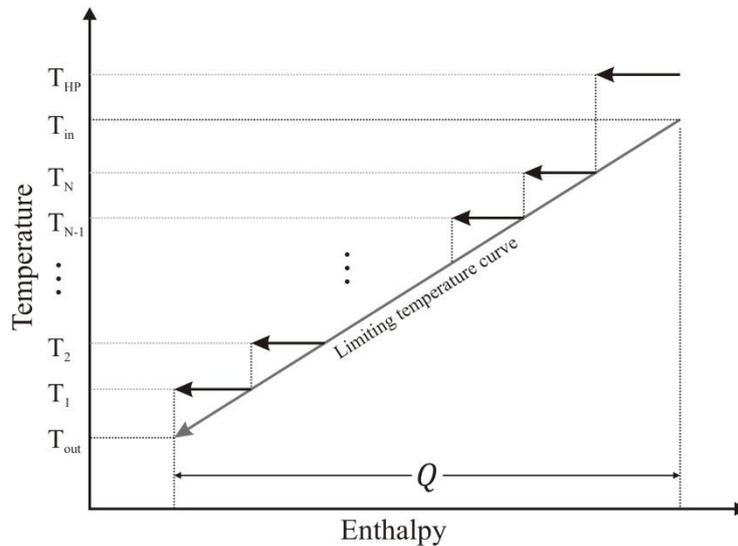


Figure 4.2: An arbitrary process heated only with latent heat from multiple steam levels.

Again, it is noted that the situation depicted in Figure 4.2, with all the intermediate steam levels forming pinches against the limiting temperature curve, represents the minimum total steam flowrate. Here, the total steam flowrate is the sum of all the individual flowrates of the different steam levels (Equation 4.14)

$$\begin{aligned}
 \dot{m}(T_i) = & \frac{(T_1 - T_{out})Q}{(T_{in} - T_{out})\lambda_1} + \dots + \frac{(T_i - T_{i-1})Q}{(T_{in} - T_{out})\lambda_i} + \dots + \frac{(T_N - T_{N-1})Q}{(T_{in} - T_{out})\lambda_N} \\
 & + \frac{(T_{in} - T_N)Q}{(T_{in} - T_{out})\lambda_{HP}} \quad i = 1..N \quad (4.14)
 \end{aligned}$$

4 Mathematical Analysis

To analyse the change in the total steam flowrate as a result of a change in the saturation temperature T_i of one of the steam levels, the first partial derivative of Equation 4.14 must be calculated for each of the N intermediate steam levels. Noting that any T_i appears in only two terms of Equation 4.14, Equation 4.15 expresses these N first partial derivatives.

$$\frac{\partial \dot{m}}{\partial T_i} = \frac{Q\lambda_i + (T_i - T_{i-1})Qb}{(T_{in} - T_{out})\lambda_i^2} - \frac{Q}{(T_{in} - T_{out})\lambda_{i+1}} \quad \forall i \in \{1, N\} \quad (4.15)$$

By setting the N expressions in Equation 4.15 to 0 and solving for T_i , the N stationary points in Equation 4.16 are obtained. Just as with Equation 4.13, these stationary points can be expressed in an alternative form (Equation 4.17). In these two equations, T_0 is used to refer to T_{out} and T_{N+1} is used to refer to T_{HP} .

$$T_i^* = -\frac{1}{b} \left(\sqrt{a^2 - ab(T_{i-1} + T_{i+1}) + b^2 T_{i-1} T_{i+1}} - a \right) \quad \forall i \in \{1, N\} \quad (4.16)$$

$$\lambda_i^* = \sqrt{\lambda_{i-1}^* \lambda_{i+1}^*} \quad \forall i \in \{1, N\} \quad (4.17)$$

To determine whether the total steam flowrate obtained at the set of saturation temperatures in Equation 4.16 is a minimum or a maximum, one must inspect the matrix of second partial derivatives of the total steam flowrate with respect to T_i . Since the first partial derivative with respect to T_i is a function of only three temperatures (T_{i-1} , T_i and T_{i+1}), the matrix will only have three non-zero elements per row. This symmetric tridiagonal Hessian matrix is shown in Matrix 4.1.

4 Mathematical Analysis

$$\left[\begin{array}{ccccccc}
 \frac{\partial^2 \dot{m}}{\partial T_1^2} & \frac{\partial^2 \dot{m}}{\partial T_1 \partial T_2} & 0 & & & & \\
 \frac{\partial^2 \dot{m}}{\partial T_2 \partial T_1} & \frac{\partial^2 \dot{m}}{\partial T_2^2} & \frac{\partial^2 \dot{m}}{\partial T_2 \partial T_3} & \dots & & 0 & 0 & 0 \\
 0 & \frac{\partial^2 \dot{m}}{\partial T_3 \partial T_2} & \frac{\partial^2 \dot{m}}{\partial T_3^2} & & & 0 & 0 & 0 \\
 & \vdots & & \ddots & & \vdots & & \\
 & & & & \frac{\partial^2 \dot{m}}{\partial T_{N-2}^2} & \frac{\partial^2 \dot{m}}{\partial T_{N-2} \partial T_{N-1}} & & 0 \\
 0 & 0 & 0 & & \frac{\partial^2 \dot{m}}{\partial T_{N-1} \partial T_{N-2}} & \frac{\partial^2 \dot{m}}{\partial T_{N-1}^2} & \frac{\partial^2 \dot{m}}{\partial T_{N-1} \partial T_N} & \\
 0 & 0 & 0 & \dots & & \frac{\partial^2 \dot{m}}{\partial T_N \partial T_{N-1}} & \frac{\partial^2 \dot{m}}{\partial T_N^2} & \\
 & & & & 0 & & &
 \end{array} \right] \quad (4.1)$$

The diagonal elements of Matrix 4.1 evaluated at the stationary point are given in Equation 4.18. The off-diagonal elements of Matrix 4.1 evaluated at the stationary point are given in Equation 4.19.

$$\left. \frac{\partial^2 \dot{m}}{\partial T_i^2} \right|_{T_i^*, T_{i-1}^*} = \frac{2(T_i^* - T_{i-1}^*)Qb^2 + 2\lambda_i^* Qb}{(T_{in} - T_{out})(\lambda_i^*)^3} \quad \forall i \in \{1, N\} \quad (4.18)$$

$$\left. \frac{\partial^2 \dot{m}}{\partial T_i \partial T_{i+1}} \right|_{T_i^*, T_{i+1}^*} = \frac{-Qb}{(T_{in} - T_{out})(\lambda_{i+1}^*)^2} \quad \forall i \in \{1, N - 1\} \quad (4.19)$$

In Appendix B, it is shown that the Hessian matrix composed of the second partial derivatives of Equation 4.14 (Matrix 4.1) is positive definite at the stationary point. As such, the stationary point represented by the temperatures in Equation 4.16 represent a minimum (Rao, 2009). In words, this states that when using only latent heat, the minimum total steam flowrate obtained with intermediate steam levels at the saturation temperatures expressed by Equation 4.16 is lower than the minimum total steam flowrate obtained using any other

4 Mathematical Analysis

set of saturation temperatures. The set of steam levels expressed in Equation 4.16 should be viewed as the optimal set of saturation temperatures for the intermediate steam levels.

4.2 Latent and Sensible Heat (Hot Liquid Reuse)

The second case to be analysed involves the use of latent heat and sensible heat. It is this case that looks at the steam flowrate minimisation techniques developed by Coetzee and Majozzi (2008) and Price and Majozzi (2010), and considers the effect of the chosen set of steam levels on the minimum total steam flowrate achieved. The analysis begins by considering an arbitrary process stream that requires a heating duty of some positive value Q . Based on the supply and target temperatures of the cold process stream, and the ΔT_{\min} value for the heat exchanger, a limiting temperature curve for the hot utility can be plotted on a temperature versus enthalpy plot (Figure 4.3) with minimum inlet and outlet temperatures of T_{in} and T_{out} respectively.

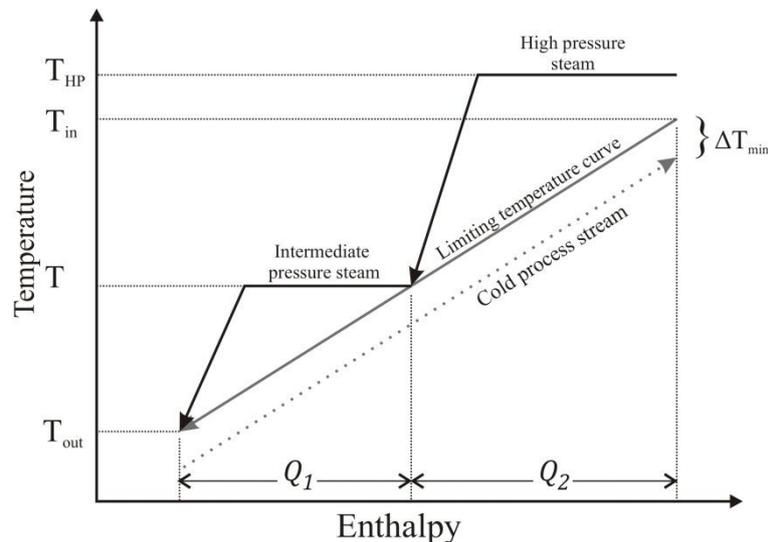


Figure 4.3: An arbitrary process heated using latent and sensible heat from two steam levels.

4 Mathematical Analysis

Again, the first steam level considered is a high pressure steam level supplied directly from the boiler. This steam level has a fixed saturation temperature of T_{HP} , determined by the boiler operation. Ultimately, this temperature is specified in the early stages of design to ensure that the HP steam level is hot enough to fulfil the highest temperature demands of the plant. In this analysis, T_{HP} can be fixed at any temperature greater than or equal to T_{in} .

The second steam level considered is an intermediate pressure steam level with an arbitrarily chosen saturation temperature T . It is this steam level that will be altered in order to view the effects of steam level selection on the minimum steam flowrate.

The system depicted in Figure 4.3 represents the minimum steam flowrate for the given steam level saturation temperatures. As in the analysis given above, the duties provided by both steam levels are calculated using similar triangles (Equations 4.6 and 4.7). In calculating the mass flowrate of the individual steam flowrates, one must remember that both saturated steam and hot condensate are used to provide heat. As such, Equation 3.4 must be used to calculate the individual steam flowrates. Summing these individual flowrates together, one obtains the minimum total steam flowrate as a function of the IP steam saturation temperature, T . Equation 4.20 gives this function, with Equation 4.9 still being used to calculate λ .

$$\dot{m}(T) = \frac{(T - T_{out})Q}{(T_{in} - T_{out})(c_p(T - T_{out}) + \lambda)} + \frac{(T_{in} - T)Q}{(T_{in} - T_{out})(c_p(T_{HP} - T) + \lambda_{HP})} \quad (4.20)$$

In order to view the effect that a change in T has on the minimum total steam flowrate achieved, one must find the first derivative of Equation 4.20 with respect to T . Equation 4.21 gives this first derivative, after simplification.

4 Mathematical Analysis

$$\frac{d\dot{m}}{dT} = \frac{Q\lambda_{out}}{(T_{in} - T_{out})(c_p(T - T_{out}) + \lambda)^2} - \frac{Q\lambda_{HP}}{(T_{in} - T_{out})(c_p(T_{HP} - T) + \lambda_{HP})^2} \quad (4.21)$$

In order to locate any stationary points, the first derivative is set equal to zero and solved for in terms of T . The temperatures at which stationary points are located, T^* , are given in Equation 4.22, with the values expressed in Equations 4.23 and 4.24 used to reduce the overall length of Equation 4.22. As in the previous analysis, it is noted that only the positive root leads to a sensible stationary point in the context of this investigation.

$$T^* = \frac{(\lambda_{out}c_p)T_{in} - (\theta - a\gamma)\lambda_{HP} \pm \{\theta - \gamma\lambda_{HP} - \gamma c_p T_{in}\}\sqrt{\lambda_{out}\lambda_{HP}}}{\lambda_{out}c_p^2 - \gamma^2\lambda_{HP}} \quad (4.22)$$

$$\gamma = (c_p - b) \quad (4.23)$$

$$\theta = (T_{out}c_p^2 - ac_p) \quad (4.24)$$

To test whether this stationary point is a maximum or a minimum, the second derivative of Equation 4.20 with respect to T must be used. This second derivative, evaluated at the stationary point, is given in Equation 4.25.

$$\left. \frac{d^2\dot{m}}{dT^2} \right|_{T^*} = \frac{-2Q(c_p - b)\lambda_{out}}{(T_{in} - T_{out})(c_p(T^* - T_{out}) + \lambda^*)^3} - \frac{2Qc_p\lambda_{HP}}{(T_{in} - T_{out})(c_p(T_{HP} - T^*) + \lambda_{HP})^3} \quad (4.25)$$

In Appendix A, it is shown that T^* lies between T_{HP} and T_{out} , implying that T^* is greater than T_{out} . Also, by definition Q , b and λ^* are all positive quantities. Thus both denominators in Equation 4.25 are positive. Since b has a value of 4.13 between 100°C and 300°C (Equation 3.1) and because the heat capacity of water between these limits is greater than 4.13 in value (Cooper & Le Fevre,

4 Mathematical Analysis

1969), the term $(c_p - b)$ is always positive. Thus, the second derivative evaluated at the stationary point is negative, indicating a maximum.

In words, this states that when utilising both latent and saturated heat, the minimum total steam flowrate achieved when the IP steam has a saturation temperature of T^* is greater than the minimum total steam flowrate achievable using any other IP steam saturation temperature. With the aid of simulations, it was found that a maximum exists for cases with more than two steam levels as well. It was also found during these simulations that the flowrate at this maximum is lower than the minimum achieved when only using latent heat.

During these simulations, it was also noted that for the case of hot liquid reuse, the lowest minimum total steam flowrate achievable occurs when the saturation temperatures of all the intermediate steam level are set to T_{out} . Since steam with this saturation temperature is unusable in the system, this indicates that only HP steam should be used when utilising both latent and sensible heat. To understand why this is, one must look at how the steam flowrate is calculated for the case of hot liquid reuse (Equation 4.26, repeated from Equation 3.4)

$$\dot{m} = \frac{Q}{\lambda + c_p(T_{sat} - T_{out})} = \frac{Q}{(a - bT_{sat}) + c_p(T_{sat} - T_{out})} \quad (4.26)$$

The question now arises concerning how this flowrate for a single steam level is affected by a change in the saturation temperature of the steam. Equation 4.27 gives the first derivative of Equation 4.26 with respect to T_{sat} . As discussed above, the term $(c_p - b)$ is positive over the range between 100°C and 300°C. This implies that the first derivative is negative.

4 Mathematical Analysis

$$\frac{d\dot{m}}{dT_{sat}} = \frac{-Q(c_p - b)}{(\lambda + c_p(T_{sat} - T_{out}))^2} \quad (4.27)$$

Since the first derivative is negative, an increase in the steam saturation temperature will result in a decrease in the required steam flowrate. This makes sense, since a 1°C increase in T_{sat} will cause 4.13 kJ/kg of latent heat to be lost, but approximately 4.3 kJ/kg of sensible heat to be gained, increasing the total energy available per unit mass of steam.

Because of this, in the case of hot liquid reuse, hotter steam will deliver more energy per kilogram of flowrate than colder steam. This is in direct contrast to the case of using only latent heat, in which steam with a lower saturation temperature delivers more energy per kilogram, but is less useful due to temperature limitations. Since hotter steam delivers more energy per mass flowrate in the case of utilising both latent and sensible heat, it would not be recommended to add any lower steam levels, as the lower available energy content of these steam levels will result in an increased mass flowrate. This explains why the best option when utilising both latent and sensible heat is to only use a single, high pressure steam level.

4.3 Discussion

The following short discussions are presented to clarify the results of the above analyses.

4.3.1 Example

An example will be used here to graphically display the results of the analyses. Consider an arbitrary cold process stream that must be heated from 100°C to 220°C, requiring 1000 kW of heat. High pressure steam from the boiler is available at a saturation temperature of 254°C, and it is assumed that the heat

4 Mathematical Analysis

capacity of water remains constant at $4.3 \text{ kJ/kg}\cdot\text{K}$. A value of 10°C is used as the ΔT_{\min} for the heat exchanger, setting the minimum inlet and outlet temperatures for any hot utility at 230°C and 110°C respectively.

Considering first the case of using only latent heat and only two steam levels (HP and IP steam), Figure 4.4 shows the locus of the minimum total steam flowrate as the saturation temperature of the IP steam level changes. One can see that when the IP steam levels has a saturation temperature of 187.45°C , the minimum total steam flowrate is lower than the minimum total steam flowrate achievable using any other saturation temperature. Figure 4.5 also shows the locus of the minimum total steam flowrate when utilising latent heat only, but this time for three steam levels. At the point where the saturation temperatures of the MP and LP steam levels are 210.77°C and 162.93°C respectively another minimum is seen. Clearly, if one were designing a steam system for this process using only latent heat, these would be the optimum saturation temperatures for the intermediate steam levels.

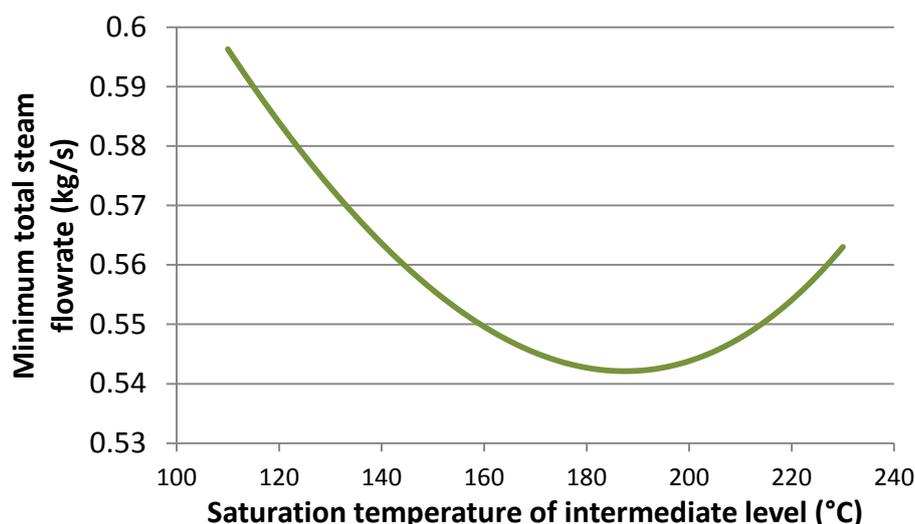


Figure 4.4: Minimum total steam flowrate as a function of IP steam saturation temperature, using only latent heat from two steam levels.

4 Mathematical Analysis

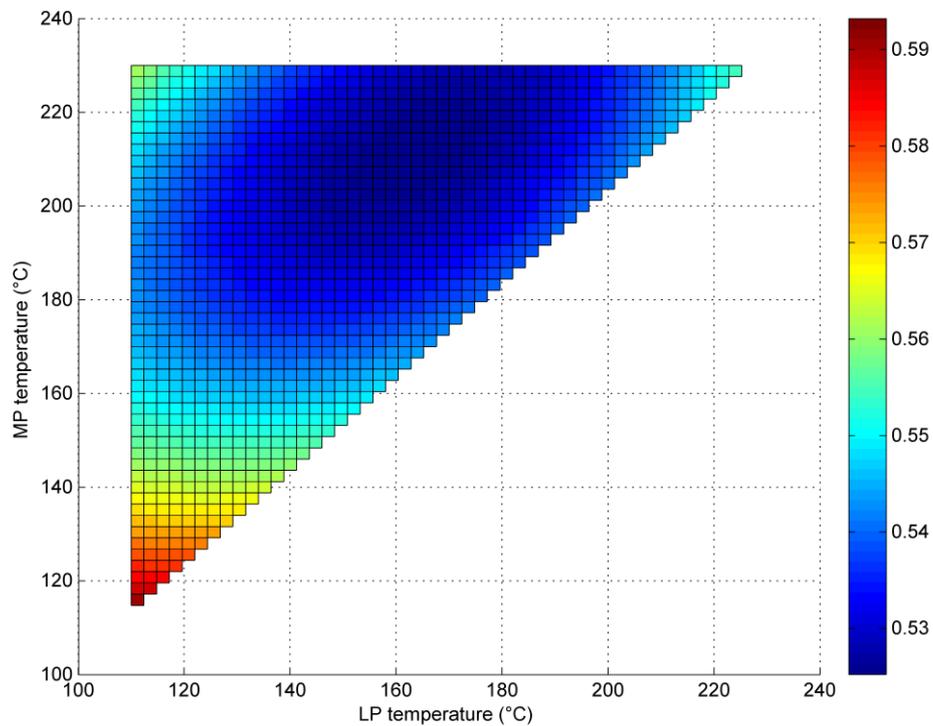
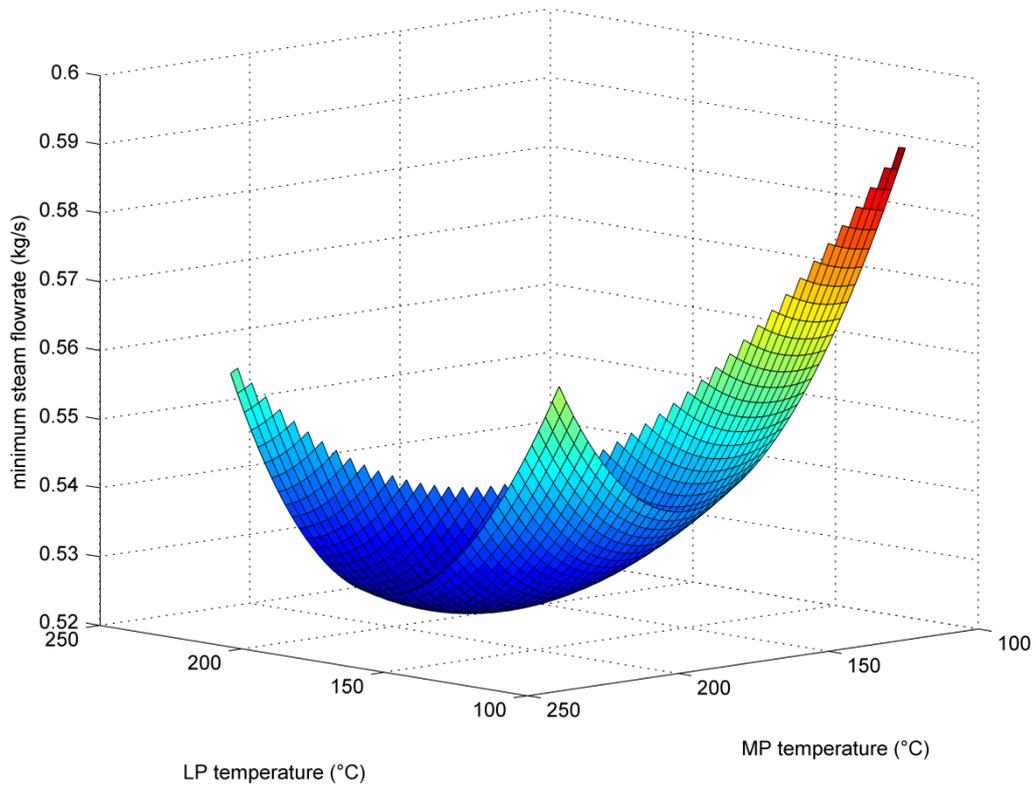


Figure 4.5: Minimum total steam flowrate as a function of MP and LP steam saturation temperatures, using only latent heat from three steam levels .

4 Mathematical Analysis

Figure 4.6 shows the locus of the minimum total steam flowrate as a function of the IP steam saturation temperature for the case of hot liquid reuse. One can see that at an IP saturation temperature of 174.08°C, the minimum total steam flowrate is greater than that achieved using any other saturation level. Figure 4.7 shows a similar maximum when the MP and LP saturation temperatures are 193.79°C and 153.62°C respectively. It is noted though, that in both these figures, the lowest minimum total steam flowrate is achieved when all the lower steam levels are set at a saturation temperature of 110°C, and only HP steam is used.

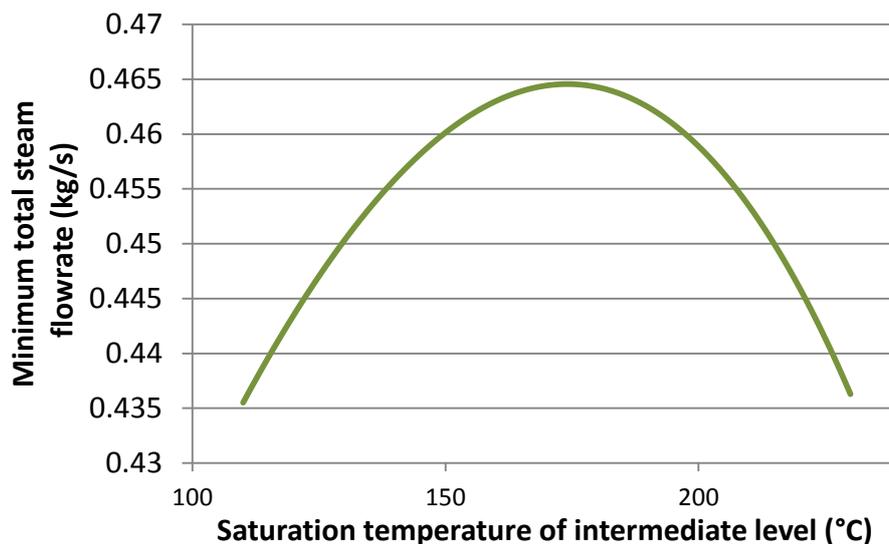


Figure 4.6: Minimum total steam flowrate as a function of IP steam saturation temperature, using latent and sensible heat from two steam levels.

4 Mathematical Analysis

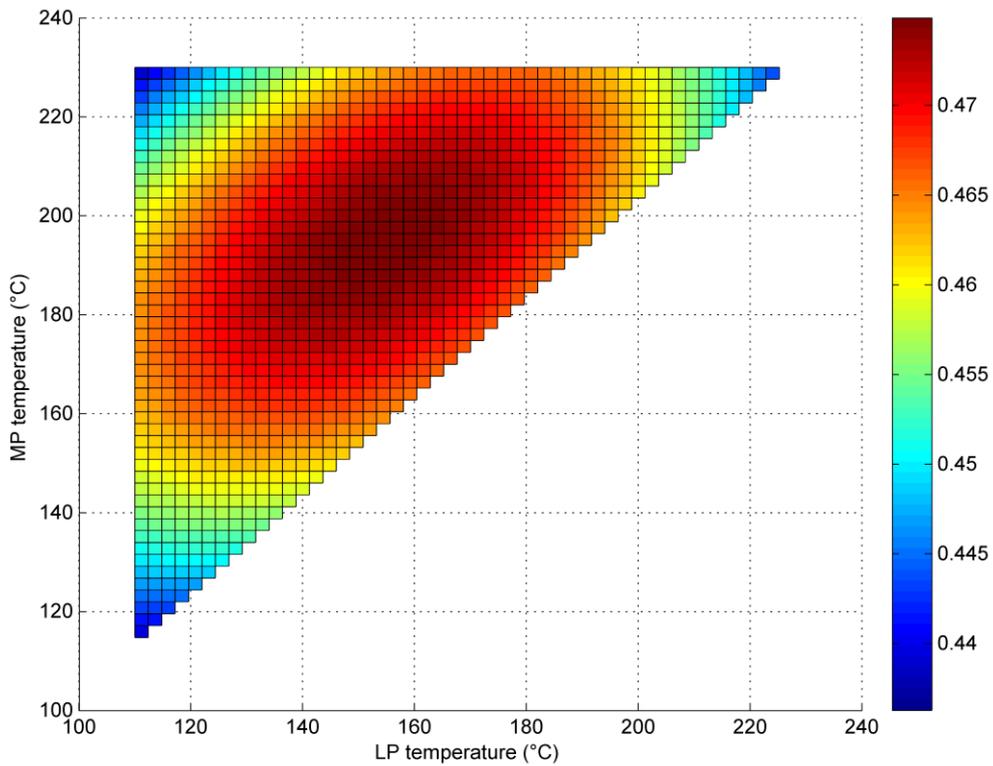
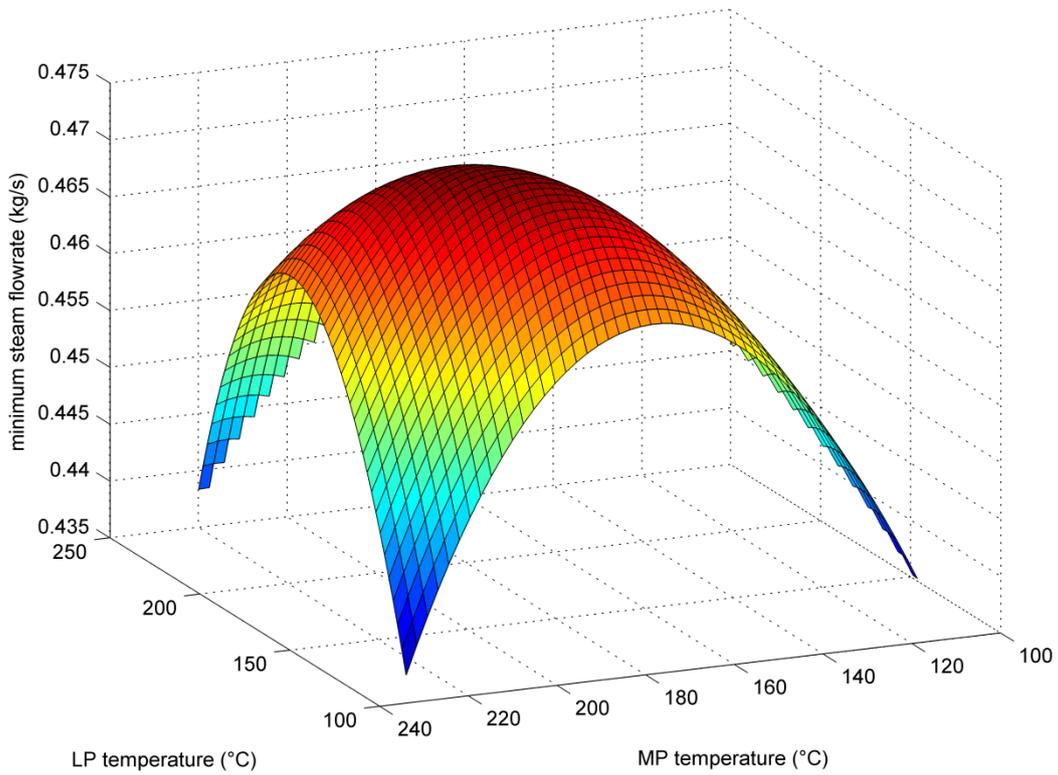


Figure 4.7: Minimum total steam flowrate as a function of MP and LP steam saturation temperatures, using latent and sensible heat from three steam levels.

4.3.2 Nonlinear Composite Curves

The analyses presented above have been for linear processes. The heating side of a grand composite curve (GCC) is, however, very rarely linear. Below is a discussion on how this might affect the results of the analyses above.

When it comes to determining the best placement of multiple steam levels for a particular problem, there are a number of heuristics that can be used. One of the more popular techniques involves inspecting the GCC for pockets and other topographical features that would suggest the placement of a steam level. Another way would be to apply the lessons learnt from the analysis for the case of latent heat only. If the heating side of the GCC lies vaguely in the region of a linear approximation between T_{in} and T_{out} (Figure 4.8) then Equation 4.17 can be used to place the intermediate steam levels.

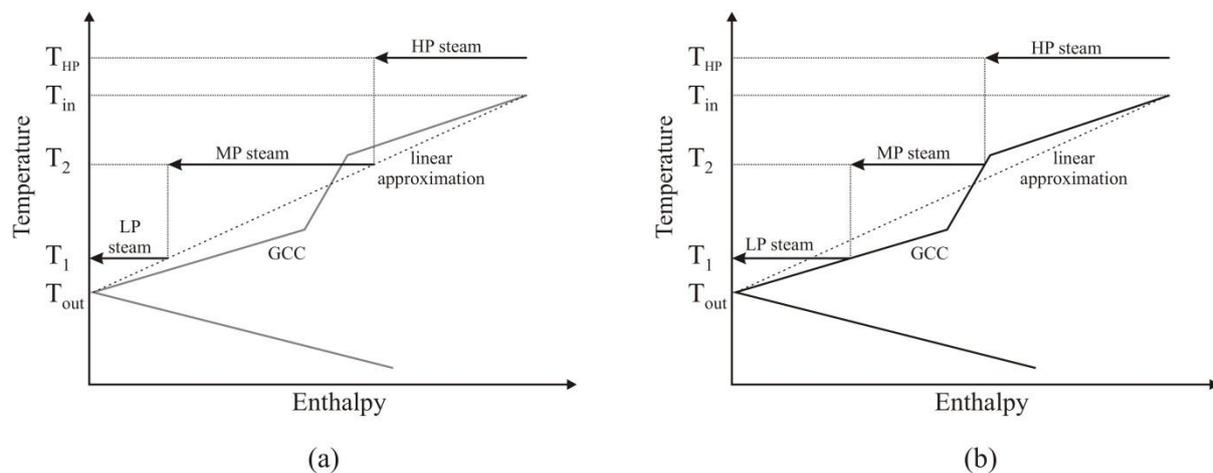


Figure 4.8: Use of a linear approximation to the GCC for the placement of intermediate steam levels (a) before adjustment (b) after adjustment.

In Figure 4.8(a), one can see the optimum placement of MP and LP steam levels against a linear approximation to the GCC between T_{in} and T_{out} . Figure 4.8(b) shows how the steam flowrates have been adjusted to the actual GCC, keeping the same saturation temperatures of the levels. In doing this, the actual steam

4 Mathematical Analysis

In the analysis for the use of both latent and sensible heat, it was stated that only a single steam level should be used to ensure a truly minimum steam flowrate. This raises the question of whether this is still true for nonlinear GCCs with pockets etc. To defend this statement, a proof by contradiction is used.

Suppose that in the event of a nonlinear GCC, using some configuration of multiple steam levels, such as in Figure 4.10(a), yields a lower flowrate than if only a single steam flowrate were used. Suppose then the saturation temperature of the IP steam level was to be increased until it were equal to the saturation temperature of the HP steam, as shown in Figure 4.10(b). As discussed above, this new IP steam level would have a lower flowrate than the IP steam level in Figure 4.10(a). The situation in Figure 4.10(b) therefore has a lower total steam flowrate than in Figure 4.10(a).

Since both the HP and IP steam levels have the same saturation temperatures in Figure 4.10(b), they are effectively the same steam level. Indeed, by adding these two identical steam levels together, one achieves the same result as if only a single steam level had been used to begin with (dashed utility curve in Figure 4.10(b)). Because using only a single steam level has produced a lower total steam flowrate than for the multiple level case assumed initially, the assumption that a multiple level solution could yield a lower total flowrate has been proven false by contradiction. It is therefore concluded that whenever both latent and sensible heat is utilised, only a single high pressure steam level should be used. This statement is not affected by nonlinearities and other topographical features of the GCC.

4 Mathematical Analysis

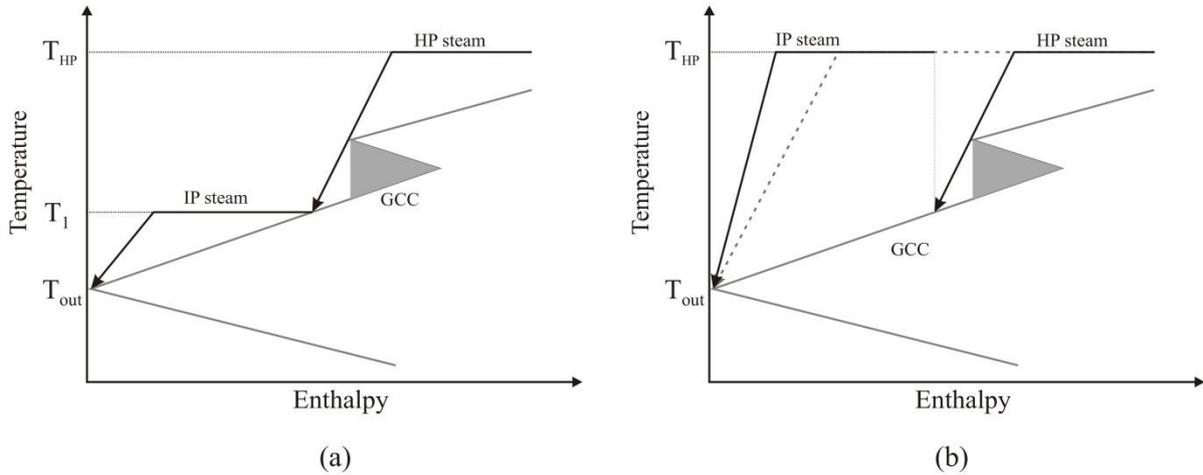


Figure 4.10: Placing steam levels when utilising latent and sensible heat (a) a possible configuration (b) showing that one steam level can satisfy both regions (overall utility line shown dashed).

4.3.3 Solving Equation 4.17

In Equation 4.17, each steam level is expressed in terms of the level directly above and below it. This will present problems if trying to solve for problems with N greater than 1, because each unknown will be expressed in terms of other unknowns. If Equation 4.17 is to be used as a heuristic for the placement of steam levels, then a simple method of solving the set of nonlinear equations is required.

If the log of both sides of Equation 4.17 is taken, then Equation 4.17 can be converted into Equation 4.28.

$$\ln(\lambda_i^*) = 0.5 \ln(\lambda_{i-1}^*) + 0.5 \ln(\lambda_{i+1}^*) \quad \forall i \in \{1, N\} \quad (4.28)$$

This set of linearized equations can be expressed in matrix notation. Matrix 4.2 shows this for N equal to 6.

4 Mathematical Analysis

$$\begin{bmatrix} -1 & 0.5 & 0 & 0 & 0 & 0 \\ 0.5 & -1 & 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & -1 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & -1 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 & -1 & 0.5 \\ 0 & 0 & 0 & 0 & 0.5 & -1 \end{bmatrix} \begin{bmatrix} \ln(\lambda_1^*) \\ \ln(\lambda_2^*) \\ \ln(\lambda_3^*) \\ \ln(\lambda_4^*) \\ \ln(\lambda_5^*) \\ \ln(\lambda_6^*) \end{bmatrix} = \begin{bmatrix} -0.5\ln(\lambda_{out}) \\ 0 \\ 0 \\ 0 \\ 0 \\ -0.5\ln(\lambda_{HP}) \end{bmatrix} \quad (4.2)$$

The vector containing the natural logarithms of the latent heats can easily be solved for using matrix mathematics. The optimum saturation temperatures of the individual intermediate steam levels can then be obtained with Equation 4.29

$$T_i^* = \frac{1}{b} (a - \exp[\ln(\lambda_i^*)]) \quad \forall i \in \{1, N\} \quad (4.29)$$

4.4 References

- Coetzee, W. A., & Majazi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Cooper, J. R., & Le Fevre, E. J. (1969). Thermophysical properties of water substance. Butterworth-Heinemann, London, UK.
- Price, T., & Majazi, T. (2010). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Rao, S. S. (2009). Engineering Optimization: Theory and Practice. Hoboken: John Wiley & Sons.

Chapter 5

Model Development

In the analyses presented in the previous chapter, it is stated that only a single high pressure steam level should be employed to ensure a minimum total steam flowrate when utilising both latent and sensible heat. This is a feasible suggestion if the only use for steam on the plant is process heating. When steam must be used to drive steam turbines to provide shaft work, then additional steam levels caused by the turbine exhaust will be present. Since it would be a waste to discard this steam, it is often used as low and medium pressure steam for heating.

This poses the question of how best to make use of this turbine exhaust steam in the heat exchanger network. The model by Price and Majozi (2010) accepts that the steam turbines have been previously designed and the steam levels fixed before the HEN design is undertaken. The model minimises the flowrate of high pressure steam supplied to the HEN, while using the fixed flowrates of turbine exhaust steam to provide as much heating as possible. As was discussed in section 3.4, the shaft work produced by a turbine is a function of the steam flowrate and the pressure drop over the turbine. There are many configurations of these two variables that will produce the same quantity of shaft work, but will yield different results in the model by Price and Majozi (2010). Clearly, a minimum steam flowrate cannot be guaranteed if the turbines are designed separately from the HEN.

The ability for the design of a turbine to affect the minimum steam flowrate required by the HEN suggests that a holistic approach must be taken in respect to the HEN and the power block. The design of the turbines should ideally be included in the model for minimising the total steam flowrate. This way, the interactions between the HEN and the power block can be accounted for, and a turbine design can be obtained that allows for a true minimum steam flowrate to be achieved for the HEN. The model presented below has been developed to address this need for a holistic coverage of the HEN and power block.

5.1 Problem Statement

The problem to be addressed here can be stated formally as follows.

Given:

- a set of cold process streams,
- the fixed duties required by each cold process stream,
- the supply and target temperatures for each cold process stream,
- the minimum temperature difference for heat exchange,
- a shaft work target.

Determine:

- the minimum total steam flowrate,
- the saturation temperatures of the intermediate steam levels required to satisfy the energy demands of the heat exchangers and shaft work requirements and
- the network of heat exchangers that will fulfil this target.

5.2 Superstructure

The superstructure used in this model (Figure 5.1) is based on the superstructure for the multiple steam level model developed by Price and Majozi (2010). The difference here is the presence of variables to account for the operation of the turbines.

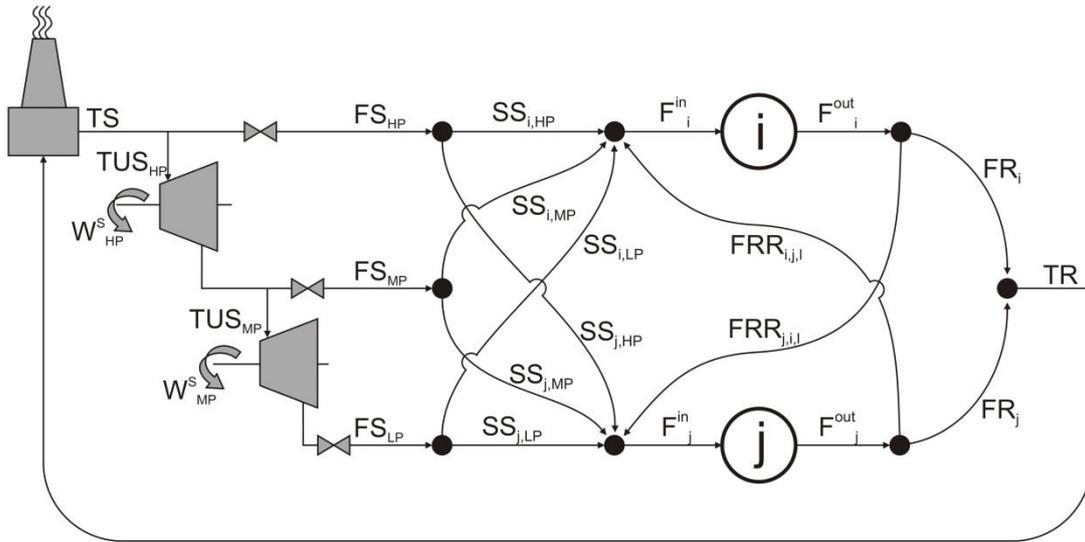


Figure 5.1: Superstructure for the present model.

In Figure 5.1, one can see that a steam boiler produces a total flowrate of high pressure steam TS . This steam is split between the HEN and the high pressure turbine. The exhaust steam from this HP turbine can be used to drive a medium pressure turbine or can be supplied to the HEN. Another option, not drawn in Figure 5.1, is to return this MP steam to the boiler after passing through a condenser, wasting potentially useful steam. A similar description applies to the low pressure turbine.

In Figure 5.1, i and j are heat exchangers belonging to the set of all heat exchangers I . There are also the individual steam levels l belonging to the set of all steam levels L . Here, it can be seen that any heat exchanger i can receive saturated steam from any one of the levels l , as well as hot liquid reuse from

any other heat exchanger j . The liquid leaving heat exchanger i can be returned to the boiler, or supplied as hot liquid to any other heat exchanger j .

5.3 Constraints

The constraints of the present model are derived from mass and energy balances over various sections of the superstructure in Figure 5.1. The first set of constraints concern mass balances over the inlet and outlet of the whole HEN. Equation 5.1 states that the total quantity of steam entering the HEN is equal to the sum of the steam flowrates of the individual steam levels supplying the HEN. Equation 5.2 states that the total quantity of liquid leaving the HEN is equal to the sum of the boiler return flowrates of the individual heat exchangers. If leakages within the HEN are negligible, then mass is conserved and Equation 5.3 must hold.

$$TS = \sum_{l \in L} FS_l \quad (5.1)$$

$$TR = \sum_{i \in I} FR_i \quad (5.2)$$

$$TS = TR \quad (5.3)$$

Considering the inlet to the HEN, Equation 5.4 states that the flowrate of each steam level is equal to the sum of the flowrates of saturated steam of that level supplied to the individual heat exchangers. It is this constraint that will serve as a link between the set of overall HEN mass balances above, and mass balances performed over individual heat exchangers.

$$FS_l = \sum_{i \in I} SS_{i,l} \quad \forall l \in L \quad (5.4)$$

5 Model Development

Just as a mass balance was performed over the entire HEN, so too can a mass balance be performed over the individual heat exchangers. Equation 5.5 states that the mass flowrate at the inlet to heat exchanger i is equal to the sum of the flowrate of saturated steam supplied to heat exchanger i from all levels, plus the sum of the flowrates of all the reuse streams being supplied to heat exchanger i from all other heat exchangers j , from all levels. Equation 5.6 states the mass flowrate at the outlet of heat exchanger i is equal to the boiler return plus the sum of the flowrates of the reuse streams supplied by i to all other heat exchangers j at all levels. Equation 5.7 ensures conservation of mass inside the heat exchangers. Equation 5.8 is used to show that each reuse stream can be made up of saturated liquid and hot liquid.

$$F_i^{in} = \sum_l SS_{i,l} + \sum_{j,l \in J,L} FRR_{i,j,l} \quad \forall i \in I \quad (5.5)$$

$$F_i^{out} = FR_i + \sum_{j,l \in J,L} FRR_{j,i,l} \quad \forall i \in I \quad (5.6)$$

$$F_i^{in} = F_i^{out} \quad \forall i \in I \quad (5.7)$$

$$FRR_{i,j,l} = SL_{i,j,l} + HL_{i,j,l} \quad \forall i, j \in I, l \in L \quad (5.8)$$

A particular heat exchanger should not be allowed to recycle hot liquid back to itself, as this will serve to cool the inlet stream, which will produce infeasibilities. To prevent local recycle, Equation 5.9 is implemented. Constraints similar to Equation 5.9 can be implemented to prevent unfavourable

5 Model Development

matches between particular streams. Here, the indices relating to the streams that may not be connected must be specified manually.

$$FRR_{i,j,l} = 0 \quad \text{if } i = j \quad \forall i, j \in I \quad (5.9)$$

Saturated liquid is the product of saturated steam condensing. Accounting for this phase change, Equation 5.10 states that the quantity of saturated liquid leaving heat exchanger i may not exceed the quantity of saturated steam with which heat exchanger i is supplied. In a similar fashion, Equation 5.11 states that the quantity of hot liquid leaving heat exchanger i may not exceed the quantity of hot liquid with which i is supplied.

$$\sum_{j \in J} SL_{i,j,l} \leq SS_{i,l} \quad \forall i \in I, l \in L \quad (5.10)$$

$$\sum_{j \in J} HL_{i,j,l} \leq \sum_{j \in J} SL_{j,i,l} + \sum_{j \in J} HL_{j,i,l} \quad \forall i \in I, l \in L \quad (5.11)$$

Energy balances can also be performed over the individual heat exchangers. Equation 5.12 states that the quantity of latent heat supplied to heat exchanger i is the sum over all levels of the flowrate of saturated steam multiplied by the latent heat of that steam level. The latent heat of each level is calculated using the correlation given by Mavromatis and Kokossis (1998) which was discussed previously. This constraint (Equation 5.13) is valid between 100°C and 300°C. Equation 5.14 states that the quantity of sensible heat supplied to heat exchanger i is equal to the product of the heat capacity, the inlet mass flowrate, and temperature change of the utility stream over the heat exchanger. Equation 5.15 shows how the temperature of the utility stream entering heat exchanger i can be calculated using a blending rule.

5 Model Development

$$Q_i^{SS} = \sum_{l \in L} SS_{i,l} \lambda_l \quad \forall i \in I \quad (5.12)$$

$$\lambda_l = 2726 - 4.13 T_l^{sat} \quad \forall l \in L \quad (5.13)$$

$$Q_i^{HL} = c_p F_i^{in} (T_i^{in} - T_i^{out}) \quad \forall i \in I \quad (5.14)$$

$$T_i^{in} = \frac{\sum_{j,l \in J,L} SL_{j,i,l} T_l^{sat} + \sum_{j,l \in J,L} HL_{j,i,l} T_j^{out}}{F_i^{in}} \quad \forall i \in I \quad (5.15)$$

Equations 5.14 and 5.15 both contain the bilinear term $F_i^{in} T_i^{in}$. Following the linearization technique used by Coetzee and Majozi (2008), Equation 5.15 is substituted into Equation 5.14, followed by setting all outlet temperatures equal to their respective minimum outlet temperatures. This second step has been shown by Savelski and Bagajewicz (2000) to be a necessary condition for optimality in waste water minimisation problems. The analogies between heat and mass transfer allow this condition to be used here also. Equation 5.16 gives the final linearized constraint. Equation 5.17 states that the sum of the latent heat and sensible heat supplied to heat exchanger i must equal the heat demand of process stream i .

$$Q_i^{HL} = \sum_{j,l \in J,L} c_p SL_{j,i,l} T_l^{sat} + \sum_{j,l \in J,L} c_p HL_{j,i,l} T_j^{out,L} - c_p F_i^{out} T_i^{out,L} \quad \forall i \in I \quad (5.16)$$

$$Q_i^{SS} + Q_i^{HL} = Q_i \quad \forall i \in I \quad (5.17)$$

As in the models by Coetzee and Majozi (2008) and Price and Majozi (2010), upper bounds can be calculated for the flowrate of hot liquid and saturated

5 Model Development

steam through each heat exchanger. Equation 5.18 calculates the upper bound on the flowrate of hot liquid through heat exchanger i . Equation 5.19 calculates the upper bound on the flowrate of saturated steam of each level through heat exchanger i . Unlike the model by Price and Majozi (2010), the present model allows for lower steam levels to heat process streams to an intermediate temperature, with higher steam levels supplying the remaining heat and bringing the stream to its target temperature.

$$FRR_i^U = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (5.18)$$

$$SS_{i,l}^U = \begin{cases} 0 & \text{if } T_l^{sat} \leq T_i^{out,L} \\ \frac{(T_l^{sat} - T_i^{out,L}) Q_i}{(T_i^{in,L} - T_i^{out,L}) \lambda_l} & \text{if } T_i^{out,L} < T_l^{sat} < T_i^{in,L} \\ \frac{Q_i}{\lambda_l} & \text{if } T_l^{sat} \geq T_i^{in,L} \end{cases} \quad \forall i \in I \quad (5.19)$$

The complicated structure of Equation 5.19 can be understood easier by considering Figure 5.2. If steam with a saturation temperature lower than or equal to $T_i^{out,L}$ is considered, such as T_1^{sat} in Figure 5.2, then no steam is capable of being used.

If steam with a saturation temperature between $T_i^{out,L}$ and $T_i^{in,L}$ were considered, such as T_2^{sat} in Figure 5.2, then the steam will only be able to supply a limited quantity of heat to the process. This quantity of heat can be calculated using similar triangles. In effect, this is using a lower steam level to preheat the process stream, and then using a high steam level to provide the outstanding duty and bring the process stream to its target temperature.

5 Model Development

Lastly, if steam with a saturation temperature greater than or equal to $T_i^{in,L}$ is considered, such as T_3^{sat} in Figure 5.2, then the steam is hot enough to raise the process stream to its target temperature. This steam level is capable of supplying the entire heat duty required by the process stream. The upper limit on the steam flowrate is simply the duty divided by the latent heat of the steam.

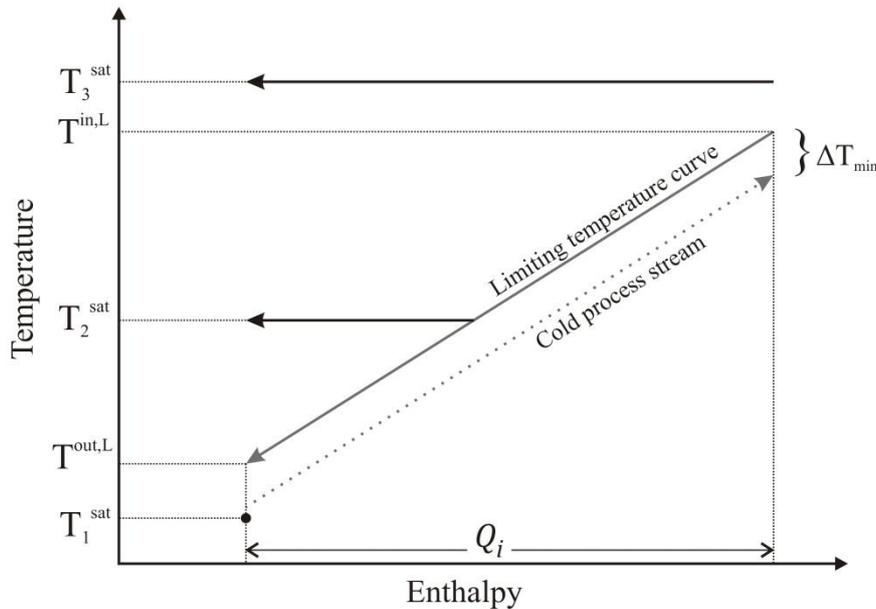


Figure 5.2: The ability of steam from different levels to provide latent heat.

To provide a means of controlling which heat exchangers are supplied with latent heat, and which with sensible heat, two binary variables are introduced. Firstly, x_i is introduced to denote whether or not heat exchanger i is using hot liquid. Secondly, $y_{i,l}$ is introduced to denote whether or not heat exchanger i is using saturated steam of level l . Both of these binary variables take on a value of 1 if the heat exchanger is using the utility in question, and 0 if it is not. Equations 5.20 and 5.21 prevent any flowrate from exceeding its upper bound whilst using the binary variables to determine the existence of streams.

$$SS_{i,l} \leq SS_{i,l}^U y_{i,l} \quad \forall i \in I, l \in L \quad (5.20)$$

5 Model Development

$$\sum_{j,l \in J,L} FRR_{i,j,l} \leq FRR_i^U x_i \quad \forall i \in I \quad (5.21)$$

The binary variables can also be used to control the number of split heat exchangers present in a design. If no split heat exchangers are desired, then Equation 5.22 must be enacted.

$$x_i + \sum_{l \in L} y_{i,l} \leq 1 \quad \forall i \in I \quad (5.22)$$

If it is permitted to split up to m heat exchangers, Equations 5.23 and 5.24 must be used in place of Equation 5.22. Doing this will raise the capital expense of the HEN, since splitting heat exchangers requires addition heat exchangers to be purchased, but will allow a lower total steam flowrate to be achieved and ultimately allow for a cheaper boiler to be purchased.

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_{i,l} \geq |I| \quad (5.23)$$

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_{i,l} \leq |I| + m \quad (5.24)$$

Having dealt with the HEN, attention is now turned to the turbines. Equation 5.25 gives a mass balance over a turbine. This constraint states that the quantity of steam supplied by a turbine to the next turbine, plus the quantity of steam supplied to the HEN may not exceed the quantity of steam entering the turbine. Note that if there are L steam levels, then there can only be $L - 1$ turbines. It is

5 Model Development

assumed that the set of steam levels is arranged in order from highest to lowest pressure, e.g. [HP, MP, LP]. Thus “HP +1” would be “MP”.

$$TUS_{l+1} + FS_{l+1} \leq TUS_l \quad \forall l \in L \quad l < |L| \quad (5.25)$$

Furthermore, Equation 5.26 must be implemented to ensure that each steam level has a saturation temperature greater than the level below it.

$$T_l^{sat} \geq T_{l+1}^{sat} \quad \forall l \in L \quad l < |L| \quad (5.26)$$

As discussed in Section 3.4, Equations 5.27 to 5.29 can be used to calculate the shaft work produced by the individual turbines. The coefficient of 3.6 has been added to convert TUS_l from kilograms per second to tons per hour, as required in Equation 3.69. The values for the coefficients in Equations 5.28 and 5.29 have already been given in Table 3.2.

$$W_l^s = \frac{1}{B_l} (3.6 \overline{\Delta H}_l^{is} TUS_l - A_l) \quad \forall l \in L \quad l < |L| \quad (5.27)$$

$$A_l = a_1 + a_2 T_l^{sat} \quad \forall l \in L \quad l < |L| \quad (5.28)$$

$$B_l = b_1 + b_2 T_l^{sat} \quad \forall l \in L \quad l < |L| \quad (5.29)$$

If it assumed that the heat load of the steam supplied to the turbine is dominated by the latent heat of the steam, then the correlation given by Singh (1997) for calculating $\overline{\Delta H}_l^{is}$ (Equation 3.70) can be rewritten as Equation 5.30.

$$\overline{\Delta H}_l^{is} = \frac{T_l^{sat} - T_{l+1}^{sat}}{391.8 + 2.215 T_l^{sat}} \quad \forall l \in L \quad l < |L| \quad (5.30)$$

Equation 5.31 states that the sum of the shaft work produced by all the turbines must equal the demand for shaft work. If particular turbines are required to drive specific pieces of machinery, then the shaft work targets can be specified per turbine, rather than as a total.

$$\sum_{l < |L|} W_l^s = W_{demand}^s \quad (5.31)$$

Lastly, the objective is to minimise the total steam flowrate produced by the boiler in order to reduce the purchase cost of the boiler. Since the flowrate of high pressure steam is made up of the flow of HP steam to the HEN and the flow of HP steam to the HP turbine the objective function can be expressed as Equation 5.32.

$$\text{minimise}(FS_{HP} + TUS_{HP}) \quad (5.32)$$

The above constraints constitute an MINLP model for Steam flowrate minimisation. The model contains elements of both design and synthesis. The sizing of the turbines represents the design element of the model, whereas determining the configuration of the HEN is synthesis, since the heat exchangers are not sized.

5.4 Solution Procedure

One of the many advantages of a linear model over a nonlinear model is that a linear model does not require a starting point. Nonlinear models on the other hand require a feasible starting point close to the optimum to ensure that the algorithm converges.

5 Model Development

In the model presented above, nonlinearities are introduced as a result of the unknown saturation temperatures of the steam levels. Equation 5.12 contains the product of the saturated steam flowrate and the latent heat of the steam level, which is a function of the steam saturation temperature. Equation 5.16 contains the product of the saturated liquid flowrate and the saturation temperature. Equations 5.27 to 5.30 also introduce numerous nonlinearities as a result of the saturation temperatures. This therefore requires that a suitable starting point be obtained.

If the saturation temperatures of the intermediate steam levels are fixed at suitable values, the model presented above becomes an MILP problem. This can then easily be solved. In this investigation, the saturation temperatures are initially fixed at typical industry standards. The exact values used here have already been discussed in Table 3.1 (Harrel, 1996). The linear model thus obtained is solved, and the resulting solution used as a starting point to the MINLP model.

5.5 References

- Coetzee, W. A., & Majazi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Harrel, G. (1996). Steam system survey guide. ORNL/TM-2001/263: Oak Ridge National Laboratory.
- Mavromatis, S. P., & Kokossis, A. C. (1998). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Price, T., & Majazi, T. (2010). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Savelski, M. J., & Bagajewicz, M. J. (2000). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.
- Singh, H. (1997). Strategies for emissions minimisation in chemical process industries. Ph.D. thesis, Department of Process Integration, UMIST, Manchester, UK.

Chapter 6

Case Study

In order to demonstrate the mathematical analysis and model presented above, a case study is presented here. The case study in question comes from a South African petrochemical company. This case study is given by Coetzee and Majozi (2008), and is also used by Price and Majozi (2010a,b,c).

6.1 Problem Description

The problem in question considers seven cold process streams that require heating. Table 6.1 gives the supply and target temperatures of these cold process streams, as well as the duty required by each. A global ΔT_{\min} value of 10°C is assumed. Using this, the limiting inlet and outlet utility temperatures can be calculated for each stream. Table 6.2 gives this limiting data for each utility stream. The limiting hot utility curve resulting from the data in Table 6.2 is shown in Figure 6.1: Limiting hot utility composite curve.

Table 6.1: Cold process stream data (Coetzee & Majozi, 2008)

Cold Stream	T_i^{supply} ($^{\circ}\text{C}$)	T_i^{target} ($^{\circ}\text{C}$)	Q_i (kW)
1	25	45	135
2	25	45	320
3	209	215	3620
4	79	185	12980
5	207	207	1980
6	44	70	635
7	44	70	330
			20000

6 Case Study

Table 6.2: Limiting hot utility data. (Coetzee & Majozi, 2008)

Cold Stream	$T_i^{in,L} (^\circ\text{C})$	$T_i^{out,L} (^\circ\text{C})$	Q_i (kW)
1	55	35	135
2	55	35	320
3	225	219	3620
4	195	89	12980
5	217	217	1980
6	80	54	635
7	80	54	330
			20000

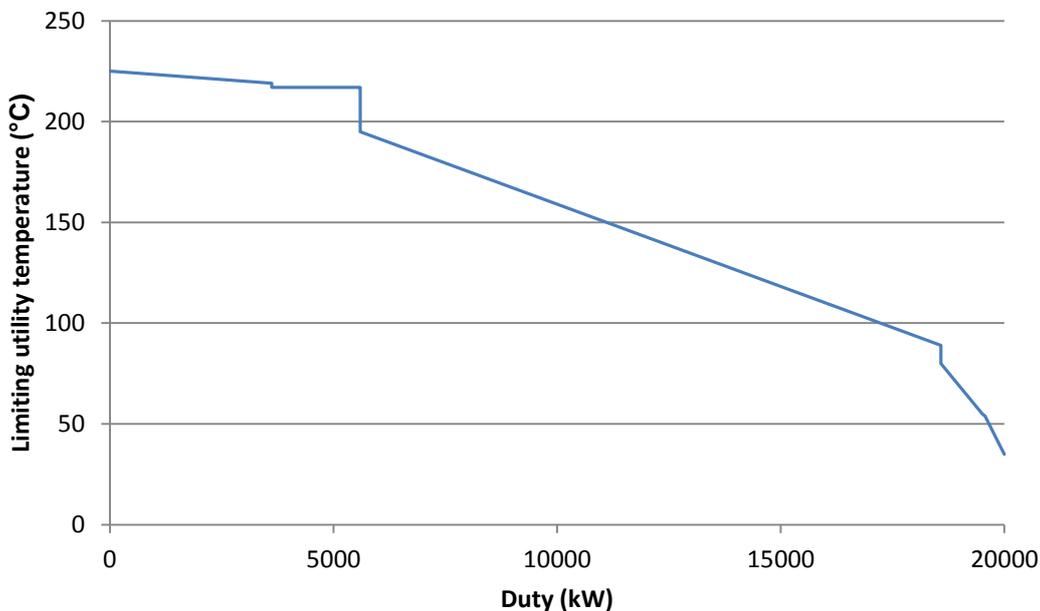


Figure 6.1: Limiting hot utility composite curve.

High pressure steam with a saturation temperature of 225°C is available from the central boiler. For the sake of this investigation, the heat capacity of water is fixed at a value of $4.3 \text{ kJ/kg}\cdot\text{K}$, a safe and typical assumption.

Price and Majozi (2010b) report the existence of two turbines providing MP and LP exhaust steam to the heat exchanger network at a rate of 2 kg/s and 0.23 kg/s respectively, with respective saturation temperatures of 197°C and 114°C . The

shaft work output of the turbines can be calculated using the turbine model discussed above, based on the operating conditions given in Price and Majози (2010b). The shaft work output of the high pressure and medium pressure turbines is 104.56 kW and 5.57 kW respectively. Therefore, for this investigation, the total shaft work target is set to be 110.13 kW.

6.2 Mathematical Analysis

Before the optimum set of steam levels is determined using the MINLP model, the effect of the choice in steam level on the minimum total steam flowrate will be investigated. This investigation will be performed for the case of utilizing latent heat only, as well as for the case of utilizing latent and sensible heat.

The first case deals with utilizing only latent heat. Three steam levels will be considered; high pressure, medium pressure and low pressure. As mentioned in the problem description, high pressure steam is available at a saturation temperature of 225°C. The saturation temperatures of the medium and low pressure steam levels need to be specified. It is the effect of this choice of steam levels on the minimum steam flowrate that must be determined.

Figure 6.2 shows the minimum steam flowrate as a function of saturation temperatures of the medium and low pressure steam levels for the case of latent heat only. This figure was generated by systematically selecting saturation temperatures for the medium pressure and low pressure steam levels between 100°C and 220 °C. With these steam levels, Figure 6.1 is used to determine the quantity of duty required of each of the three steam levels. The flowrate of each steam level is calculated by dividing the duty required of each level by its respective latent heat. The sum of these three flowrates gives the minimum steam flowrate required for that particular set of steam levels. Figure 6.2

therefore shows the locus traced by the minimum steam flowrate as the medium and low pressure saturation temperatures are systematically changed.

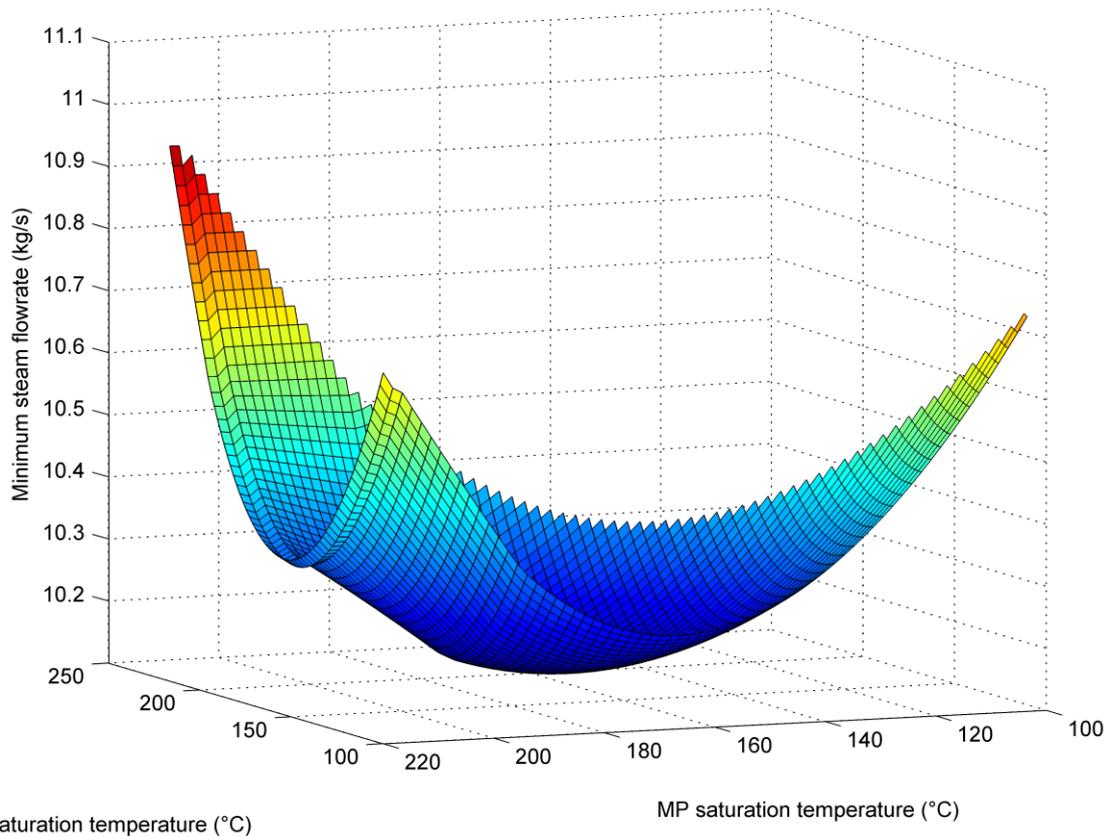


Figure 6.2: Minimum steam flowrate for the case study problem as a function of MP and LP steam level saturation temperatures using latent heat only.

As can be seen in Figure 6.2, there is an optimum set of steam levels. This occurs when the HP, MP and LP steam level saturation temperatures are 225°C, 180.5°C and 131.4°C respectively, with a minimum steam flowrate of 10.17 kg/s. If any other saturation temperatures are used for the MP or LP steam levels, then the minimum total steam flowrate achievable will be greater than 10.17 kg/s.

It must be noted that Figure 6.2 is similar in form to Figure 4.5. This confirms that the conclusions drawn from the mathematical analysis developed for a hypothetical linear process are valid for real problems. Although the composite

6 Case Study

curve in Figure 6.1 is dominated by a large linear region between 89°C and 195°C, the non-linear features of Figure 6.1 at the higher temperatures present themselves in Figure 6.2 as sudden changes in slope. Despite this, Figure 6.2 is still approximately convex as predicted by the analysis. The non-linear features of Figure 6.1 at temperatures lower than 89°C do not feature in Figure 6.2 since the stem levels were restricted to be greater than 100°C.

Since an optimum point for the case study has been found, for the situation utilizing only latent heat, it can be compared to the steam levels determined using the heuristic presented in Chapter 4. Once again, HP steam is available at a saturation temperature of 225°C. The task is to determine the optimal saturation temperatures for the MP and LP steam levels. For this case study, T_{HP} and T_{out} are 225°C and 35°C respectively. This makes λ_{HP} and λ_{out} take values 1834 kJ/kg and 2418.5 kJ/kg respectively. The matrix equation to be solved is given in Equation 6.1. The solution to Equation 6.1 indicates that λ_{MP} and λ_{LP} should be 2011.2 kJ/kg and 2205.4 kJ/kg respectively. This implies that T_{MP}^{sat} and T_{LP}^{sat} should be 180.8°C and 119.1°C respectively. It must be noted that in this calculation, for greater accuracy, steam tables were used to obtain latent heat values rather than using the linear approximation discussed previously. The calculations are shown in Appendix C.

$$\begin{bmatrix} -1 & 0.5 \\ 0.5 & -1 \end{bmatrix} \begin{bmatrix} \ln(\lambda_{MP}) \\ \ln(\lambda_{LP}) \end{bmatrix} = \begin{bmatrix} -0.5\ln(1834) \\ -0.5\ln(2418.5) \end{bmatrix} \quad (6.1)$$

Figure 6.3 shows the limiting hot utility composite curve for this case study, along with the linear approximation used for the heuristic, and the steam levels obtained using the heuristic. The total flowrate of steam required is 10.19 kg/s, only 0.2% greater than the minimum steam flowrate obtained using the optimum steam levels. This low deviation can be accredited to the relatively flat

6 Case Study

region in the area surrounding the optimum in Figure 6.2, and to the fact that the composite curve in Figure 6.3 lies close to the linear approximation.

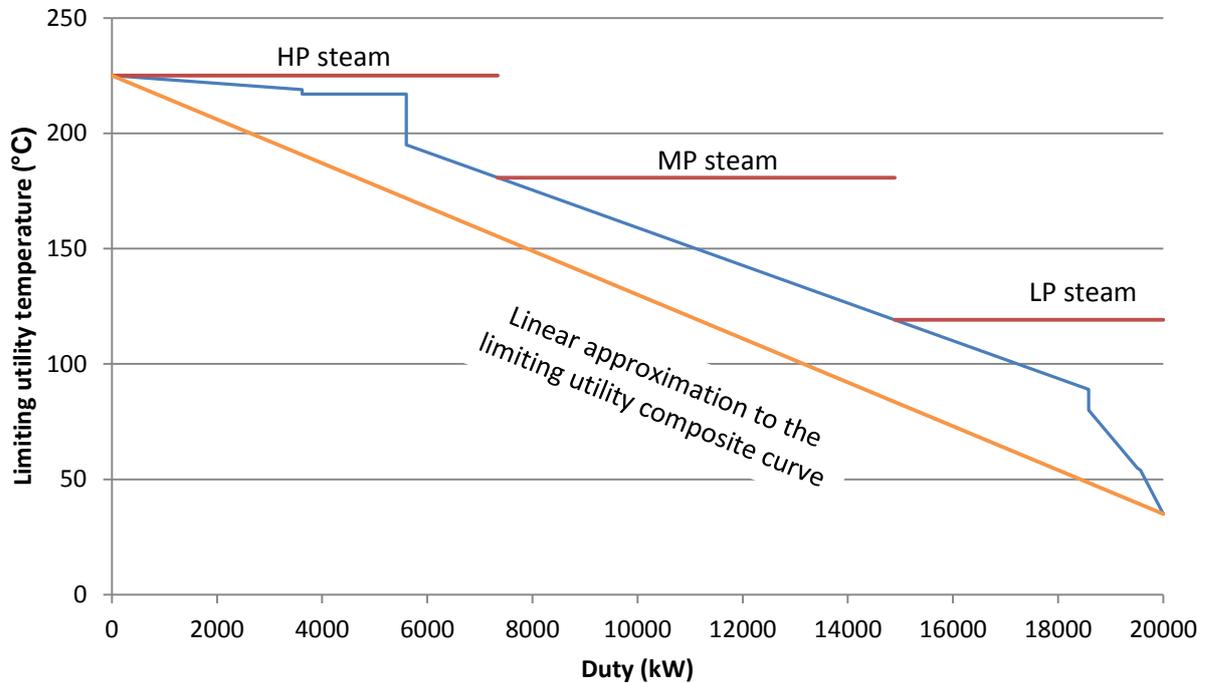


Figure 6.3: Placement of steam levels according to the new heuristic.

A similar analysis can be performed on the case study problem for the case of hot liquid reuse. Again, the aim is to observe how the choice in MP and LP steam saturation temperatures affects the minimum steam flowrate required. The saturation temperature of the HP steam remains fixed while the saturation temperatures of the MP and LP steam levels are systematically changed. A minimum steam flowrate is then calculated for each set of steam levels, for the case of hot liquid reuse. Figure 6.4 shows the minimum steam flowrate for the various selections of T_{MP}^{sat} and T_{LP}^{sat} .

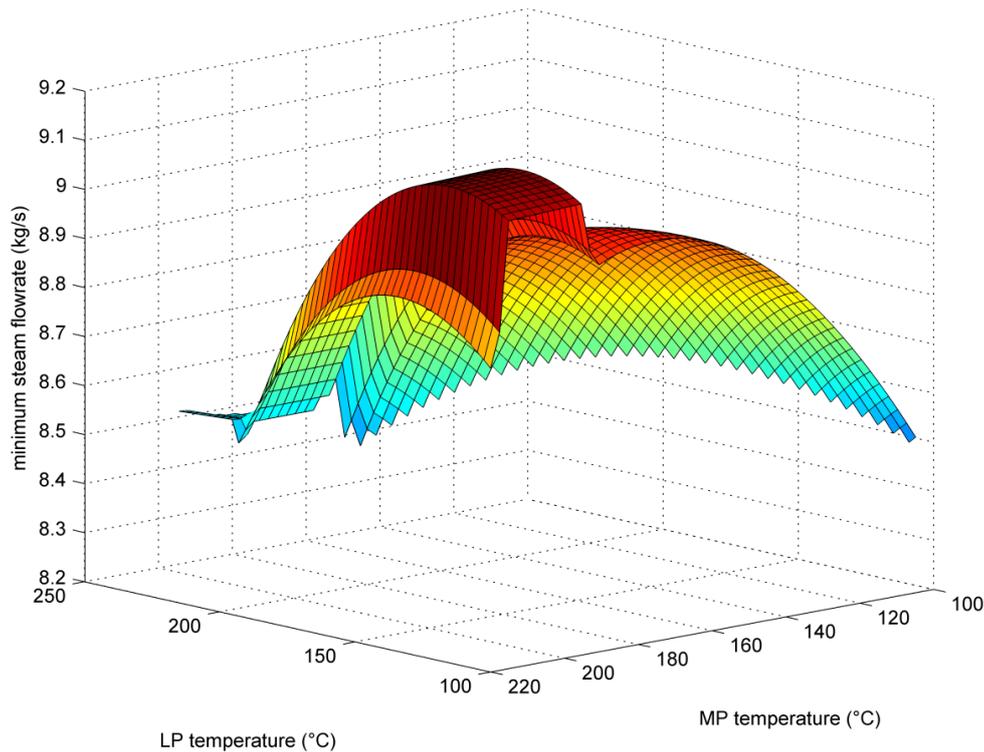


Figure 6.4: Minimum steam flowrate for the case study problem as a function of MP and LP steam level saturation temperatures using latent heat only.

Figure 6.4 shows that a maximum occurs in the minimum steam flowrate when the MP and LP steam levels have a saturation temperature of 208.8°C and 124.5°C respectively, with an associated steam flowrate of 9.16 kg/s. If any other set of steam levels is selected, then a lower minimum steam flowrate can be achieved.

Comparing the shape of Figure 6.4 to that of Figure 4.7 again confirms that the conclusions drawn from the mathematical analysis developed for a hypothetical linear process are valid for real problems. Although the non-linear features in Figure 6.1 are present in Figure 6.4 at high temperatures, the graphs still have a general concave form, as predicted by the analysis.

Figure 6.4 also shows that the lowest minimum steam flowrate is achieved when both the MP and LP steam levels are forced to their lowest allowable

levels. This confirms the statement made earlier that when utilizing hot liquid reuse, only a single high pressure steam level should be used. It must also be noted that the highest minimum steam flowrate achieved with hot liquid reuse is still lower than the lowest minimum steam flowrate achieved using only latent heat.

These analyses show that the lowest steam flowrate possible for the case study is achieved using hot liquid reuse and a single steam level. This can be compared with two results from literature for the same case study problem. Coetzee and Majozi (2008) obtained a minimum steam flowrate of 7.67 kg/s using only a single steam level and hot liquid reuse. Using multiple steam levels and hot liquid reuse, Price and Majozi (2010b) obtained a flowrate of 5.68 kg/s for HP steam, 2.00 kg/s for MP steam and 0.23 kg/s for LP steam, giving a total of 7.91 kg/s. These two examples from literature confirm the prediction that introducing additional steam levels increases the minimum steam flowrate achievable.

6.3 MINLP Model Results

The conclusions drawn in the previous section do not address the fact that additional steam levels must be introduced in the form of turbine exhaust due to the need to meet shaft work requirements. Here, the MINLP model developed in Chapter 5 will be used to target the minimum total steam flowrate, whilst synthesising the heat exchanger network as well as specifying the turbine dimensions to meet the shaft work requirements.

Before developing the HEN for minimum total steam flowrate, a base case for comparison will first be developed using the conventional practice of only utilising latent heat. In Price and Majozi (2010b), it is stated that 2 kg/s of MP steam is available to the HEN at a saturation temperature of 197°C, as well as

6 Case Study

0.23 kg/s of LP steam at a saturation temperature of 114°C. If only latent heat is to be used, then a further 8.71 kg/s of HP steam is required to fulfil the energy demands of the cold process streams, giving a total steam requirement of 10.94 kg/s. The two existing turbines fulfil the shaft work target of 110.13kW. Figure 6.5 shows the HEN for this base case scenario.

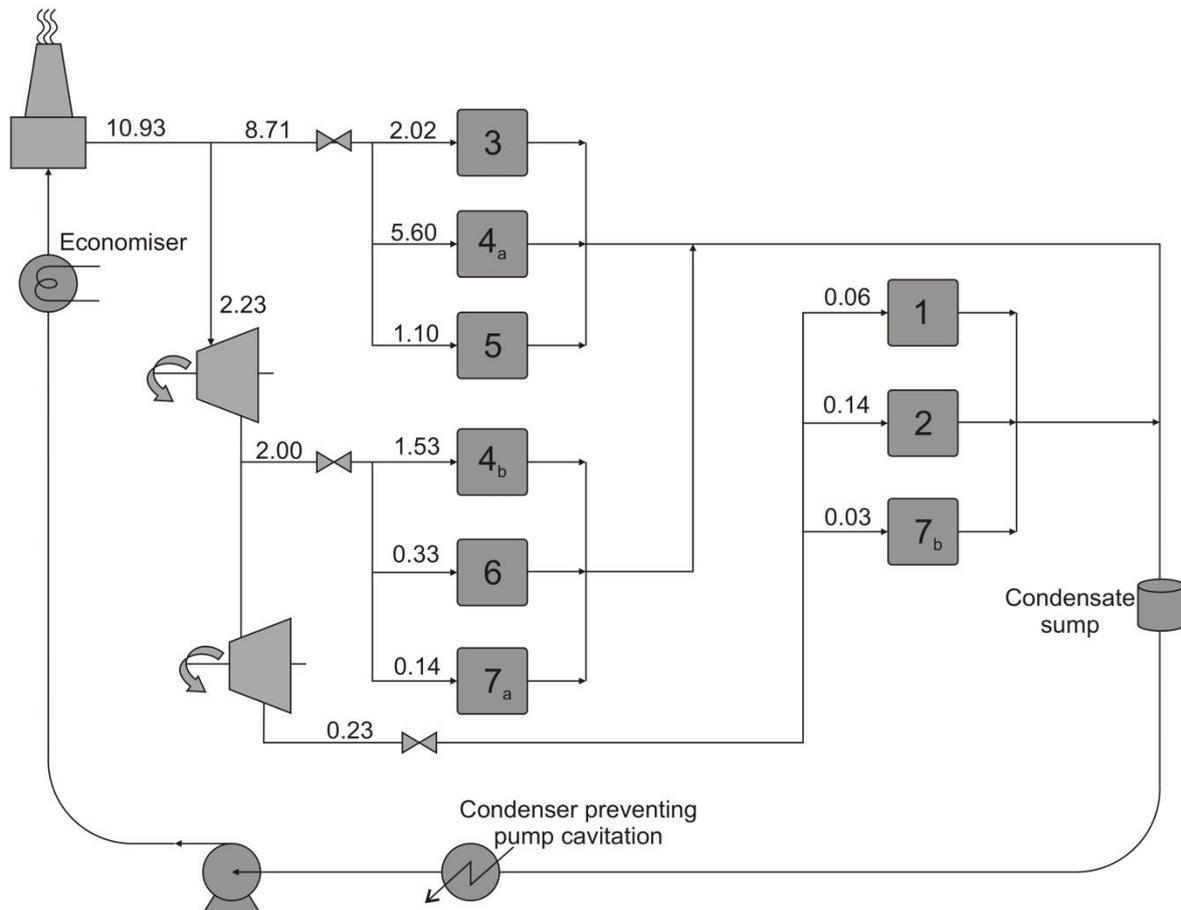


Figure 6.5: Base case HEN.

Using the new model, which utilises both latent and sensible heat, a total minimum steam flowrate of 7.81 kg/s is obtained. The model was solved in GAMS v22.0 on a Intel® Core™ i3-2100 3.1GHz processor and 2 GB of RAM, using Dicopt as the MINLP solver, with Conopt as the NLP solver and Cplex as the MIP solver. Since the Dicopt algorithm requires a feasible starting point, the temperatures of the steam levels were fixed at levels recommended by

6 Case Study

Harrel (1996) and the resulting MILP problem solved. The solution to this MILP was used as the starting point for the MINLP problem with variable temperatures. A CPU time of 0.01s was required for the MILP and 0.52s for the MINLP, giving a total of 0.53s. Three major iterations were required between the NLP and MIP solvers. The model involved 127 equations and 255 variables.

The steam flowrate of 7.81 kg/s represents a 28.6% reduction in steam flowrate compared to the base case. Figure 6.6 shows the HEN obtained using the new model. Figure 6.7 shows the placement of the utilities above the limiting hot utility composite curve, and the location of the pinch. A significant observation is that this solution only includes two steam levels and one turbine. Despite the fact that the model in this instance was set up to consider three steam levels and two turbines, the solver chose to eliminate one steam level and one turbine. Only one turbine is required, with a steam flowrate of 0.90 kg/s and an outlet saturation temperature of 148.3°C.

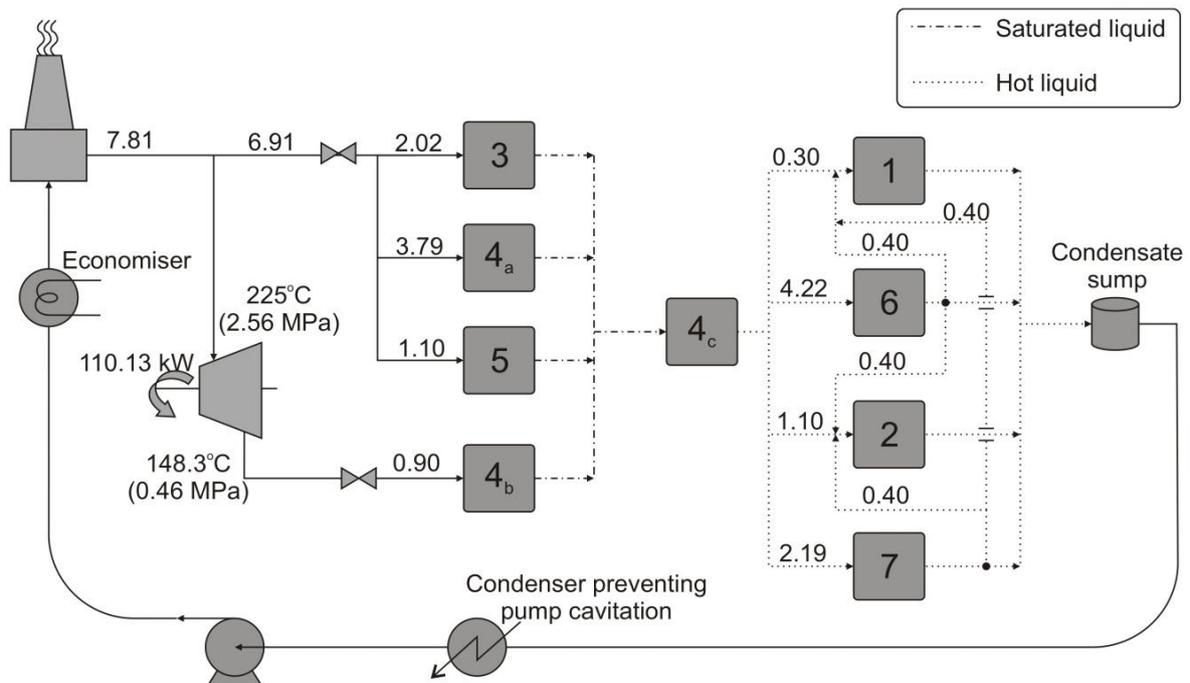


Figure 6.6: HEN obtained using new model.

6 Case Study

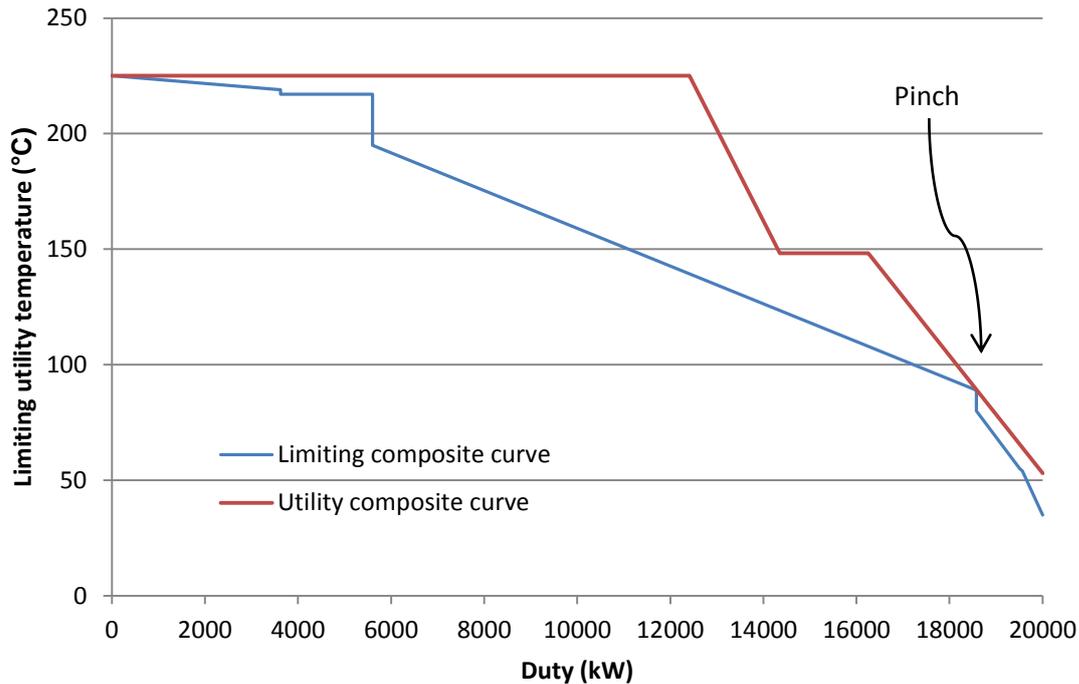


Figure 6.7: Placement of the utilities above the limiting hot utility composite curve.

This observation can be explained by reconsidering the results of the mathematical analysis. When using both latent and sensible heat, only a single steam level must be used. In this case, an extra steam level had to be added in order to drive the turbine and meet the shaft work requirements. The effect that adding this steam level has on the flowrate can be seen by comparing the result of 7.81 kg/s to the flowrate of 7.69 kg/s obtained by Coetzee and Majozi (2008) using only a single steam level. Since adding additional steam levels raises the minimum steam flowrate, the logical decision is to only have one additional steam level, and to meet the shaft work requirement using one large turbine, which is exactly what the solver did.

A last observation that is seen in Figure 6.6 is that only two heat exchanger splits are required, the same as for the base case in Figure 6.5. Here, heat exchanger 4 has been split twice, bringing the number of heat exchangers to a total of 9. This is interesting, because in keeping with Price and Majozi (2010b),

6 Case Study

the maximum number of splits allowed (m) was set to 3. Despite this, the solver only required two heat exchanger splits. If m is set to any value greater than 2, the same result is obtained, indicating that two heat exchanger splits is the maximum number of splits required to give a minimum steam flowrate. If m is given a value less than 2, the model becomes limited in its ability to fully utilise the available heat. This will in turn require higher steam flowrates. Table 6.3 gives the minimum steam flowrate required for the case study when different values of m are chosen. The decision as to how many heat exchanger splits to allow must ultimately be supported by a thorough economic analysis, considering that reducing the total steam flowrate will incur additional heat exchanger costs, but will also lower the boiler purchase cost.

Table 6.3: Minimum steam flowrate based on the number of allowed heat exchanger splits

m	Flowrate (kg/s)
0	10.95
1	8.40
2	7.81
3+	7.81

Thus it is seen that the model has successfully met the goals set out in the problem statement in Chapter 5. The model has targeted the minimum total steam flowrate that is required to both heat the cold process streams, and to supply shaft work. The model has selected the optimum set of steam levels, and has designed the turbine between the steam levels. Lastly, the model has also synthesised the HEN, placing all the series and parallel connection required to make the network feasible.

6.4 References

- Coetzee, W. A., & Majozi, T. (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Harrel, G. (1996). Steam system survey guide. ORNL/TM-2001/263: Oak Ridge National Laboratory.
- Price, T., & Majozi, T. (2010a). On Synthesis and Optimization of Steam System Networks. 1. Sustained Boiler Efficiency. *Ind. Eng. Chem. Res.*, 49, 9143-9153.
- Price, T., & Majozi, T. (2010b). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Price, T., & Majozi, T. (2010c). On Synthesis and Optimization of Steam System Networks. 3. Pressure Drop Consideration. *Ind. Eng. Chem. Res.*, 49, 9165-9174.

Chapter 7

Conclusions and Recommendations

In this work, the effect that the selection of intermediate steam levels has on the minimum total steam flowrate required by a HEN, and on the shaft work production, has been extensively studied. This addresses a number of critical features of steam systems that previous works of this nature fail to consider. Through the use of mathematical analysis and mathematical programming, interesting characteristics of steam systems have been discovered, and conclusions have been drawn.

Observing that the minimum total steam flowrate achievable is dependent on the set of steam levels employed, a mathematical analysis was undertaken to determine the effect that changing the set of steam levels has on the minimum steam flowrate. This analysis was carried out for the conventional method of utilising only latent heat, as well as for the method of reducing steam flowrate by utilising sensible heat. Equations to calculate the minimum steam flowrate required as a function of the steam level saturation temperatures were used to plot the locus traced by the minimum steam flowrate as the set of steam levels changed. First and second derivatives were used to locate and classify any local optima. The following are the conclusions drawn from this analysis:

- For the case of latent heat use only, an optimum set of steam levels exists that results in the lowest minimum total steam flowrate.

7 Conclusions and Recommendations

- When using only latent heat, using any set of steam levels other than the optimum set results in a minimum total steam flowrate higher than the minimum total steam flowrate achieved at the optimum.
- For the case utilising hot liquid reuse, a concave surface is drawn as the minimum total steam flowrate changes with the set of steam levels.
- For the case utilising hot liquid reuse, an undesirable set of steam levels exists with a minimum total steam flowrate higher than that achieved using any other set of steam levels.
- The highest minimum total steam flowrate obtained while utilising hot liquid reuse is lower than the lowest minimum total steam flowrate obtained using only latent heat.
- The lowest minimum total steam flowrate for the case of hot liquid reuse is achieved when only a single high pressure steam level is used. This indicates that when employing the method of hot liquid reuse, only a single high pressure steam level should be considered.

The mathematical analysis was applied to a case study from literature. The results for this real world example reflected the results obtained for the idealised case. From this it is concluded that the observations listed above hold for real problems.

Since a desirable optimum set of steam levels exists when using only latent heat, a heuristic was developed that enables one to quickly determine a set of steam levels that lies close to this optimum. This heuristic was applied to a case study in which it successfully determined a satisfactory set of steam levels. The minimum total steam flowrate achieved using the heuristic was 0.2% greater than the steam flowrate achieved at the mathematical optimum.

7 Conclusions and Recommendations

Because additional steam levels result from the need to include steam turbines to provide shaft work, a novel MINLP model was formulated to optimise the entire steam system network, comprising the boiler, the heat exchanger network and the power block. The model targets the minimum total steam flowrate required from the boiler, while selecting the required addition steam levels, synthesising the heat exchanger network to meet heating requirements and designing the turbines required to meet shaft work requirements. Application of the new model to a case study from literature yielded the following results:

- A minimum total steam flowrate of 7.81 kg/s was obtained, representing a 28.6% reduction when compared to the minimum total steam flowrate obtained when following the conventional practice of designing for latent heat use only.
- A feasible HEN was synthesised to meet the heating demands of the cold process streams.
- Only one steam turbine and one additional steam level is required to meet shaft work requirements.
- Two heat exchanger splits is the maximum number of splits required for this case study.
- Reducing the maximum number of allowed heat exchanger splits below two increases the minimum total steam flowrate achievable.

The observation that only one large turbine is required, despite the fact that the model was set up to include two turbines and three steam levels, is rather profound. This confirms the observation made in the mathematical analysis that incorporating additional steam levels increases the minimum total steam flowrate achievable.

7 Conclusions and Recommendations

Based on these observations, it is concluded that the shortcomings of previous works of this nature have been successfully addressed. In doing so, valuable insight into the behaviour of steam systems has been gained, especially when hot liquid reuse is utilised. Furthermore, it is concluded that the novel MINLP model successfully achieved a reduction in the total steam flowrate required from the boiler, while meeting the heating and shaft work requirements of the process.

Thus far, the model developed in this work, and its predecessors, have only considered steady state operation. A steam system designed with all heat exchangers in parallel is capable of handling disturbances in the process streams by simply opening or closing individual control valves, without affecting the performance of other heat exchangers. In systems which involve series connections between heat exchangers, increasing or decreasing the steam flowrate to one heat exchanger to address a process disturbance can negatively affect the performance of other heat exchangers to which it is connected. It is therefore recommended that further research be conducted into developing a model to synthesize networks that are feasible in dynamic situations.

Appendices

Appendix A

The analyses presented in Chapter 4 require that it be shown that T^* lies between T_{out} and T_{HP} . If T^* were any less, it would be too cold to heat the process, and if any more, then it would be hotter than the high pressure steam from which it is derived, which is not physically realisable. In order to prove that at least one value of T^* lies in this range for both cases, the first derivative of steam flowrate with respect to temperature will be used.

A.1 Latent heat only

To begin, T_{out} is substituted into Equation 4.10, which yields

$$\left. \frac{d\dot{m}}{dT} \right|_{T_{out}} = \frac{Q(\lambda_{HP} - \lambda_{out})}{(T_{in} - T_{out})\lambda_{HP}\lambda_{out}} \quad (A1)$$

Because λ_{out} is greater than λ_{HP} (since T_{out} is less than T_{HP}), and since all other terms are positive figures, it is seen that the first derivative at T_{out} is negative. Likewise, if T_{HP} is substituted into Equation 4.10 one gets

$$\left. \frac{d\dot{m}}{dT} \right|_{T_{HP}} = \frac{Q(\lambda_{out} - \lambda_{HP})}{(T_{in} - T_{out})\lambda_{HP}^2} \quad (A2)$$

Noting that all the terms are positive, it is concluded that the second derivative at T_{HP} is positive.

Now, since the first derivative is positive at one end of the range, negative at the other and continuous in between, there must be an odd number of roots in that range. According to Equation 4.11, Equation 4.10 only has two roots. It is thus concluded that Equation 8 has only one root between T_{out} and T_{HP} which occurs at T^* . The other root, which lies outside the range, is meaningless.

A.2 Latent and Sensible heat

Similar to above, substitution of T_{out} into Equation 4.21 yields

$$\left. \frac{d\dot{m}}{dT} \right|_{T_{out}} = \frac{Q \left[(c_p(T_{HP} - T_{out}) + \lambda_{HP})^2 - \lambda_{HP}\lambda_{out} \right]}{(T_{in} - T_{out})\lambda_{out}(c_p(T_{HP} - T_{out}) + \lambda_{HP})^2} \quad (A3)$$

Here, the denominator is positive, but the nature of the term in square brackets is uncertain. Using Equation 4.9, it can be shown that

$$\lambda_{out} = \lambda_{HP} + b(T_{HP} - T_{out}) \quad (A4)$$

Applying this substitution to Equation A3, the term inside the square brackets expands to give

$$c_p^2(T_{in} - T_{out})^2 + \lambda_{HP}(T_{HP} - T_{out})(2c_p - b) \quad (A5)$$

Since c_p is greater than b , this expression is positive, and it is seen that the first derivative evaluated at T_{out} (Equation A3) is positive. The same procedure applied to the other boundary, T_{HP} , yields

$$\left. \frac{d\dot{m}}{dT} \right|_{T_{HP}} = \frac{-Q \left[(c_p(T_{HP} - T_{out}) + \lambda_{HP})^2 - \lambda_{HP}\lambda_{out} \right]}{(T_{in} - T_{out})\lambda_{HP}(c_p(T_{HP} - T_{out}) + \lambda_{HP})^2} \quad (A6)$$

which means that the first derivative at T_{HP} is negative.

Again, since the first derivative differs in sign between the two boundaries, and is continuous, there must be an odd number of roots between T_{out} and T_{HP} . Since Equation 4.22 states that there are only two roots for Equation 4.21, there can only be one root between T_{out} and T_{HP} , which occurs at T^* . The other root, which lies outside the range, is meaningless.

Appendix B

In Chapter 4, it is required to prove that the Hessian matrix given in Matrix 4.1 is positive definite. One method of showing that a matrix is positive definite is to show that the determinants of all the leading principal minors are positive (Rao, 2009). For the matrix A below, the leading principal minor A_n is the square matrix made up of the first n rows and columns of A , as below.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix}$$

$$A_1 = [a_{11}]$$

$$A_2 = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

$$A_3 = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

etc

Matrix 4.1 in Chapter 4 is tridiagonal, with the diagonal and off-diagonal terms expressed as Equations 4.18 and 4.19. These can be rewritten in terms of Matrix A above as Equations B1 to B3. It must be remembered that λ_i^* is the latent heat of a steam level calculated at the optimal saturation temperature T_i^* .

$$a_{i,i} = \frac{2\lambda_{i-1}^* Qb}{(T_{in} - T_{out})(\lambda_i^*)^3} \quad (B1)$$

Appendices

$$a_{i,j} = a_{j,i} = \frac{-Qb}{(T_{in} - T_{out})(\lambda_{i+1}^*)^2} \quad \forall j = i + 1 \quad (B2)$$

$$a_{i,j} = a_{j,i} = 0 \quad \forall j > i + 1 \quad (B2)$$

The proof begins by considering the determinant of the first principal minor. Since this is simply the first element of Matrix A , which is positive, the determinant of the first principal minor is positive.

$$\det(A_1) = a_{11} = \frac{2\lambda_{out}^* Qb}{(T_{in} - T_{out})(\lambda_1^*)^3} \quad (B3)$$

The calculation of the determinant of the second principal minor is shown below.

$$\begin{aligned} \det(A_2) &= \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21} \\ &= \frac{4\lambda_0^* \lambda_1^* Q^2 b^2}{(T_{in} - T_{out})^2 (\lambda_1^*)^3 (\lambda_2^*)^3} - \frac{Q^2 b^2}{(T_{in} - T_{out})^2 (\lambda_2^*)^4} \\ &= \frac{4\lambda_0^* \lambda_1^* \lambda_2^* Q^2 b^2 - \lambda_1^{*3} Q^2 b^2}{(T_{in} - T_{out})^2 (\lambda_1^*)^3 (\lambda_2^*)^4} \end{aligned}$$

A transformation, shown in Equation B4, can be obtained from Equation 4.17.

$$\lambda_0^* \lambda_2^* = \lambda_1^{*2} \quad (B4)$$

This can be applied to the step above, to reach the determinant in Equation B5 below

Appendices

$$\det(A_2) = \frac{3\lambda_1^{*3}Q^2b^2}{(T_{in} - T_{out})^2(\lambda_1^*)^3(\lambda_2^*)^4} \quad (B5)$$

Since all the terms in Equation B5 are positive terms, it is concluded that the determinant of the second principal minor is positive.

The determinant of the third principal minor can be calculated as follows

$$\begin{aligned} \det(A_3) &= \begin{vmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{vmatrix} = a_{33} \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} - a_{23}(0 - a_{32}|a_{11}|) \\ &= \frac{6\lambda_1^{*3}\lambda_2^*Q^3b^3}{(T_{in} - T_{out})^3(\lambda_1^*)^3(\lambda_2^*)^4(\lambda_3^*)^3} + \frac{2\lambda_0^*Q^3b^3}{(T_{in} - T_{out})^3(\lambda_1^*)^3(\lambda_3^*)^4} \\ &= \frac{6\lambda_1^{*3}\lambda_2^*\lambda_3^*Q^3b^3 + 2\lambda_0^*\lambda_2^{*4}Q^3b^3}{(T_{in} - T_{out})^3(\lambda_1^*)^3(\lambda_2^*)^4(\lambda_3^*)^4} \end{aligned}$$

Applying the transformations

$$\lambda_0^*\lambda_2^* = \lambda_1^{*2} \quad \text{and} \quad \lambda_1^*\lambda_3^* = \lambda_2^{*2}$$

one gets Equation B6.

$$\det(A_3) = \frac{8\lambda_1^{*2}\lambda_2^{*3}Q^3b^3}{(T_{in} - T_{out})^3(\lambda_1^*)^3(\lambda_2^*)^4(\lambda_3^*)^4} \quad (B6)$$

Since Equation B6 is made up of only positive terms, it is concluded that the determinant of the third principal minor is positive.

An interesting pattern can be seen from the calculation of the determinant of the third principal minor, resulting from the fact that Matrix A is tridiagonal. The large number of zero terms allows the determinant of the n^{th} principal minor to be calculated as

$$\begin{aligned} \det(A_n) &= a_{n,n} \cdot \det(A_{n-1}) - a_{n,n+1} (0 - a_{n+1,n} \cdot \det(A_{n-2})) \\ &= a_{n,n} \cdot \det(A_{n-1}) + a_{n,n+1}^2 \cdot \det(A_{n-2}) \end{aligned} \quad (B7)$$

Since $a_{n,n}$ and $a_{n,n+1}^2$ are both positive, knowing that $\det(A_1)$ and $\det(A_2)$ are positive, Equation B7 shows that $\det(A_3)$ is positive. Likewise, if $\det(A_2)$ and $\det(A_3)$ are positive, then $\det(A_4)$ is positive. This can be repeated for all the leading principal minors. Since, through induction, the determinants of all the leading principal minors of Matrix A have been shown to be positive, it is concluded that the Hessian matrix in Matrix 4.1 is positive definite.

Appendix C

$$\begin{bmatrix} -1 & 0.5 \\ 0.5 & -1 \end{bmatrix} \begin{bmatrix} \ln(\lambda_{MP}) \\ \ln(\lambda_{LP}) \end{bmatrix} = \begin{bmatrix} -0.5\ln(1834) \\ -0.5\ln(2418.5) \end{bmatrix}$$

$$\begin{bmatrix} -1 & 0.5 \\ 0.5 & -1 \end{bmatrix} \begin{bmatrix} \ln(\lambda_{MP}) \\ \ln(\lambda_{LP}) \end{bmatrix} = \begin{bmatrix} -3.7571 \\ -3.8955 \end{bmatrix}$$

$$\begin{bmatrix} \ln(\lambda_{MP}) \\ \ln(\lambda_{LP}) \end{bmatrix} = \begin{bmatrix} -1.3333 & -0.6667 \\ -0.6667 & -1.3333 \end{bmatrix} \begin{bmatrix} -3.7571 \\ -3.8955 \end{bmatrix}$$

$$\begin{bmatrix} \ln(\lambda_{MP}) \\ \ln(\lambda_{LP}) \end{bmatrix} = \begin{bmatrix} 7.6065 \\ 7.6987 \end{bmatrix}$$

$$\begin{bmatrix} \lambda_{MP} \\ \lambda_{LP} \end{bmatrix} = \begin{bmatrix} \exp(7.6065) \\ \exp(7.6987) \end{bmatrix}$$

$$\begin{bmatrix} \lambda_{MP} \\ \lambda_{LP} \end{bmatrix} = \begin{bmatrix} 2011.2 \\ 2205.4 \end{bmatrix}$$

From steam tables

$$\begin{bmatrix} T_{MP}^{sat} \\ T_{LP}^{sat} \end{bmatrix} = \begin{bmatrix} 180.8 \text{ }^\circ\text{C} \\ 119.1 \text{ }^\circ\text{C} \end{bmatrix}$$

Appendix D

*full model non linear

Sets

i Heat exchangers /1*7/

l Steam Levels /HP,MP,LP/;

Alias (i,j);

Parameters

Q(i) Heat exchanger duty

/1	135
2	320
3	3620
4	12980
5	1980
6	635
7	330/

TinL(i) Minimum inlet temperature

/1	55
2	55
3	225
4	195
5	217.1
6	80
7	80/

ToutL(i) Minimum outlet temperature

/1	35
----	----

$$A(l) = -0.131 + 0.00117 * T_{sat}(l);$$

$$B(l) = 0.989 + 0.00152 * T_{sat}(l);$$

$$\Delta H(l) = (T_{sat}(l) - T_{sat}(l+1)) / (391.8 + 2.215 * T_{sat}(l));$$

Binary Variables

$x(i)$ the use of liquid in HE i

$y(i,l)$ the use of steam level l in HE i ;

Variable

z total steam flow supply ;

Positive variables

FRT total return

FST total steam supply to HEs

FS(l) total steam flow of each level

SS(i,l) supply of steam of level l to HE i

Fin(i) total flow into i

Fout(i) total flow out of HE i

SL(j,i,l) saturated liquid from j to i on level l

HL(j,i) hot liquid from j to i

FRS(i,l) saturated liquid return to boiler from HE i

FRL(i) hot liquid return to boiler from HE i

QSS(i,l) latent heat supplied to i from level l

QL(i) sensible heat supplied to i

TUS(l) Steam supply to turbine k

WS(l) shaftwork of turbine k

Temps(l) Variable steam level temperature

Lam(l) Variable latent heat

- delHiso(1) isentropic enthalpy change
coefA(1) turbine parameter
coefB(1) turbine parameter ;

Equations

- e1(1) sum of steam in each level
e2(i) Total flow into HE i
e3(i) total flow out of HE i
e4 total supply
e5 total out
e6 total balance
e7(i) individual HE balance
e8(i) liquid balance
e9(i,l) Steam balance over HE
e10(1) steam level balance

e11(i) Total duty
e12(i,l) heat delivered as latent to i from level l
e13(i) heat delivered as sensible to i
e14(i,l) limit steam flowrate of level l to HE i
e15(i) limit on liquid
e16(i) no recycle

e17 turbine limits
e18(1) Turbine power output
e19 Total power
e20 objective function

e21(i) each HE must have heat

e22 restricting splits

*nonlinear addition

e23(i,l) heat delivered as latent to i from level l

e24(l) calculates latent heat

e25(i) heat delivered as sensible to i

e26(l) turbine shaft work

e27(l) isentropic enthalpy change

e28(l) turbine coefficient

e29(l) turbine coefficient

e30 top level steam set point

e31(l) steam level lower bounds;

*=====

*linear part

*=====

*material balances

e1(l).. $FS(l) = e = \text{sum}(i, SS(i,l));$

e2(i).. $Fin(i) = e = \text{sum}(l, SS(i,l)) + \text{sum}(j,l, SL(j,i,l)) + \text{sum}(j, HL(j,i));$

e3(i).. $Fout(i) = e = \text{sum}(j,l, SL(i,j,l)) + \text{sum}(j, HL(i,j)) + \text{sum}(l, FRS(i,l)) +$
 $FRL(i);$

e4.. $FST = e = \text{sum}(l, FS(l));$

e5.. $FRT = e = \text{sum}(i,l, FRS(i,l)) + \text{sum}(i, FRL(i));$

e6.. $FST = e = FRT;$

e7(i).. $Fin(i) = e = Fout(i);$

e8(i).. $\text{sum}(j,l, SL(j,i,l)) + \text{sum}(j, HL(j,i)) = e = \text{sum}(j, HL(i,j)) + FRL(i);$

e9(i,l).. $SS(i,l) = e = \text{sum}(j, SL(i,j,l)) + FRS(i,l);$

e10(l).. $FS(l) = e = \text{sum}(i,j, SL(i,j,l)) + \text{sum}(i, FRS(i,l));$

*energy balances

$$e11(i).. \quad QL(i) + \text{sum}(l, QSS(i,l)) = e= Q(i);$$

$$e12(i,l).. \quad QSS(i,l) = e= SS(i,l)*\lambda(l);$$

$$e13(i).. \quad QL(i) = e= \text{sum}((j,l), SL(j,i,l)*T_{sat}(l)*c_p) + \\ \text{sum}(j, HL(j,i)*c_p*T_{outL}(j)) - \text{sum}((j,l), SL(j,i,l)*T_{outL}(i)*c_p) - \\ \text{sum}(j, HL(j,i)*c_p*T_{outL}(i));$$

$$e14(i,l).. \quad SS(i,l) = l= SS_{sup}(i,l)*y(i,l);$$

$$e15(i).. \quad \text{sum}((j,l), SL(j,i,l)) + \text{sum}(j, HL(j,i)) = l= L_{up}(i)*x(i);$$

$$e16(i).. \quad HL(i,i) = e= 0;$$

*Turbine equations

$$e17(l) \$(\text{ord}(l) < \text{card}(l)).. \quad TUS(l+1) + FS(l+1) = l= TUS(l);$$

$$e18(l) \$(\text{ord}(l) < \text{card}(l)).. \quad WS(l) = e= (\Delta H(l)*3.6*TUS(l) - A(l))/B(l);$$

$$e19.. \quad \text{sum}(l \$(\text{ord}(l) < \text{card}(l)), WS(l)) = e= WSR;$$

$$e20.. \quad z = e= FS('HP') + TUS('HP');$$

$$e21(i).. \quad \text{sum}(l, y(i,l)) + x(i) = g= 1;$$

$$e22.. \quad \text{sum}(i, x(i)) + \text{sum}((i,l), y(i,l)) = l= 7 + \text{splits};$$

*=====

*non linear part

*=====

*energy balances

$$e23(i,l).. \quad QSS(i,l) = e= SS(i,l)*\lambda(l);$$

$$e24(l).. \quad \lambda(l) = e= 2726 - 4.13*T_{emps}(l);$$

$$e25(i).. \quad QL(i) = e= \text{sum}((j,l), SL(j,i,l)*T_{emps}(l)*c_p) +$$

Appendices

$$\text{sum}(j, \text{HL}(j,i) * \text{cp} * \text{ToutL}(j)) - \text{sum}((j,1), \text{SL}(j,i,1) * \text{ToutL}(i) * \text{cp}) - \text{sum}(j, \text{HL}(j,i) * \text{cp} * \text{ToutL}(i));$$

*Turbine equations

$$\text{e26}(1) \$(\text{ord}(1) < \text{card}(1)).. \quad \text{WS}(1) = \text{e} = (\text{delHiso}(1) * 3.6 * \text{TUS}(1) - \text{coefA}(1)) / \text{coefB}(1);$$

$$\text{e27}(1) \$(\text{ord}(1) < \text{card}(1)).. \quad \text{delHiso}(1) = \text{e} = (\text{Temps}(1) - \text{Temps}(1+1)) / (391.8 + 2.215 * \text{Temps}(1));$$

$$\text{e28}(1).. \quad \text{coefA}(1) = \text{e} = -0.131 + 0.00117 * \text{Temps}(1);$$

$$\text{e29}(1).. \quad \text{coefB}(1) = \text{e} = 0.989 + 0.00152 * \text{Temps}(1);$$

$$\text{e30}.. \quad \text{Temps}('HP') = \text{e} = \text{Tsat}('HP');$$

$$\text{e31}(1).. \quad \text{Temps}(1) = \text{g} = 100;$$

model linear /e1,e2,e3,e4,e5,e6,e7,e8,e9,e10,e11,e12,e13,e14,e15,e16,e17,e18,
e19,e20,e21,e22/;

model nonlinear /e1,e2,e3,e4,e5,e6,e7,e8,e9,e10,e11,e14,e15,e16,e17,e19,e20,
e21,e22,e23,e24,e25,e26,e27,e28,e29,e30,e31/;

solve linear using MIP minimizing z;

$$\text{delHiso.l}(1) = \text{delH}(1);$$

$$\text{coefA.l}(1) = \text{A}(1);$$

$$\text{coefB.l}(1) = \text{B}(1);$$

solve nonlinear using MINLP minimising z;

display z.l, Temps.l;