

A Unified Approach to Heat Integration in Continuous Chemical Processing Plants

Sheldon Grant Beangstrom

A Unified Approach to Heat Integration in Continuous Chemical Processing Plants

by

Sheldon Grant Beangstrom

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

**Doctor of Philosophy
(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

July 2015

Synopsis

Heat integration is a popular method for minimising the energy needs of a chemical plant, and also for optimising the accompanying utility systems. In conventional practice, the regions of process-process heat integration, cooling water system design, and steam system design are treated in isolation from one another. Methods have been developed specific to each region, but fail to properly acknowledge the existence of the other regions, or the interaction between various regions of an energy system. This separated approach to process integration leads to suboptimal results.

In this work, a new unified approach to heat integration on chemical plants is presented. Models are developed that simultaneously consider the process-process heat exchanger network together with the cooling water and steam networks. The operation of the cooling tower and steam turbines is also included, providing a holistic coverage of the associated utility systems, leading to a comprehensive utility system design. The models can be applied to two specific design cases. The first case involves existing utility systems, with the objective of designing an energy system that best utilises these utilities. The second case considers a grass roots design, in which the utility systems are optimised together with the heat exchanger networks. The advantage of the first case is that systems can be debottlenecked, including systems already debottlenecked using current techniques. The advantage of the second case is that new plants can exploit the improvements by reducing the construction costs of the utility systems.

The new models were applied to two case studies to demonstrate their performance. The results show that the new unified approach provides consistent reductions in utility flowrates, compared to the case when the utilities are optimised separately from the process. In all cases, the minimum energy requirement of the process was not compromised in achieving these reductions. These results indicate that a unified approach to heat integration on chemical plants is a feasible method which is superior to current separated techniques.

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 thesis 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

To my supervisor, Prof Thoko Majozi - if I have managed to see further, it is because I have stood on the shoulders of a giant.

To my parents and sister - thank you for all the support over the years, and the regular shipments of chocolate chip biscuits.

To the choir of Christ Church, Arcadia, and especially George King - thank you for giving me a reason to sing, and for keeping me busy on Thursday evenings.

To the members of the Pretoria Highlanders Pipe Band - thank you for your words of encouragement (and advice on title length) after band practice.

To Dr Carol Steyn - thank you for always enquiring about my progress every Sunday morning at tea, and for offering words of consolation during tough times.

To my neighbours: Alan and Cathy Cordes, and Heidi Kohn – thank you for sharing great evenings around the braai with a glass of wine.

To my close friends, Ruan Pieterse, Marius le Roux, George Hatting and Bern Alberts – thank you for being my friends. We have shared many great laughs together, without which I would not have had the sanity to complete this work.

To all my colleagues, especially Bola Adekola, Jane Stamp, Tim Price and Vincent Gololo - thank you for many insightful discussions and good laughs.

To all others that a very tired brain now fails to remember - thank you for all of your contributions, no matter how small.

A.M.D.G.

In loving memory of
Robert Davidson McKee
1 Oct 1923 – 29 Nov 2014

RAF Spitfire pilot, generous Scotsman and awesome grandpa.



Contents

1	Introduction.....	1
1.1	Background.....	1
1.2	Motivation	3
1.3	Objective of Investigation	6
1.4	Structure	7
1.5	References	8
2	Literature Survey I - Fundamentals of Process Integration.....	9
2.1	Process-Process Heat Integration	9
2.1.1	Pinch Techniques.....	11
2.1.2	Mathematical Programming Techniques.....	17
2.2	Mass Integration	24
2.3	Cooling Water System Design	30
2.4	Cooling Tower Models.....	36
2.5	Steam System Design.....	40
2.6	Relaxation techniques.....	45
2.7	References	49
3	Literature Survey II – Specific Technical Details	60
3.1	Process-Process Heat Integration	61
3.1.1	Problem Statement.....	61
3.1.2	Superstructure	62
3.1.3	The Method of Yee and Grossmann (1990)	63

3.1.4	The Method of Zhu <i>et al</i> (1995)	71
3.1.5	The Method of Isafiade and Fraser (2008)	74
3.2	Steam System Design.....	77
3.2.1	Problem Statement.....	77
3.2.2	The Method of Coetzee and Majozi (2008).....	77
3.2.3	The Method of Beangstrom (2013)	84
3.3	Cooling Water System Design	92
3.3.1	Problem Statement.....	92
3.3.2	The Method of Gololo and Majozi (2011)	93
3.4	Cooling Tower Model	97
3.5	Steam levels.....	103
3.6	Shaft Work Estimation	105
3.7	Solving Differential Equations.....	109
3.7.1	The Runge-Kutta Method	109
3.7.2	The Adams-Bashforth Method	111
3.8	References	115
4	Model Development.....	118
4.1	Problem Statement	119
4.2	Regions of Application.....	120
4.3	Superstructures	123
4.3.1	Above Pinch Superstructure	124
4.3.2	Below Pinch Superstructure.....	126
4.4	Existence Matrices	129
4.5	Model Constraints	133

4.5.1	Above Pinch Model	134
4.5.2	Below Pinch Model.....	146
4.6	Solution Procedure	162
4.7	References	164
5	Illustrative Examples	167
5.1	First Example	167
5.1.1	Problem description	167
5.1.2	Base Case	170
5.1.3	New Model.....	172
5.1.4	Summary	184
5.2	Second Example	186
5.2.1	Problem description	186
5.2.2	Base Case	189
5.2.3	New Model.....	191
5.2.4	Summary	204
5.3	References	206
6	Conclusions and Recommendations	207
	Appendix A: Steam levels and hot liquid reuse.....	212
	Appendix B: GAMS codes	217

List of Figures

Figure 1.1 Basic composite curves to determine regions of application for heat integration.	2
Figure 1.2: Cooling tower effectiveness	4
Figure 1.3: Steam boiler purchase cost as a function of steam flowrate	4
Figure 2.1: Onion diagram for the above mentioned design steps, with a focus on heat integration.....	10
Figure 2.2: Heat availability diagram.	12
Figure 2.3: Grand Composite Curve showing the proper placement of multiple utilities.....	14
Figure 2.4: Use of the grid diagram in designing HENs.	16
Figure 2.5: Removing a heat exchanger	17
Figure 2.6: The three sections of a total processing plant	19
Figure 2.7: Superstructure used to synthesize the utility system.....	20
Figure 2.8: Targeting the minimum water flowrate.....	25
Figure 2.9: Two-dimensional grid diagram	29
Figure 2.10: Targeting the minimum cooling water flowrate.....	31
Figure 2.11: Water mains superstructure	32
Figure 2.12: Stage wise superstructure.	33
Figure 2.13: Two methods of preserving boiler efficiency	43
Figure 3.1: Process-process heat integration superstructure.....	62
Figure 3.2 Demonstration of how variable temperatures can be used to alter which stages a stream exists	64
Figure 3.3: Superstructure for the method of Yee and Grossmann	65
Figure 3.4: Example of a block interval on the composite curves.	72
Figure 3.5 Superstructure repeated over the intervals created by two hot and two cold streams.....	75

Figure 3.6: The importance of ΔT_{\min} in determining feasible and infeasible hot utilities.....	78
Figure 3.7: Superstructure for simultaneously targeting flowrate and synthesizing the HEN.....	79
Figure 3.8: Superstructure used for HEN synthesis utilising multiple steam levels and satisfying shaft work requirements.	84
Figure 3.9: Superstructure used for cooling water network design with multiple cooling towers.	93
Figure 3.10: Differential slice across cooling tower packing.	97
Figure 3.11: Latent heat of steam and heat capacity of water as a function of saturation temperature.....	104
Figure 3.12: The Willans line for a simple turbine.....	105
Figure 3.13: Nonlinear variation of turbine efficiency with operating conditions	106
Figure 4.1: Old paradigm in which hot and cold composite curves define the boundaries of three regions of application.....	120
Figure 4.2: New paradigm in which the pinch defines the boundary between two regions of application.....	122
Figure 4.3: Above Pinch superstructure	125
Figure 4.4: Below Pinch superstructure.....	127
Figure 4.5: Relationship between the cold stream and the maximum hot liquid flowrate	141
Figure 4.6: Simplified cooling tower shell with proportions.....	160
Figure 5.1: First example - composite curves.....	169
Figure 5.2: First example – grand composite curve.	169
Figure 5.3: First example – relative stream positions and interval placement.	173
Figure 5.4: First example – graphical targeting.....	173
Figure 5.5: First example - above pinch HEN for Case 1.	175
Figure 5.6: First example - below pinch HEN for Case 1.	177

Figure 5.7: First example - above pinch HEN for Case 2.	180
Figure 5.8: First example - below pinch HEN for Case 2.	182
Figure 5.9: Second example - composite curve.....	187
Figure 5.10: Second example - grand composite curve.....	188
Figure 5.11: Second example – relative stream positions and interval placement.	192
Figure 5.12: Second example – graphical targeting.	192
Figure 5.13: Second example - above pinch HEN for Case 1.....	194
Figure 5.14: Second example - below pinch HEN for Case 1.....	196
Figure 5.15: Second example - HEN for refrigerated section.	198
Figure 5.16: Second example - above pinch HEN for Case 2.....	200
Figure 5.17: Second example - below pinch HEN for Case 2.....	202

List of Tables

Table 3.1: Typical steam levels	103
Table 3.2: Turbine model coefficients	108
Table 5.1: Stream data for first example.....	168
Table 5.2: Hot and cold utility requirements.	170
Table 5.3: Duties for Figure 5.5 in kW.....	176
Table 5.4: Duties for Figure 5.6 in kW.....	178
Table 5.5: Duties for Figure 5.7 in kW.....	181
Table 5.6: Duties for Figure 5.8 in kW.....	183
Table 5.7: Summary of first example, Case 1.....	184
Table 5.8: Summary of first example, Case 2.....	185
Table 5.9: Stream data for second example	186
Table 5.10: Hot and cold utility requirements.	190
Table 5.11: Duties for Figure 5.13 in kW.....	195
Table 5.12: Duties for Figure 5.14 in kW.....	197
Table 5.13: Duties for Figure 5.16 in kW.....	201
Table 5.14: Duties for Figure 5.17 in kW.....	203
Table 5.15: summary of second example, Case 1.....	204
Table 5.16: Summary of second example, Case 2.....	205

Nomenclature

Sets

C	Set of all cold streams
C'	Set of all cold streams (alias)
H	Set of all hot streams
H'	Set of all hot streams (alias)
K	Set of all intervals
L	Set of all steam levels
Z	Set of slices along height of cooling tower.

Parameters

A	Steam turbine parameter	[-]
A_{CS}	Cooling tower cross sectional area	[m ²]
B	Steam turbine parameter	[-]
Cp_a	Heat capacity of air	[kJ/kg·K]
Cp_v	Heat capacity of water vapour	[kJ/kg·K]
Cp_w	Heat capacity of water liquid	[kJ/kg·K]
$HL_{c,k}^U$	Upper limit on hot liquid to c in interval k	[kg/s]
$L_{h,k}^U$	Upper limit on cooling water to h in interval k	[kg/s]
M	Maximum number of heat exchanger splits	[-]
s_{step}	Step size for cooling tower slice	[m]
$SS_{c,k,l}^U$	Upper limit on steam of level l to c in interval k	[kg/s]
T^{limit}	Temperature limit for cooling tower packing	[°C]

Continuous Variables

B	Cooling tower blow down	[kg/s]
CP_c	Heat capacity flowrate of cold stream c	[kW/K]
CP_h	Heat capacity flowrate of hot stream h	[kW/K]
$CW_{h,k}$	Cooling water supplied to h in interval k	[kg/s]
E	Evaporative losses in cooling tower	[kg/s]
$F_{c,k}^{in}$	Mass flowrate into utility heater for c in k	[kg/s]
$F_{c,k}^{out}$	Mass flowrate out of utility heater for c in k	[kg/s]
$F_{h,k}^{in}$	Mass flowrate into utility cooler for h in k	[kg/s]
$F_{h,k}^{out}$	Mass flowrate out of utility cooler for h in k	[kg/s]

$FR_{c,k}$	Condensate returned from c in interval k	[kg/s]
$FR_{h,k}$	Cooling tower return from h in interval k	[kg/s]
$FRR_{c',k',c,k}$	Hot liquid reuse from c' in k' to c in k	[kg/s]
$FRR_{h',k',h,k}$	Cold liquid reuse from h' in k' to h in k	[kg/s]
G	Gas flowrate per area inside cooling tower	[kg/m ² ·s]
$h_a a_f$	Cooling tower mass transfer coefficient	[kg/m ² ·s]
$\overline{\Delta H}_l^{is}$	Specific isentropic enthalpy change between levels	[MWh/t]
i_z^{ma}	Air enthalpy in slice z of the cooling tower	[kJ/kg]
i_z^{masw}	Saturated air enthalpy in slice z of the tower	[kJ/kg]
L	Liquid flowrate per area inside the cooling tower	[kg/m ² ·s]
Le_z^f	Lewis factor in slice z of the cooling tower	
M	Cooling tower make up	[kg/s]
m_a	Total mass flowrate of air in cooling tower	[kg/s]
m_w	Total mass flowrate of water in cooling tower	[kg/s]
Me	Merkel number	[-]
$p_z^{sat,w}$	Saturation pressure of water in slice z	[kPa]
$Q_{h,k}^{CU}$	Cold utility heat from h in interval k	[kW]
$Q_{c,k}^{HL}$	Sensible heat supplied to c in interval k	[kW]
$Q_{c,k}^{HU}$	Hot utility heat to c in interval k	[kW]
$Q_{c,h,k}^{PP}$	Heat transferred from h to c in interval k	[kW]
$Q_{c,k}^{SS}$	Latent heat supplied to c in interval k	[kW]
QC_c	Heat to be supplied to cold stream c	[kW]
QH_h	Heat to be removed from hot stream h	[kW]
R_b	Cooling tower base radius	[m]
$SL_{c,k,l}$	Saturated liquid of level l supplied to c in k	[kg/s]
$SS_{c,k,l}$	Saturated steam of level l supplied to c in k	[kg/s]
W^s	Shaft work produced by turbine	[MW]
T^{cw}	Cooling water temperature	[°C]
$T_{c,k}^C$	Temperature of stream c on left side of interval k	[°C]
$T_{h,k}^H$	Temperature of stream h on left side of interval k	[°C]
T^M	Temperature of make-up water	[°C]
T_l^{sat}	Saturation temperature of steam level l	[°C]
T_c^{sup}	Supply temperature of cold stream c	[°C]
T_c^{tar}	Target temperature of cold stream c	[°C]

T_h^{sup}	Supply temperature of hot stream h	[°C]
T_h^{tar}	Target temperature of hot stream h	[°C]
T^{ret}	Return temperature to cooling tower	[°C]
TR	Total condensate returned to boiler	[kg/s]
TR	Total water returned to cooling tower	[kg/s]
TS_l	Total steam of level l supplied to HEN	[kg/s]
TUS	Steam supplied to turbine of level l	[kg/s]
TW	Total water from cooling tower	[kg/s]
T_z^w	Water temperature in slice z of the cooling tower	[°C]
W_z	Humidity in slice z of the cooling tower	[kg/kg]
W_z^{sw}	Saturated humidity in slice z of the cooling tower	[kg/kg]

Binary Variables

$pp_{c,h,k}$	Match between c and h exists in interval k	[-]
$x_{c,k,l}$	Stream c in interval k uses steam of level l	[-]
$y_{c,k}$	Stream c in interval k uses hot liquid	[-]
$y_{h,k}$	Stream h in interval k uses cooling water	[-]

Greek

Γ	Large Number	[-]
ε	Cooling tower effectiveness	[-]
λ_l	Latent heat of steam level l	[kJ/kg]

Abbreviations

GA	Genetic Algorithm
GCC	Grand Composite Curve
HEN	Heat Exchanger Network
LP	Linear Programming
MEN	Mass Exchanger Network
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
MSA	Mass Separating Agent
NLP	Non-Linear Programming
NTU	Number of Transferred Units

Chapter 1

Introduction

1.1 Background

The primary objective of process integration is to analyse, synthesize and optimise the performance of a chemical plant by means of the systematic consideration of the interactions between various unit operations. From the 1970s to the present, the pressures of overpopulation and diminishing fuel sources have caused numerous process integration methods to be developed and implemented to reduce energy consumption in chemical plants.

Through process integration, a number of economic and environmental advantages can be achieved. Utility minimisation, steam system design, cooling water system design and wastewater minimisation improve the profitability of a plant through reduced capital costs, reduced operating costs, and reduced environmental legislation charges due to 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 effect each unit has on other units. Process integration therefore uses a holistic and systematic approach to exploit the interactions between process units and bring about an optimally operating process.

The field of heat integration came to the fore during the 1970's energy crisis, when the Arab Organisation of Petroleum Exporting Countries (AOPEC) placed

1 Introduction

embargos on the exportation of oil. Rapidly escalating energy costs forced companies to reconsider energy efficiency in their processes, seeking less wasteful methods of operation. Arguably the first work of this nature was that of Hohmann (1971), in which the trade-off between utility cost and heat exchanger area was considered. Not long after, many improvements upon this idea were published.

Following the success of process-process heat integration, similar methods were developed to apply pinch techniques to the regions of cooling water systems and steam systems, as determined by the balanced composite curves (Figure 1.1). Although these are not necessarily focused on minimising the use of energy, the utility flowrate can be reduced, reducing the size and cost of the related equipment, or debottlenecking existing processes.

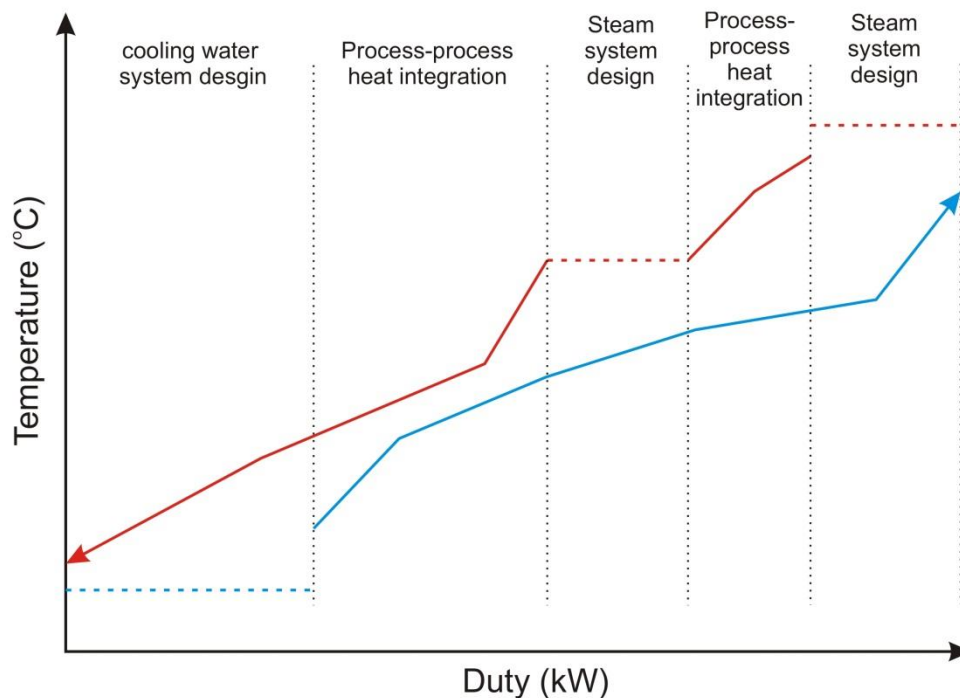


Figure 1.1 Basic balanced composite curves to determine regions of application for heat integration and utility system design.

A common streak to all of these utility optimization methods is that they each operate in isolation to each other. Process-process methods focus on the

1 Introduction

processes, assuming that the utility systems will be designed in the traditional manner. Cooling water system and steam system design methods only consider the streams that require cooling or heating. Often, the methods of cooling water system design and steam system design are only applied after process-process heat integration has been applied, and the regions for hot and cold utility have been fixed. Such an approach has the consequence that the methods of process-process heat integration, cooling water system design and steam system design remain isolated. Furthermore, the techniques in published literature tend to focus on the design and optimisation of the system at hand, while the accompanying utility operations, i.e. the boilers, steam turbines, and cooling towers are ignored. This indicates a definite need for a method which considers the interactions between the three systems and the accompanying utility systems, to optimise the process further than what is possible using the isolated approach, hence this contribution.

1.2 Motivation

The motivation behind the individual methods of process-process heat integration, cooling water system design, and steam system design are all applicable to the present study. Process-process heat integration is motivated by the simultaneous reduction in the amount of hot and cold utility required, resulting in reduced energy costs and physically smaller utility systems. Pinch techniques for cooling water systems are motivated by the observation that reducing the circulating water flowrate or increasing the water return temperature results in increased cooling tower effectiveness (Figure 1.2). Likewise, the motivation behind the application of pinch techniques to steam systems lies in the observation that the purchase cost of a steam boiler increases rapidly with an increase in the required steam flowrate (Figure 1.3). In addition, the reduced cooling water and steam flowrates serve to debottleneck a process. All of these observations, collectively, can also be considered as motivating

1 Introduction

factors to the present study, which aims to perform all three tasks simultaneously.

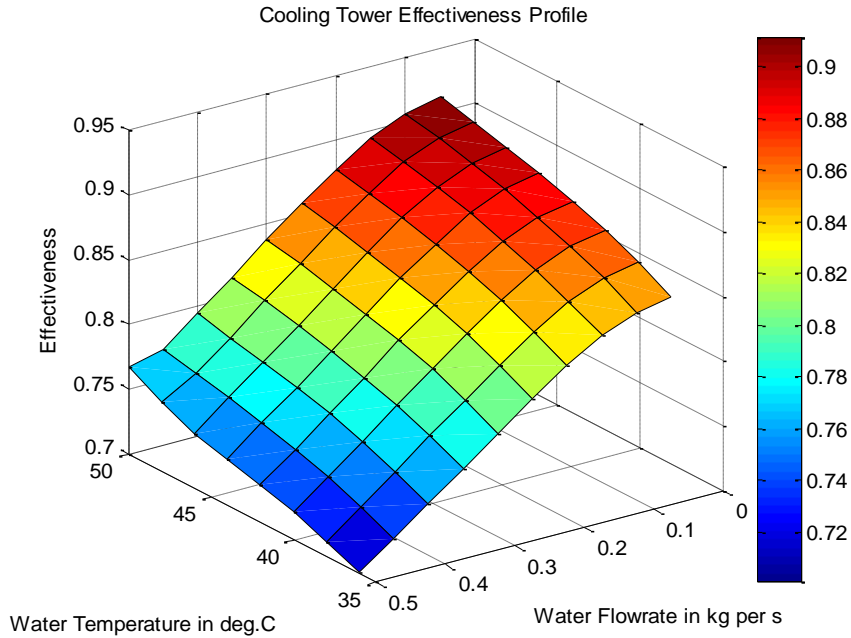


Figure 1.2: Cooling tower effectiveness (Kim & Smith, 2001; after Bernier, 1994).

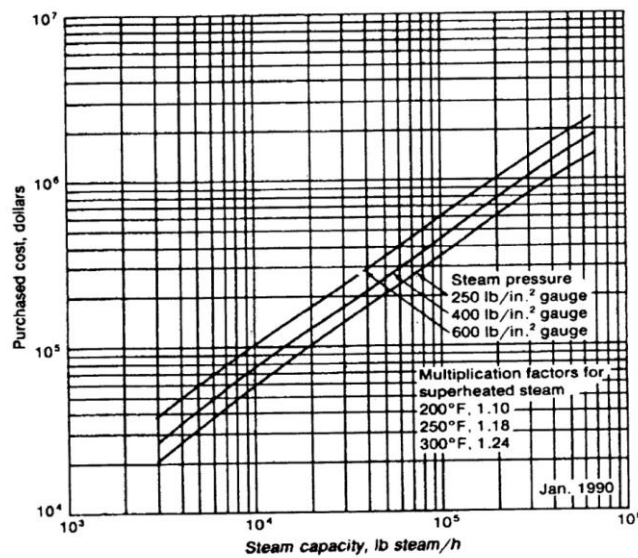


Figure 1.3: Steam boiler purchase cost as a function of steam flowrate (Peters & Timmerhaus, 1991).

1 Introduction

More importantly, this work is motivated by the observation that the above three classes of process integration techniques are still largely treated in isolation, with little regard for the interaction between the three systems or the accompanying utility systems. Even the most popular framework, the Grand Composite Curve, which is used to select utility levels best suited for a particular set of process streams, does not take into account the recent advances in utility stream reuse, nor does it take into account the design and optimisation of the accompanying utility systems.

Cooling water system design and steam system design techniques are built upon the concept of reusing a utility stream from one process unit to another, seeking out feasible matches based on the temperature requirements of the individual streams. If the region of application for cooling water system design and steam system design are determined and fixed after performing process-process heat integration, the methods of cooling water system and steam system heat integration are restricted to operate within a narrow temperature band, limiting their potential for utility flowrate reduction. This isolated approach to process integration often leads to suboptimal results.

Unit operations such as cooling towers, boilers, and steam turbines should be optimised together with the process to exploit the potential savings afforded by their interactions. For this reason, it is necessary to develop a comprehensive framework for utility system design that simultaneously performs process-process heat integration, cooling water system design, and steam system design, while designing and optimising the accompanying utility operations.

1.3 Objective of Investigation

In light of the separated nature of previously published work, the objective of this work is to develop a comprehensive design framework that simultaneously takes into account process-process heat integration, cooling water system design, and steam system design, as well as the design and optimisation of the accompanying utility operations.

The proposed method does not alter the minimum energy requirements of the process. The aim is to minimise the flowrates of cooling water and steam further than what is possible if previous methods are applied in isolation to the three regions of heat integration. This ultimately increases the cooling tower effectiveness and reduces the steam boiler size. Alternatively, the extra capacity can be used for increased production, avoiding the expense of building new utility systems.

In addition to optimizing the utility flowrates, the proposed method is capable of synthesizing the heat exchanger network that will achieve these targets. This includes all process-process matches, as well as connections to hot and cold utilities at the appropriate levels and the reuse streams for each utility. Furthermore, the proposed method is capable of designing and optimising the accompanying cooling towers, boilers, and steam turbines, taking into account the interaction between these units and the process streams.

1.4 Structure

This thesis is divided into six chapters as follows:

- Chapter 1 is the introduction presented above.
- Chapter 2 gives a detailed survey of the available literature. The purpose here is to give a broad outline of the various methods available, and how they relate to each other.
- Chapter 3 gives a technical background to a number of key methods. These are the methods upon which the current work is built, and an understanding of these methods is required to follow the development of the proposed model.
- Chapter 4 contains the development of the proposed model. A detailed discussion of the applicable constraints is given as the model is derived.
- Chapter 5 presents two examples to demonstrate the effectiveness of the present model.
- Chapter 6 gives the conclusion of this study. Here the results are summed up, and recommendations for future work proposed.

1.5 References

Bernier MA (1994). Cooling tower performance: Theory and experiments. *ASHRAE Trans. Res.*, 100, 114-121.

Hohmann EC (1971). Optimum networks for heat exchange. PhD Thesis: University of Southern California, USE.

Kim JK & Smith R (2001). Cooling water system design. *Chem. Eng. Sci.*, 56, 3641-3658.

Peters MS & Timmerhaus KD (1991). Plant Design and Economics for Chemical Engineers. USA: McGraw-Hill.

Chapter 2

Literature Survey I – Fundamentals of Process Integration

In this chapter, a brief overview will be given of the various contributions that have led up to this present work.

2.1 Process-Process Heat Integration

When designing chemical processes, there are a number of sequential steps to be followed in the design process. The following list (after 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) Eliminate differences in composition (decide on the type and proper placement of separation units)
- 3) Eliminate differences in temperature, pressure and phase (decide where heating, cooling and pumping etc. is required)
- 4) Integrate the tasks (develop the HEN and assign utilities)

Process-process heat integration is concerned with the last two of these steps; identifying the streams that require heating and cooling, and integrating these

2 Literature Survey

streams in a heat exchanger network (HEN) that minimises the use of hot and cold utilities.

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

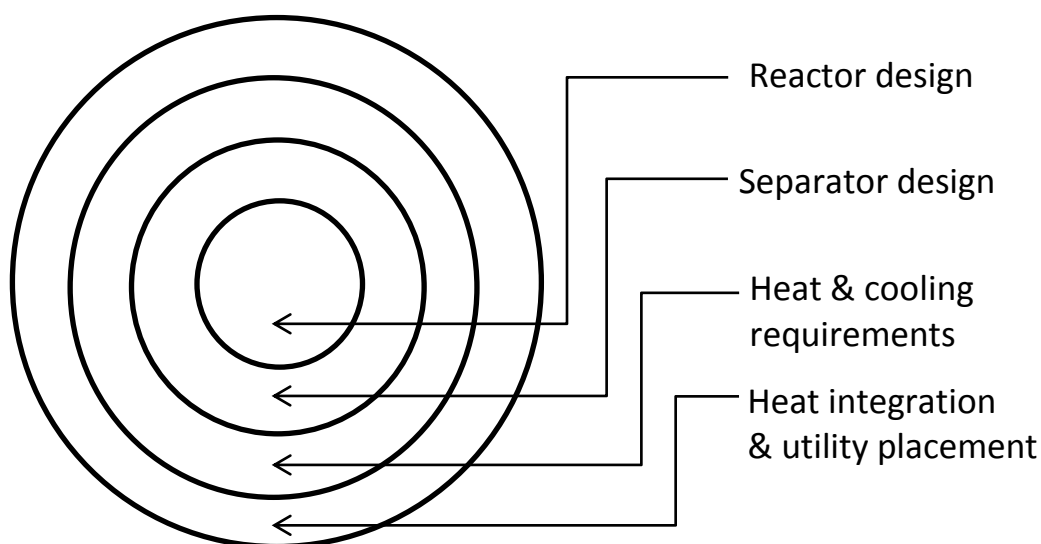


Figure 2.1: Onion diagram for the above mentioned design steps, with a focus on heat integration. (after Kemp, 2007)

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 and optimal. The only task remaining is to optimise the heat exchanger network. A number of techniques have been developed to do this, as will now be discussed.

2 Literature Survey

2.1.1 Pinch Techniques

The earliest works on process-process heat integration were graphical methods, using the designer's knowledge of the system to guide the process towards an optimal solution. Hohmann (1971) considered 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 technique was performed on a diagram of temperature versus enthalpy (or duty), and sought to reduce the quantity of utilities required. Hohmann (1971) showed how the minimum temperature difference for heat exchange (ΔT_{\min}) affected the quantity of utilities required, and also developed the N-1 rule to predict the smallest number of heat exchanger units that satisfy the problem.

Umeda *et al* (1979) used the concept of thermodynamically available energy in order to minimise the energy requirements. The aim was 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) expressed all the stream data as a single pair of hot and cold composite curves.

With this definition for the axes of the graph, Umeda *et al* (1979) showed that the area under a composite curve represents the energy of the constituent process streams available for transfer to cooler streams, with the area between the composite curves representing the quantity of useful energy that is lost.

2 Literature Survey

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 together until they meet.

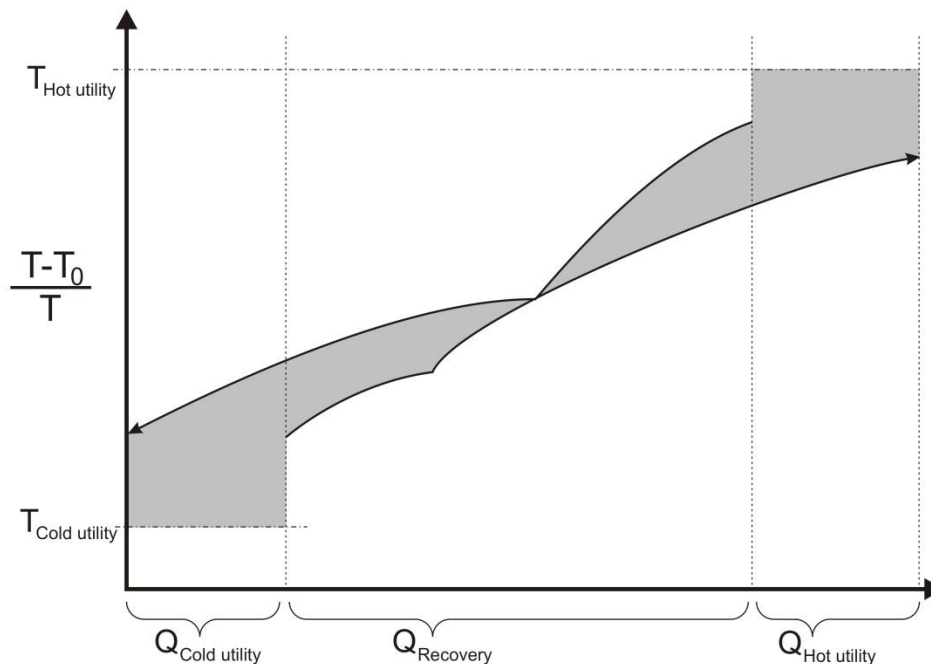


Figure 2.2: Heat availability diagram. The shaded region represents lost available energy (Umeda et al, 1979)

Umeda *et al* (1979) called the point at which the two composite curves meet the ‘pinch point’ and explained that it represented a bottleneck in the process. It is this point that prevents further energy savings, and if changes could be made that would smooth the composite curves, a better energy target could be realised. Umeda *et al* (1979) briefly discussed 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) was their use of computer aided calculations. Two programmes used in applying the method are mentioned. The first programme targeted the maximum quantity of energy recovery using the concepts illustrated in Figure 2.2, while the second

2 Literature Survey

synthesised the network for minimum area. The authors gave little information as to how the programmes performed these tasks.

Linnhoff and Flower (1978a) developed a mathematical method of locating the pinch temperature (now known as the Problem Table Algorithm), rather than obtaining it graphically. A set of temperature intervals is created based on the supply and target temperatures of the streams. The duty of all hot streams present in a particular temperature interval is summed, with the same done for the cold streams. 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 may 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 quantity vanishes and becomes zero, that is, when no interval has an energy deficit. The temperature at which this zero 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 (1978b) went on to 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). Rather than using an unwieldy PFD, Linnhoff and Flower (1978b) made 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 were matched by linking them with vertical lines connected at the relevant temperatures. This produced a clean and uncluttered diagram on which one could easily keep track of the energy being transferred and the resulting temperatures of the streams.

2 Literature Survey

Townsend and Linnhoff (1983b) developed what is now known as the Grand Composite Curve (although originally called 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, as in Figure 2.3. The advantage of the GCC lay in its ability to show at which temperature energy must be supplied to or removed from the process. This aided in the proper placement of multiple high and low value utilities, and the determination of the duty required of each utility. Furthermore, regions of pure process-process integration could be easily identified as pockets in the GCC (shaded in Figure 2.3).

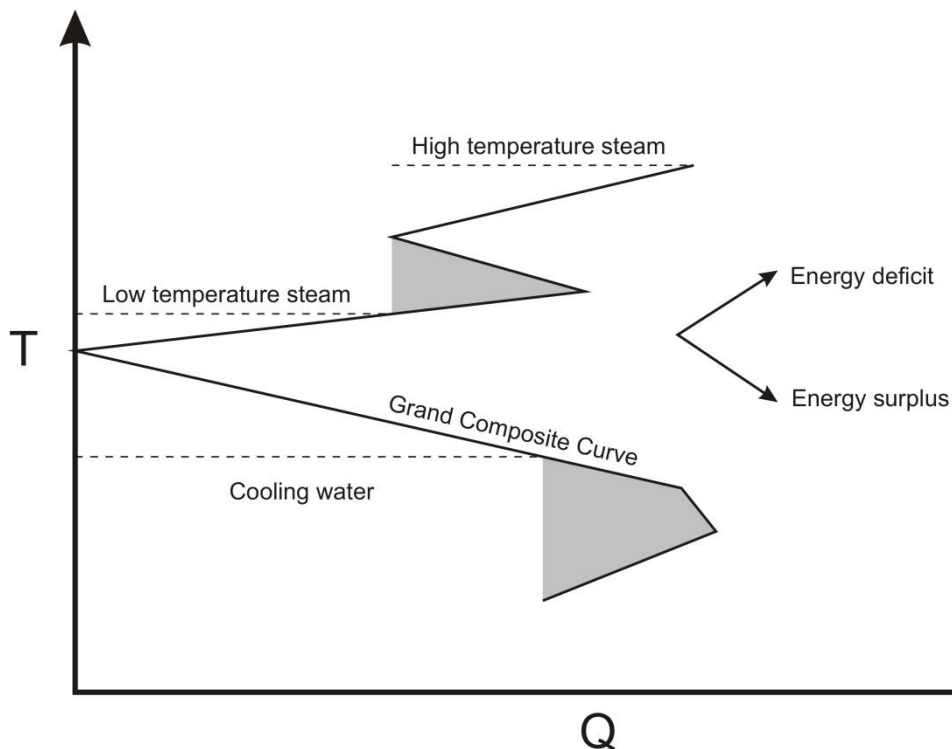


Figure 2.3: Grand Composite Curve showing the proper placement of multiple utilities. (Kemp, 2007)

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

2 Literature Survey

application”. They explained how a method that is flexible and “helps the user think” rather than “think for the user” is more desirable in industry. With a formula for predicting the minimum number of units, it was proposed that all synthesis methods should first attempt to design for the minimum number of units at maximum energy recovery. Linnhoff, Mason and Wardle (1979) concluded by solving a number of problems from literature, including one that was previously deemed unsolvable.

Linnhoff and Hindmarsh (1983) combined the best aspects of the above methods into a clear, systematic and accessible design procedure. The use of process-process heat integration was popularised as a means of saving energy and capital by creating one clear and simple procedure out of all the available knowledge. 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 was determined before any design was 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) proceed to synthesise the layout of the heat exchanger network. This is accomplished on the grid diagram, introduced by Linnhoff and Flower (1978). Linnhoff and Hindmarsh (1983) explained that the pinch represented the most constrained region inside the processes, and as such, the design should begin at the pinch and move outwards towards the hot and cold ends. Because of the

2 Literature Survey

three rules regarding the pinch, the design of the HEN could be broken into two independent sub-networks connected at the pinch, each is designed separately and then combined to give the final network (Figure 2.4).

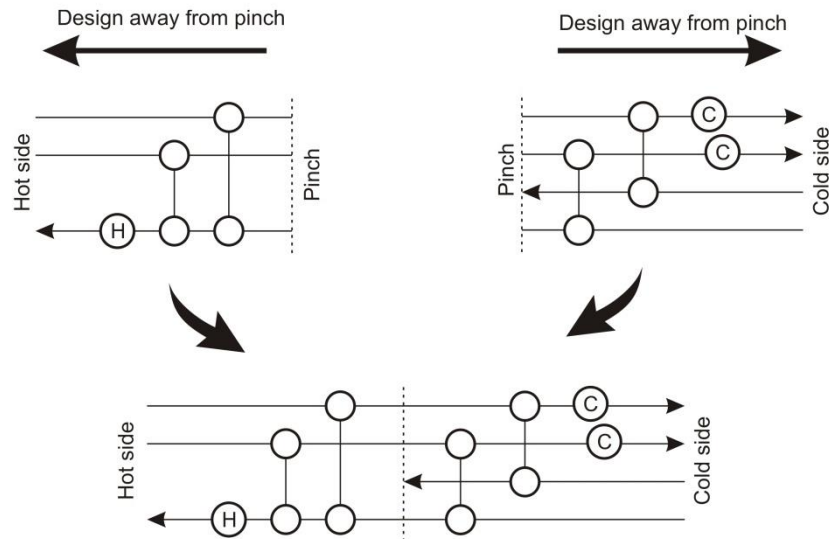


Figure 2.4: Use of the grid diagram in designing HENs.

Although Figure 2.4 looks relatively simple, it is not always easy to identify which streams to match. Linnhoff and Hindmarsh (1983) gave a set of rules to aid in identifying feasible stream matches involving the heat capacity flowrate (CP) of the streams. In addition to this, Linnhoff and Hindmarsh (1983) also provided several rules based on the CP of the streams that allowed 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, leaving it to the designer to choose the relative importance of energy savings versus capital savings. The number of units is reduced by removing one or more heat exchangers that form “heat loops” when the two halves of the HEN are joined together (Figure 2.5)

2 Literature Survey

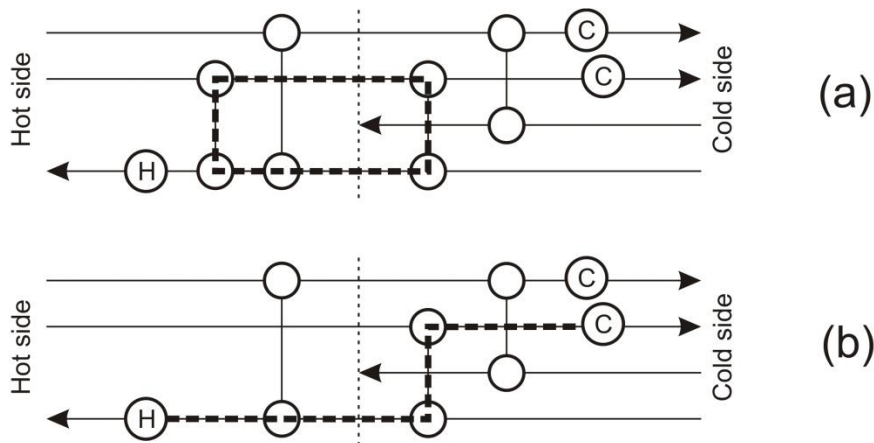


Figure 2.5: Removing a heat exchanger. (a) identifying a heat loop (b) correcting for temperature infeasibilities.

Using the techniques of heat integration discussed above, Ahmad and Polley (1990) discussed how pinch techniques can be applied to debottleneck existing processes, with an emphasis on the cost of retrofitting. Hui and Ahmad (1994) further proposed that heat available in one region of a plant could be transported to another distant region using the existing steam headers. Here, surplus energy in one region of a plant was indirectly supplied to another region using steam raised in a waste heat boiler. Hui and Ahmad (1994) used the GCCs of the individual regions to target how much low and intermediate level steam could be raised, and how much was in demand.

2.1.2 Mathematical Programming Techniques

The manual techniques discussed above often require repetitive calculations to be performed. After the introduction of the personal computer, researchers sought to automate these calculations to speed up the design process. With the ability to handle multiple dimensions, computer models soon proved their worth by taking more into account than what was possible graphically. This, however, came at the expense of accepting black box design procedures, with the designer and his insight being further and further removed from the process.

2 Literature Survey

Some of the earliest models for mathematically synthesising system designs use heuristic and thermodynamic insights to simplify the models. In a series of three papers (Rudd, 1968; Musso & Rudd, 1969; Sirola, Powers & Rudd, 1971), knowledge and insight were used to decompose the problem into smaller sub-problems. The methods did not make use of any initial structure, but instead attempted to use artificial intelligence along with the heuristics. Similar to this is the method of Nishio *et al* (1980) which used 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 may preclude the true optimum, leading to a suboptimal solution.

Grossmann and Santibanez (1980) demonstrated the power of binary variables when they developed 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. In this way, Grossmann and Santibanez (1980) could include several options in the mathematical formulation, and the optimisation routine could select between options. This, however, can only be done if these options are present in the problem formulation. For this, a superstructure had to be developed which encompassed many options, as demonstrated by Papoulias and Grossmann (1983a, 1983b, 1983c).

Papoulias and Grossmann (1983a) developed a technique for finding the optimal structure of the utility section of a total process system. The system was divided into three sections: the chemical plant, the heat recovery network and the utility systems, with the relation between these sections shown in Figure 2.6. The design of a chemical plant was optimised to meet the production objectives;

2 Literature Survey

to produce the required products at the required rate and quality. After the chemical plant had been specified, the supporting systems were designed and optimised.

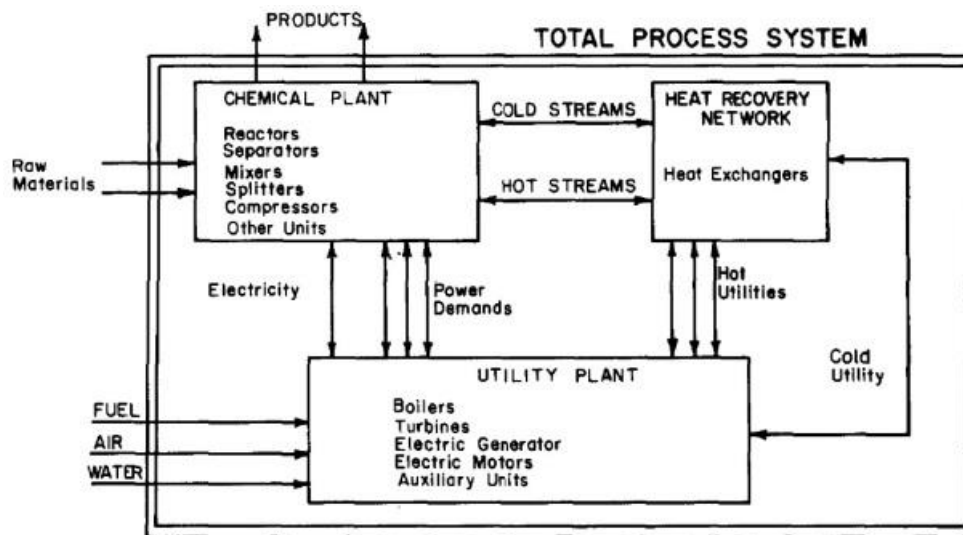


Figure 2.6: The three sections of a total processing plant. (Papoulias & Grossmann, 1983c)

In the first of three papers, Papoulias and Grossmann (1983a) considered the synthesis of the utility plant. A superstructure (Figure 2.7) that included most of the possible units one would find in a utility plant was developed. Using this, an MILP model of the process was developed, with the objective to minimise the cost of the plant while ensuring that the required utilities are provided. Where more than one option was available for supplying a utility, binary variables were used to select between options. Binary variables were also used to select between various discrete operating conditions for a particular unit. In the formulation, Papoulias and Grossmann (1983a) included constraints that ensured that if two operations were dependent on one another, the existence of one operation forced the existence of the other.

2 Literature Survey

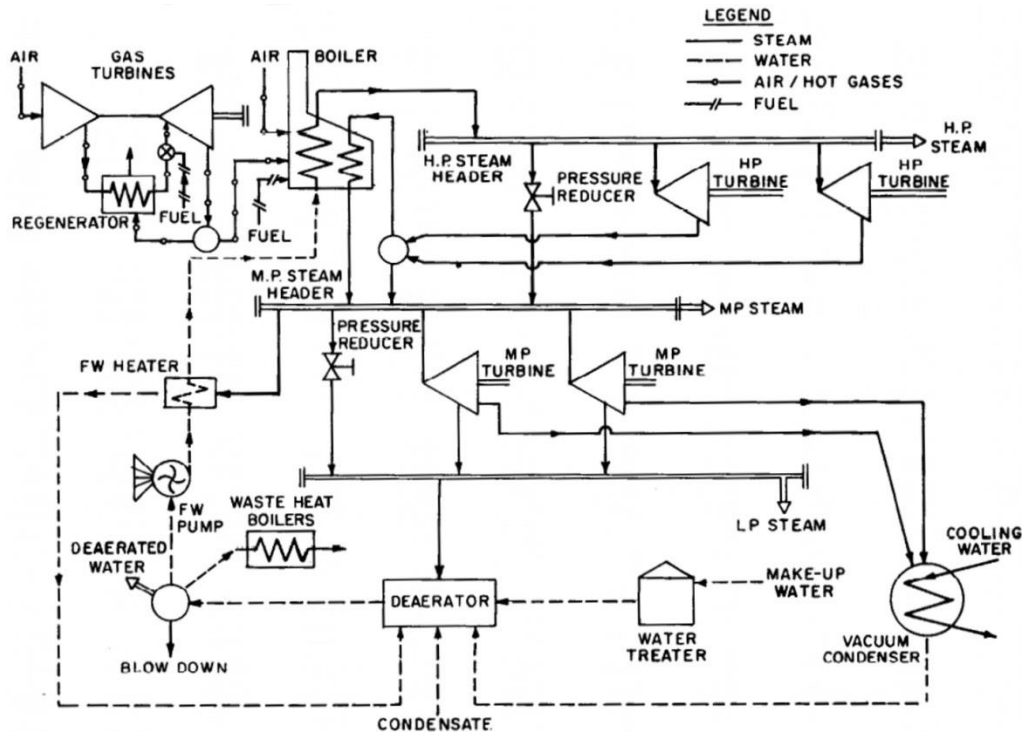


Figure 2.7: Superstructure used to synthesize the utility system. (Papoulias & Grossmann, 1983a)

In the second of three papers, Papoulias and Grossmann (1983b) looked at the synthesis of the heat recovery network. An LP formulation was first developed to target the minimum utility costs for the case where there were no forbidden matches, using a transshipment model to ensure thermodynamic feasibility. In the transshipment model, heat was transferred from the hot streams to the cold stream via a number of intermediate temperature intervals. The Problem Table Algorithm (Linnhoff and Flower, 1978) may be used to obtain these intervals, but Papoulias and Grossmann (1983b) claimed that intervals obtained using the methods of Grimes (1980), Cerda *et al* (1981) and Cerda *et al* (1983) yielded smaller and faster transshipment models.

Papoulias and Grossmann (1983b) went on 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 provided a number of steps in which all of the above

2 Literature Survey

mentioned models were linked together and used to synthesize the optimal total utility system.

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

Papalexandri and Pistikopoulos (1994) used 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 was developed, based on a multiperiod MINLP model. A total annualised cost was used as the objective function, but the model incorporated a number of very important additional constraints. Given that the operation was multiperiod, the resulting network must be capable of handling changes in the flow and temperatures of the streams. Papalexandri and Pistikopoulos (1994) emphasised the controllability of the resulting network, considering process disturbances and heat exchanger fouling.

In an attempt to move away from cumbersome transshipment models, Yee *et al* (1990) considered the transfer of heat directly from the hot streams to the cold streams without passing through an intermediary temperature interval. The hot and cold streams were divided into a number of theoretical stages, and a superstructure applied to each stage that made provision for a match between every hot stream and every cold stream. Yee *et al* (1990) assigned binary

2 Literature Survey

variables to denote the existence of these matches, and developed an MINLP model to synthesise the HEN. Since the model was non-linear, an initialisation technique was provided.

The stage wise decomposition method of Yee *et al* (1990) resulted in stages with no physical meaning. Zhu *et al* (1995) refined this with a block wise decomposition technique, in which the composite curves were used to determine blocks with physical meaning. The same superstructure developed by Yee *et al* (1990) was applied within each block, and an MINLP model used to synthesise the HEN. A relaxed MILP model was also provided, the solution of which could be used as the initial point for the MINLP model.

Taking the best aspects of these two methods, Isafiade and Fraser (2008) developed an interval based method of decomposing the process streams. Here, one set of streams was divided into abstract stages, while the other set was divided into blocks with physical meaning. The same superstructure as above was used, along with an MINLP model. Isafiade and Fraser (2008) claimed that no special initialisation procedures were required.

The classical optimisation routines used in many of the above methods rely on gradient based methods to steer the solver towards the optimum. This can cause serious problems when the feasible region is highly non-linear, or contains discontinuities. One method of overcoming this is to use modern optimisation techniques, such as Genetic Algorithms (GA). In GA techniques, the solution vector is discretised as a binary string, representing the DNA string of a theoretical species. As the technique progresses, the species evolve towards the optimum value. Random genetic mutations allow the algorithm to “jump” around the feasible space, overcoming the obstacles of non-linearity and discontinuity.

2 Literature Survey

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

Ma *et al* (2008) used 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 were 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, yielding the final result.

2.2 Mass Integration

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

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

Since heat and mass transfer share these characteristics, one can adapt the tools developed for heat integration to perform mass integration and vice versa.

El-Halwagi and Manousiouthakis (1990) developed a model to automatically synthesize a Mass Exchanger Network (MEN) for a single contaminant. The model considered the transfer of a single component from a set of rich streams to a set of lean streams using a variety of mass separating agents (MSAs) as the lean streams. If the minimum permissible concentrations difference was specified globally, an LP model for minimum annual cost could be used, but if the minimum permissible concentration differences were specified per match, an MILP model was obtained.

The method of El-Halwagi and Manousiouthakis (1990) assumed that a variety of MSAs are considered. In many cases, only water is used as the MSA. Wang and Smith (1994) developed a graphical method of minimising the quantity of wastewater produced when water is the only lean stream. The method worked on the grounds that not all water using processes require absolutely clean water, and could tolerate a certain maximum level of contamination. On a plot of contaminant concentration versus contaminant mass load, a limiting concentration profile described the limitations of the various water using

2 Literature Survey

operations (Figure 2.8). A water utility line, the gradient of which is inversely proportional to the flowrate, was gradually shifted closer to the limiting concentration profile until a pinch was formed. At this point the minimum wastewater flowrate had been targeted.

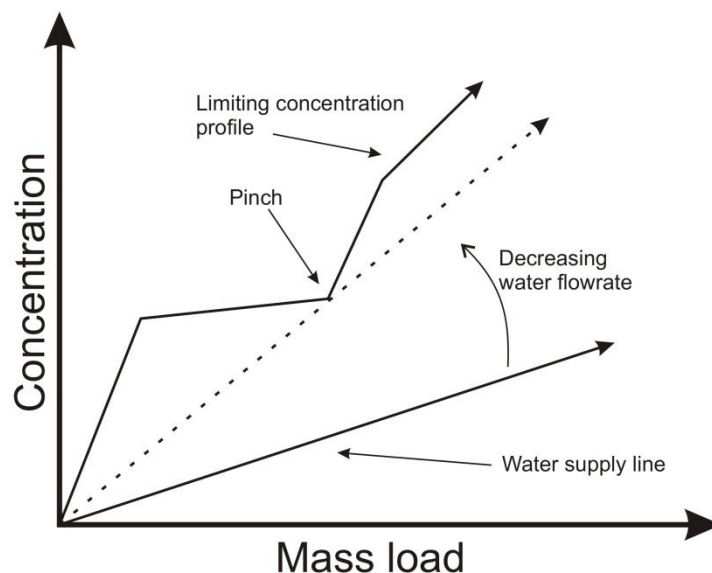


Figure 2.8: Targeting the minimum water flowrate. (Wang & Smith, 1994)

Wang and Smith (1994) also considered the possibility of regenerating the water, while distinguishing between reusing and recycling this regenerated water. Wang and Smith (1994) went on to expand their graphical method further to incorporate multiple contaminants, but the method was complicated and not well suited to large industrial scale problems.

Olesen and Polley (1997) observed that in cases of regeneration-reuse, there were instances where the method of Wang and Smith (1994) required some operations to be split in two. A simplified procedure was proposed for targeting and designing wastewater networks using a “load table”, which expressed the contaminant load above and below the pinch for each process. The design procedure was based on inspection and intuition, and the authors themselves

2 Literature Survey

stated that the method could become complex and was best suited to small problems

Doyle and Smith (1997) developed a mathematical programming method for targeting the maximum water reuse in a system, based on the concepts of Wang and Smith (1994). Two cases were considered, the first based on a fixed mass load and the second based on a fixed outlet concentration. In the first case, the problem resulted in an NLP formulation, while in the second case the problem resulted in an LP formulation. Since many processes require that a fixed mass load be exchanged, a combined method was proposed wherein the LP problem was solved first, and the solution used as the starting point of the NLP problem.

Kuo and Smith (1998a) developed 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 was that some effluent treatment systems might work better if contaminant concentrations are kept within an ideal operating range. Kuo and Smith (1998a) also developed the “water mains” method for use in determining the layout of the water network. Kuo and Smith (1998b) expanded upon these developments to include regeneration-reuse and regeneration-recycling.

Savelski and Bagajewicz (2000a) presented and proved a number of necessary conditions for the optimality of water using systems. This stemmed from their belief that the mathematical methods in existence up until that point were over-complicated and usually resulted in NLP models. These necessary conditions were intended to help linearize the models. Savelski and Bagajewicz (2000b) used these necessary conditions in an algorithmic method for designing the water network for minimum flowrate. Savelski and Bagajewicz (2001a) further refined this method into a non-iterative algorithmic method. Through the use of

2 Literature Survey

necessary and sufficient conditions, it was claimed that the method provided a globally optimal design without the need to target the minimum water flowrate first. The authors also claimed that the procedure was sufficiently simple to be carried out by hand for problems of any size. Savelski and Bagajewicz (2003) provided a number of necessary conditions for optimality in the presence of multiple contaminants, similar to those of the single contaminant case.

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

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, such as the ideal water temperature for a cleaning operation. Srinivas and El-Halwagi (1994) considered the problem of combining heat integration and reactive mass transfer, proposing a method that started by defining sets of rich and lean streams with specified flowrates and supply and target temperatures. Each lean stream was divided into a number of lean sub-streams, each characterised by a variable composition and temperature. Srinivas and El-Halwagi (1994) made use of an MINLP formulation to solve the problem for minimum operating cost. A simplified LP formulation was also given which may be used to generate a starting point for the MINLP.

Savulescu, Kim and Smith (2005a,b) developed a graphical method for simultaneous integration of heat and mass, with consideration for single

2 Literature Survey

contaminant systems. Savulescu *et al* (2005a) developed a method of designing the heat exchanger network for the system while stipulating that there was no water reuse. Minimising the flowrate of water simply becomes a matter of maximising the outlet concentration of each operation. A graphical method was used to design the heat exchanger network to meet the energy demands. This was based largely on the grid diagram method, the major difference being that in the grid diagram method, only sub streams that resulted from the splitting of the same process stream were allowed to be mixed, whereas the method of Savulescu *et al* (2005a) allows the mixing of unrelated water streams, but not processes streams.

Savulescu *et al* (2005b) introduced the option for the reuse of water from one operation to another. Two important aspects of the reuse problem were considered: multiple designs attaining the same minimum target, and the trade-off between direct and indirect heat transfer. The first aspect stemmed from the observation that different reuse connections can result in the same water target, but different energy targets. The second aspect looked 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. Savulescu *et al* (2005b) developed a two-dimensional grid diagram to obtain this design.

The two-dimensional grid diagram is similar to the water mains method of Kuo and Smith (1998a), but included a temperature scale on the vertical axis in addition to the concentration scale on the horizontal axis (Figure 2.9). Here, the operations were 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 represented cold streams that required heating and water streams

2 Literature Survey

moving downwards represented hot stream requiring cooling. This allowed matches between the hot and cold streams to be made while exploring the different reuse connections. Again, this method was limited to single contaminant problems, and being a graphical method, it became tedious for large problems.

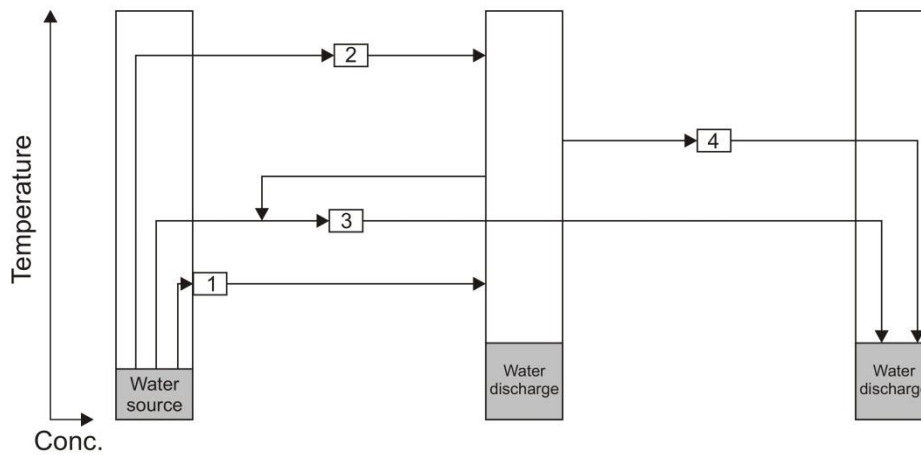


Figure 2.9: Two-dimensional grid diagram. (Kuo & Smith, 1998a)

2.3 Cooling Water System Design

With the exception of a few specialised cases, the dominant cold utility on the typical plant is invariably cooling water. Cold water is used to remove heat from a hot stream, and passes this heat 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 important factors that influence the effectiveness 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 circulating flowrate was decreased or the return temperature increased, the cooling tower effectiveness improved (Figure 1.2). This is convenient, since for a fixed heat load, as the flowrate is decreased the return temperature increases simultaneously. Kim and Smith (2001) confirmed these observations using a mathematical model of a cooling tower.

Using the findings of Bernier (1994), Kim and Smith (2001) showed 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 directly from the cooling tower. Kim and Smith (2001) adapted the graphical wastewater minimisation method by Wang and Smith (1994), gradually increasing the outlet water temperature until a pinch was formed. Kim and Smith (2001) further adapted the water mains method of Kuo and Smith (1998) to design the heat exchanger network that would accomplish this target.

The method of Kim and Smith (2001) was a graphical method that systematically targeted the minimum flowrate of cooling water. The procedure

2 Literature Survey

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 2.10, the cooling water supply line begins at the temperature supplied by the cooling tower, with a gradient inversely proportional to the flowrate. The flowrate is reduced 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.

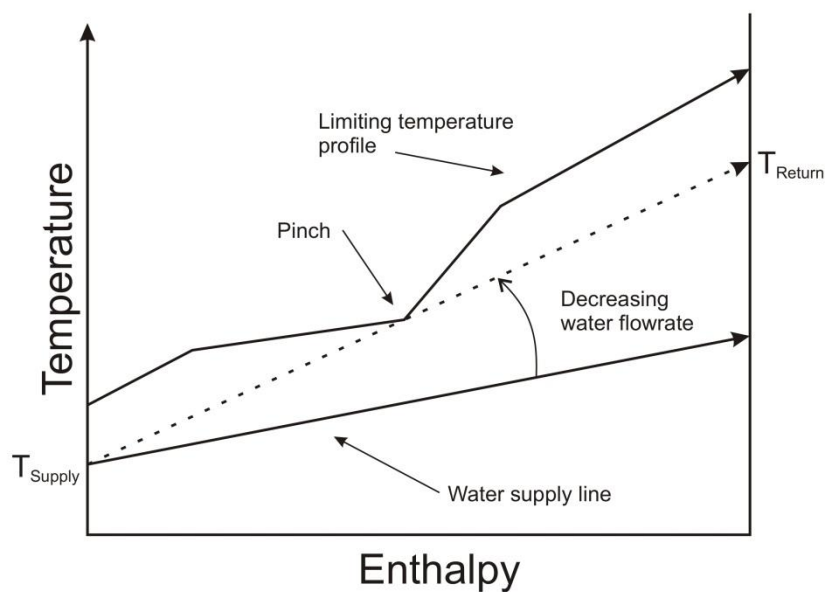


Figure 2.10: Targeting the minimum cooling water flowrate. (Kim & Smith, 2001).

Kim and Smith (2003) converted the graphical method of Kim and Smith (2001) into a mathematical formulation. An MINLP formulation was presented for the automatic synthesis of cooling water systems in retrofit projects. Of special interest in this work was the inclusion of pressure drop correlations. Kim and Smith (2003) used the Critical Path Algorithm, commonly used in project management, to minimise the total pressure drop of the system.

Feng *et al* (2005) developed a model for reusing cooling water using a different superstructure (Figure 2.11). Here, three water mains were established: a

2 Literature Survey

cooling water supply main, an intermediate main, and a return main. A water using operation may be supplied with cooling water from both the supply main and the intermediate main, and may return its cooling water to either the intermediate main or the return main. The advantage to using water mains to indirectly reuse cooling water is that variations in cooling water flowrate due to process disturbances are dampened out. This results in a more controllable system. The drawback is that higher circulating flowrates are required compared to methods with direct reuse.

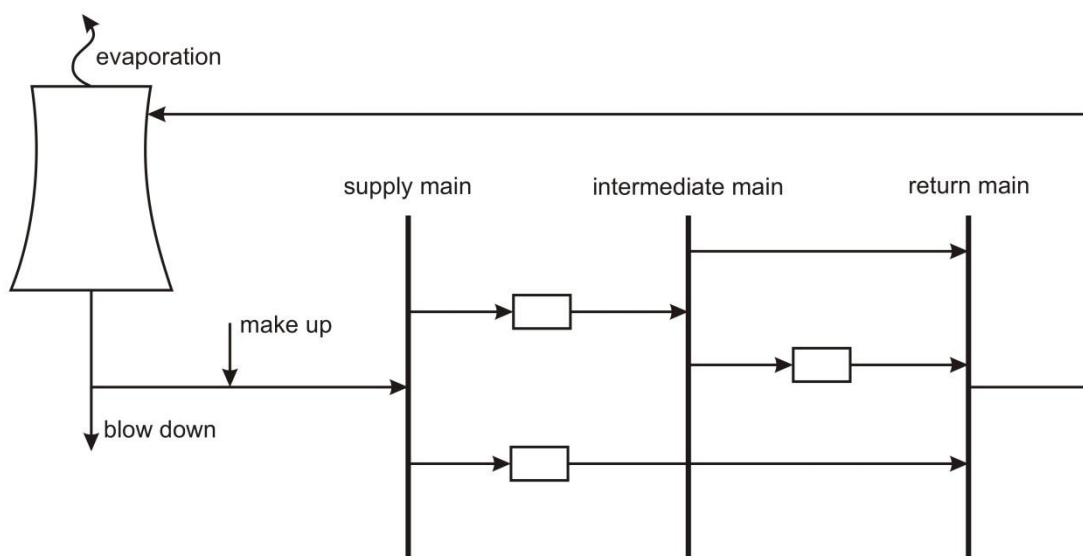


Figure 2.11: Water mains superstructure used by Feng *et al* (2005).

Ponce-Ortega *et al* (2007) extended this concept by dividing the set of hot streams into a set of stages (Figure 2.12). Each stage could be considered as having its own main, supplied by the previous stage. In addition to this, each stage could receive fresh cooling water, and could return water to the cooling tower. The increased number of stages showed improvements, but the stage wise method resulted in a non-convex nonlinear model. Ponce-Ortega *et al* (2010) improved upon this model by including consideration for the cooling tower, using the Merkel equation.

2 Literature Survey

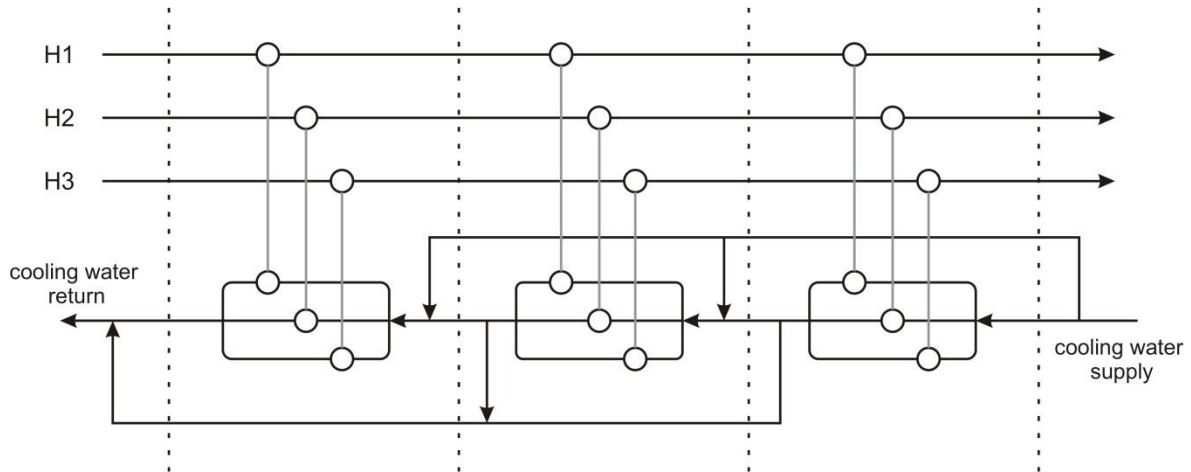


Figure 2.12: Stage wise superstructure used by Ponce-Ortega *et al* (2007).

The above methods assume that there is only one cooling tower supplying the cold utility. This makes it possible to use a graphical procedure. Majozi and Nyathi (2007) developed a method for synthesising cooling water networks supplied by multiple cooling towers. Two cases were considered. In the first case, there were no limitations on either the return temperature or the network topology. In the second case, no limitations were placed on the return temperature of the water, but each water-using process had a specified source and sink.

Majozi and Moodley (2008) expanded upon the method of Majozi and Nyathi (2007) with a rigorous mathematical optimization model. In addition to the two cases considered by Majozi and Nyathi (2007), Majozi and Moodley (2008) consider two additional cases by incorporating return temperature limitations to the original cases. Four models were developed, one for each case. Case 1 resulted in an LP problem, case 2 in an MILP problem, while cases 3 and 4 both resulted in MINLP problems. One of the conditions proven by Savelski and Bagajewicz (2000a) was used to remove some non-linear terms. Further 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.

2 Literature Survey

Panjeshahi and Ataei (2008) expanded the work of Kim and Smith (2001) to include a cooling tower model, as well as ozone treatment of the cooling water. By treating the cooling water with ozone, biological growth was inhibited, lowering the amount of blow down and make up required. Panjeshahi *et al* (2009) expanded upon this by including pinch migration, while Ataei *et al* (2010) accounted for the rain and spray zones in the cooling tower model

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

Gololo and Majozi (2013) expanded upon this by considering the pressure drop within the cooling water network. Where multiple network configurations existed that achieve the same minimum cooling water flowrate, the Critical Path Algorithm was used to select the configuration with the minimum total pressure drop. Gololo and Majozi (2013) also compared the effects of solving the differential equations of the cooling tower model simultaneously within the optimisation platform, with the results obtained when the differential equations were solved iteratively in a second platform. Since more information was

2 Literature Survey

available to the optimisation procedure when all equations were solved within the optimisation platform, it was found that a simultaneous solution procedure resulted in better objective functions.

2.4 Cooling Tower Models

Cooling towers are used to reject waste heat to the atmosphere. Since their operation is intrinsically linked to the prevailing atmospheric conditions, they can quite easily be the most temperamental unit operation on a plant. None the less, a number of models have been created to describe the function of cooling towers and to aid in their design.

One of the earliest models for predicting the temperature of cooling water leaving a cooling tower was proposed by Merkel (1925). Merkel proposed characterising the cooling tower performance using a single number, now referred to as the Merkel number (Equation 2.1). The integral on the right of Equation 2.1 can be seen to be the area between the saturated air curve, and the tower operating line on a plot of air enthalpy versus temperature. For a cooling tower with a known Merkel number, the outlet temperature of the cooling water can be deduced by evaluating the integral graphically.

$$Me = \frac{h_d a_f \cdot L}{G} = \int_{T_{w,in}}^{T_{w,out}} \frac{c_{pw}}{(i_{masw} - i_{ma})} dT_w \quad (2.1)$$

Merkel (1925) made number of simplifying assumptions in deriving his model:

- The Lewis factor for the air-water system was unity (1)
- The air stream leaving the tower is saturated
- The evaporative losses are negligible, implying a constant water flowrate.

The Merkel model is useful for determining the temperature of the cooling water leaving the tower, but provides no other information. Furthermore, with the simplifying assumptions made, there will always be some discrepancy between the predicted temperature and the actual temperature achieved.

2 Literature Survey

Noting that a cooling tower is in fact an exceptionally large heat exchanger between a hot water stream and a cold air stream, Jaber and Webb (1989) developed the effectiveness-NTU (e-NTU) method. The method is based upon the NTU (number of transferred units) method used in heat exchanger design. The e-NTU method made use of the same simplifying assumptions used by Merkel (1925), but did not require the evaluation of an integral function. This reduced the computational difficulties of the model, since a numerical method would otherwise be required to evaluate an integral. Soleymez (2004) extended the effectiveness method to include forced draught cooling towers as well.

In contrast to the effectiveness based methods above, Poppe and Rogener (1991) developed a differential equation based model of a cooling tower. Using a cross sectional slice of the cooling tower with differential height as a control volume, Poppe and Rogener (1991) performed a mass and an enthalpy balance, resulting in two differential equations. Most importantly, rather than using Lewis factor of 1, a correlation given by Bosnjakovic (1965) was used to calculate the actual Lewis factor.

Bernier (1994) studied the performance of a natural draught counter current cooling tower by performing energy balances over a water droplet falling inside the tower. It was found that as much as 90% of the cooling achieved by a cooling tower is due to evaporation, and that changes in the wet bulb temperature of air had a greater effect on performance than the dry bulb temperature. Most importantly, Bernier (1994) found that reducing the circulating water flowrate or raising the return temperature both brought about an improvement in the tower effectiveness. Here, effectiveness was the actual quantity of heat rejected to the atmosphere compared to the theoretical

2 Literature Survey

maximum quantity of heat that can be rejected. This is the same effectiveness that forms part of the e-NTU method (Equation 2.2).

$$\varepsilon = \frac{m_w c_{pw} (T_{w,in} - T_{w,out})}{C_{min} (i_{masw,in} - T_{ma,in})} \quad (2.2)$$

Kim and Smith (2001) confirmed the observations of Bernier (1994) using their own cooling tower model. A cross sectional slice with differential height was used to as the control volume, and it was assumed that the only gradients that existed were one dimensional, varying along the height of the tower. Three differential equations were derived, expressing the changes in humidity, water temperature and air temperature along the height of the tower. Sadly, in this model, the Lewis factor was once again assumed to be unity.

Fisenko, Petrushik and Solodukhin (2002) developed a model for natural draught cooling towers, taking into account the evaporative losses. The model was developed in two sections, a spray region and a film region. The film region model was developed using a water film flowing down vertical surface as the control volume. Four differential equations were derived to describe the change in film thickness due to evaporative losses, water temperature, air temperature, and moist air density. The spray region model was developed using a falling water droplet as the control volume. Five differential equations were derived to describe the change in droplet radius due to evaporative losses, the velocity of the falling droplet, water temperature, air temperature, and the density of moist air.

Kröger (2004) developed a simplified cooling tower model along similar lines to Kim and Smith (2001), with many of the variables lumped together in a heat or mass transfer coefficient. Again a cross sectional slice of the cooling tower

2 Literature Survey

was used as the control volume. Three differential equations were derived to express the changes in humidity, water temperature, and air enthalpy along the height of the tower. Most importantly, Kröger (2004) did not assume the Lewis factor to be unity. The correlation by Bosnjakovic (1965) was built into the model equations to account for changes in the Lewis factor as conditions inside the tower changed. The model did, however, neglect evaporative losses, assuming a constant water flowrate.

Qureshi and Zubair (2006) developed a model similar to Fisenko *et al* (2002). The model encompassed both a spray zone and a fill zone. Qureshi and Zubair (2006), however, compensate for fouling in the cooling tower fill. This is important since evaporation in the tower encourages mineral deposition, and the warm, moist environment is ideal for algae growth.

2.5 Steam System Design

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 saturated steam to furnaces. The most common form of hot utility in use is steam. In practice, steam is raised in a boiler and 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 2.1.2, Papoulias and Grossmann (1983) developed a superstructure that contained a variety of utilities. Included in the superstructure were three levels of steam. The mathematical model selected, amongst other things, whether the steam should be supplied by a boiler, by turbine exhaust or by letting down higher steam levels.

Marechal and Kalitventzeff (1998) discussed 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 were used as a means to transport energy from one process on the site to another. As such, the levels of the utility had to 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) considered the interactions between the various levels of steam and the turbines used to provide mechanical power. Models were 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 was also developed, which was subsequently used by Shang and Kokossis (2004).

2 Literature Survey

Shang and Kokossis (2004) developed an MILP formulation to optimise the steam levels of a total site utility for multiperiod operation, using a transshipment model as the basis of the formulation. Constraints were added to this 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) was used, and a new boiler hardware model (BHM) was developed. Abdallah & Ismail (2001) further explained how proper consideration for the efficiency of a boiler and the correct insulation was 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), developed a method of minimising the flowrate of steam through the HEN by utilising hot liquid condensate and reuse streams. The motivation for this came from the observation that the cost of a boiler increased rapidly with required flowrate. Coetzee and Majozi (2008) developed both a graphical method and a mathematical model for targeting the minimum steam flowrate for single level problems. In the case of the graphical method, a separate LP model was used to synthesize the HEN after the minimum steam flowrate had been targeted. In the second MILP model, the targeting and synthesis were performed simultaneously.

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

2 Literature Survey

Price and Majozi (2010a) included the boiler efficiency model developed by Shang and Kokossis (2004) in their formulation to minimise the loss in boiler efficiency. Two possibilities were considered to maintain return temperature: using sensible heat from the superheated steam (Figure 2.13a), or using a dedicated preheater (Figure 2.13b). In both cases, the model allowed 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.

Price and Majozi (2010b) included the possibility of multiple steam levels in the above model. An adapted version of the superstructure developed by Coetzee and Majozi (2008) was used to minimise the total flowrate of steam across the multiple levels while maintaining boiler efficiency. Here, the lower steam levels were the result of steam turbine exhausts, each having a fixed flowrate and saturation temperature.

2 Literature Survey

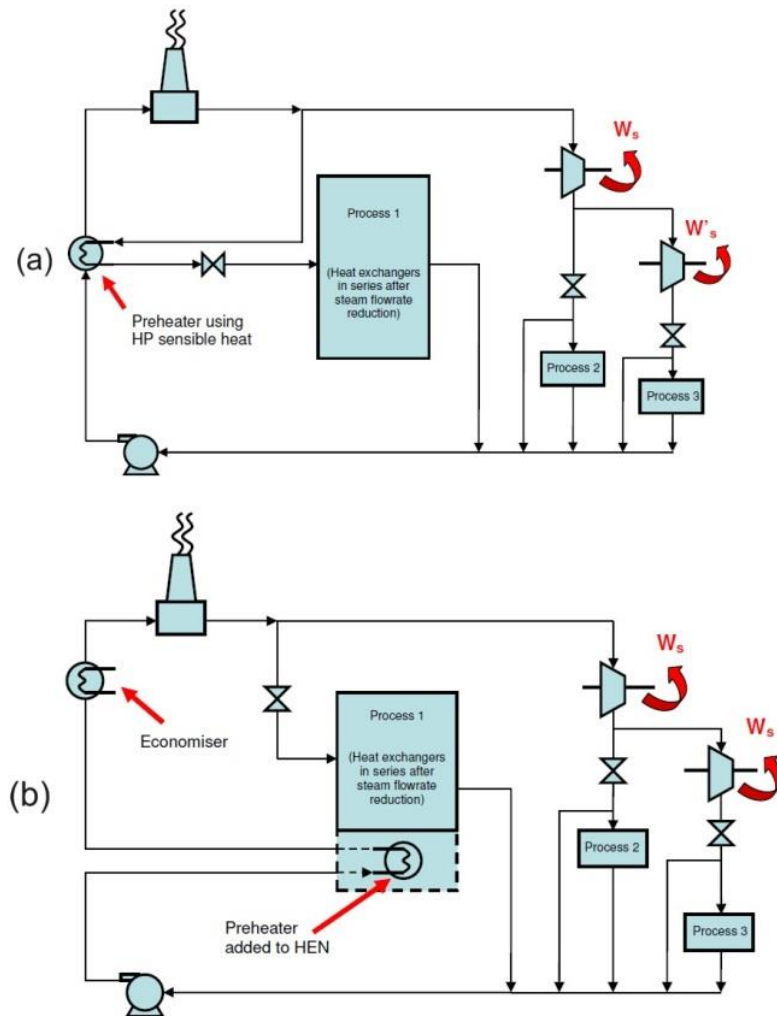


Figure 2.13: Two methods of preserving boiler efficiency: (a) using sensible heat (b) using a dedicated preheater. (Price & Majozi, 2010a)

Coetzee and Majozi (2008) noted that in some instances, multiple network configurations exist that are capable of attaining the same minimum flowrate. Price and Majozi (2010c) therefore used 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 used pressure drop correlations developed by Nie (1998), Nie and Zhu (1999) and Zhu and Nie (2002)

Chen and Lin (2012) developed a model for designing entire energy systems for chemical plants. The model considers multiple steam levels with turbines

2 Literature Survey

between them. Steam can be raised in a boiler, or can be raised in a heat recovery steam generator. Chen and Lin (2012) do not, however, consider the reuse of hot liquid condensate.

Price and Majozi (2010b) assumed that the operation of the steam turbines within the power block was already fixed before optimising the multiple steam level HEN. Realising that different configurations of flowrate and pressure drop within a steam turbine can produce the same quantity of shaft work, Beangstrom (2013) developed an MINLP model that simultaneously optimised the HEN and power block. Here, the flowrate and saturation temperature of the lower steam levels were treated as variables that had to be determined by the model. Beangstrom (2013) further showed that when hot liquid reuse was employed as a strategy for reducing steam flowrate, it was best to utilise only two steam levels with a single steam turbine between them providing shaft work.

2.6 Relaxation techniques.

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.

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 escape 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 guess is to solve a relaxed form of the original problem. If the original problem can be relaxed, 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) introduced a novel method of removing non-linearities occurring due to the product of a binary variable and a continuous variable. Here, x is a continuous variable and y a binary variable, both defined as

$$x \in \mathbb{R}, y \in [0,1] \quad (2.3)$$

2 Literature Survey

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

$$xy \equiv \Gamma \quad (2.4)$$

It is seen that Γ assumes a value of 0 when y is 0, and a value of x when y is equal to 1. Furthermore, if x has upper and lower bounds

$$X^L \leq x \leq X^U \quad (2.5)$$

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

$$X^L \cdot y \leq \Gamma \leq X^U \cdot y \quad (2.6)$$

$$x - X^U(1 - y) \leq \Gamma \leq x + X^L(1 - y) \quad (2.7)$$

It can be seen that Equations 2.6 and 2.7 are linear in terms of x and y . Using Equation 2.4 to remove non-linear terms and adding Equations 2.6 and 2.7 to the existing constraints is an effective method of removing non-linear terms 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, based on the work of McCormick (1979). A bilinear term arises from the product of two continuous variables, defined as

$$x \in \mathbb{R}, \quad y \in \mathbb{R} \quad (2.8)$$

2 Literature Survey

Again the following substitution is made, bearing in mind that now two continuous variables are being dealt with:

$$xy \equiv \Gamma \quad (2.9)$$

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

$$X^L \leq x \leq X^U \quad (2.10)$$

$$Y^L \leq y \leq Y^U \quad (2.11)$$

then the following constraints arise

$$x - X^L \geq 0 \text{ and } X^U - x \geq 0 \quad (2.12)$$

$$y - Y^L \geq 0 \text{ and } Y^U - y \geq 0 \quad (2.13)$$

Taking the product of the first constraint in both Equations 2.12 and 2.13 one gets

$$X^U Y^U - x Y^U - X^U y + xy \geq 0 \quad (2.14)$$

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

$$\Gamma \geq x Y^U + X^U y - X^U Y^U \quad (2.15)$$

A further three constraints can be derived in a similar fashion using different combinations of Equations 2.12 and 2.13. These are given below.

$$\Gamma \leq x Y^U + X^L y - X^L Y^U \quad (2.16)$$

$$\Gamma \leq x Y^L + X^U y - X^U Y^L \quad (2.17)$$

2 Literature Survey

$$\Gamma \geq xY^L + X^L y - X^L Y^L \quad (2.18)$$

The bilinear term can thus be removed by substituting the term xy for Γ , and adding the above 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. The result of the linearized problem is then used as the initial starting point for the rigorous non-linear problem. Quesada and Grossmann (1995) showed that if the solutions to both the linear and non-linear models match exactly, the solution is globally optimal. If the solutions do not match, no guarantee is made that the local optimum found is also globally optimal.

2.7 References

- Abdallah AM & Ismail AL (2001). Saving energy lost from steam boiler vessels. *Renewable Energy*, 23, 537–550.
- Ahmad S & Polley GT (1990). Debottlenecking of heat exchanger networks. *Heat Recovery Systems & CHP*, 10(4), 369-385.
- Androulakis IP & Venkatasubramanian V (1991). A genetic algorithmic framework for process design and optimisation. *Comp. Chem. Eng.*, 15, 217-228.
- Ataei A, Gharaie M, Parand R & Panjeshahi MH (2010). Application of ozone treatment and pinch technology in cooling water system design for water and energy conservation. *Int. J. of Energy Res.*, 34, 494-506.
- Bernier MA (1994). Cooling tower performance: Theory and experiments. *ASHRAE Trans. Res.*, 100, 114-121.
- Bosnjakovic F (1965). *Technical thermodynamics*, translated by Blackshear PI, 1-80, Holt, Reinhart and Wilson, New York.
- Cerda J, Westerberg AW, 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 AW, Mason D & Linnhoff B (1983). Minimum utility usage in heat exchanger network synthesis: a transportation problem. *Chem. Eng. Sci.*, 38(3), 373-387.
- Chen CL & Lin CY (2012). Design of entire energy systems for chemical plants. *Ind. Eng. Chem. Res.*, 51, 9980-9996.

2 Literature Survey

- Coetzee WAS & Majozi T (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Doyle SJ & Smith R (1997). Targeting water reuse with multiple contaminants. *Trans IChemE*, 78(B3), 181-189.
- El-Hawagi MM & Manousiouthakis V (1990). Automatic synthesis of mass-exchange networks with single-component targets. *Chem. Eng. Sci.*, 45(9), 2813-2831.
- Feng X, Shen R & Wang B (2005). Recirculation cooling-water network with an intermediate cooling-water main. *Energy & Fuel*, 19, 1723-1728.
- Fisenko SP, Petrushik AI & Solodukhin AD (2002). Evaporative cooling of water in a natural draft cooling tower. *Int. J. of Heat & Mass Trans.*, 45, 4683-4694.
- Floudas CA & Grossmann IE (1986). Synthesis of flexible heat exchanger networks for multiperiod operation. *Comp. Chem. Eng*, 10(2), 153-168.
- Glover F (1975). Improved linear integer programming formulations of nonlinear integer problems. *Management Science*, 22(4), 455-460.
- Gololo KV & Majozi T (2011). On synthesis and optimization of cooling water systems with multiple cooling towers. *Ind. Eng. Chem. Res.*, 50, 3775-3787.
- Gololo KV & Majozi T (2013). Complex cooling water systems optimisation with pressure drop considerations. *Ind. Eng. Chem. Res.*, 52, 7056-7065.
- Grimes LE (1980). The synthesis and evaluation of networks of heat exchangers that feature the minimum number of units. MSc Thesis: Carnegie-Mellon University.

2 Literature Survey

- Grossmann IE & 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 JK & Smith R (2005). Automated design of total water systems. *Ind. Eng. Chem. Res.*, 44, 588-599.
- Hohmann EC (1971). Optimum networks for heat exchange. PhD Thesis: University of Southern California.
- Huang F & Elshout RV (1976). Optimizing the heat recovery of crude units. *Chem. Eng. Progr.*, 72, 68-74.
- Hui CW & Ahmad S (1994). Total site heat integration using the utility system. *Comp. Chem. Eng.*, 18(8), 729-742.
- Isafiade AJ & Fraser DM (2008). Interval-based MINLP superstructure synthesis of heat exchange networks. *Chem. Eng. Res. & Design*, 86, 245-257.
- Jaber H & Webb RL (1989). Design of cooling towers by the effectiveness-NTU method. *J. of Heat Transfer*, 111, 837-843.
- Kemp IC (2007). Pinch Analysis and Process Integration: a User Guide on Process Integration for the Efficient Use of Energy. Great Britain: Butterworth-Heinemann.
- Kim JK & Smith R (2001). Cooling water system design. *Chem. Eng. Sci.*, 56, 3641-3658.
- Kim JK & Smith R (2003). Automated retrofit Design of cooling-water systems. *AIChE J.*, 49(7), 1712-1730.

2 Literature Survey

- Kröger DG (2004). *Air-cooled heat exchangers and cooling towers*, Penn Well Corporation, USA.
- Kuo WC & Smith R (1998a). Designing for the interactions between water-use and effluent treatment. *Trans IChemE*, 76(Part A), 287-301.
- Kuo WC & Smith R (1998b). Design of water-using systems involving regeneration. *Trans IChemE*, 76(Part B), 94-114.
- Lewin DR (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 DR, 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 & Flower JR (1978a). Synthesis of heat exchanger networks: I. systematic generation of energy optimal networks. *AICHE J.*, 24(4), 633-642.
- Linnhoff B & Flower JR. (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 DR & Wardle I (1979). Understanding heat exchanger networks. *Comp. & Chem. Eng.*, 3, 295-302.

2 Literature Survey

- 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 & Moodley A (2008). Simultaneous targeting and design for cooling water systems with multiple cooling water supplies. *Comp. Chem. Eng.*, 32, 540-551.
- Majozi T & Nyathi N (2007). On cooling-water systems design for South African industry: two recent developments. *S. African J. of Sci.*, 103, 239-244.
- Marechal F & Kalitventzeff B (1998). Energy integration of industrial sites: tools, methodology and application. *App. Therm. Eng.*, 18, 921-933.
- Mavromatis SP & Kokossis AC (1998a). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Mavromatis SP & Kokossis AC (1998b). Conceptual optimisation of utility networks for operational variations -II. Network development and optimisation. *Chem. Eng. Sci.*, 53(8), 1609-1630.
- McCormick GP (1979). Computability of global solutions to factorable non-convex programs: Part I – Convex underestimating problems. *Math. Programming*, 10, 147-175.
- Merkel F (1925). Verdunstungskühlung. *VDI-Zeitschrift*, 70, 123-128.
- Musso AH & Rudd DF (1969). The synthesis of system designs: II Heuristic Structuring. *AIChE J.*, 15, 10-17.

2 Literature Survey

- Nie X (1998). Heat exchanger network retrofit considering pressure drop and heat transfer enhancement. PhD Thesis: UMIST, Manchester.
- Nie X & Zhu XX (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 SG & Polley GT (1997). A simple methodology for the design of water networks handling single contaminants. *Trans. IChemE*, 75(Part A), 420-426.
- Panjeshahi MH & Ataei A (2008). Application of an environmentally optimum cooling water system design in water and energy conservation. *Int. J. of Env. Sci and Tech.*, 5(2), 251-262.
- Panjeshahi MH, Ataei A, Gharaie M & Parand R (2009). Optimum design of cooling water systems for energy and water conservation. *Chem. Eng. Res. & Design*, 87, 200-209.
- Papalexandri KP & Pistikopoulos EN (1994a). Synthesis and retrofit of operable heat exchanger networks.1. Flexibility and structural controllability aspects. *Ind. Eng. Chem. Res.*, 33, 1718-1737.
- Papalexandri KP & Pistikopoulos EN (1994b). Synthesis and retrofit of operable heat exchanger networks.2. Dynamics and control structure considerations. *Ind. Eng. Chem. Res.*, 33, 1738-1755.
- Papoulias SA & Grossmann IE (1983a). A structural optimization approach in process synthesis - I Utility systems. *Comp. Chem. Eng.*, 7(6), 695-706.

2 Literature Survey

Papoulias SA & Grossmann IE (1983b). A structural optimization approach in process synthesis - II Heat recovery networks. *Comp. Chem. Eng.*, 7(6), 707-721.

Papoulias SA & Grossmann IE (1983c). A structural optimization approach in process synthesis - III Total processing systems. *Comp. Chem. Eng.*, 7(6), 723-734.

Pintaric ZN & Kravanja Z (2004). A strategy for MINLP synthesis of flexible and operable processes. *Comp. Chem. Eng.*, 28, 1105-1119.

Ponce-Ortega JM, Serna-González M & Jiménez-Gutiérrez A (2007). MINLP synthesis of optimal cooling networks. *Chem. Eng. Sci.*, 62, 5728-2735.

Ponce-Ortega JM, Serna-González M & Jiménez-Gutiérrez A (2010). Optimization model for re-circulating cooling water systems. *Comp. Chem. Eng.*, 34, 177-195.

Poppe M & Rogener H (1991). Berechnung von Ruckkuhlwerken. *VDI-armeatlas*, 1-15.

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.

2 Literature Survey

- Quesada I & Grossmann IE (1995). Global optimisation of bilinear process networks with multi component flows. *Comp. Chem. Eng.*, 19(12), 1219-1242.
- Qureshi BA & Zubair SM (2006). A complete model of wet cooling towers with fouling fills. *Applied Thermal Engineering*, 26, 1982-1989.
- Rao SS (2009). *Engineering Optimization: Theory and Practice*. Hoboken: John Wiley & Sons.
- Rudd DF (1968). The synthesis of system designs: I. Elementary decomposition theory. *AIChE J.*, 14, 343-349.
- Savelski MJ & Bagajewicz MJ (2000a). On the optimality conditions of water utilization systems in process plants with single contaminants. *Chem. Eng. Sci.*, 55, 5035-5048.
- Savelski MJ & Bagajewicz MJ (2000b). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.
- Savelski MJ & Bagajewicz MJ (2001a). Algorithmic procedure to design single component water utilization systems in process plants. *Chem. Eng. Sci.*, 56(5), 1897-1912.
- Savelski MJ & Bagajewicz MJ (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 MJ & Bagajewicz MJ (2003). On the optimality conditions of water utilization systems in process plants with multiple contaminants. *Chem. Eng. Sci.*, 58, 5349-5362.

2 Literature Survey

- Savulescu L, Kim JK & 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 JK & 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 WD, Seader JD & Lewin DR (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 JJ, Powers GJ & Rudd DF (1971). The synthesis of system designs: III Toward a process concept generator. *AIChE J.*, 17, 677-682.
- Soleymez MS (2004). On the optimum performance of forced draft counter flow cooling towers. *Energy Conversion and Management*, 45, 2335-2341.
- Srinivas BK & El-Halwagi MM (1994). Synthesis of combined heat and reactive mass-exchange networks. *Chem. Eng. Sci.*, 49, 2059-2074.
- Townsend DW & 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 DW & Linnhoff B (1983b). Heat and power networks in process design. II. Design procedure for equipment selection and process matching. *AIChE J.*, 29, 748-771.

2 Literature Survey

- 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.
- Wang YP & Smith R (1994). Wastewater minimisation. *Chem. Eng. Sci.*, 49(7), 981-1006.
- Yee TF, Grossmann IE & Kravanja Z (1990a). Simultaneous optimization models for heat integration - I. Area and energy targeting and modelling of multi-stream exchangers. *Comp. Chem. Eng.*, 14(10), 1151-1164.
- Yee TF & Grossmann IE (1990b). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comp. Chem. Eng.*, 14(10), 1165-1184.
- Yee TF, Grossmann IE & Kravanja Z (1990c). Simultaneous optimization models for heat integration - III. Process and heat exchanger network optimization. *Comp. Chem. Eng.*, 14(11), 1185-1200.
- Zhu XX (1997). Automated design method for heat exchanger network using block decomposition and heuristic rules. *Comp. Chem. Eng.*, 21(10), 1095-1104.
- Zhu XX & Nie X (2002). Pressure drop considerations for heat exchanger network grassroots design. *Comp. Chem. Eng.*, 26, 1661-1676.
- Zhu XX, O'Neill BK, Roach JR & Wood RM (1995a). A new method for heat exchanger network synthesis using targeting procedures. *Comp. Chem. Eng.*, 19(2), 197-222.
- Zhu XX, O'Neill BK, Roach JR & Wood RM (1995b). Area-targeting methods for the direct synthesis of heat exchanger networks with unequal film coefficients. *Comp. Chem. Eng.*, 19(2), 223-239.

2 Literature Survey

Zhu XX, O'Neill BK, Roach JR & Wood RM (1995c). A method for automated heat exchanger network synthesis using block decomposition and non-linear optimization. *Trans. IChemE*, 73(A), 919-930.

Chapter 3

Literature Survey II – Specific Technical Details

In the previous chapter, a brief survey of the available literature was presented. The purpose of this chapter is to provide specific background information on topics that will be useful 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.

Introduced first will be the three fields of heat integration: process-process heat integration, steam system design, and cooling water system design. In each section, the recent models that are to be built upon in the chapters to come will be discussed. Following that, descriptions of other relevant systems and mathematical techniques will be discussed.

3.1 Process-Process Heat Integration

Many mathematical models have been developed for process-process heat integration, owing largely to the fact that it is the oldest and most studied branches of heat integration. The majority of these methods share similarities with other methods, particularly when both methods are based on a common predecessor. Each method, however, will have its own unique set of advantages and shortcomings.

In this section, three of the leading methods for synthesising process-process heat exchanger networks will be discussed. These methods provide the foundation for this work, and the methods to come. For the sake of consistency, all variables will be written using the notation for this work, rather than the different notational styles used in each of the original works.

3.1.1 Problem Statement

The general problem that is addressed by the process-process heat integration methods to be discussed can be stated broadly as:

Given:

- A set of cold streams that require heating,
- A set of hot streams that require cooling,
- The supply and target temperatures of each stream,
- The heat capacity flowrate of each stream,
- The minimum temperature difference for heat transfer.

Determine:

- The minimum hot and cold utilities required,
- The location of the pinch,

3 Technical Background

- The heat exchanger network configuration that will achieve the minimum energy requirements.

3.1.2 Superstructure

The superstructure used by the methods to be discussed is quite common amongst heat integration models. This superstructure was first presented by Grossmann and Sargent (1978), and remains popular in models considering process-process interactions. Consider a set of H hot streams that require cooling, and a set of C cold streams that require heating. Figure 3.1a shows the superstructure as originally developed, and as used in some of the early works, wherein each hot stream in H and each cold stream C is present. Figure 3.1b shows an alternative view of the same superstructure using a simpler format, where vertical lines have been used to represent matches between hot and cold streams. Within this work, the latter format will be used, as it leads to more readable designs, especially when the problems at hand become large.

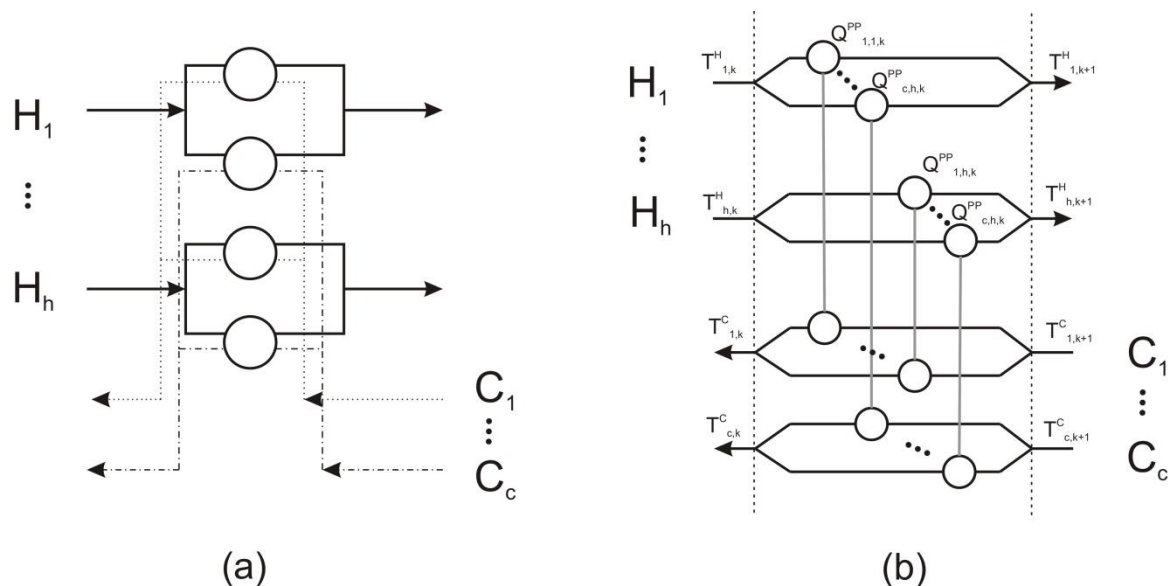


Figure 3.1: Process-process heat integration superstructure. a) Original format b) simplified format.

3 Technical Background

In the superstructure presented in Figure 3.1, provision is made for each hot stream to have the opportunity to exchange heat with each cold stream. In order to make this possible, each hot stream is hypothetically split into as many parallel streams as there are cold streams, and vice versa. This does not imply that all of these parallel streams and heat exchangers will be present in the final design, since the model will eliminate any unnecessary features.

In order to make series connections possible, the superstructure has to be repeated several times in succession, once in each stage or block. These repetitions create a set of K stages. By convention, stages are numbered in order of decreasing temperature. When considering the two temperatures of a stream at the boundaries of a stage, the hotter of the two receives the stage number, while the cooler will receive the number of the following stage.

There are various ways to define the stages over which the superstructure in Figure 3.1 will be repeated. Yee and Grossmann (1990) propose the heuristic in which the number of hot streams and the number of cold streams are considered, setting the number of stages to be used equal to the larger of the two. Zhu *et al* (1995) propose using the hot and cold composite curves to aid in creating several blocks placed in logical positions. Isafiade and Fraser (2008) define intervals based on the supply and target temperatures of one of the sets of streams.

3.1.3 The Method of Yee and Grossmann (1990)

The method of Yee and Grossmann (1990) involves repeating the superstructure in Figure 3.1 over several stages, with hot and cold utilities placed at the extremities of the respective streams. The number of stages to be used must be chosen by the designer before further work is done. Yee and Grossmann suggest

3 Technical Background

a heuristic where the number of stages to be used should be equal to the number of hot or cold streams in the problem, whichever is the larger of the two.

Each stream, whether hot or cold, is divided across all of the stages. The temperature of each stream as it crosses from one stage to the next is a variable unique to each stream, and as such the concept of a stage has no physical meaning. Here the stages are no more than an ordered set of subdivisions of the various streams. The advantage of this is that the model can control in which stage a stream exists, and consequently where heat is exchanged. Figure 3.2 illustrates this concept for a few cases.

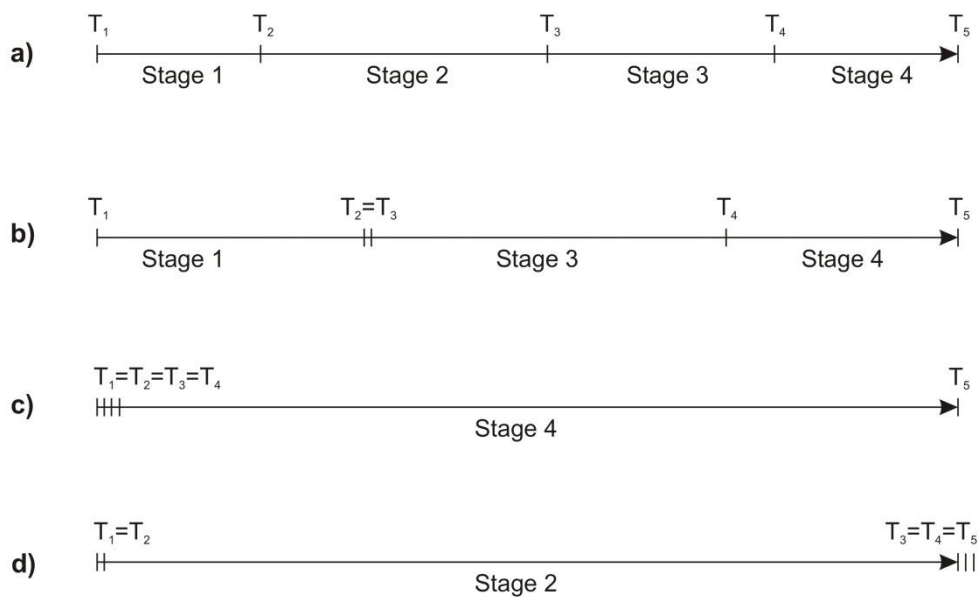


Figure 3.2 Demonstration of how variable temperatures can be used to alter which stages a stream exists in (a) stream exists in all four stages (b) stream exists in stages 1,3 and 4 only (c) stream exists in stage 4 only (d) stream exists in stage 2 only.

In Figure 3.2a, a stream has been divided into four stages. By manipulating the temperatures as the stream transitions from one stage to the next, one can arrive at the case shown in Figure 3.2b. Here, the stream does not participate in Stage 2, and consequently, since no heat is transferred in that stage, the temperature of the stream at both boundaries is identical. This does not, however, mean that

3 Technical Background

Stage 2 has disappeared; other streams may be exchanging heat in Stage 2. In a similar fashion, by manipulating the transition temperatures for a stream, the stream may be made to transfer all of its heat within a single stage, as in Figure 3.2c & d.

The ability for the model to shift streams between stages is a powerful technique. It allows the model to compare many potential designs that would have been precluded if streams were limited to stages that had physical meaning. This does, however, come at the cost of many additional variables, additional constraints to control temperature feasibility, and nonlinearities in constraints.

The superstructure on which the model by Yee and Grossmann (1990) is based (Figure 3.3), is made by repeating the superstructure in Figure 3.1 several times, once for each stage. Each hot and cold stream exists in every stage. Hot and cold utilities are placed at the extremities of the streams to ensure that target temperatures are met.

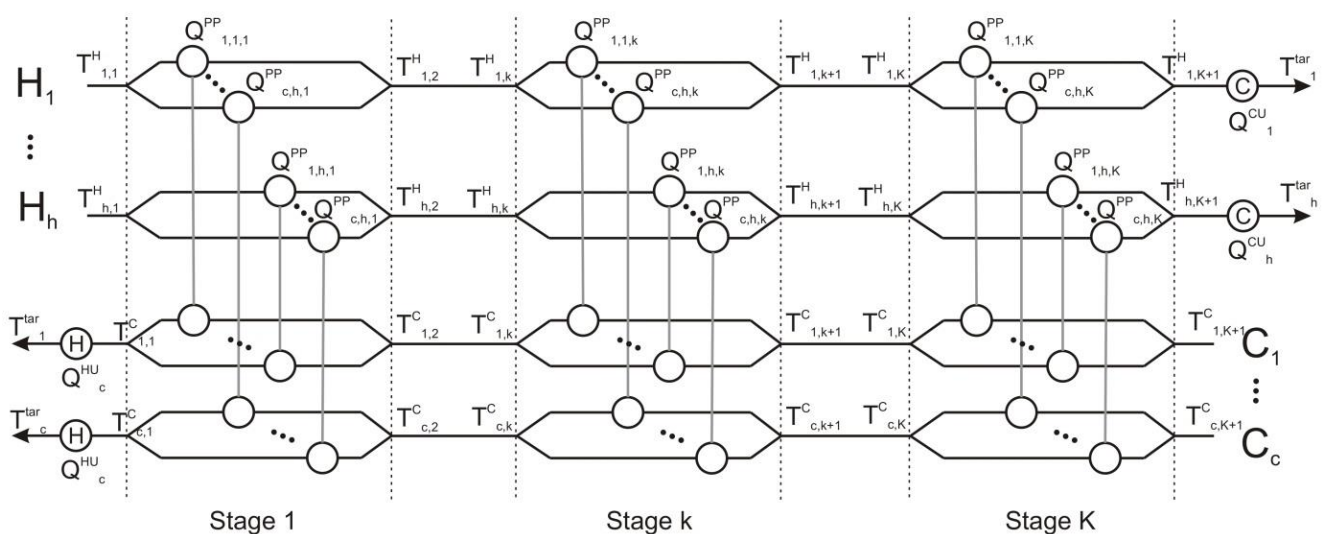


Figure 3.3: Superstructure for the method of Yee and Grossmann (1990)

3 Technical Background

The model is comprised of a number of mass and energy balances performed over the stages as well as the individual streams and utilities. Equations 3.1 and 3.2 represent total heat balances over each stream. Equation 3.1 states that the total quantity of heat that must be removed from a hot stream, cooling the stream down from its supply temperature to its target temperature, is equal to the sum of the heat transferred to all cold streams across all stages, plus the heat removed by a cold utility. Likewise, Equation 3.2 states that the total quantity of heat that must be supplied to a cold stream is equal to the sum of all the heat received from all the hot streams across all the stages, plus the heat received from a hot utility.

$$(T_h^{sup} - T_h^{tar}) \cdot CP_h = \sum_{c,k} Q_{c,h,k}^{PP} + Q_h^{CU} \quad \forall h \in H \quad (3.1)$$

$$(T_c^{tar} - T_c^{sup}) \cdot CP_c = \sum_{h,k} Q_{c,h,k}^{PP} + Q_c^{HU} \quad \forall c \in C \quad (3.2)$$

Equations 3.3 and 3.4 represent heat balances for each stream within a single stage. Equation 3.3 states that the total quantity of energy removed from a particular hot stream in a particular stage is equal to the sum of the heat transferred to all of the cold streams within that stage. Likewise, Equation 3.4 states that the total quantity of heat supplied to a particular cold stream in a particular stage is equal to the sum of heat received from all of the hot streams within that stage.

$$(T_{h,k}^H - T_{h,k+1}^H) \cdot CP_h = \sum_c Q_{c,h,k}^{PP} \quad \forall h, k \in H, K \quad (3.3)$$

3 Technical Background

$$(T_{c,k}^C - T_{c,k+1}^C) \cdot CP_c = \sum_h Q_{c,h,k}^{PP} \quad \forall c, k \in C, K \quad (3.4)$$

Similar to the energy balances performed over the individual stages, energy balances must also be performed over the individual utilities. Equations 3.5 and 3.6 show how the quantity of heat removed from or supplied to a particular stream, is equal to the amount of heat required to cool or heat the stream from the temperature of the last stage it was in (Stage K for hot streams and Stage 1 for cold streams), to the target temperature of that stream.

$$(T_{h,K}^H - T_h^{tar}) \cdot CP_h = Q_h^{CU} \quad \forall h \in H \quad (3.5)$$

$$(T_c^{tar} - T_{c,1}^C) \cdot CP_c = Q_c^{HU} \quad \forall c \in C \quad (3.6)$$

While Equations 3.5 and 3.6 handle the target temperatures of each stream, Equations 3.7 and 3.8 ensure that the stage temperature for each stream in the first stage it encounters (Stage 1 for hot streams and Stage K for cold streams) is equal to the supply temperature of the stream.

$$T_{h,1}^H = T_h^{sup} \quad \forall h \in H \quad (3.7)$$

$$T_{c,k+1}^C = T_c^{sup} \quad \forall c \in C \quad (3.8)$$

As mentioned above, the temperatures of the streams as they transition from one stage to the next are variables. In order to ensure that the temperatures are monotonically decreasing as the stage numbers increase, Equations 3.9 to 3.12 must be imposed.

3 Technical Background

$$T_{h,k}^H \geq T_{h,k+1}^H \quad \forall h, k \in H, K \quad (3.9)$$

$$T_{c,k}^C \geq T_{c,k+1}^C \quad \forall c, k \in C, K \quad (3.10)$$

$$T_h^{tar} \leq T_{h,K+1}^H \quad \forall h \in H \quad (3.11)$$

$$T_c^{tar} \geq T_{c,1}^C \quad \forall c \in C \quad (3.12)$$

Having performed a number of energy balances, logical constraints must be added to control which heat exchangers exist, and that there is sufficient temperature difference for heat transfer. To make this possible, binary variables are introduced to represent the existence of matches between hot and cold streams, as well as matches with one of the utilities. Yee and Grossmann (1990) also introduce a large number, Ω , which is meant to represent the largest anticipated quantity of heat transferred in the system. In Equation 3.13, if the binary variable denoting whether heat is transferred between hot stream h and cold stream c in stage k takes on a value of 0, then the variable representing quantity of heat transferred between h and c is forced to take on a value of 0. If the binary variable has a value of 1, then the variable representing the quantity of heat transferred between h and c is free to take on any value below the upper bound Ω . Equations 3.14 and 3.15 control the existence of matches between hot and cold utilities in a similar fashion.

$$Q_{c,h,k}^{PP} \leq \Omega \cdot x_{c,h,k}^{PP} \quad \forall c, h, k \in C, H, K \quad (3.13)$$

$$Q_h^{CU} \leq \Omega \cdot x_h^{CU} \quad \forall h \in H \quad (3.14)$$

$$Q_c^{HU} \leq \Omega \cdot x_c^{HU} \quad \forall c \in C \quad (3.15)$$

3 Technical Background

To ensure that there is always sufficient temperature difference for heat transfer when matches exist, a second large number, Γ , must be introduced. Equations 3.16 and 3.17 are used to ensure that if a match exists between stream h and stream c in stage k , then the temperature difference between the two streams at both sides of stage k is greater than ΔT_{min} . When the binary variable takes on a value of 1, the large number Γ falls away and the two temperature differences are forced to take on values greater than ΔT_{min} . If the binary variable takes on a value of 0, the temperature differences at both ends of the stage are not constrained to meet ΔT_{min} requirements. Equations 3.18 and 3.19 perform that same function, ensuring there is sufficient temperature difference between the streams and the utilities.

$$T_{h,k}^H - T_{c,k}^C \geq \Delta T_{min} - \Gamma(1 - x_{c,h,k}^{PP}) \quad \forall c, h, k \in C, H, K \quad (3.16)$$

$$T_{h,k+1}^H - T_{c,k+1}^C \geq \Delta T_{min} - \Gamma(1 - x_{c,h,k}^{PP}) \quad \forall c, h, k \in C, H, K \quad (3.17)$$

$$T^{HU} - T_c^{tar} \geq \Delta T_{min} - \Gamma(1 - x_c^{HU}) \quad \forall c \in C \quad (3.18)$$

$$T_h^{tar} - T^{CU} \geq \Delta T_{min} - \Gamma(1 - x_h^{CU}) \quad \forall h \in H \quad (3.19)$$

The heat exchanger area required for each match can be calculated using Equation 3.20, where U is a general heat transfer coefficient, and ΔT^{lm} is the logarithmic mean temperature difference. Yee and Grossmann (1990) recommend using the Chen equation (Chen, 1987) to approximate the logarithmic mean temperature difference (Equation 3.21). This is necessary to avoid the singularity caused by the logarithm when the temperature differences on both sides of the stage are identical.

3 Technical Background

$$Q_{c,h,k}^{PP} = UA_{c,h,k} \Delta T_{c,h,k}^{lm} \quad \forall c, h, k \in C, H, K \quad (3.20)$$

$$\Delta T_{c,h,k}^{lm} = \left[0.5(T_{h,k}^H - T_{c,k}^C)(T_{h,k+1}^H - T_{c,k+1}^C)(T_{h,k}^H + T_{h,k+1}^H - T_{c,k}^C - T_{c,k+1}^C) \right]^{1/3} \quad (3.21)$$

A number of objective functions can be used with this model. One can design for minimum utilities by summing the heat transfer to the hot and cold utilities or one can design for minimum heat exchange area, by summing the areas of the individual heat exchangers. Yee and Grossmann (1990) combine these objectives by assigning cost indices and minimising for total annualised cost (Equation 3.22).

$$\begin{aligned} \min & \left(\sum_c C^{HU} Q_c^{HU} + \sum_h C^{CU} Q_h^{CU} + \sum_c (C^F x_c^{HU} + C^A A_{c,HU}) \right. \\ & \left. + \sum_{c,h,k} (C^F x_{c,h,k}^{PP} + C^A A_{c,h,k}) + \sum_h (C^F x_h^{CU} + C^A A_{h,CU}) \right) \quad (3.22) \end{aligned}$$

The above equations represent a MINLP model. As such, it is important to have a good starting point from which the nonlinear solver can start. It is also important to remember that since the stream temperatures between stages were variables, the pinch will be located where all the temperature differences are equal to ΔT_{\min} .

3 Technical Background

3.1.4 The Method of Zhu *et al* (1995)

One of the major drawbacks of the method of Yee and Grossmann (1990) is that, like all other non-linear optimization problems, it requires a feasible starting point if it is to be solved using conventional nonlinear solvers. This is not an easy task, and adds significant difficulties to using the method of Yee and Grossmann (1990). Zhu *et al* (1995) note that since the concept of a stage has no physical meaning. The initialisation procedure supplied by Yee and Grossmann (1990) does not correspond to real life networks and the initial solution obtained might not be good.

For this reason, Zhu *et al* (1995) developed a method of decomposing the problem into a number of linear sub-problems which can be solved easily. The solutions to these sub problems are then used as the starting point for a more rigorous non-linear problem. In this decomposition method, the hot and cold composite curves are used to aid in dividing the problem into a number of small blocks.

In Figure 3.4, after the hot and cold composite curves have been shifted together, the pinch identified, and the hot and cold utilities placed, the remaining region of process-process heat integration is divided into a number of blocks. No heuristic is given regarding how many blocks should be created. It is expected that one will use the shape of the composite curves to suggest the ideal number and placement of the blocks.

3 Technical Background

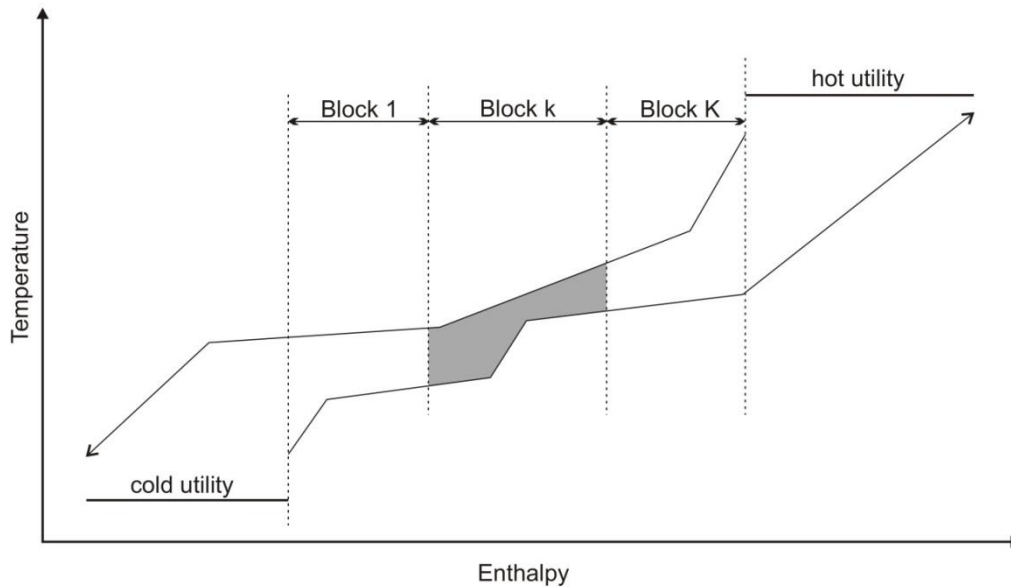


Figure 3.4: Example of a block interval on the composite curves.

After establishing the blocks, each block becomes a process-process heat exchange problem that can be solved independently from the other blocks. The superstructure presented in Figure 3.1 is applied once in each block. Note that within each block, the heating and cooling duties required match exactly. Furthermore, the inter-block temperatures are fixed by the definition of the stage boundaries and are not variables as in the method of Yee and Grossmann (1990). This also ensures that there are no temperature infeasibilities within a block, since as can be seen from Figure 3.4, the temperatures at the block boundaries will always be equal to or greater than ΔT_{\min} .

The mathematical model used by Zhu *et al* (1995) is based largely on the model of Yee and Grossmann (1990). Equations 3.3, 3.4, 3.16 and 3.17 form the body of the model and perform the same functions as described above. Note that since the inter-block temperatures are fixed, no additional constraints are required to ensure temperature feasibilities. These equations function to select where and how much heat is exchanged between particular hot and cold streams.

3 Technical Background

Zhu *et al* (1995) also used a constraint similar to Equation 3.21 to approximate the log mean temperature difference. Here, however, Paterson's approximation (Paterson, 1984) is used to avoid the singularity inherent in logarithms (Equation 3.23). Again it should be noted that since the inter-block temperatures are fixed, the log mean temperature differences calculated in Equation 3.23 are constant.

$$\Delta T_{c,h,k}^{lm} = \frac{2}{3} \sqrt{(T_{h,k}^H - T_{c,k}^C)(T_{h,k+1}^H - T_{c,k+1}^C)} + \frac{1}{3} \frac{T_{h,k}^H + T_{h,k+1}^H - T_{c,k}^C - T_{c,k+1}^C}{2} \quad (3.23)$$

Zhu *et al* (1995) provide two objective functions to be used in conjunction with the five constraints that make the model. The first objective function (Equation 3.24) aims to minimise the total heat transfer area required for the particular block. The use of this objective function results in a MILP model, which does not require an initial solution. The second objective function (Equation 3.25) aims to minimise the total capital cost of the heat exchangers for a particular block, taking into account the fixed cost of the units as well as the cost of heat exchanger area. The use of this objective function results in an MINLP model. It is intended that the solution to the MILP model be used as the initial solution when solving the MINLP model.

$$\min \left(\sum_{c,h} \frac{Q_{c,h,k}^{PP}}{U \cdot \Delta T_{c,h,k}^{lm}} \right) \quad (3.24)$$

$$\min \left(\sum_{c,h} \left[a \cdot x_{c,h,k}^{PP} + b \left(\frac{Q_{c,h,k}^{PP}}{U \cdot \Delta T_{c,h,k}^{lm}} \right)^{c_1} \right] \right) \quad (3.25)$$

3 Technical Background

Once a solution has been obtained for each block, the solutions are recombined into the final design. A further advantage of this method is that if data for a particular stream changes, only the blocks in which that stream participated need to be redesigned.

3.1.5 The Method of Isafiade and Fraser (2008)

A drawback to the method of Zhu *et al* (1995) is that streams are restricted to participate within particular predetermined blocks. This prevents certain potentially beneficial options from being explored. By combining the best features of the stage-wise and block-wise decomposition methods, Isafiade and Fraser (2008) developed the interval based method for the synthesis of heat exchanger networks. Here, an interval is a hybrid between a stage and a block, with boundaries defined by the supply and target temperatures of one of the sets of process streams.

In the interval based method, either the set of hot or cold process streams is chosen to be the reference set. The reference streams are divided between the intervals in a similar fashion to block-wise decomposition. Rather than manually placing blocks, Isafiade and Fraser (2008) stipulate that intervals be defined by the supply and target temperatures of the reference streams. In doing so, not every stream in the reference set will participate in every interval. With the exception of the supply and target temperatures of the reference streams, all of the boundary temperatures between intervals are treated as variables.

After establishing the intervals using the reference streams, the non-reference streams are dealt with in a similar fashion to stage-wise decomposition. Each of the non-reference streams are permitted to exist in each of the intervals, with all of the boundary temperatures being variable. This does not mean that each non-reference stream will participate in each of the intervals, but that the model has

3 Technical Background

the freedom to place these streams where needed. Having defined the intervals and which streams exist within each, the superstructure in Figure 3.1 is applied once to each interval.

To illustrate how Isafiade and Fraser (2008) define an interval, consider two hot streams and two cold streams. Taking the hot streams as the reference, Figure 3.5 shows how the supply and target temperatures are used to define the intervals. As per definition, the intervals are numbered in the direction from hot side to cold side. In the first interval, only hot stream 2 is present, since the entire interval is hotter than the supply temperature of hot stream 1. Likewise, only hot stream 1 is present in the third interval. Since the cold streams were not used as the reference streams, they are made to exist across all the intervals. Thus, using the method of Isafiade and Fraser (2008), the superstructure and model equations will be applied differently in each interval based on which streams are present in that interval.

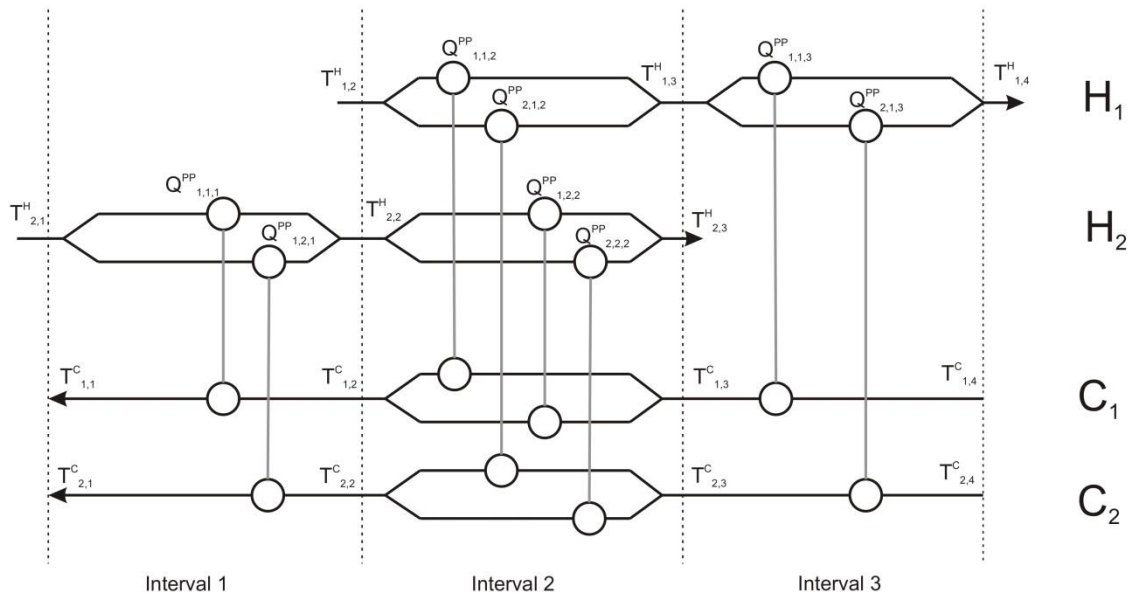


Figure 3.5 Superstructure repeated over the intervals created by two hot and two cold streams (Isafiade & Fraser, 2008).

3 Technical Background

Isafiade and Fraser (2008) use the same constraints as Yee and Grossmann (1990) in their model, along with the uniquely created intervals described above. The resulting formulation is a MINLP model. Isafiade and Fraser (2008) state that this method, unlike other non-linear methods, does not require a particular initialisation procedure in order to obtain an optimal design.

3.2 Steam System Design

Like with process-process interactions, heat integration principles have also been applied to the utility systems. In doing so, better use is made of the utility systems, resulting in debottlenecking of existing utilities or more cost effective designs. In this section, methods of applying heat integration principles to steam system networks will be discussed.

3.2.1 Problem Statement

The general problem that is addressed by the steam system design methods to be discussed can be formally stated as:

Given:

- A set of cold streams that require heating,
- The supply and target temperature of each cold stream,
- The heat capacity flowrate of each cold stream,
- The minimum temperature difference for heat transfer,
- The thermophysical properties of the steam utility.

Determine:

- The minimum steam flowrate required,
- The heat exchanger network that will achieve this flowrate.

3.2.2 The Method of Coetzee and Majozi (2008)

The method developed by Coetzee and Majozi (2008) uses the principles of heat integration to minimise the flowrate of steam required to heat the cold process streams. The motivation behind this is twofold. On existing plants, minimising the steam flowrate will debottleneck the boiler, making steam available for further uses. In new designs, minimising the steam flowrate will greatly reduce

3 Technical Background

the required size, and hence purchase cost of the boiler. In order to facilitate the reduction of steam flowrate, sensible heat from hot condensate is used to provide heating to the cold process streams in addition to the latent heat provided by the steam.

The method begins by considering the function of a heat exchanger. In order for a heat exchanger to provide the necessary heat transfer, there must be sufficient driving force (ΔT_{\min}). Figure 3.6 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.

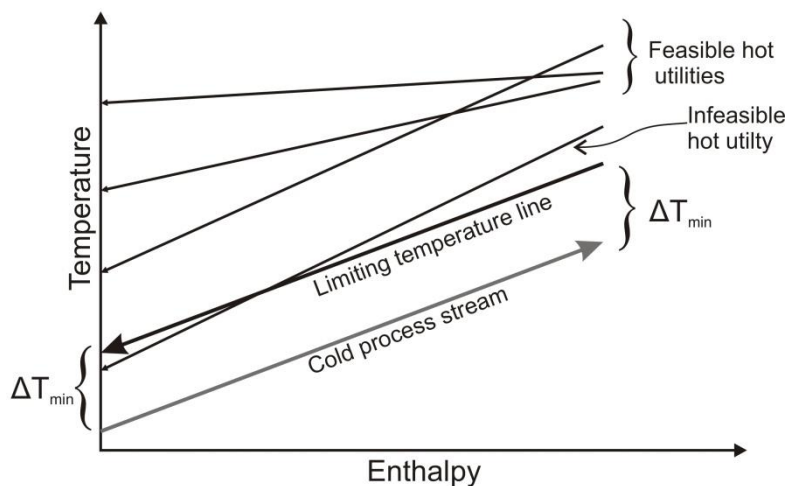


Figure 3.6: The importance of ΔT_{\min} in determining feasible and infeasible hot utilities.

From this understanding, one can see that a minimum inlet and outlet temperature for the hot utility stream can be obtained by adding ΔT_{\min} to the

3 Technical Background

target and supply temperatures of the cold streams respectively. Using this data, a limiting hot utility profile can be created in the same way in which the cold composite curve is drawn. This limiting hot utility curve creates a boundary between feasible and infeasible utilities, which is used by Coetzee and Majozi (2008) to graphically target the minimum steam flowrate. The limiting hot utility temperatures are also used in mathematical models to ensure feasibility with regards to temperature differences between the hot utility and the cold process streams.

In addition to the graphical targeting procedure presented by Coetzee and Majozi (2008), a mathematical model was also presented which simultaneously targets the minimum steam flowrate and synthesises the HEN. The superstructure used (Figure 3.7) has the ability to allow for both series and parallel connections between heat exchangers, and also allows for the use of latent heat from steam, as well as sensible heat from hot liquid. Consider the set of I heat exchangers that will heat the cold streams. In Figure 3.7, heat exchanger i has the potential to be supplied with saturated steam, and also with hot liquid reused from any other heat exchanger j . Heat exchanger i can also return its hot liquid to the boiler, or supply it as hot liquid to any other heat exchanger j .

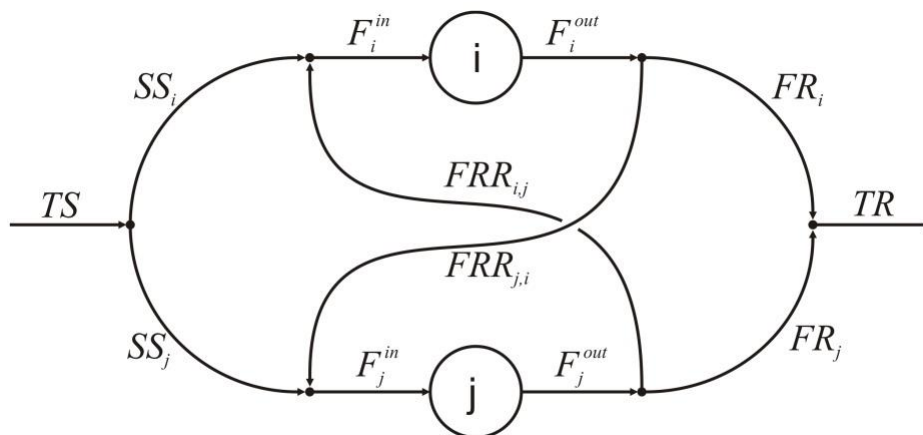


Figure 3.7: Superstructure for simultaneously targeting flowrate and synthesizing the HEN.

3 Technical Background

Coetzee and Majozi (2008) begin by calculating an upper bound on the saturated steam flowrate (Equation 3.26) and the hot liquid flowrate (Equation 3.27) to heat exchanger i , where $T_i^{in,L}$ and $T_i^{out,L}$ are the limiting inlet and outlet temperatures for the hot utility to cold stream i .

$$SS_i^U = \frac{Q_i}{\lambda} \quad \forall i \in I \quad (3.26)$$

$$FRR_i^U = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (3.27)$$

The constraints of the model are made up of a number of mass and energy balances performed over various nodes of the superstructure. Equation 3.26 states that the sum of the saturated steam supplied to the individual heat exchangers must equal the total steam flowrate. Equation 3.27 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 3.28).

$$TS = \sum_{i \in I} SS_i \quad (3.26)$$

$$TR = \sum_{i \in I} FR_i \quad (3.27)$$

$$TS = TR \quad (3.28)$$

3 Technical Background

Since this model must account for both saturated steam and hot liquid, Equation 3.29 states that the flowrate into a particular heat exchanger is equal to the 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 made up of saturated condensate and hot liquid (Equation 3.30). Equation 3.31 prevents a heat exchanger from recycling hot liquid back to itself.

$$F_i^{in} = SS_i + \sum_{j \in I} FRR_{i,j} \quad \forall i \in I \quad (3.29)$$

$$FRR_{i,j} = SL_{i,j} + HL_{i,j} \quad \forall i, j \in I, J \quad (3.30)$$

$$HL_{i,i} = 0 \quad \forall i \in I \quad (3.31)$$

Since saturated liquid is formed through the condensation of steam, Equation 3.32 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 3.33 states that the flowrate of hot liquid supplied by heat exchanger i to all other heat exchangers may not exceed the total flowrate of reuse liquid that entered heat exchanger i .

$$\sum_{j \in I} SL_{j,i} \leq SS_i \quad \forall i \in I \quad (3.32)$$

$$\sum_{j \in I} HL_{j,i} \leq \sum_{j \in I} FRR_{i,j} \quad \forall i \in I \quad (3.33)$$

3 Technical Background

In order to control which heat exchangers use steam and which use liquid, Coetzee and Majozi (2008) introduced 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 3.26 and 3.27 to limit the flowrate of saturated steam (Equation 3.34) and hot liquid reuse (Equation 3.35).

$$SS_i \leq SS_i^U y_i \quad \forall i \in I \quad (3.34)$$

$$\sum_{j \in I} FRR_{i,j} \leq FRR_i^U x_i \quad \forall i \in I \quad (3.35)$$

The binary variables also give control over split heat exchangers. If Equation 3.36 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.

$$x_i + y_i \leq 1 \quad \forall i \in I \quad (3.36)$$

If one were to permit a total of m heat exchangers to be split between hot liquid and saturated steam, then Equations 3.37 and 3.38 must be implemented in place of Equation 3.36. Here, $|i|$ represents the number of elements in set I .

$$\sum_{i \in I} x_i + \sum_{i \in I} y_i \geq |i| \quad (3.37)$$

$$\sum_{i \in I} x_i + \sum_{i \in I} y_i \leq |i| + m \quad (3.38)$$

3 Technical Background

Using Equation 3.39 allows the duty required of each heat exchanger to be supplied as both latent heat for steam, and sensible heat from hot liquid. Equation 3.40 models the quantity of heat provided as latent heat, while Equation 3.41 models the quantity of heat provided as sensible heat. Coetzee and Majazi (2008) linearized Equation 3.41 by setting all of the outlet temperatures to their limiting values ($T_i^{out,L}$), in accordance with an optimality condition proven by Savelski and Bagajewicz (2000).

$$Q_i = Q_i^{SS} + Q_i^{HL} \quad \forall i \in I \quad (3.39)$$

$$Q_i^{SS} = SS_i \lambda \quad \forall i \in I \quad (3.40)$$

$$Q_i^{HL} = c_p \sum_{j \in I} (SL_{i,j} T^{sat}) + c_p \sum_{j \in I} (HL_{i,j} T_j^{out,L}) - F_i^{in} c_p T_i^{out,L} \quad \forall i \in I \quad (3.41)$$

The above constraints constitute an MILP model for the simultaneous targeting of the minimum steam flowrate and HEN synthesis. The objective function, given in Equation 3.42 is simply to minimise the total steam flowrate supplied to the HEN.

$$\text{minimise}(TS) \quad (3.42)$$

3 Technical Background

3.2.3 The Method of Beangstrom (2013)

The method of Coetzee and Majozi (2008) is simplistic in that it only considers a single steam level. Beangstrom (2013) presents a method of applying heat integration principles to steam systems that include multiple steam levels, as well as steam turbines that are required to meet shaft work requirements. Here, the saturation temperatures and turbine sizes are not determined beforehand, but are optimised together with the HEN, providing a holistic approach to the steam system.

The superstructure used by Beangstrom (2013) is given in Figure 3.8 below. In Figure 3.8, 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 shown in Figure 3.8, 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.

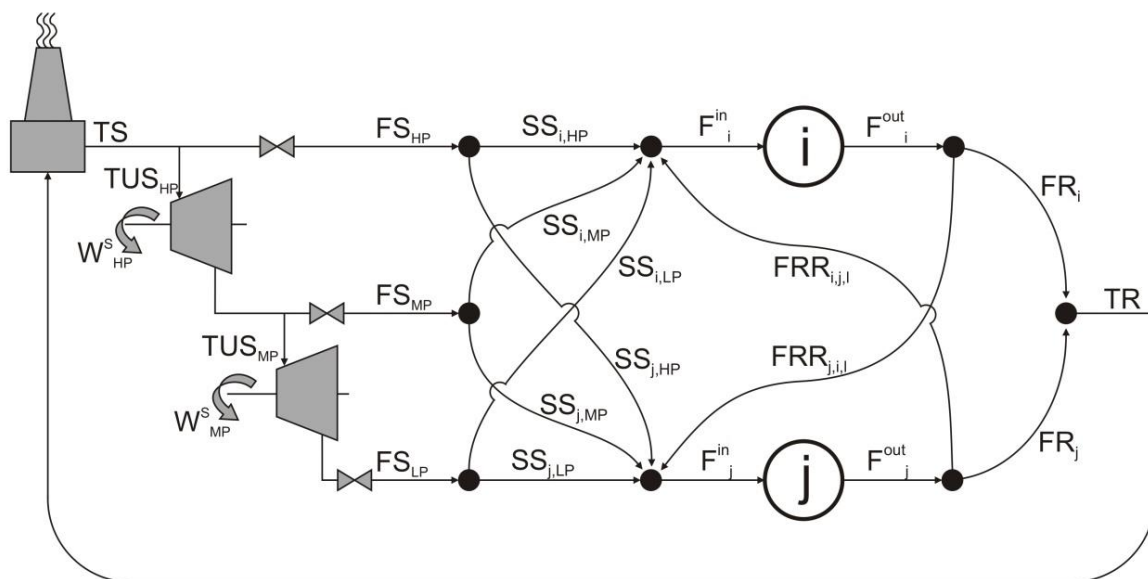


Figure 3.8: Superstructure used for HEN synthesis utilising multiple steam levels and satisfying shaft work requirements.

3 Technical Background

In Figure 3.8, i and j are heat exchangers belonging to the set of all heat exchangers I . 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 .

As in the models by Coetzee and Majozi (2008), upper bounds are calculated for the flowrate of hot liquid and saturated steam through each heat exchanger. Equation 3.43 calculates the upper bound on the flowrate of hot liquid through heat exchanger i . Equation 3.44 calculates the upper bound on the flowrate of saturated steam of each level through heat exchanger i . Equation 3.44 takes into account the fact that a particular steam level may not be hot enough to heat a particular cold stream, or that it may only be hot enough to heat it to a certain point, after which a higher steam level is required to reach the target temperature.

$$FRR_i^U = \frac{Q_i}{c_p(T_i^{in,L} - T_i^{out,L})} \quad \forall i \in I \quad (3.43)$$

$$SS_{i,l}^U = \begin{cases} 0 & \text{if } T_l^{sat} \leq T_i^{out,L} \\ \frac{(T_l^{sat} - T_i^{out,L}) Q_i}{(T_i^{in,L} - T_i^{out,L}) \lambda_l} & \text{if } T_i^{out,L} < T_l^{sat} < T_i^{in,L} \\ \frac{Q_i}{\lambda_l} & \text{if } T_l^{sat} \geq T_i^{in,L} \end{cases} \quad \forall i \in I \quad (3.44)$$

The constraints of the model are derived from mass and energy balances over various sections of the superstructure in Figure 3.8. The first set of constraints concern mass balances over the inlet and outlet of the whole HEN.

3 Technical Background

Equation 3.45 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 3.46 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, mass is conserved and Equation 3.47 must hold.

$$TS = \sum_{l \in L} FS_l \quad (3.45)$$

$$TR = \sum_{i \in I} FR_i \quad (3.46)$$

$$TS = TR \quad (3.47)$$

Considering the inlet to the HEN, Equation 3.48 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.

$$FS_l = \sum_{i \in I} SS_{i,l} \quad \forall l \in L \quad (3.48)$$

Performing mass balances over the individual heat exchangers, Equation 3.49 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 3.50 states that 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

3 Technical Background

all other heat exchangers j at all levels. Equation 3.51 ensures the conservation of mass inside the heat exchangers. Equation 3.52 details how each reuse stream can be made up of saturated liquid and hot liquid.

$$F_i^{in} = \sum_l SS_{i,l} + \sum_{j,l \in J,L} FRR_{i,j,l} \quad \forall i \in I \quad (3.49)$$

$$F_i^{out} = FR_i + \sum_{j,l \in J,L} FRR_{j,i,l} \quad \forall i \in I \quad (3.50)$$

$$F_i^{in} = F_i^{out} \quad \forall i \in I \quad (3.51)$$

$$FRR_{i,j,l} = SL_{i,j,l} + HL_{i,j,l} \quad \forall i,j \in I, l \in L \quad (3.52)$$

To prevent local recycle, Equation 3.53 is implemented. Constraints similar to Equation 3.53 can be added manually on a case by case basis to prevent unfavourable matches between particular streams.

$$FRR_{i,j,l} = 0 \quad \text{if } i = j \quad \forall i,j \in I \quad (3.53)$$

Accounting for the phase change that occurs when saturated steam condenses, Equation 3.54 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 3.55 states that the quantity of hot liquid leaving heat exchanger i may not exceed the quantity of hot liquid with which i is supplied.

3 Technical Background

$$\sum_{j \in J} SL_{i,j,l} \leq SS_{i,l} \quad \forall i \in I, l \in L \quad (3.54)$$

$$\sum_{j \in J} HL_{i,j,l} \leq \sum_{j \in J} SL_{j,i,l} + \sum_{j \in J} HL_{j,i,l} \quad \forall i \in I, l \in L \quad (3.55)$$

Performing energy balances over the heat exchanges, Equation 3.56 states that the sensible heat provided from hot liquid, and the latent heat from steam together must satisfy the energy demand of each cold stream. Equation 3.57 calculates the sum of the sensible heats provided by the various steam levels, while Equation 3.58 approximates the latent heat of condensation for each steam level based on its saturation temperature (Mavromatis and Kokossis, 1998). Equation 3.59 calculates the quantity of sensible heat supplied to heat exchanger i from all of the hot liquid reuse streams. As in the model by Coetzee and Majozi (2008), Equation 3.59 has been linearized by setting the outlet temperatures to their limiting values, and proven necessary by Savelski and Bagajewicz (2000).

$$Q_i^{SS} + Q_i^{HL} = Q_i \quad \forall i \in I \quad (3.56)$$

$$Q_i^{SS} = \sum_{l \in L} SS_{i,l} \lambda_l \quad \forall i \in I \quad (3.57)$$

$$\lambda_l = 2726 - 4.13T_l^{sat} \quad \forall l \in L \quad (3.58)$$

$$Q_i^{HL} = \sum_{j,l \in J,L} c_p SL_{j,i,l} T_l^{sat} + \sum_{j,l \in J,L} c_p HL_{j,i,l} T_j^{out,L} - c_p F_i^{out} T_i^{out,L} \quad \forall i \in I \quad (3.59)$$

3 Technical Background

Two binary variables are introduced to control which heat exchangers are supplied with latent heat, and which with sensible heat. 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 . In Equation 3.60, if $y_{i,l}$ takes on a value of 1, then heat exchanger i may be supplied with any quantity of saturated steam of level l below the upper bound. If $y_{i,l}$ takes on a value of 0, then the flow of steam is not permitted. Equation 3.61 performs in a similar fashion, permitting or restricting the supply of hot liquid to heat exchanger i .

$$SS_{i,l} \leq SS_{i,l}^U y_{i,l} \quad \forall i \in I, l \in L \quad (3.60)$$

$$\sum_{j,l \in J,L} FRR_{i,j,l} \leq FRR_i^U x_i \quad \forall i \in I \quad (3.61)$$

The binary variables are also used to control the number of split heat exchangers present in the design. Either Equation 3.62 or Equations 3.63 and 3.64 must be implemented, depending on whether no splits or a maximum of m splits are permitted.

$$x_i + \sum_{l \in L} y_{i,l} \leq 1 \quad \forall i \in I \quad (3.62)$$

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_{i,l} \geq |I| \quad (3.63)$$

$$\sum_{i \in I} x_i + \sum_{i,l \in I,L} y_{i,l} \leq |I| + m \quad (3.64)$$

3 Technical Background

Beangstrom (2013) also includes constraints dealing with the steam turbines to ensure that the shaft work requirements are met. Equation 3.65 states that the exhaust steam of a particular level supplied to a turbine, as well as to the HEN, may not exceed the quantity of steam supplied to the higher level turbine generating the exhaust steam. Equation 3.66 ensures that the saturation temperatures of steam levels decrease as the steam levels decrease.

$$TUS_{l+1} + FS_{l+1} \leq TUS_l \quad \forall l \in L \quad l < |L| \quad (3.65)$$

$$T_l^{sat} \geq T_{l+1}^{sat} \quad \forall l \in L \quad l < |L| \quad (3.66)$$

Beangstrom (2013) uses a steam turbine model by Mavromatis and Kokossis (1998) to estimate the shaft work produced by the steam turbine. Equation 3.67 calculates the amount of shaft work produced by each turbine, using parameters calculated from Equations 3.68 to 3.70. These equations will be discussed in greater detail later on in this chapter. Lastly, Equation 3.71 states that the sum of shaft work produced must satisfy the total demand. If required, the shaft work targets can be set for each turbine individually.

$$W_l^s = \frac{1}{B_l} (3.6 \overline{\Delta H}_l^{is} TUS_l - A_l) \quad \forall l \in L \quad l < |L| \quad (3.67)$$

$$A_l = a_1 + a_2 T_l^{sat} \quad \forall l \in L \quad l < |L| \quad (3.68)$$

$$B_l = b_1 + b_2 T_l^{sat} \quad \forall l \in L \quad l < |L| \quad (3.69)$$

$$\overline{\Delta H}_l^{is} = \frac{T_l^{sat} - T_{l+1}^{sat}}{391.8 + 2.215 T_l^{sat}} \quad \forall l \in L \quad l < |L| \quad (3.70)$$

3 Technical Background

$$\sum_{l \in |L|} W_l^S = W_{demand}^S \quad (3.71)$$

Lastly, the objective is to minimise the total steam flowrate produced by 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 3.72.

$$\text{minimise}(FS_{HP} + TUS_{HP}) \quad (3.72)$$

The above constraints constitute an MINLP model for steam flowrate minimisation. Since the nonlinearities are caused by variable steam level saturation temperatures, Beangstrom (2013) first fixes the steam levels at industrial standard levels and solves the resulting MILP problem. The solution to this then serves as the starting point for the full MINLP problem.

3.3 Cooling Water System Design

Like with steam systems, heat integration principles can be applied to cooling water systems to reduce the total cooling water flowrate. The motivation is based on the observation by Bernier (1994) that the effectiveness of a cooling tower increases as the flowrate is decreased and the return temperature is increased. Like as with steam systems, this reduction in flowrate is achieved through liquid reuse, but here, no phase change needs to be accounted for.

3.3.1 Problem Statement

The general problem that is addressed by the cooling water heat integration methods to be discussed can be formally stated as:

Given:

- A set of hot streams that require cooling,
- The supply and target temperature of each hot stream,
- The heat capacity flowrate of each hot stream,
- The minimum temperature difference for heat transfer,
- The supply and limiting return temperatures for cooling water,
- The dimensions and physical properties associated with the cooling towers.

Determine:

- The minimum flowrate of cooling water required,
- The heat exchanger network configuration that will achieve this flowrate,
- The cooling tower performance variables.

3 Technical Background

3.3.2 The Method of Gololo and Majozi (2011)

The method presented by Gololo and Majozi (2011) presents a general coverage of the topic of applying heat integration to the cooling water system. The model developed takes into account multiple cooling towers, and allows for the possibility that cooling water may be returned to a different tower from the one which supplied the cold water. Also, Gololo and Majozi (2011) make use of a cooling tower model to predict the performance of the cooling towers.

The superstructure used by Gololo and Majozi (2011) is given in Figure 3.9. Here, a set of I hot processes are cooled using cooling water from a set of N cooling towers. In Figure 3.9, one can see that a particular hot process i can be supplied with cooling water from any one of the cooling towers, as well as with reused liquid from any of the other hot processes. The liquid leaving hot process i can also be reused in another process, or can be returned to any one of the cooling towers. Each cooling tower also has its associated make up, blow down and evaporative losses.

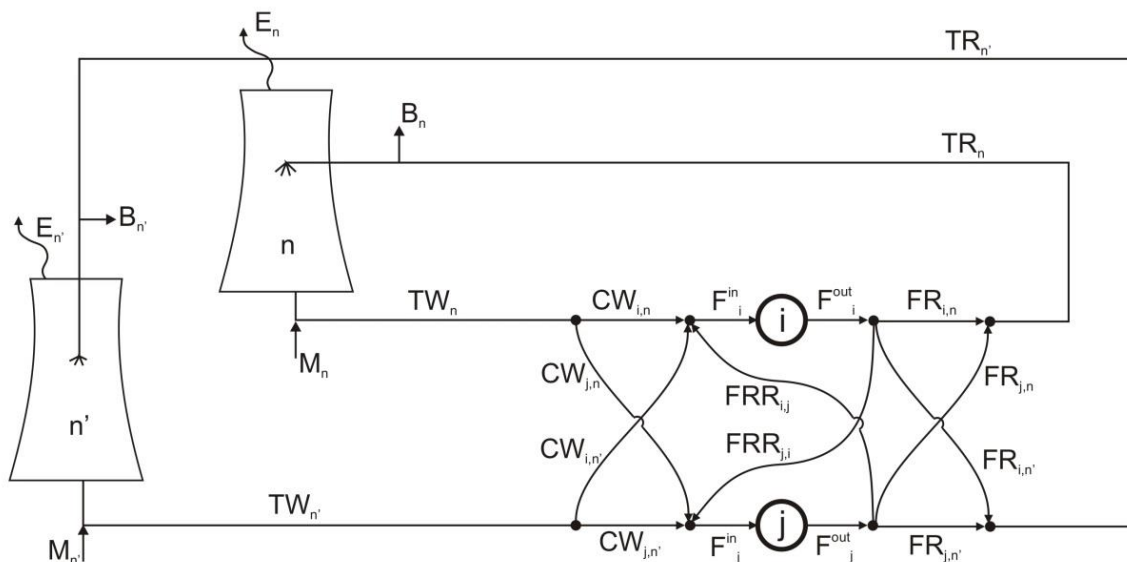


Figure 3.9: Superstructure used for cooling water network design with multiple cooling towers.

3 Technical Background

As with the models described above, the model by Gololo and Majazi (2011) comprises of a number of mass and energy balances performed over the various nodes in Figure 3.9. Beginning with the individual heat exchangers, Equation 3.73 states that the flowrate into the heat exchanger is made up of cooling water from each of the towers as well as reuse liquid from each of the other heat exchangers. Equation 3.74 states that the liquid leaving the heat exchanger can be reused in any of the other heat exchangers, or returned to any one of the cooling towers. Equation 3.75 states that mass must be conserved in each heat exchanger.

$$F_i^{in} = \sum_{n \in N} CW_{i,n} + \sum_{j \in I} FRR_{i,j} \quad \forall i \in I \quad (3.73)$$

$$F_i^{out} = \sum_{n \in N} RW_{i,n} + \sum_{j \in I} FRR_{j,i} \quad \forall i \in I \quad (3.74)$$

$$F_i^{in} = F_i^{out} \quad \forall i \in I \quad (3.75)$$

Gololo and Majazi (2011) also performed mass balances over the cooling towers. Equations 3.76 and 3.77 show how the water supplied from and returned to each tower is made up of the sum of the individual flows associated with each heat exchanger. Equation 3.78 makes provision for evaporative and blow down losses, as well as for the addition of fresh make up water.

$$TW_n = \sum_{i \in I} CW_{i,n} \quad \forall n \in N \quad (3.76)$$

$$TR_n = \sum_{i \in I} FR_{i,n} \quad \forall n \in N \quad (3.77)$$

3 Technical Background

$$TW_n = TR_n - B_n - E_n + M_n \quad \forall n \in N \quad (3.78)$$

Unlike in the methods concerning steam networks discussed above, where two phases are used, only one liquid phase is used within cooling water networks. As such, only Equation 3.79 is required to ensure that the cooling demand of process i is met by the various supplies of cooling water and reuse streams. In addition to this, since for practical reasons the return temperature cannot exceed a certain threshold, Equation 3.80 is included to calculate the return temperature to each cooling tower, and Equation 3.81 ensures that the return temperature to each cooling tower does not exceed the limit for that tower.

$$Q_i = c_p F_i^{in} T_i^{out,L} - c_p \sum_{n \in N} CW_{i,n} T^{cw} - c_p \sum_{j \in I} FRR_{i,j} T_j^{out,L} \quad \forall i \in I \quad (3.79)$$

$$T_n^{ret} = \frac{\sum_{i \in I} FR_{i,n} T_i^{out,L}}{TR_n} \quad \forall n \in N \quad (3.80)$$

$$T_n^{ret} \leq T_n^{ret,Limit} \quad \forall n \in N \quad (3.81)$$

It must be noted that since only a single phase has been employed, no binary variables are required. Binary variables and their associated constraints would need to be added if it were desired to add extra control, such as prohibiting a processes from receiving or supplying cooling water from/to more than one cooling tower.

In addition to the above constraints developed for the cooling water network, Gololo and Majozi (2011) make use of a cooling tower model developed by Kröger (2004) to predict the performance of each cooling tower. The cooling

3 Technical Background

tower model takes the form of several differential equations, which will be discussed in detail in the next section. The output of the cooling tower model not only allows the cooling water temperature to be predicted, but is also used to predict the overall effectiveness of the collection of cooling towers (Equation 3.82). Here, effectiveness is defined as the ratio of the actual total quantity of heat rejected by the cooling towers, to the maximum theoretical total quantity of heat that could be rejected under the present operating conditions.

$$\varepsilon_{overall} = \frac{\sum_{n \in N} Q_n^{actual}}{\sum_{n \in N} Q_n^{maximum}} \quad (3.82)$$

Lastly, Gololo and Majozi (2011) define the objective function (Equation 3.83), where the aim is to maximise the overall effectiveness of the collection of cooling towers.

$$Max(\varepsilon_{overall}) \quad (3.83)$$

Since the cooling tower model by Kröger (2004) contains differential equations, Gololo and Majozi (2011) used an iterative approach to solving the models. An assumption was first made with respect to the cooling tower output variables. These assumed values were then used in conjunction with the network model to optimise the network. With the results of the network optimisation, the cooling tower model was then solved using a Runge-Kutta algorithm. These two steps would be repeated until convergence in order to obtain the final solution.

3 Technical Background

3.4 Cooling Tower Model

The cooling tower model used by Gololo and Majozi (2011), and also in this work, was developed by Kröger (2004). In this cooling tower model, an analysis of a differential slice of the packing inside a cooling tower is used to develop the equations describing the performance of the cooling tower.

The development of the cooling tower model, as given by Kröger (2004), is discussed below. The differential slice taken across the cross sectional area of the cooling tower packing is shown in Figure 3.10. Here, the counter current nature of the cooling tower is seen, with the water trickling down over the packing, while the air rises up. A number of assumptions are also made with regard to the model:

- All properties are the same across the cross sectional area
- The interface temperature at the surface of water droplets is the same as the bulk water temperature
- The area for mass transfer and heat transfer are identical
- The water and air flowrates remain constant.

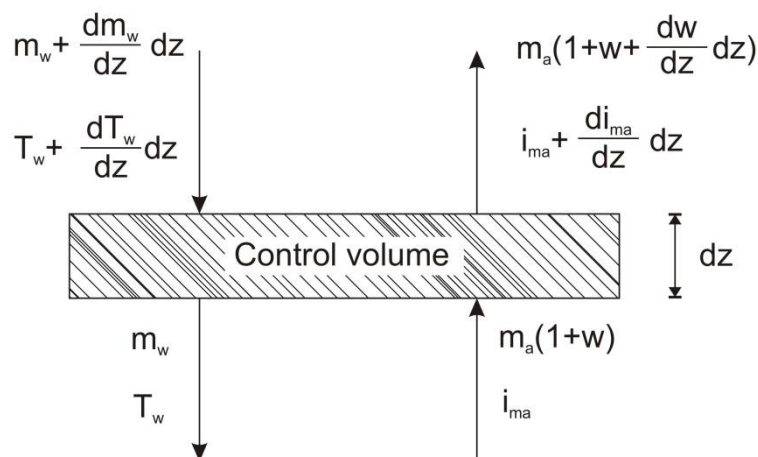


Figure 3.10: Differential slice across cooling tower packing.

3 Technical Background

Performing a mass balance over the control volume results in Equation 3.84. By cancelling out like terms, Equation 3.85 is obtained.

$$m_a(1 + w) + \left(m_w + \frac{dm_w}{dz} dz\right) = m_a \left(1 + w + \frac{dw}{dz} dz\right) + m_w \quad (3.84)$$

$$\frac{dm_w}{dz} = m_a \frac{dw}{dz} \quad (3.85)$$

In a similar fashion, Equation 3.86 is the result of performing an energy balance over the control volume. After simplifying, and also after ignoring second order derivatives, Equation 3.87 is obtained.

$$m_a i_{ma} + \left(m_w + \frac{dm_w}{dz} dz\right) c_{p,w} \left(T_w + \frac{dT_w}{dz} dz\right) = m_a \left(i_{ma} + \frac{di_{ma}}{dz} dz\right) + m_w c_{p,w} T_w \quad (3.86)$$

$$\frac{dT_w}{dz} = \frac{m_a}{c_{p,w} m_w} \left(\frac{1}{c_{p,w}} \frac{di_{ma}}{dz} - T_w \frac{dw}{dz}\right) \quad (3.87)$$

In the above equations, the enthalpy of humid air per mass of dry air, i_{ma} , can be calculated using Equation 3.88.

$$i_{ma} = c_{p,a} T_a + w(\lambda_0 + c_{p,v} T_a) \quad (3.88)$$

3 Technical Background

Within the control volume, one can examine the transfer of mass and enthalpy between air and water across the liquid surface. The enthalpy transfer in particular is made up of two parts: enthalpy transfer as a result of mass transfer, and enthalpy transfer due to convective heat transfer (Equation 3.89).

$$dQ = dQ_m + dQ_c \quad (3.89)$$

The quantity of water transferred as vapour from the bulk liquid to the air is proportional to the difference between the saturation humidity and the actual humidity (Equation 3.90). Since this mass has enthalpy, the transfer of mass also represents an enthalpy transfer across the surface. The quantity of enthalpy can be determined by multiplying the vapour mass flux with the enthalpy of water vapour (Equation 3.91). In both of these expressions, A refers to the area available for transfer between the water and air.

$$\frac{dm_w}{dz} dz = h_d(w_{sw} - w)dA \quad (3.90)$$

$$dQ_m = i_v \frac{dm_w}{dz} dz = i_v h_d(w_{sw} - w)dA \quad (3.91)$$

The enthalpy transfer due to convective heat transfer is driven by the temperature difference between the water and the air (Equation 3.92).

$$dQ_c = h(T_w - T_a)dA \quad (3.92)$$

Using Equation 3.88 the enthalpy of saturated air at the bulk water temperature is evaluated (Equation 3.93), which can be rewritten as Equation 3.94.

3 Technical Background

$$i_{masw} = c_{p,a}T_w + w_{sw}(\lambda_0 + c_{p,v}T_w) \quad (3.93)$$

$$i_{masw} = c_{p,a}T_w + wi_v + (w_{sw} - w)i_v \quad (3.94)$$

By subtracting Equation 3.88 from Equation 3.94, and rearranging terms, Equation 3.95 is obtained.

$$T_w - T_a = \frac{1}{c_{p,ma}} [(i_{masw} - i_{ma}) - (w_{sw} - w)i_v] \quad (3.95)$$

$$\text{where } c_{p,ma} = c_{p,a} + w \cdot c_{p,v}$$

By substituting this last equation along with Equations 3.91 and 3.92 into Equation 3.89, one obtains Equation 3.96.

$$dQ = h_d \left[\frac{h}{c_{p,ma}h_d} (i_{masw} - i_{ma}) + \left(1 - \frac{h}{c_{p,ma}h_d} \right) i_v (w_{sw} - w) \right] dA \quad (3.96)$$

It must be noted in Equation 3.96 that one of the groups of terms, shown in Equation 3.97, is better known as the Lewis factor. Furthermore, if a_f is the wetted area per unit fill inside the cooling tower, and A_{CS} is the cross sectional area of the cooling tower packing, then the amount of transfer area between air and water can be related to the thickness of the horizontal slice in Figure 3.10 using Equation 3.98.

$$\frac{h}{c_{p,ma}h_d} = Le_f \quad (3.97)$$

3 Technical Background

$$dA = a_f A_{cs} dz \quad (3.98)$$

With this in mind, and noting that the enthalpy change of the air must be equal to the amount of enthalpy transferred between air and water, the third differential equation in the model by Kröger (2004) is given in Equation 3.99.

$$\frac{di_{ma}}{dz} = \frac{1}{m_a} \frac{dQ}{dz} = \frac{h_d a_f A_{cs}}{m_a} [Le_f (i_{masw} - i_{ma}) + (1 - Le_f) i_v (w_{sw} - w)] \quad (3.99)$$

The differential equations expressed as Equations 3.85, 3.87 and 3.99 constitute the cooling tower model developed by Kröger (2004). A number of additional algebraic equations must be added to facilitate the solution of these equations. Bosnjakovic (1965) gives an expression (Equation 3.100) for calculating the Lewis factor for the combination of air and water.

$$Le_f = 0.866^{0.667} \frac{\left(\frac{w_{sw} + 0.622}{w + 0.622} - 1\right)}{\ln\left(\frac{w_{sw} + 0.622}{w + 0.622}\right)} \quad (3.100)$$

To calculate the saturation humidity, w_{sw} , used in Equation 3.99 and others, a close approximation given by Coulson and Richardson (1996) can be used (Equation 3.101). To calculate the vapour pressure of water, Lyderson (1983) gives constants for an Antoine equation (Equation 3.102) valid between 0°C and 57°C, a range suitable for the temperatures that will be experienced inside a cooling tower.

$$w_{sw} = \frac{18}{29} \frac{P_W^{sat}}{P_{atm} - P_W^{sat}} \quad (3.101)$$

3 Technical Background

$$P_W^{sat} = \exp \left[23.7093 - \frac{4111}{237.7 + T_w} \right] \quad (3.102)$$

Finally, Lemouari, Boumaza and Kaabi (2009) provide a correlation for calculating the mass transfer properties required in Equation 3.99, using the mass flowrate of water and air per unit cross sectional area. This correlation (Equation 3.103) was determined experimentally for vertical counter current flow in the pellicular regime, that is, water trickling over the packing inside the tower.

$$h_a a_f = 1.880952381 \cdot \left(\frac{m_w}{A_{CS}} \right)^{0.52} \cdot \left(\frac{m_a}{A_{CS}} \right)^{0.48} \quad (3.103)$$

3 Technical Background

3.5 Steam levels

There is no fixed method for determining the ideal temperatures of the individual steam levels present on a chemical processing plant. Ultimately, the steam levels must be chosen to satisfy the requirements of the plant, but a number of heuristics do exist to aid in the initial selection of steam levels. 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 utilising multiple steam levels on a chemical processing plant arises from variations in the latent heat of steam. Figure 3.11 shows how the latent heat of steam increases as the saturation temperature decreases. With this in mind, it makes sense that each unit operation that requires heat should be supplied with steam from the lowest feasible steam level.

3 Technical Background

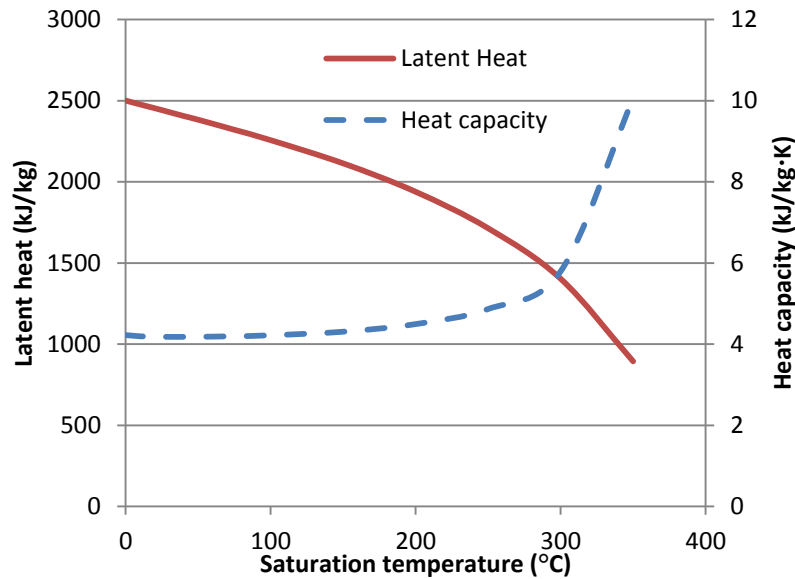


Figure 3.11: Latent heat of steam and heat capacity of water as a function of saturation temperature. (Cooper & Le Fevre, 1969)

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 the 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.

$$\lambda = 2726 - 4.13T^{sat} \quad (3.104)$$

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

3 Technical Background

3.6 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 unit operations. This allows the optimization algorithm 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 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 3.12), a common tool for describing simple turbines. From this, it can be seen that the Willans line can be expressed as:

$$E = nM - E^{loss} \tag{3.105}$$

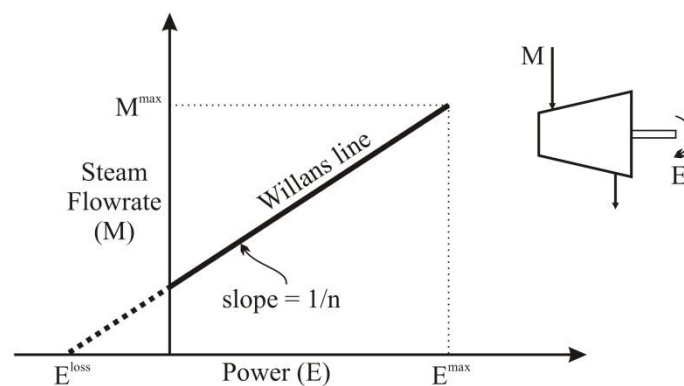


Figure 3.12: The Willans line for a simple turbine. (Mavromatis & Kokossis, 1998)

3 Technical Background

Mavromatis and Kokossis (1998) note that the slope of a line from the origin to any operating point on the Willans line (Figure 3.13a) 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 3.13b). The shape obtained in Figure 3.13b agrees well with actual turbine data collected by Peterson and Mann (1985).

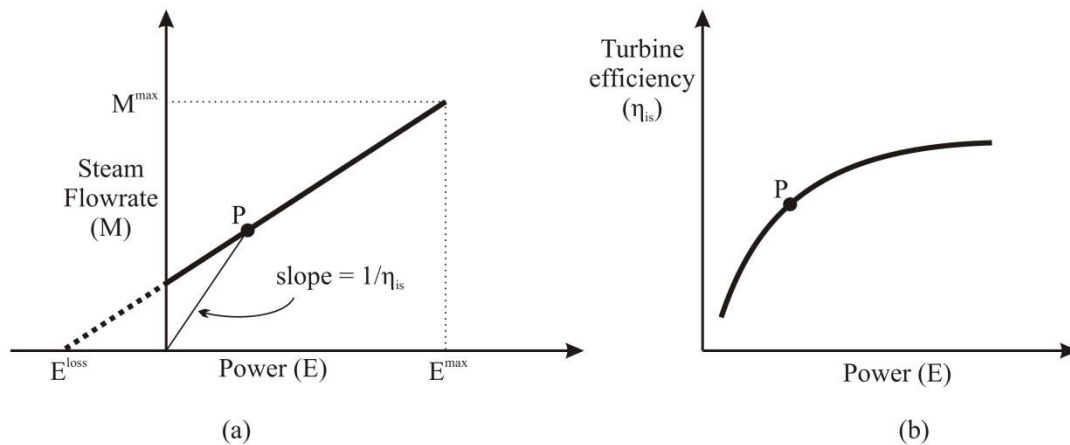


Figure 3.13: Nonlinear variation of turbine efficiency with operating conditions. (Mavromatis & Kokossis, 1998)

The data in Figure 3.13b, through a change in axes, can be expressed as a linear function (Equation 3.106). 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 3.107 and 3.108)

$$\frac{E^{max}}{\eta_{is}^{max}} = A + B E^{max} \quad (3.106)$$

$$A = a_1 + a_2 T_{in}^{sat} \quad (3.107)$$

$$B = b_1 + b_2 T_{in}^{sat} \quad (3.108)$$

3 Technical Background

Using the definition of isentropic efficiency (Equation 3.109), Equation 3.110 is obtained, which is substituted into Equation 3.106. 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 3.111).

$$\eta_{is} = \frac{\bar{E}}{\Delta\bar{H}_{is}} = \frac{E}{\Delta\bar{H}_{is}M} \quad (3.109)$$

$$\frac{E^{max}}{\eta_{is}^{max}} = \Delta\bar{H}_{is}M^{max} \quad (3.110)$$

$$E^{loss} = 0.2E^{max} \quad (3.111)$$

Using Equations 3.105, 3.106, 3.110 and 3.111, Mavromatis and Kokossis (1998) obtained the following two expressions for the parameters n and E^{loss} in Equation 3.105.

$$n = \frac{5}{6} \frac{1}{B} \left(\Delta\bar{H}_{is} - \frac{A}{M^{max}} \right) \quad (3.112)$$

$$E^{loss} = \frac{1}{5} \frac{1}{B} (\Delta\bar{H}_{is}M^{max} - A) \quad (3.113)$$

By substituting Equations 3.112 and 3.113 into Equation 3.105, Mavromatis and Kokossis (1998) obtain Equation 3.114, 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 3.107 and 3.108. 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 3.114 reduces to Equation 3.115.

3 Technical Background

$$E = \frac{5}{6} \frac{1}{B} \left(\overline{\Delta H}_{is} - \frac{A}{M^{max}} \right) \left(M - \frac{1}{6} M^{max} \right) \quad (3.114)$$

$$E^{max} = \frac{1}{B} (\overline{\Delta H}_{is} M^{max} - A) \quad (3.115)$$

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 3.115 requires the term $\overline{\Delta H}_{is}$ to be calculated. Singh (1997) provides a correlation for approximating this isentropic enthalpy change (Equation 3.116). 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.

$$\overline{\Delta H}^{is} = \frac{\Delta T^{sat}}{1854 - 1931 \cdot q^{in}} \quad (3.116)$$

3.7 Solving Differential Equations

It is rare that the differential equations encountered in engineering practice will have easily determined analytic solutions. For this reason, a number of techniques have been developed to solve differential equations numerically. It is, however, important to have an understanding of the available techniques so that the best technique can be selected for the task at hand.

Two techniques will be discussed in this section: the Runge-Kutta method and the Adams-Bashforth method. Both of these methods can be used to numerically solve initial value ordinary differential equations of the form given in Equation 3.117.

$$\frac{dy}{dt} = f(y, t); \quad y(t_0) = y_0 \quad (3.117)$$

3.7.1 The Runge-Kutta Method

The Runge-Kutta method is a family of predictor-corrector methods, meaning that each new point is first predicted before a second step corrects this prediction. These methods, and in particular the “classic” fourth order Runge-Kutta method, represent some of the most popular techniques for numerically solving differential equations (Rice & Do, 1994). This popularity is in part due to the fact that the technique achieves good accuracy without the need to calculate and evaluate derivatives of $f(y, t)$ (Burden & Fairs, 2005).

The Runge-Kutta method is a fourth order method, therefore the accumulative error is of the order $O(s^4)$, where s represents the step size between successive points. As such, the desired accuracy can be achieved by selecting a sufficiently small step size. One must bear in mind though that with smaller step sizes, a

3 Technical Background

greater number of computations is required to achieve the desired result. Thus one must be ever mindful of the trade-off between accuracy and computational speed.

To execute the Runge-Kutta method, four predictors must first be calculated, utilising information about the last known point (Equation 3.118). In essence, each one of these values predicts the change in y moving from the current time point to the next. After that, Equation 3.119 calculates the new value of y by adding a weighted average of these four predictions to the last known value of y .

$$k_{1,n} = s \cdot f(y_n, t_n) \quad (3.118)$$

$$k_{2,n} = s \cdot f\left(y_n + \frac{1}{2}k_{1,n}, t_n + \frac{s}{2}\right)$$

$$k_{3,n} = s \cdot f\left(y_n + \frac{1}{2}k_{2,n}, t_n + \frac{s}{2}\right)$$

$$k_{4,n} = s \cdot f(y_{n+1}, t_{n+1})$$

$$y_{n+1} = y_n + \frac{1}{6}(k_{1,n} + 2k_{2,n} + 2k_{3,n} + k_{4,n}) \quad (3.119)$$

The Runge-Kutta method is very simple to implement by repeating the two steps described above until the desired time point is reached. Furthermore, since each iteration only requires information about the current point, the method is easy to start with only a single initial value. This method does, however, require the platform to be able to loop over these two steps, a feature not always available in optimisation software. For example, in the work of Gololo and Majosi (2011), the bulk of the model was solved in Gams, but the differential equations involved in predicting the performance of the cooling tower were solved using the Runge-Kutta method in Matlab. Information regarding the state

3 Technical Background

of the model had to be passed back and forth between the two platforms while the two sections of the model were solved iteratively.

3.7.2 The Adams-Bashforth Method

One of the downsides to the Runge-Kutta method is that the four predictions calculated in Equation 3.118 are only used once, and then discarded. This is computationally wasteful, since valuable processing time is used in calculating each value. One way around this is to employ a multistep method, such as the Adams-Bashforth method.

The Adams-Bashforth method is a family of multistep methods, the simplest of which is better known as the Euler method (Rice & Do, 1994). Here, the term multistep refers to the fact that information about multiple previous point is used to determine the next value of y . Equation 3.120 gives the fourth order Adams-Bashforth method which, as its name implies, has an accumulative error of the order $O(s^4)$. Here, $f(y_n)$ is used as a simplified form of $f(y_n, t_n)$ for ease of reading.

$$y_{n+1} = y_n + \frac{s}{24} [55f(y_n) - 59f(y_{n-1}) + 37f(y_{n-2}) - 9f(y_{n-3})] \quad (3.120)$$

Note that in the right hand side of Equation 3.120, only one new function evaluation must performed, $f(y_n)$, as the others are already know from previous iterations of Equation 3.120. Unlike the Runge-Kutta method, where multiple function evaluations are required to calculate the predictors and are then discarded, the Adams-Bashforth method reuses old function evaluations in each new iteration. This makes the Adams-Bashforth method more computationally efficient.

3 Technical Background

The drawback to the Adams-Bashforth method lies in the fact that four known previous points are required. This makes the Adams-Bashforth method a difficult method to initiate, since often only one initial value is known. This can be overcome by using another method to determine the first three points, such as the Runge-Kutta method or the Euler method. The Euler method (Equation 3.121) is quite attractive, since it is already a member of the Adams-Bashforth family of methods, and because the function evaluations required in the right hand side of Equation 3.121 can be stored for reuse in Equation 3.120 after sufficient initial points have been determined.

$$y_{n+1} = y_n + s \cdot f(y_n) \quad (3.121)$$

Another attractive feature of the Adams-Bashforth method, in the context of this work, is that it allows the numeric solution of an ordinary differential equation to be decomposed into a system of simultaneous algebraic equations. If the Euler method is used to determine the first three unknown points before employing the Adams-Bashforth method, then the system of simultaneous equations can be expressed in matrix notation as follows

3 Technical Background

Another advantage to expressing the solution to a set of differential equations as a system of simultaneous algebraic equations is that the initial point supplied need not necessarily be the beginning point. When solving differential equations in the usual manner, one begins at the initial point, and each successive point is calculated from the last. When the differential equation is expressed as a system of simultaneous equations, all points exist as variables which are functions of the surrounding variables. Any one of these points could be specified, not only the first point. This is of special advantage to the cooling tower model described above, since the inlet enthalpy and humidity of air are known at the bottom of the tower, but the water temperature is known at the top of the tower, being the return temperature. If the cooling tower model were to be solved in the traditional unidirectional manner, the outlet temperature of the cooling water would need to be guessed, the model solved, and the predicted inlet water temperature compared with the actual water temperature. These steps would have to be iterated over until the model converged, adding additional computational time, since there is already the back and forth iteration between the differential model solver and the optimisation solver. By expressing the cooling tower model as a system of simultaneous algebraic equations, the known points can be substituted in where they belong, and no iteration is required.

3.8 References

- Beangstrom SG (2013). *Steam system network analysis, synthesis and optimisation*. Master's thesis, Department of Chemical Engineering, University of Pretoria, South Africa.
- Bernier MA (1994). Cooling tower performance: Theory and experiments. *ASHRAE Trans. Res.*, 100, 114-121.
- Bosnjakovic F (1965). *Technical thermodynamics*, translated by Blackshear PI, 1-80, Holt, Reinhart and Wilson, New York.
- Burden RL & Faires JD (2005). *Numerical analysis*, 8th Ed, Brooks/Cole, USA.
- Chen JJJ (1987). Letter to the editors: Comments on improvement on a replacement for the logarithmic mean. *Chem. Eng. Sci.*, 42, 2488-2489.
- Coetzee WAS & Majozi T (2008). Steam System Network Synthesis using Process Integration. *Ind. Eng. Chem. Res.*, 47, 4405-4413.
- Cooper JR & Le Fevre EJ (1969). *Thermophysical properties of water substance*. Butterworth-Heinemann, London, UK.
- Coulson JM & Richardson JF (1996). *Chemical engineering: Fluid flow, heat transfer and mass transfer*, 5th Ed, Pergamon Press, Oxford.
- Gololo KV & Majozi T (2011). On synthesis and optimization of cooling water systems with multiple cooling towers. *Ind. Eng. Chem. Res.*, 50, 3775-3787.
- Grossmann IE & Sargent RWH (1978). Optimum design of heat exchanger networks. *Comp. Chem. Eng.*, 2, 1-7.
- Harrel G (1996). Steam system survey guide. ORNL/TM-2001/263: Oak Ridge National Laboratory.

3 Technical Background

- Isafiade AJ & Fraser DM (2008). Interval-based MINLP superstructure synthesis of heat exchange networks. *Chem. Eng. Res. & Design*, 86, 245-257.
- Kröger DG (2004). *Air-cooled heat exchangers and cooling towers*, Penn Well Corporation, USA.
- Lemouari M, Boumaza M & Kaabi A (2009). Experimental analysis of heat and mass transfer phenomena in a direct contact evaporative cooling tower. *Energy Conservation & Management*, 50, 1610-1617.
- Lydersen AL (1983). *Mass transfer in engineering practice*, Wiley, New York.
- Mavromatis SP & Kokossis AC (1998). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Paterson WR (1984). A replacement for the logarithmic . *Chem. Eng. Sci.*, 39, 1635.
- Peterson JF & Mann WL (1985). Steam-system design: how it evolves. *Chem. Eng. Sci.*, 92(21), 62-74.
- Price T & Majozi T (2010). On Synthesis and Optimization of Steam System Networks. 2. Multiple Steam Levels. *Ind. Eng. Chem. Res.*, 49, 9154-9164.
- Rice RG & Do DD (1994). *Applied mathematics and modelling for chemical engineers*, Wiley, USA.
- Savelski M J & Bagajewicz MJ (2000). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.

3 Technical Background

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

Yee F & Grossmann IE (1990). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comp. Chem. Eng.*, 14(10), 1165-1184.

Zhu XX, O'Neill BK, Roach JR & Wood RM (1995). A method for automated heat exchanger network synthesis using block decomposition and non-linear optimization. *Trans. IChemE*, 73(A), 919-930.

Chapter 4

Model Development

In this chapter, the new models will be developed for the simultaneous heat integration of the utilities and the process-process interactions. Before the new models are presented a number of preliminary topics must first be discussed.

In the models, it will be assumed that only one cooling tower is present. If, however, it is essential that two or more towers must be included and cannot be approximated as one large tower, then the models presented below can easily be modified to accommodate multiple cooling in a similar fashion to Gololo and Majozi (2011, 2013).

A further assumption is that only two steam levels are employed. This stems from the observation (outlined in Appendix A) that if hot liquid reuse is utilised as a strategy for reducing steam flowrate, then only a single high pressure steam level should be used to ensure minimum steam flowrate. If, however, a steam turbine must be present to fulfil shaft work requirements, then the turbine exhaust constitutes a second steam level. Although the models presented below will be solved using only two steam levels, additional steam levels can easily be included by simply noting that the set of steam levels will contain additional elements.

In this study, objective functions with cost factors are avoided when possible. The reasoning here is that cost factors are subjective, and vary both with regard to location and point in time. It is better to develop a model that looks at physical properties to better understand the process. Such an approach provides a flexible model, allowing future designers to customise the model and to utilise objective functions specific to the unique situations encountered.

4.1 Problem Statement

The problem to be addressed by this work can be stated more formally as:

Given:

- a set of cold process streams that require heating,
- a set of hot process streams that require cooling,
- the fixed heating/cooling duty required by each process stream,
- the supply and target temperatures for each process stream,
- the minimum temperature difference for heat transfer (ΔT_{\min}),
- the atmospheric conditions relevant to the operation of cooling towers,
- the design constraints on cooling towers,
- the thermophysical properties of the steam levels,
- a shaft work target required from steam turbines.

Determine:

- the minimum cooling water flowrate, resulting in increased cooling tower effectiveness,
- the minimum steam flowrate, resulting in reduced boiler purchase cost,
- the heat exchanger network layout that will achieve these objectives whilst maintaining the minimum energy requirements, through the

4 Model Development

simultaneous application of process-process heat integration, cooling water system design, and steam system design.

4.2 Regions of Application

As has been mentioned above, the current paradigm divides heat integration of chemical processes into three distinct regions: process-process heat integration, cooling water system design, and steam system design. This has been a convenient division, because the respective techniques can be applied individually to each region with minimal regard for the operation of the other regions. Visually, the natural placement of the three regions can be seen in Figure 4.1, where the hot and cold composite curves define the boundaries of the three regions. In the centre exists the region for process-process heat integration. To the left and right exist regions for cooling and heating respectively, where cooling water system design and steam system design are confined.

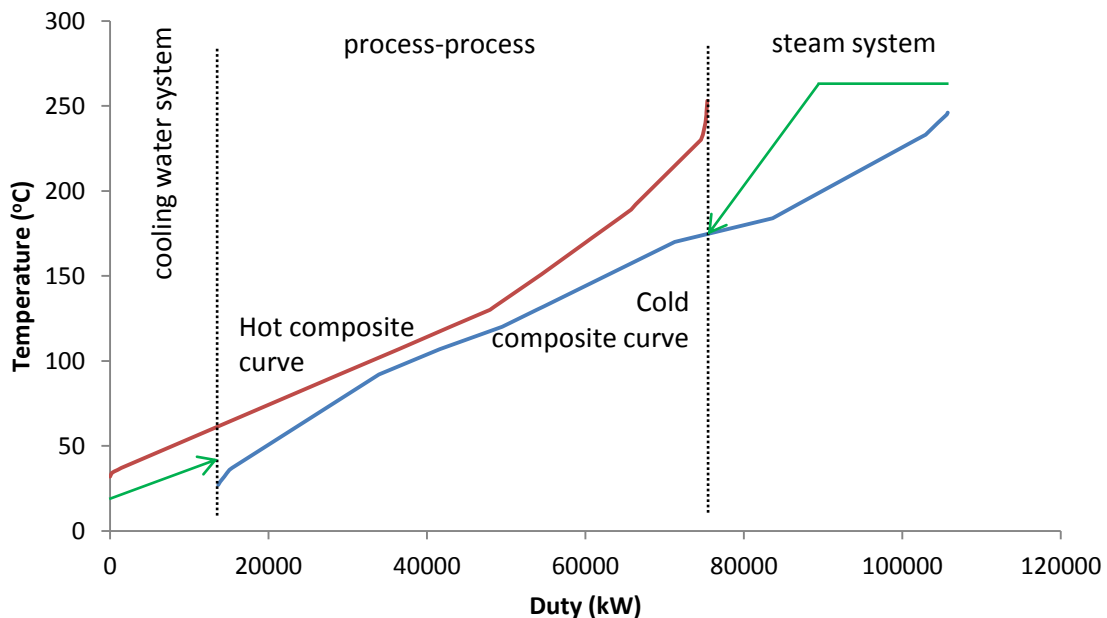


Figure 4.1: Old paradigm in which hot and cold composite curves define the boundaries of three regions of application.

4 Model Development

In process-process heat integration though, there are three “golden rules” (Kemp, 2007):

- Do not apply a cold utility above the pinch
- Do not apply a hot utility below the pinch
- Do not transfer heat across the pinch

These three rules suggest a new paradigm, one in which there are only two regions: “above pinch” and “below pinch”. Above the pinch, the steam system and half of the process-process interactions are treated in a holistic manner. Likewise, below the pinch, the cooling water system and the process-process interactions are treated holistically. Furthermore, because hot and cold utilities are confined to separate regions, and because heat should not be transferred over the pinch, the above and below pinch regions are independent of each other.

Just as the three regions in the old paradigm can be best visualised on the hot and cold composite curves, the new paradigm can best be visualised on the grand composite curve (Figure 4.2). Here, for example one can see how the hot utility needs to cooperate with the hot process streams in heating the cold process streams. Because of this, further trade-offs between the utility and the process streams can be exploited, which are not available if the utilities are confined to their own regions at the extremities of the processes.

4 Model Development

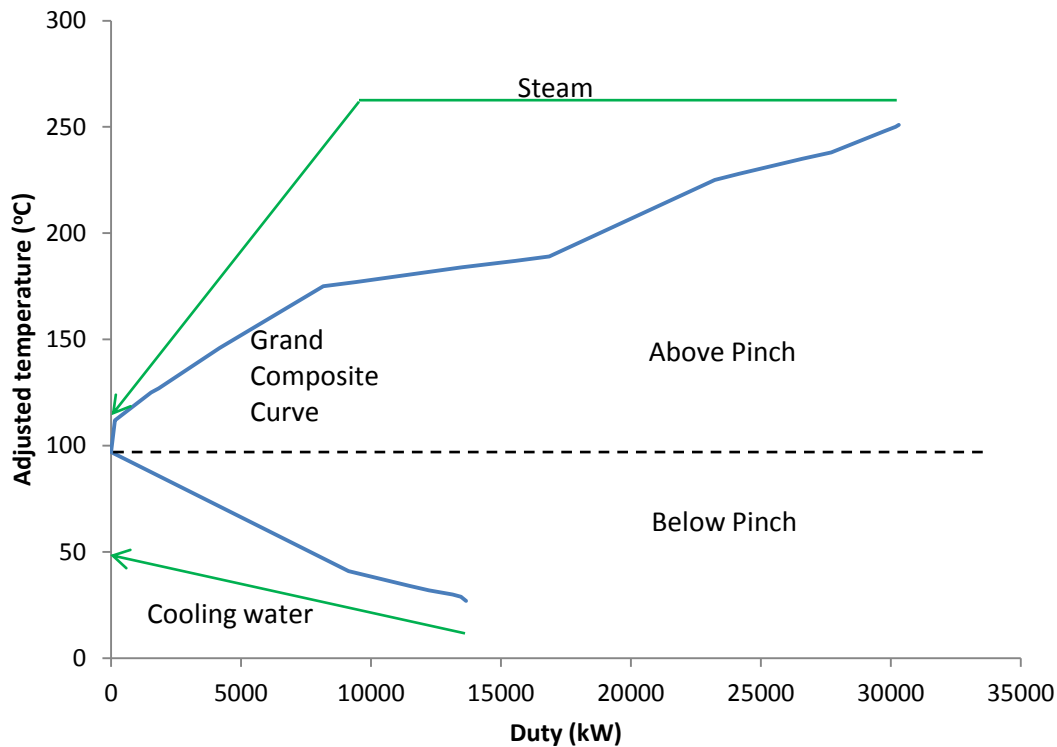


Figure 4.2: New paradigm in which the pinch defines the boundary between two regions of application.

In this work the new paradigm will be utilised. Since both regions contain only either a hot or a cold utility, and because the original problem can be decomposed into two separate sub problems, two models will be developed. The two models will naturally be very similar to each other, but will contain unique elements that address the specific needs encountered above and below the pinch.

On a last note, it must be stated that there are numerous methods of determining the location of the pinch point. Methods such as the graphical shifting of composite curves, problem table algorithm and process-process integration models can all be used.

4.3 Superstructures

The superstructures that will be presented here provide a generic visualisation of the system. Because the superstructures are generic, models can be developed that can accommodate many different processes, rather than a model developed specifically for a single case.

The superstructures presented here are built from elements of the superstructures of the methods on which they were based, those discussed in Chapter 3. Special mention must be made regarding the process-process heat integration method though. In this work, a modified version of the interval based method by Isafiade and Fraser (2008) will be used. The interval based method is desirable because having one set of process streams fixed is convenient for integrating the process-process heat integration model with the utility heat integration model. Leaving the other set of process streams variable gives the model the flexibility to explore many options.

One issue with the interval based method is the way in which intervals are defined. Isafiade and Fraser (2008) suggest that the supply and demand temperatures of the fixed set of process streams be used to define the boundaries of the intervals. This approach will lead to many intervals being created, some with only a small temperature change. Besides for the fact that having many small intervals greatly increases the number of variables that must be solved for by the model, it is impractical to expect that many small heat exchangers must be purchased to cater for these small intervals.

Inspired by the block decomposition method of Zhu *et al* (1995), the intervals in the present work will be defined similar to the way in which blocks are defined, rather than in the way described by Isafiade and Fraser (2008). This will lead to intervals that have more physical meaning, a reduction in the number of

4 Model Development

variables that must be solved for as well as preventing impractically small heat exchangers being called for.

4.3.1 Above Pinch Superstructure

The super structure for the Above Pinch Model is given in Figure 4.3. Here a set of K intervals are created, numbered in order of decreasing temperature. A set of C cold process streams that require heating are present, and will be the fixed set of process streams. As such, not each cold stream c exists in each interval k . The presence or absence of stream c in interval k is determined by the supply and target temperatures of c in relation to the boundary temperatures of interval k .

A set of H hot process streams that require cooling are also present. Since the hot streams are not the fixed streams, they exist across all of the intervals, at least hypothetically. In Figure 4.3, three intervals are shown to demonstrate how the hot streams exist across all intervals, whereas cold streams only exist in certain intervals. Here, the centre interval, interval k , represents the general case, and will be the reference when developing the mathematical model.

In Figure 4.3, one can see that within each interval, each hot stream is permitted to exchange heat with each cold stream, provided that the cold stream exists within that particular interval.

4 Model Development

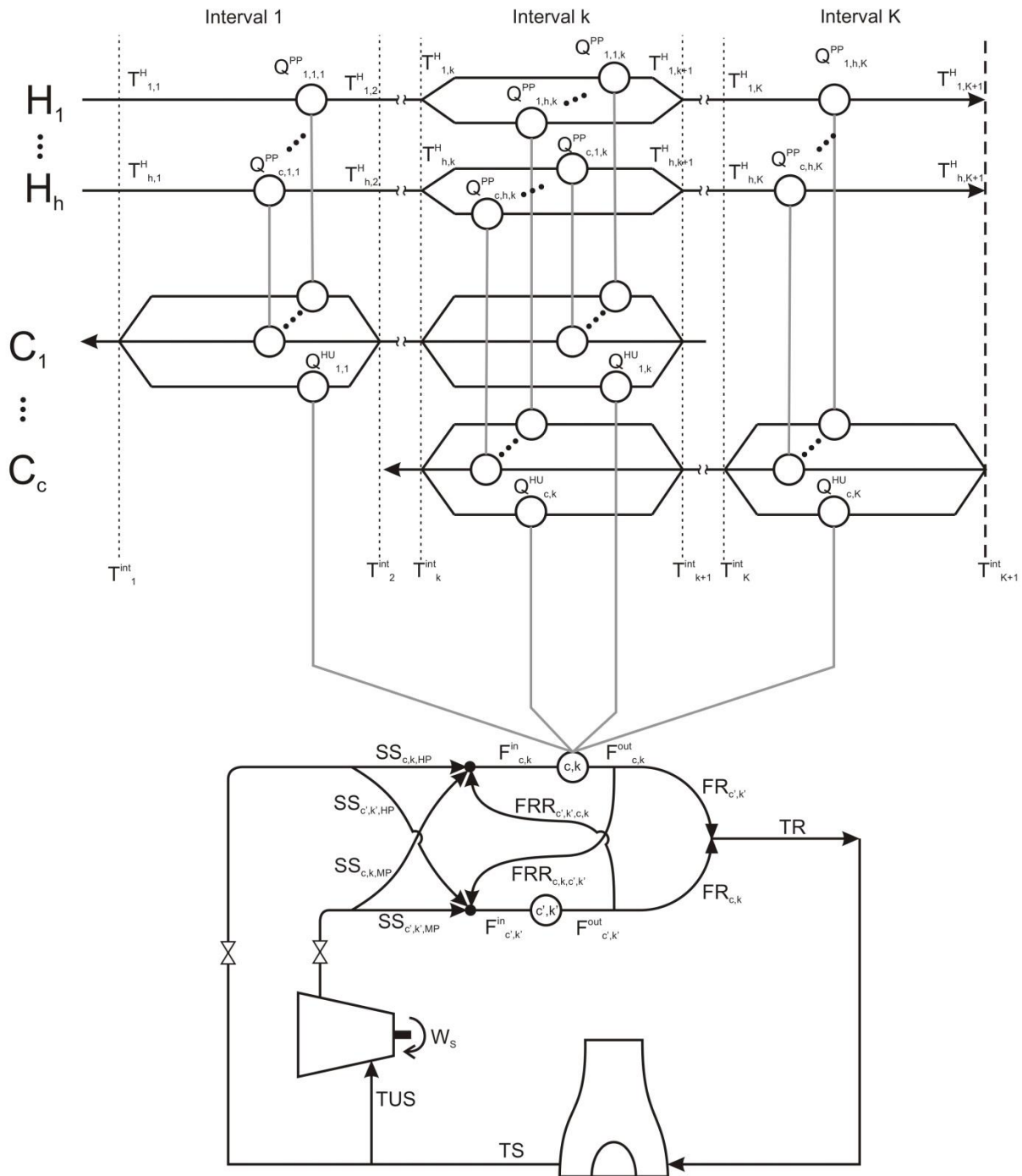


Figure 4.3: Above Pinch superstructure

In addition to the process-process interactions, Figure 4.3 also contains the steam system that will supply utility heat to the cold process streams. In this steam system, a boiler generates high pressure steam, which is the highest steam level in the set L . Part of the steam is supplied as high pressure steam for use in heating the cold process streams, and part is supplied to a high pressure steam

4 Model Development

turbine. After extracting shaft work from the steam turbine, the exhaust steam is supplied as medium pressure steam to the cold processes. Only two steam levels are employed here, in accordance with the findings of Beangstrom (2013). It is, however, a simple matter to modify the superstructure should additional steam levels and steam turbines be unavoidable.

Each cold stream c is permitted to receive utility heat within each interval k . This creates a set of (C, K) process heaters. As can be seen in Figure 4.3, process heater (c, k) can be supplied with high pressure saturated steam and medium pressure saturated steam, as well as hot liquid reuse from any other process heater (c', k') in the set. The liquid leaving a process heater (c, k) can be returned to the boiler, or if hot enough, can be supplied for reuse in any other process heater (c', k') in the set. The collected boiler return streams are then returned to the boiler before repeating the cycle.

4.3.2 Below Pinch Superstructure

The superstructure employed in the Below Pinch Model is similar to that of the Above Pinch Model, but with the necessary changes for cooling rather than heating. The superstructure for the Below Pinch Model is given in Figure 4.4. Here a set of K intervals are created, numbered in order of decreasing temperature. A set of H hot process streams that require cooling are present, and will be the fixed set of process streams. As such, not each hot stream h exists in each interval k . The presence or absence of stream h in interval k is determined by the supply and target temperatures of h in relation to the boundary temperatures of interval k .

A set of C cold process streams that require heating are also present. Since the cold streams are not the fixed streams, they exist across all of the intervals, at

4 Model Development

least hypothetically. In Figure 4.4, three intervals are shown to demonstrate how the cold streams exist across all intervals, whereas hot streams only exist in certain intervals. Here, the centre interval, interval k , represents the general case, and will be the reference when developing the mathematical model.

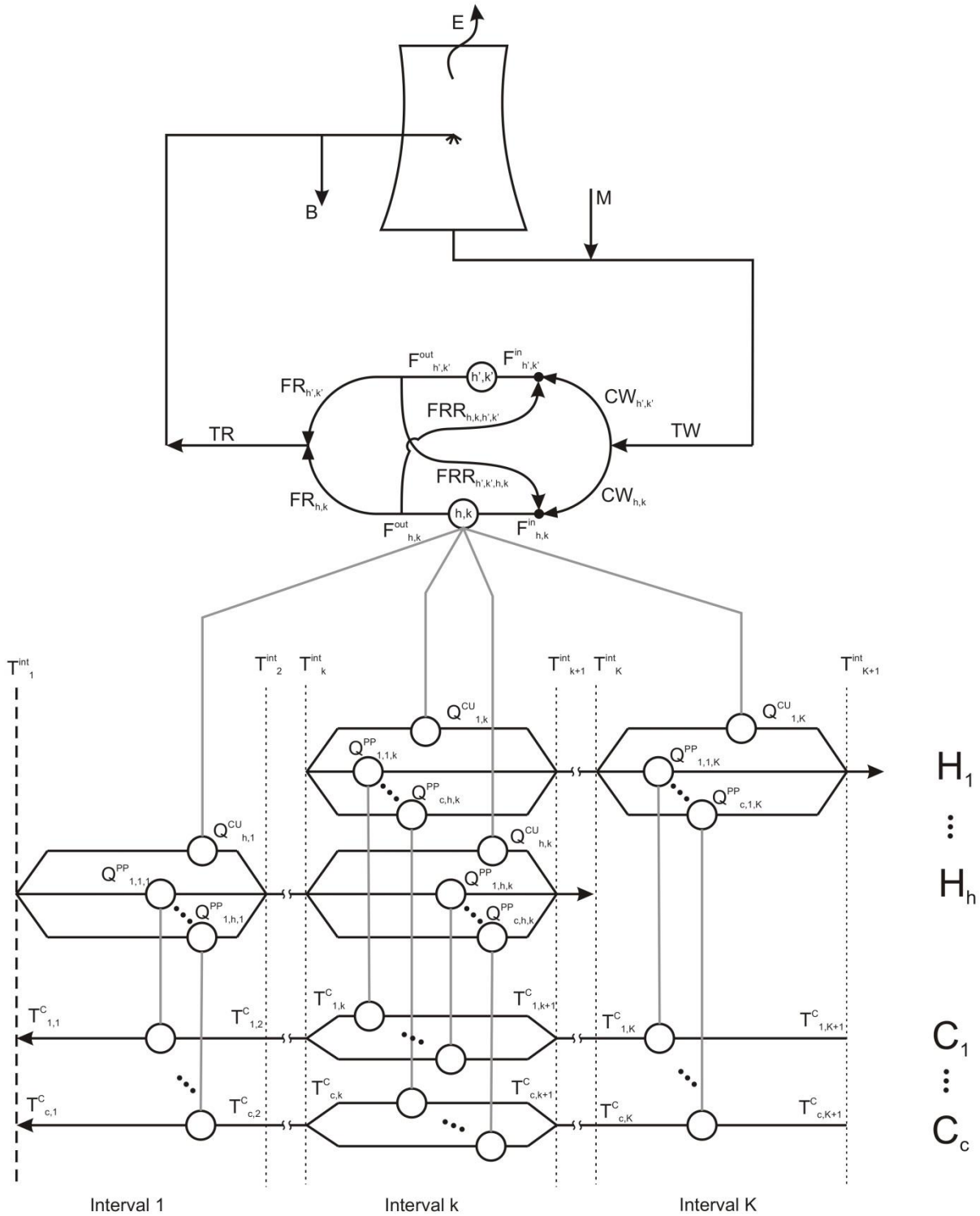


Figure 4.4: Below Pinch superstructure

4 Model Development

In Figure 4.4, one can see that within each interval, each hot stream is permitted to exchange heat with each cold stream, provided that the hot stream exists within that particular interval.

In addition to the process-process interactions, Figure 4.4 also contains the cooling water network that will supply utility cooling to the hot process streams. In this network, a counter current natural draught cooling tower is employed to cool the cooling water. A warm blow-down stream is removed before the water enters the tower, in order to limit the accumulation of dissolved salts. Within the cooling tower, further water losses are encountered due to evaporation losses. Following that, cold fresh make-up water is added to the cooling water to make up for the losses, before the cooling water is supplied to the process coolers.

Each hot stream h is permitted to receive utility cooling within each interval k . This creates a set of (H, K) process coolers. As can be seen in Figure 4.4, process cooler (h, k) can be supplied with cooling water directly from the cooling tower, as well as with reuse water from any other process cooler (h', k') in the set. The water leaving process cooler (h, k) can be returned to the cooling tower or, if cold enough, supplied for reuse in any other process cooler (h', k') . The collected return streams are returned to the cooling tower for cooling, before repeating the cycle.

In the Below Pinch Model, another set must be introduced to handle the discretisation of the cooling tower. A set Z is introduced representing points progressing up the height of the packing inside the cooling tower. This set is used when solving the differential equations of the cooling tower to index the properties located at a specific height within the cooling tower packing.

4.4 Existence Matrices

In both the Above Pinch Model and the Below Pinch Model, one set of process streams is fixed. The streams in the fixed set only exist in certain intervals, dependent on their supply and target temperatures. Since the supply and target temperatures for all of the streams are known *a priori*, as well as the interval boundary temperatures, it is possible to predetermine in which intervals a particular process stream will participate in.

In the Above Pinch Model and the Below Pinch Model, an existence matrix will be used to indicate the existence of one of the fixed streams within a particular interval. Although a mathematical model will be able to determine this for itself, by predetermining this matrix, the number of variables that must be solved for can be reduced.

In the Above Pinch Model, the term $E(c, k)$ will be used to denote whether cold process stream c exists in interval k or not. If the stream exists, $E(c, k)$ will have a value of 1, and if not, it will have a value of 0. This matrix of 1s and 0s should not be confused with binary variables. The matrix is a predetermined parameter, the elements of which will be used in Boolean logic operators to reduce the number of variables and equations that need to be solved. The method for constructing this matrix is simple and is given in pseudo code below. The procedure begins by creating a $C \times K$ matrix containing only 0s. Thereafter, the following nested loop is executed:

4 Model Development

```

Loop over C
  Loop over K
    If ( $T_c^{tar} > T_{k+1}^{int}$ ) and ( $T_c^{sup} < T_k^{int}$ )
       $E(c, k) = 1$ 
    End If
  End Loop
End Loop

```

As has been mentioned, in the Above Pinch Model the set of cold streams represents the fixed set of process streams. As such, the temperatures $T_{c,k}^C$ are fixed and can be calculated as parameters before the model is executed. By making use of the existence matrix developed above as a logic operator, the pseudo code given below can be used to assign these temperatures, taking note of the supply and target temperatures of the cold streams.

```

Loop over C
  Loop over K
    If ( $E(c, k)$ ) and ( $T_c^{tar} < T_k^{int}$ )
       $T_{c,k}^C = T_c^{tar}$ 
    Else If ( $E(c, k)$ ) and ( $T_c^{tar} \geq T_k^{int}$ )
       $T_{c,k}^C = T_k^{int}$ 
    End If

    If ( $E(c, k)$ ) and ( $T_c^{sup} \geq T_{k+1}^{int}$ )
       $T_{c,k+1}^C = T_c^{sup}$ 
    End If
  End Loop
End Loop

```

4 Model Development

Similar to the Above Pinch Model, in the Below Pinch Model the existence matrix $E(h, k)$ will be used to denote if hot stream h exists in interval k . To create this existence matrix, an $H \times K$ matrix of 0s is first created. Thereafter, the following nested loop is executed:

```
Loop over  $H$ 
  Loop over  $K$ 
    If  $(T_h^{sup} > T_{k+1}^{int})$  and  $(T_h^{tar} < T_k^{int})$ 
       $E(h, k) = 1$ 
    End If
  End Loop
End Loop
```

In the Below Pinch Model the set of hot streams represents the fixed set of process streams. As such, the temperatures $T_{h,k}^H$ are fixed and can be calculated as parameters before the model is executed. Making use of the existence matrix developed above as a logic operator, the pseudo code given below can be used to assign these temperatures, taking note of the supply and target temperatures of the hot streams.

4 Model Development

Loop over H

Loop over K

If $(E(h, k))$ and $(T_h^{sup} < T_k^{int})$

$$T_{h,k}^H = T_h^{sup}$$

Else If $(E(h, k))$ and $(T_h^{sup} \geq T_k^{int})$

$$T_{h,k}^H = T_k^{int}$$

End If

If $(E(h, k))$ and $(T_h^{tar} \geq T_{k+1}^{int})$

$$T_{h,k+1}^H = T_h^{tar}$$

End If

End Loop

End Loop

4.5 Model Constraints

The mathematical constraints for the two models employed on both sides of the pinch will be presented below. These constraints arise from performing mass and energy balances over the various nodes in the superstructures, as well as equations describing the function of other unit operations.

When solving these models, two cases will be considered. In the first case, the utility systems exist, and the models are required to determine the heat exchanger network that minimises the utility flowrates and debottlenecks the process. In the second case, the model must optimise the utility system and the heat exchanger network simultaneously. The specifics of both cases will be discussed below.

Case 1- In the first case, the steam turbine and cooling tower have been designed beforehand. Above the pinch, the saturation temperatures and pressures for the HP and MP steam levels have been selected. A steam turbine has been sized to supply the required quantity of shaft work, producing a fixed the flowrate of MP steam. The task of the Above Pinch Model is to synthesize a heat exchanger network that will best utilise the available MP steam while minimising the flowrate of HP steam required, debottlenecking the boiler. Below the pinch, the cooling tower has been sized beforehand. The task of the Below Pinch Model is to synthesize the heat exchanger network to minimise the cooling water flowrate, thereby debottlenecking and raising the effectiveness of the cooling tower.

Case 2- In the second case, the utility systems and heat exchanger networks are optimised simultaneously. Above the pinch, the saturation temperature of the HP steam level has been selected to ensure that it is high enough to meet all process requirements. The Above Pinch Model must size the steam turbine and

4 Model Development

select the MP steam level, while at the same time synthesizing the heat exchanger network to minimise the total steam flowrate demanded of the boiler. The task of the Below Pinch Model is synthesize the heat exchanger network while at the same time to sizing the cooling tower to ensure minimum construction costs for the cooling tower.

It should be noted that when the problem is split at the pinch, the minimum energy targets become intrinsically fixed. These energy targets are not affected by the subsequent application of heat integration principles to the two separate sub-problems. The goal of the two models is therefore not to reduce energy consumption, but to either debottleneck the process or design for minimum capital expenditure.

4.5.1 Above Pinch Model

The Above Pinch Model begins with energy balances performed over the hot and cold process streams in the superstructure presented in Figure 4.3. Equation 4.1 states that the total quantity of heat that must be removed from hot stream h is equal to the sum of heat transferred to all cold streams across all intervals. Here the condition used in the summation, $c, k|E(c, k)$, states that the summation must be performed over all c and all k , provided that the element (c, k) exists, denoted by the value 1 in the existence matrix. In doing this, variables that represent non-existent entities are excluded from the model during the compilation stage, rather than expecting the solver to essentially confirm that the variables are indeed zero. This reduces the size and complexity of the model.

$$QH_h = \sum_{c, k|E(c, k)} Q_{c, h, k}^{PP} \quad \forall h \in H \quad (4.1)$$

4 Model Development

Similar to Equation 4.1, Equation 4.2 states that the total quantity of heat that must be supplied to cold stream c is equal to the sum of heat received from all hot streams across all intervals, with the addition that heat may also be received from the hot utility.

$$QC_c = \sum_{h,k|E(c,k)} Q_{c,h,k}^{PP} + \sum_{k|E(c,k)} Q_{c,k}^{HU} \quad \forall c \in C \quad (4.2)$$

Just as energy balances can be performed over entire streams, energy balances can be performed over individual intervals. Equation 4.3 states that the quantity of heat removed from hot stream h in interval k , measured by the change in the temperature of the stream between the interval boundaries, is equal to the sum of heat transferred to all cold streams within that interval. Equation 4.4 states that the quantity of heat received by cold stream c in interval k is equal to the sum of the heat received from all hot streams in the interval, as well as the heat received from the hot utility. Note that similar to above, where the existence matrix was used to determine which variables need not be included in the constraint, the existence matrix is used here to prevent the model including unnecessary constraints.

$$(T_{h,k}^H - T_{h,k+1}^H) \cdot CP_h = \sum_{c|E(c,k)} Q_{c,h,k}^{PP} \quad \forall h, k \in H, K \quad (4.3)$$

$$(T_{c,k}^C - T_{c,k+1}^C) \cdot CP_c = \sum_h Q_{c,h,k}^{PP} + Q_{c,k}^{HU} \quad \forall c, k \in \{C, K|E(c,k)\} \quad (4.4)$$

In the Above Pinch Model, the set of cold process streams is set as the fixed set of process streams. As such, the temperatures of these streams as they transition from one interval to the next are known and constant. The hot streams, however,

4 Model Development

exist hypothetically across all of the intervals, and the temperatures at the interval boundaries are variables. This requires that constraints be introduced to ensure that the supply and target temperatures are met. Equation 4.5 states that the temperature of hot stream h as it enters the first interval must be equal to the supply temperature of that hot stream. Likewise, Equation 4.6 states that the temperature of hot stream h as it leaves the last interval must be equal to the target temperature of that hot stream. Note that since the Above Pinch Model represents a subsection of the total problem, this target temperature will either be the true target temperature of the hot stream (if the hot stream terminates above the pinch) or the pinch temperature (acting as a pseudo target temperature if the hot stream transitions over the pinch).

$$T_{h,1}^H = T_h^{sup} \quad \forall h \in H \quad (4.5)$$

$$T_{h,K+1}^H = T_h^{tar} \quad \forall h \in H \quad (4.6)$$

In addition to setting the end points of the hot streams, it is important to ensure that the temperature of the hot streams decrease monotonically as the stage number increases. This is accomplished in Equation 4.7.

$$T_{h,k}^H \geq T_{h,k+1}^H \quad \forall h, k \in H, K \quad (4.7)$$

In order for heat exchange to occur, there must be sufficient driving force for exchange. To ensure this, one must first establish a binary variable $pp_{c,h,k}$ denoting whether or not heat exchange is occurring between cold stream c and hot stream h in interval k . If $pp_{c,h,k}$ is 1, denoting that heat exchange is occurring, then Equation 4.8 states that at the left hand boundary of interval k , the difference between the hot and cold stream temperatures must be greater

4 Model Development

than ΔT_{\min} . By choosing Γ as some sufficiently large value, Equation 4.8 will automatically be satisfied when $pp_{c,h,k}$ is 0, denoting no heat exchange between this pair. Equation 4.9 performs the same function with the temperatures at the right hand boundary of interval k . Together, Equations 4.8 and 4.9 ensure that when a heat exchanger is installed between hot stream h and cold stream c in interval k , the temperature difference between the hot and cold stream is greater than or equal to ΔT_{\min} on both sides of the heat exchanger.

$$T_{h,k}^H - T_{c,k}^C \geq \Delta T_{\min} - \Gamma(1 - pp_{c,h,k}) \quad \forall c, h, k \in \{C, H, K | E(c, k)\} \quad (4.8)$$

$$T_{h,k+1}^H - T_{c,k+1}^C \geq \Delta T_{\min} - \Gamma(1 - pp_{c,h,k}) \quad \forall c, h, k \in \{C, H, K | E(c, k)\} \quad (4.9)$$

In order to link the binary variable used in Equations 4.8 and 4.9 to the occurrence of heat exchange, Equation 4.10 is used. Here, if $pp_{c,h,k}$ takes on a value of 0, $Q_{c,h,k}^{PP}$ is forced to take on a value of 0 too. If $pp_{c,h,k}$ takes on a value of 1, $Q_{c,h,k}^{PP}$ is free to take on some positive value. Since the cold stream should not receive more heat than what is required within that interval, the interval temperatures are used to calculate the upper bound on heat transfer within that interval.

$$Q_{c,h,k}^{PP} \leq pp_{c,h,k} \cdot [CP_c(T_{c,k}^C - T_{c,k+1}^C)] \quad \forall c, h, k \in \{C, H, K | E(c, k)\} \quad (4.10)$$

The above constraints handle the process-process interactions of superstructure. Similar mass and energy balances must also be performed over the steam system, bearing in mind that the two systems are interacting.

In the steam system, there are two phases that must be accounted for: the gaseous steam phase and the liquid condensate phase. In addition to this, special

4 Model Development

consideration must be made for the fact that there is both high pressure steam and medium pressure steam. These considerations are all taken into account in the mass and energy balances performed over the steam system.

Beginning with mass balances over the total steam system, Equation 4.11 states that the total quantity of steam supplied of a particular level is equal to the sum of the quantity of steam of that level supplied to each cold stream c in each interval k in which it exists. Equation 4.12 states that the total flowrate of liquid returned to the boiler is equal to the sum of the liquid return from each cold stream c in each interval k . Since mass must be conserved, these two quantities must be equal (Equation 4.13). Furthermore, since saturated liquid is a product of condensing saturated steam, Equation 4.14 ensures that the total amount of saturated liquid of a specific level supplied to the various process heaters does not exceed the quantity of steam supplied at that level.

$$TS_l = \sum_{c,k|E(c,k)} SS_{c,k,l} \quad \forall l \in L \quad (4.11)$$

$$TR = \sum_{c,k|E(c,k)} FR_{c,k} \quad (4.12)$$

$$\sum_l TS_l = TR \quad (4.13)$$

$$\sum_{c,k|E(c,k)} SL_{c,k,l} \leq TS_l \quad \forall l \in L \quad (4.14)$$

4 Model Development

Turning to the individual utility heaters, Equation 4.15 states that if cold stream c exists in interval k , the total mass flowrate of utility flowing into the utility heater dedicated to that process is equal to the sum of saturated steam and saturated liquid condensate supplied at the various levels to that process heater, plus the sum of hot liquid reused from all other process heaters. Likewise, Equation 4.16 states that the total mass flowrate flowing out of the particular process heater is equal to the flowrate of saturated liquid as a direct consequence of the saturated steam condensing, plus the reuse streams sent to all other process heaters and the boiler return stream. Conservation of mass requires that these two flowrates be equal (Equation 4.17). To prevent a process heater recycling hot liquid back to itself, Equation 4.18 is implemented.

$$F_{c,k}^{in} = \sum_l SS_{c,k,l} + \sum_l SL_{c,k,l} + \sum_{c'k'|E(c'k')} FRR_{c',k',c,k} \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.15)$$

$$F_{c,k}^{out} = \sum_l SS_{c,k,l} + \sum_{c'k'|E(c'k')} FRR_{c,k,c',k'} + FR_{c,k} \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.16)$$

$$F_{c,k}^{in} = F_{c,k}^{out} \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.17)$$

$$FRR_{c,k,c,k} = 0 \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.18)$$

At this point, two binary variables $x_{c,k,l}$ and $y_{c,k}$ are introduced to indicate which processes are utilising saturated steam of a particular level, and which are

4 Model Development

utilising hot liquid. Equation 4.19 states that when $x_{c,k,l}$ is 0, no steam of level l is supplied to that process, but when it is 1, steam of level l is permitted up to a value lower than an upper bound. Equation 4.20 performs the same function for the use of hot liquid. Equation 4.21 ensures that at least one source of utility heat is available to each cold stream c .

$$SS_{c,k,l} \leq x_{c,k,l} \cdot SS_{c,k,l}^U \quad \forall c, k, l \in \{C, K, L | E(c, k)\} \quad (4.19)$$

$$\sum_l SL_{c,k,l} + \sum_{c'k' | E(c'k')} FRR_{c',k',c,k} \leq y_{c,k} \cdot HL_{c,k}^U \quad \forall c, k \in \{C, K | E(c, k)\} \quad (4.20)$$

$$\sum_{k,l | E(c,k)} x_{c,k,l} + \sum_{k | E(c,k)} y_{c,k} \geq 1 \quad \forall c \in C \quad (4.21)$$

It may happen that a particular process heater might be split between two steam levels, or between saturated steam and hot liquid. To prevent this, Equation 4.22 must be implemented. If a maximum of M splits are permitted per process heater per interval, then Equation 4.23 should be implemented instead.

$$\sum_l x_{c,k,l} + y_{c,k} \leq 1 \quad \forall c, k \in \{C, K | E(c, k)\} \quad (4.22)$$

$$\sum_l x_{c,k,l} + y_{c,k} \leq M \quad \forall c, k \in \{C, K | E(c, k)\} \quad (4.23)$$

The upper bound on the flowrate of saturated steam of level l supplied to cold stream c in interval k is given in Equation 4.24. This upper bound is based on the observation that within an interval. It is possible for the entire heat

4 Model Development

requirement of a cold stream to be satisfied by saturated steam. The upper bound on the flowrate of hot liquid to cold stream c in interval k is given in Equation 4.25. This can be understood by considering Figure 4.5, in which it can be seen that the maximum liquid flowrate occurs when the hot liquid is separated from the cold process by ΔT_{\min} on both ends of the heat exchanger.

$$SS_{c,k,l}^U = \frac{CP_c(T_{c,k}^C - T_{c,k+1}^C)}{\lambda_l} \quad \forall c, k, l \in \{C, K, L|E(c, k)\} \quad (4.24)$$

$$HL_{c,k}^U = \frac{CP_c(T_{c,k}^C - T_{c,k+1}^C)}{Cp_w(T_{c,k}^C - T_{c,k+1}^C)} = \frac{CP_c}{Cp_w} \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.25)$$

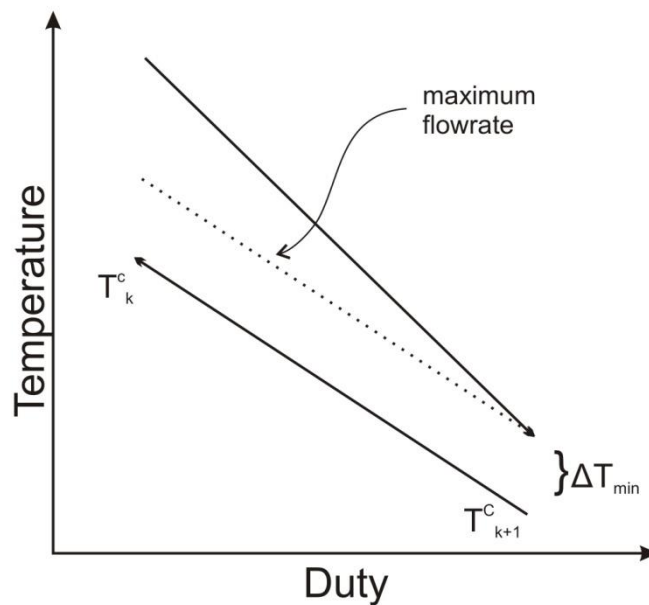


Figure 4.5: Relationship between the cold stream and the maximum hot liquid flowrate

The upper bound on the hot liquid flowrate in Equation 4.25 makes provision for the fact that cold stream c may be heated only by hot liquid in interval k .

4 Model Development

This upper bound works well in conjunction with Equation 4.20. When the heat requirements of cold stream c in interval k are split between hot liquid and other heat sources, then the upper bound in Equation 4.25 is somewhat higher than what is required. For this reason Equation 4.26 is added to ensure that the liquid flowrate into a process heater is never greater than what is required to supply the part load.

$$\sum_l SL_{c,k,l} + \sum_{c'k'|E(c'k')} FRR_{c',k',c,k} \leq \frac{Q_{c,k}^{HU}}{Cp_w(T_{c,k}^C - T_{c,k+1}^C)} \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.26)$$

Having taken care of mass balances within the steam system, energy balances must be performed to ensure the steam system is capable of performing the requisite heating. Equation 4.27 states that the amount of latent heat supplied to a cold stream c in interval k is equal to the sum of the latent heat supplied by the various steam levels. Equation 4.28 is used to determine the latent heat of condensation of the steam levels based on the saturation temperatures of the steam levels (Mavromatis & Kokossis, 1998).

$$Q_{c,k}^{SS} = \sum_l (SS_{c,k,l} \cdot \lambda_l) \quad \forall c, k \in \{C, K|E(c, k)\} \quad (4.27)$$

$$\lambda_l = 2726 - 4.13 \cdot T_l^{sat} \quad \forall l \in L \quad (4.28)$$

Note that in Case 1, the saturation temperatures of the steam levels are fixed, and the values determined by Equation 4.28 represent parameters. In Case 2, where the steam levels are to be optimised, the values in Equation 4.28 are

4 Model Development

variables and Equation 4.28 must be included as a model constraint. Equation 4.29 is used to ensure that if the saturation temperature of a particular steam level is lower than the minimum temperature required to heat cold stream c in interval k , the binary variable for that steam level is forced to be 0, prohibiting the use of that steam level in that instance.

$$(T_{c,k}^C + \Delta T_{min}) \cdot x_{c,k,l} \leq T_l^{sat} \quad \forall c, k, l \in \{C, K, L | E(c, k)\} \quad (4.29)$$

The quantity of heat supplied to cold stream c in interval k as sensible heat is determined using Equation 4.30. This sensible heat arises from both the saturated liquid supplied to the process heater, as well as the hot liquid reuse stream supplied from other process heaters. It must be noted that the outlet temperature for each process heater has been set to the limiting outlet temperature $(T_{h,k+1}^C + \Delta T_{min})$ in accordance with the optimality condition proven by Savelski and Bagajewicz (2000). Here, ΔT_{min} has been used to ensure that there is always sufficient temperature difference for heat exchange. Equation 4.31 states that the sum of the latent heat and sensible heat must fulfil the utility heat required by stream c in interval k .

$$Q_{c,k}^{HL} = Cp_w \cdot \sum_l (SL_{c,k,l} \cdot T_l^{sat}) + Cp_w \cdot \sum_{c'k' | E(c'k')} FRR_{c',k',c,k} \cdot (T_{h',k'+1}^C + \Delta T_{min}) - Cp_w \cdot F_{c,k}^{in} \cdot (T_{h,k+1}^C + \Delta T_{min}) \quad \forall c, k \in \{C, K | E(c, k)\} \quad (4.30)$$

$$Q_{c,k}^{HU} = Q_{c,k}^{SS} + Q_{c,k}^{HL} \quad \forall c, k \in \{C, K | E(c, k)\} \quad (4.31)$$

4 Model Development

The last section of the steam systems that must be covered is the steam turbine. Note that in Case 1, the steam levels and turbine have already been designed, and the following values and equations represent parameters that are calculated beforehand. In Case 2, where the steam levels are optimised together with the process, the following are model constraints.

Equation 4.32 relates the shaft work target to the turbine steam supply flowrate, and the isentropic enthalpy change between the steam levels. This isentropic enthalpy change is determined using Equation 4.33. Furthermore, since the medium pressure steam level is a product of the steam turbine, the total mass flowrate of MP steam supplied to the steam system must be less than or equal to the mass flowrate of HP steam supplied to the turbine (Equation 4.34).

$$W^s = \frac{1}{B} (3.6 \cdot \overline{\Delta H}^{is} \cdot TUS - A) \quad (4.32)$$

$$\overline{\Delta H}^{is} = \frac{T_{HP}^{sat} - T_{MP}^{sat}}{391.8 + 2.215T_{HP}^{sat}} \quad (4.33)$$

$$TS_{MP} \leq TUS \quad (4.34)$$

The two parameters A and B in Equation 4.32 are calculated using Equations 4.35 and 4.36. The coefficients here were given in Table 3.2 as discussed in Section 3.6. If more than two steam levels are utilised, with additional steam turbines, then Equations 4.35 and 4.36 must be adjusted accordingly for each new turbine

4 Model Development

$$A = a_1 + a_2 T_{HP}^{sat} \quad (4.35)$$

$$B = b_1 + b_2 T_{HP}^{sat} \quad (4.36)$$

The above constraints constitute the Above Pinch Model. In Case 1, where the steam levels and turbine are designed beforehand, Equations 4.24, 4.25, 4.28, 4.32, 4.33, 4.35 and 4.36 represent parameters that are calculated prior to executing the model. All of the steam level saturation temperatures T_i^{sat} are parameters, as well as the flowrate of MP steam issuing from the exhaust of the steam turbine. As such, the remaining equations which form the model to be optimised are linear.

Since in Case 1, the flowrate of MP steam is fixed, the supply of HP steam to the process heaters can be manipulated to influence the boiler size, thereby reducing the boiler purchase cost, or debottlenecking the process. The objective function for Case 1 is therefore simply to minimise the total flowrate of HP steam supplied to the network of process heaters (Equation 4.37). This, together with the constraints, constitutes an MILP model.

$$\text{Min}(TS_{HP}) \quad (4.37)$$

In Case 2, the steam levels and steam turbine (with the exception of the saturation temperature of the HP steam level directly from the boiler) are variables that must be optimised together with the process. Only Equations 4.24, 4.25, 4.35 and 4.36 represent parameters that must be calculated prior to executing the model. The remainder of the equations above form the model to be optimised. Due to the variable steam levels, a number of these equations are now nonlinear.

4 Model Development

In Case 2, the supply of HP steam to the process heaters, as well as the supply of HP steam to the steam turbine can be manipulated to influence the boiler size, thereby reducing the boiler purchase cost, or debottlenecking the process. Reducing the total steam flowrate not only reduces boiler size, but will favour smaller turbines as well. The objective function for Case 2 is therefore to minimise the total steam flowrate required from the boiler (Equation 4.38). This, together with the constraints, constitutes an MINLP model.

$$\text{Min}(TS_{HP} + TUS) \quad (4.38)$$

4.5.2 Below Pinch Model

The Below Pinch Model is developed in much the same way as the Above Pinch Model was developed, with the exception that a cooling water system replaces the steam system. The Below Pinch Model begins by performing energy balances over the hot and cold streams in Figure 4.4. Equation 4.39 states that the total quantity of heat that must be removed from hot stream h is equal to the sum of heat transferred to all cold streams across all intervals, plus the heat removed by the cold utility in all intervals. Here the condition used in the summation, $h, k|E(h, k)$, states that the summation must be performed over all h and all k , provided that the element (h, k) exists, denoted by the value 1 in the existence matrix. In doing this, variables that represent non-existent entities are excluded from the model during the compilation stage, rather than expecting the solver to essentially confirm that the variables are indeed zero. This reduces the size and complexity of the model.

$$QH_h = \sum_{c,k|E(h,k)} Q_{c,h,k}^{PP} + \sum_{k|E(h,k)} Q_{h,k}^{CU} \quad \forall h \in H \quad (4.39)$$

4 Model Development

Equation 4.40 states that the total quantity of heat that must be supplied to cold stream c is equal to the sum of heat received from all hot streams across all intervals.

$$QC_c = \sum_{h,k|E(h,k)} Q_{c,h,k}^{PP} \quad \forall c \in C \quad (4.40)$$

Energy balances are also performed over the streams within the separate intervals. Equation 4.41 states that the quantity of heat removed from hot stream h in interval k , measured by the change in the temperature of the stream between the interval boundaries, is equal to the sum of heat transferred to all cold streams within that interval, as well as to the cold utility. Note that similar to above, the existence matrix is used to prevent unnecessary constraints from being included in the model. Equation 4.42 states that the quantity of heat received by cold stream c in interval k is equal to the heat received from all hot streams within the interval.

$$(T_{h,k}^H - T_{h,k+1}^H) \cdot CP_h = \sum_c Q_{c,h,k}^{PP} + Q_{h,k}^{CU} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.41)$$

$$(T_{c,k}^C - T_{c,k+1}^C) \cdot CP_c = \sum_{h|E(h,k)} Q_{c,h,k}^{PP} \quad \forall c, k \in C, K \quad (4.42)$$

Just as the set of cold process streams was designated as the fixed set of streams in the Above Pinch Model, in the Below Pinch Model the set of hot process streams is the fixed set of streams. As such, the temperatures of the hot streams as they transition from one interval to the next are known and constant. The cold streams, however, exist hypothetically across all of the intervals, and the temperatures at the interval boundaries are variables. Equation 4.43 ensures that the temperature of the cold stream, as it leaves the process through interval 1, is

4 Model Development

equal to the target temperature of the cold stream. Likewise, Equation 4.44 ensures that the temperature of the cold stream, as it enters the last interval, is equal to the supply temperature of the cold stream. Note that since the Below Pinch Model represents a subsection of the total problem, the target temperature in Equation 4.43 will either be the true target temperature of the cold stream (if the cold stream terminates below the pinch) or the pinch temperature (acting as a pseudo target temperature if the cold stream transitions over the pinch).

$$T_{c,1}^C = T_c^{tar} \quad \forall c \in C \quad (4.43)$$

$$T_{c,K+1}^C = T_c^{sup} \quad \forall c \in C \quad (4.44)$$

In addition to setting the end points of the cold streams, it is important to ensure that the temperature of the cold streams decrease monotonically as the stage number increases. This is accomplished in Equation 4.45.

$$T_{c,k}^C \geq T_{c,k+1}^C \quad \forall c, k \in C, K \quad (4.45)$$

In order for heat exchange to occur, there must be sufficient driving force for exchange. For this reason, a binary variable $pp_{c,h,k}$ is introduced, denoting whether or not heat exchange occurs between cold stream c and hot stream h in interval k . If $pp_{c,h,k}$ is 1, denoting that heat exchange is occurring, then Equation 4.46 states that at the left hand boundary of interval k , the difference between the hot and cold stream temperatures must be greater than ΔT_{\min} . By choosing Γ as some sufficiently large value, Equation 4.46 will automatically be satisfied when $pp_{c,h,k}$ is 0, denoting no heat exchange between this pair. Equation 4.47 performs the same function with the temperatures at the right hand boundary of interval k . Together, Equations 4.46 and 4.47 ensure that

4 Model Development

when a heat exchanger is installed between hot stream h and cold stream c in interval k , the temperature difference between the hot and cold stream is greater than or equal to ΔT_{\min} on both sides of the heat exchanger.

$$T_{h,k}^H - T_{c,k}^C \geq \Delta T_{\min} - \Gamma(1 - pp_{c,h,k}) \quad \forall c, h, k \in \{C, H, K | E(h, k)\} \quad (4.46)$$

$$T_{h,k+1}^H - T_{c,k+1}^C \geq \Delta T_{\min} - \Gamma(1 - pp_{c,h,k}) \quad \forall c, h, k \in \{C, H, K | E(h, k)\} \quad (4.47)$$

In order to link the binary variable used in Equations 4.46 and 4.47 to the occurrence of heat exchange, Equation 4.48 is introduced. Here, if $pp_{c,h,k}$ takes on a value of 0, $Q_{c,h,k}^{PP}$ is forced to take on a value of 0 too. If $pp_{c,h,k}$ takes on a value of 1, $Q_{c,h,k}^{PP}$ is free to take on some positive value below an upper bound. Since the hot stream should not reject more heat than what is required within that interval, the interval temperatures are used to calculate the upper bound on heat transfer within that interval.

$$Q_{c,h,k}^{PP} \leq pp_{c,h,k} \cdot [CP_h(T_{h,k}^H - T_{h,k+1}^H)] \quad \forall c, h, k \in \{C, H, K | E(c, k)\} \quad (4.48)$$

The above constraints handle the process-process interactions of the superstructure. Similar mass and energy balances must also be performed over the cooling water network, bearing in mind that the two systems are interacting.

The equations developed for the cooling water network are simpler than their steam system counterparts, because only a single liquid phase is considered when dealing with cooling water. The differential equations describing the operation of the cooling tower do add an increased level of difficulty though. The equations below will be developed to include only a single cooling tower, as this represents a general case for many small plants. If multiple cooling

4 Model Development

towers do exist, and their operation is substantially different to the point that they cannot be approximated as one large tower, then the model can be modified to include multiple cooling water sources in a fashion similar to the method developed by Gololo and Majozi (2011).

Beginning with mass balances over the total cooling water network, Equation 4.49 states that the total quantity of cooling water supplied to the cooling water network is equal to the sum of cooling water supplied to the individual process coolers. Likewise, Equation 4.50 states that the total amount of water returned to the cooling tower is equal to the sum of the individual return flowrates. By necessity, these two flowrates are equal (Equation 4.51).

$$TW = \sum_{h,k|E(h,k)} CW_{h,k} \quad (4.49)$$

$$TR = \sum_{h,k|E(h,k)} FR_{h,k} \quad (4.50)$$

$$TW = TR \quad (4.51)$$

Performing mass balances over the individual process coolers, Equation 4.52 states that the mass flowrate entering a process cooler associated with a particular hot stream within a particular interval is equal to the flowrate of cooling water supplied to that cooler plus the sum of reuse streams from all other coolers. Likewise, Equation 4.53 states that the mass flowrate out of the cooler is equal to the return to the cooling tower, plus the sum of reuse streams sent to all other coolers. Conservation of mass requires that these two flowrates be identical (Equation 4.54). Equation 4.55 is imposed to ensure that a particular cooler does not recycle water back to itself.

4 Model Development

$$F_{h,k}^{in} = CW_{h,k} + \sum_{h'k'|E(h'k')} FRR_{h',k',h,k} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.52)$$

$$F_{h,k}^{out} = FR_{h,k} + \sum_{h'k'|E(h'k')} FRR_{h,k,h',k'} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.53)$$

$$F_{h,k}^{in} = F_{h,k}^{out} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.54)$$

$$FRR_{h,k,h,k} = 0 \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.55)$$

To control which coolers are active, a binary variable, $y_{h,k}$, is introduced. In equation 4.56, the flow into a particular cooler is forced to be 0 if the associated binary variable is 0, and may take any value below an upper bound if the associated binary variable is 1. Equation 4.57 ensures that at least one option for utility cooling is available to each hot stream.

$$F_{h,k}^{in} \leq y_{h,k} \cdot L_{h,k}^U \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.56)$$

$$\sum_{k|E(h,k)} y_{h,k} \geq 1 \quad \forall h \in H \quad (4.57)$$

As in the Above Pinch Model, the upper bounds on the liquid flowrate are determined by considering the limiting feasible water flowrate. Equation 4.58 is therefore used to determine the constant upper boundary on the liquid flowrate. Equation 4.59 must be included to further limit the flow of water to the process cooler when only a part of the cooling duty is provided by the cooling water network.

4 Model Development

$$L_{h,k}^U = \frac{CP_H(T_{h,k}^H - T_{h,k+1}^H)}{Cp_w(T_{h,k}^H - T_{h,k+1}^H)} = \frac{CP_H}{Cp_w} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.58)$$

$$F_{h,k}^{in} \leq \frac{Q_{h,k}^{CU}}{Cp_w(T_{h,k}^H - T_{h,k+1}^H)} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.59)$$

When considering the energy balance across the individual process coolers, unlike in the steam system, only sensible heat is available in the cooling water network. This sensible heat, which must provide all the utility cooling to hot stream h in interval k , is made available through the supply of fresh cooling water to the process cooler, as well as though cold liquid reuse form other coolers (Equation 4.60). Note that the outlet temperature for each process cooler has been set to the limiting outlet temperature ($T_k^H - \Delta T_{min}$) in accordance with the optimality condition proven by Savelski and Bagajewicz (2000).

$$Q_{h,k}^{CU} = Cp_w \cdot F_{h,k}^{in} \cdot (T_k^H - \Delta T_{min}) - Cp_w \cdot \sum_{h'k'|E(h,k)} FRR_{h',k',h,k} \cdot (T_{k'}^H - \Delta T_{min}) - Cp_w \cdot CW_{h,k} \cdot T^{cw} \quad \forall h, k \in \{H, K|E(h, k)\} \quad (4.60)$$

Equation 4.61 is used to determine the temperature of the water returning to the cooling tower. This is one of the required inputs to the cooling tower model, as well as in Equation 4.62 to limit the return temperature to the cooling tower. The limitation on the cooling water return temperature is dependent on the packing material inside the tower.

$$T^{ret} = \frac{\sum_{h,k|E(h,k)} FR_{h,k} \cdot (T_{h,k}^H - \Delta T_{min})}{TR} \quad (4.61)$$

4 Model Development

$$T^{ret} \leq T^{limit} \quad (4.62)$$

The cooling tower model employed to predict the operation of the cooling tower is that developed by Kroger (2004). The model was developed from an analysis of a differential slice across the cooling tower, resulting in three differential equations representing the rate of change in water temperature, air enthalpy and humidity at any height in the tower. These differential equations must be solved numerically over the height of the column to predict its performance. In the present work, the fourth order Adams-Bashforth numerical method is used to discretise the differential equations in a manner that is acceptable to optimisation solvers. In doing so, the black box approach wherein the differential equations are solved externally to the optimisation solver is avoided. Furthermore, by including the discretised differential equations within the model, the solver has access to more information regarding the cooling tower, aiding the solution of the problem.

In discretizing the differential equations, the cooling tower must be divided into a set of Z slices, each with height s_{step} . The local rate of change in water temperature, air enthalpy and humidity over each slice can then be expressed using Equations 4.63, 4.64 and 4.65 respectively.

$$dT_z^w = \frac{G \cdot A_{cs}}{L_z} \left(\frac{1}{Cp_w} di_z^{ma} - T_z^w dW_z \right) \quad \forall Z \in Z \quad (4.63)$$

$$di_z^{ma} = \frac{h_a a_{f,z}}{G} \left(Le_z^f (i_z^{masw} - i_z^{ma}) + (1 - Le_z^f) i_z^v (W_z^{sw} - W_z) \right) \quad \forall Z \in Z \quad (4.64)$$

4 Model Development

$$dW_z = \frac{h_d a_{f,z}}{G} (W_z^{sw} - W_z) \quad \forall z \in Z \quad (4.65)$$

One of the assumptions made by Kröger (2004) is that the liquid flowrate inside the cooling tower is constant. This is, strictly speaking, not true since evaporative losses will cause the liquid flowrate to decrease as the water cascades down the packing. Furthermore, by modelling the reduction in the liquid flowrate, the evaporative losses can be estimated more accurately.

By noting that the loss of liquid flowrate is accounted for in the increase in humidity, Equation 4.66 is introduced to model the variable liquid flowrate inside the tower. Since this model has been developed for natural draught cooling towers, the dry air mass flowrate per area G is a function of the shell geometry and the prevailing weather conditions. Since the amount of air that will dissolve in water is substantially smaller than the bulk movement of air, G can be assumed to be constant over the height of the cooling tower packing.

$$dL_z = G \cdot dW_z \quad \forall z \in Z \quad (4.66)$$

Using the rate of change in cooling water temperature calculated in Equation 4.63, the water temperature in each slice can be determined using the fourth order Adams-Bashforth method. Since this method requires three known points in addition to the initial condition, the Euler method is used to calculate the water temperature in the first three slices (Equation 4.67). After this, Equation 4.68 implements the Adams-Bashforth method over the remainder of the tower height.

$$T_z^w = T_{z-1}^w + s_{step} \cdot dT_{z-1}^w \quad \forall z \in \{1,2,3\} \quad (4.67)$$

4 Model Development

$$T_z^w = T_{z-1}^w + \frac{S_{step}}{24} \cdot (55dT_{z-1}^w - 59dT_{z-2}^w + 37dT_{z-3}^w - 9dT_{z-4}^w) \quad \forall z \geq 4 \quad (4.68)$$

This procedure of using the Euler method to determine the first three points, and thereafter switching to the Adams-Bashforth method can be applied to the remaining differential equations. These are expressed in Equations 4.69 to 4.74.

$$i_z^{ma} = i_{z-1}^{ma} + S_{step} \cdot di_{z-1}^{ma} \quad \forall z \in \{1,2,3\} \quad (4.69)$$

$$i_z^{ma} = i_{z-1}^{ma} + \frac{S_{step}}{24} \cdot (55di_{z-1}^{ma} - 59di_{z-2}^{ma} + 37di_{z-3}^{ma} - 9di_{z-4}^{ma}) \quad \forall z \geq 4 \quad (4.70)$$

$$W_z = W_{z-1} + S_{step} \cdot dW_{z-1} \quad \forall z \in \{1,2,3\} \quad (4.71)$$

$$W_z = W_{z-1} + \frac{S_{step}}{24} \cdot (55dW_{z-1} - 59dW_{z-2} + 37dW_{z-3} - 9dW_{z-4}) \quad \forall z \geq 4 \quad (4.72)$$

$$L_z = L_{z-1} + S_{step} \cdot dL_{z-1} \quad \forall z \in \{1,2,3\} \quad (4.73)$$

$$L_z = L_{z-1} + \frac{S_{step}}{24} \cdot (55dL_{z-1} - 59dL_{z-2} + 37dL_{z-3} - 9dL_{z-4}) \quad \forall z \geq 4 \quad (4.74)$$

In addition to discretising the differential equations of the cooling tower model, the additional variables discussed in Section 3.4 must also be discretised, allowing the variables to be solved for in each slice of the cooling tower. Firstly,

4 Model Development

using the Antoine coefficients given by Lydersen (1983), Equation 4.75 describes the vapour pressure of water in each slice of the cooling tower. With this, the approximation given by Coulson and Richardson (1996) is used to calculate the saturated humidity within each slice (Equation 4.76)

$$P_z^{sat,w} = \exp \left[23.7093 - \frac{4111}{237.7 + T_z^w} \right] \quad \forall z \in Z \quad (4.75)$$

$$W_z^{sw} = \frac{18}{29} \frac{P_z^{sat,w}}{P_{atm} - P_z^{sat,w}} \quad \forall z \in Z \quad (4.76)$$

Equation 4.77 calculates the enthalpy of saturated air within each slice of the cooling tower (Kröger, 2004). Also, since the cooling tower model used does not assume a Lewis factor of 1, Equation 4.78 (Bosnjakovic, 1965) is used to calculate the Lewis factor for the air-water mixture. Lastly, by no longer treating the water flowrate as a constant, Equation 4.79 is used to adjust the mass transfer coefficient as the water flowrate varies down the height of the packing.

$$i_z^{masw} = C p_a T_z^w + W_z^{sw} \cdot (\lambda_0 + C p_v \cdot T_z^w) \quad \forall z \in Z \quad (4.77)$$

$$Le_z^f = 0.866^{0.667} \left(\frac{W_z^{sw} + 0.622}{W_z + 0.622} + 1 \right) / \ln \left(\frac{W_z^{sw} + 0.622}{W_z + 0.622} \right) \quad \forall z \in Z \quad (4.78)$$

$$h_d a_{f,z} = 1.881 \cdot G^{0.48} \left(\frac{L_z}{A_{CS}} \right)^{0.52} \quad \forall z \in Z \quad (4.79)$$

4 Model Development

Having outlined the equations relating to the operation of the cooling tower, it is important to link the variables in the cooling water network to the appropriate boundary values in the discretised cooling tower model. The first two boundary variables that must be specified are the enthalpy and humidity of the ambient air entering at the bottom of the cooling tower. In Equations 4.80 and 4.81, typical values are shown for a summer day in Pretoria, South Africa. It is important to make sure that conservative values are chosen for the location of interest, ensuring that the cooling tower will operate well in all seasons. The temperature of the water entering at the top of the tower must also be set equal to the return temperature of the cooling water coming from the cooling water network (Equation 4.82).

$$i_0^{ma} = 49.19 \frac{kJ}{kg} \quad (4.80)$$

$$W_0 = 0.00949 \frac{kg}{kg} \quad (4.81)$$

$$T_Z^w = T^{ret} \quad (4.82)$$

Since the change in water flowrate has been modelled in using Equation 4.66, the evaporation losses can be estimated as the difference between the incoming and outgoing liquid flowrates (Equation 4.83). Since it is advisable to draw off the blow-down stream before the circulating water enters the cooling tower, Equation 4.84 shows how the incoming flowrate relates to the total cooling water flowrate.

4 Model Development

$$E = L_Z - L_0 \quad (4.83)$$

$$L_Z = TW - B \quad (4.84)$$

The make-up and blow-down flowrates are both determined by the rate of evaporative losses inside the cooling tower. Once it has been decided how many cycles of concentration the circulating water may undergo, the make-up can be calculated using Equation 4.85. With that, the blow-down can be calculated to ensure that the circulating water flowrate is maintained (Equation 4.86). Lastly, the temperature of the cooling water supplied to the cooling water network is a function of both the water from the cooling tower and the make-up water (Equation 4.87)

$$M = E \cdot \frac{CC}{CC - 1} \quad (4.85)$$

$$B + E = M \quad (4.86)$$

$$T^{cw} = \frac{T_0^w \cdot (CW - M) + T^M \cdot M}{CW} \quad (4.87)$$

The above equations constitute the Below Pinch Model. In Case 1, where the cooling tower has already been designed, the cross sectional area and height of the packing inside the cooling tower are constant. In this case, the objective function is simply to minimise the circulating cooling water flowrate (Equation 4.88). In doing so, the return temperature will simultaneously increase, the effect of which will be increased tower effectiveness, as noted by Bernier (1994). This objective function together with the model constraints constitutes a MINLP model.

4 Model Development

$$\text{Min}(TW) \quad (4.88)$$

In Case 2, the cross sectional area and height of the cooling tower packing are variable. As such, A_{cs} and s_{step} are variables that must be solved within the model. In the Above Pinch Model, it was sufficient to minimise the total steam flowrate in order to reduce the boiler purchase cost. Here, however, the relationship between cooling tower size and cooling water flowrate is not as clean cut. The best option for Case 2 is to develop a cost function for the cooling tower that can be minimised.

The crucial element in the cooling tower is the packing, which occupies only the lowest region of a natural draught cooling tower. The concrete shell of the cooling tower is mostly empty, and serves to establish the natural draught through the packing. By inspecting the cooling tower model given by Kröger (2004), one would see that if unconstrained, the model would favour shallow packing with a large cross sectional surface area. This large cross sectional surface area would, however, require very large and costly shells to be erected over the packing. For this reason it is important to ensure that the cost function for the cooling tower properly accounts for the effects of the packing costs and the shell costs.

Kloppers and Kröger (2004) state that a typical fill will cost about $\$25/\text{m}^3$, while the cost of concrete will cost $\$200/\text{m}^3$ including the cost of construction. By knowing the cross sectional area and height of the cooling tower packing, it is a simple matter to determine the packing cost. To calculate the volume of concrete required by the shell, the product of the shell surface area and the shell thickness can be used. Kloppers and Kröger (2004) approximate the cooling tower as a cylinder, using the average of the base and top diameters. This,

4 Model Development

however, appreciably underestimates the surface area of the hyperbolic cooling tower shell and skews the relationship between packing and shell costs.

In this work the shell of the cooling tower will be approximated as the intersection of two conic surfaces, shown in Figure 4.6. Kröger (2004) states that to prevent cold inflow in the top of the cooling tower, the radius of the top opening should be 60% of the base radius. Chilton (1952) further states that cooling towers usually have a height to width ratio of 3:2. If it is assumed that the cooling tower base radius R_b is the same as the radius of the packing area, then the height and top radius of the tower are $3R_b$ and $0.6R_b$ respectively. Furthermore, by comparing a number of published designs (Form, 1986; Niemann & Zerna, 1986; Eckstein *et al*, 1987; Busch *et al*, 2002), it can be seen that the narrowest part of the shell lies approximately 70 % up the tower, with a diameter roughly 55% of the base diameter. The average wall thickness was also noted to be approximately 200mm thick.

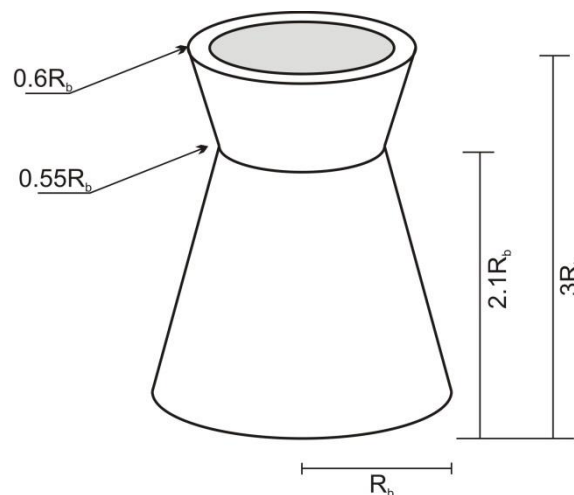


Figure 4.6: Simplified cooling tower shell with proportions.

Using the proportions shown in Figure 4.6, Equation 4.89 gives the profile of the cooling tower shell in terms of the base radius. Using the standard formula for the surface of revolution (Equation 4.90) and substituting this profile in

4 Model Development

(Equation 4.91) the surface area of the cooling tower shell in terms of the base radius is given in Equation 4.92.

$$r(z) = \begin{cases} R_b - \frac{13}{14}z & 0 \leq z < 2.1R_b \\ \frac{13}{30}R_b + \frac{1}{18}z & 2.1R_b \leq z \leq 3R_b \end{cases} \quad (4.89)$$

$$SA = 2\pi \int_0^{3R_b} r \sqrt{1 + \left(\frac{dr}{dz}\right)^2} dz \quad (4.90)$$

$$\begin{aligned} SA &= 2\pi \sqrt{1 + \left(\frac{3}{14}\right)^2} \cdot \left[R_b z - \frac{3}{28} z^2 \right]_0^{2.1R_b} \\ &+ 2\pi \sqrt{1 + \left(\frac{1}{18}\right)^2} \cdot \left[\frac{13}{30} R_b z + \frac{1}{36} z^2 \right]_{2.1R_b}^{3R_b} \end{aligned} \quad (4.91)$$

$$SA = 13.715(R_b)^2 \quad (4.92)$$

Using this information, the cost function to be minimised in Case 2 is given in Equation 4.93. This objective function, together with the model constraints constitutes a MINLP model.

$$\text{Min}(\$200 \cdot [0.2 \cdot 13.715R_b^2] + \$25 \cdot [\pi R_b^2 \cdot Z \cdot s_{step}]) \quad (4.93)$$

4.6 Solution Procedure

In the models described above, for Case 1 the Above Pinch Model yielded an MILP model. As such, no initiation procedures are required, and the model can be solved as it is with minimum effort. In addition, since the model is linear, one is assured that the optimum achieved is globally optimal.

The MINLP models described above present more of a challenge. Nonlinear solvers require that a feasible initial point be specified before solving the problem. Furthermore, in the case of non-convex problems, great care must be taken in selecting the initial point, as the solver will converge to the nearest local optimum. Below, a number of methods will be discussed for finding feasible initial points for the MINLP models developed in this work.

In the Above Pinch Model for Case 2, the nonlinearities in the model are introduced due to the presence of variable saturation temperatures for the lower steam levels. If these steam levels were to be fixed, the model would be reduced to that of Case 1, which is MILP. Therefore, following the procedure used by Beangstrom (2013), it is recommended that steam levels be temporarily fixed at typical industry standards, such as the values in Table 3.1 for example. The resulting MILP can be solved easily, the results of which will be a feasible starting point for the full MINLP model.

For both cases, the Below Pinch Model yields MINLP models. The constraints for the heat exchanger networks, both process-process and cooling water, are mixed integer linear. The nonlinearities in the model are introduced by nonlinear equations in the cooling tower model. To obtain a feasible initial point for these models, it is recommended that a subsection of the Below Pinch Model be solved first. By using an assumed temperature for the cooling water, only the constraints concerning the heat exchanger networks are solved for minimum

4 Model Development

flowrate as an MILP model. The results of this are used as the boundary conditions to the cooling tower model, which can be solved numerically as normal differential equations. The results of heat exchanger network and the cooling tower model together form a feasible starting point for the MINLP models.

4.7 References

- Beangstrom SG (2013). *Steam system network analysis, synthesis and optimisation*. Master's thesis, Department of Chemical Engineering, University of Pretoria, South Africa.
- Bernier MA (1994). Cooling tower performance: Theory and experiments. *ASHRAE Trans. Res.*, 100, 114-121.
- Busch D, Harte R, Krätzig WB & Montag U (2002). New natural draft cooling tower of 200m of height. *Eng. Struct.*, 24, 1509-1521.
- Bosnjakovic F (1965). *Technical thermodynamics*, translated by Blackshear PI, 1-80, Holt, Reinhart and Wilson, New York.
- Coulson JM & Richardson JF (1996). *Chemical engineering: Fluid flow, heat transfer and mass transfer*, 5th Ed, Pergamon Press, Oxford.
- Chilton CH (1952). Performance of natural-draught cooling towers. *Proc. Inst. Elec. Engrs.*, 99, 440.
- Eckstein U, Harte R, Krätzig WB & Wittek U (1987). Simulation of static and kinetic buckling of unstiffened and stiffened cooling tower shells. *Eng. Struct.*, 9, 9-18.
- Form J (1986). The ring-stiffened shell of the ISAR II nuclear power plant natural-draught cooling tower. *Eng. Struct.*, 8, 199-207.
- Gololo KV & Majozi T (2011). On synthesis and optimization of cooling water systems with multiple cooling towers. *Ind. Eng. Chem. Res.*, 50, 3775-3787.
- Gololo KV & Majozi T (2013). Complex cooling water systems optimisation with pressure drop considerations. *Ind. Eng. Chem. Res.*, 52, 7056-7065.

4 Model Development

- Harrel G (1996). Steam system survey guide. ORNL/TM-2001/263: Oak Ridge National Laboratory.
- Isafiade AJ & Fraser DM (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.
- Kloppers JC & Kröger DG (2004). Cost optimization of cooling tower geometry. *Engineering Optimization*, 36(5), 575-584
- Kröger DG (2004). *Air-cooled heat exchangers and cooling towers*, Penn Well Corporation, USA.
- Lyderson AL (1983). *Mass transfer in engineering practice*, Wiley, New York.
- Mavromatis SP & Kokossis AC (1998). Conceptual optimisation of utility networks for operational variations - I. Targets and level optimisation. *Chem. Eng. Sci.*, 53(8), 1585-1608.
- Niemann HJ & Zerna W (1986). Impact of research on development of large cooling towers. *Eng. Struct.*, 8, 74-86.
- Savelski M J & Bagajewicz MJ (2000). Design of water utilization systems in process plants with single contaminants. *Waste Management*, 58, 659-664.
- Yee F & Grossmann IE (1990). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comp. Chem. Eng.*, 14(10), 1165-1184.

4 Model Development

Zhu XX, O'Neill BK, Roach JR & Wood RM (1995). A method for automated heat exchanger network synthesis using block decomposition and non-linear optimization. *Trans. IChemE*, 73(A), 919-930.

Chapter 5

Illustrative Examples

To demonstrate the benefits of the proposed methods, two examples will be presented. These problems will be decomposed into above pinch and below pinch sub-problems, and will be solved for both Case 1 and Case 2 scenarios. Care has been taken to select data sets with a sufficient number of streams to prevent trivial solutions being obtained. The examples will also be solved using no hot and cold utility heat integration, and using segregated application of heat integration to the three regions. This will provide the base case against which the results of the proposed methods can be compared.

The models were 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 LP and MIP solver.

5.1 First Example

5.1.1 Problem description

The first example was composed for the purpose of this work. In this problem, there are 7 hot streams that require cooling, and 6 cold streams that require heating. The stream data are given in Table 5.1. High pressure steam is available at 270°C, which is hot enough to ensure that there is sufficient

5 Illustrative Examples

temperature difference to meet the hottest demands of the process. A shaft work target of 500 kW is required of the steam turbine. Furthermore, there is an upper limit on the cooling water return temperature of 55 °C for tower fill considerations.

Using the problem table algorithm and a ΔT_{\min} value of 10 °C, it was found that the hot and cold pinch temperatures are 102 °C and 92 °C respectively, while the minimum heating and cooling duties are 30307.8 kW and 13660.4 kW respectively. Figure 5.1 and Figure 5.2 show the composite curves and the grand composite curve, respectively.

Table 5.1: Stream data for first example.

	T_{supp} (°C)	T_{tar} (°C)	CP (kW/K)	Q (MW)
Hot streams				
1	240	132	25.8	2.79
2	130	34	213.7	20.52
3	233	37	42.4	8.31
4	230	35	128.9	25.14
5	253	192	19.3	1.18
6	151	35	15.2	1.76
7	189	32	100.1	15.72
Cold streams				
1	36	233	171.0	33.69
2	27	246	124.3	27.22
3	107	245	98.0	13.52
4	29	172	41.8	5.98
5	170	184	485.9	6.80
6	92	120	172.8	4.84

5 Illustrative Examples

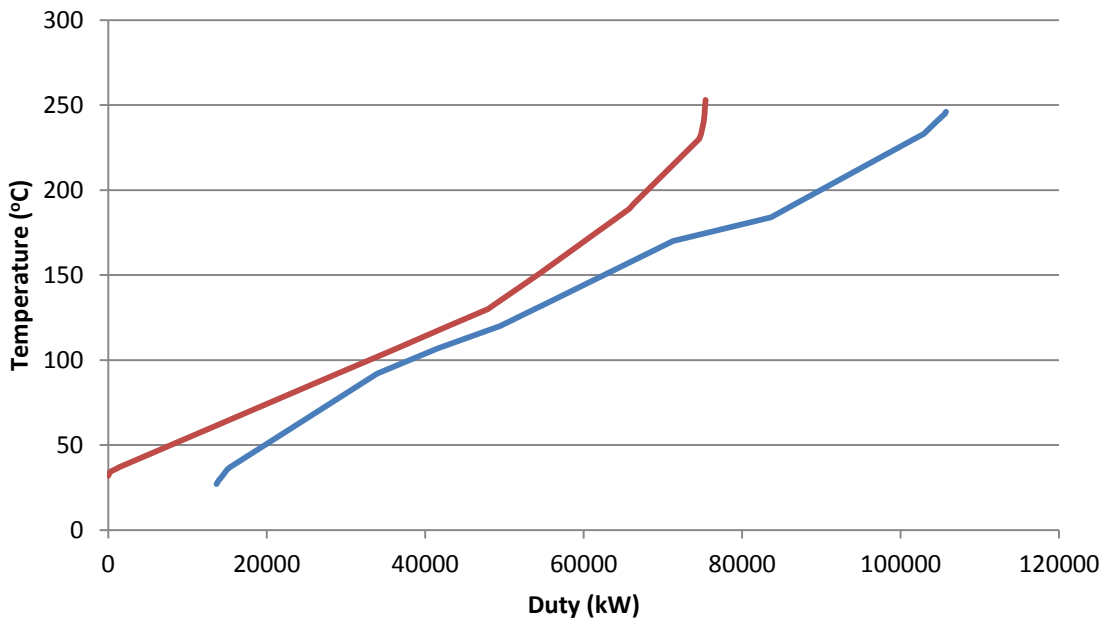


Figure 5.1: First example - composite curves.

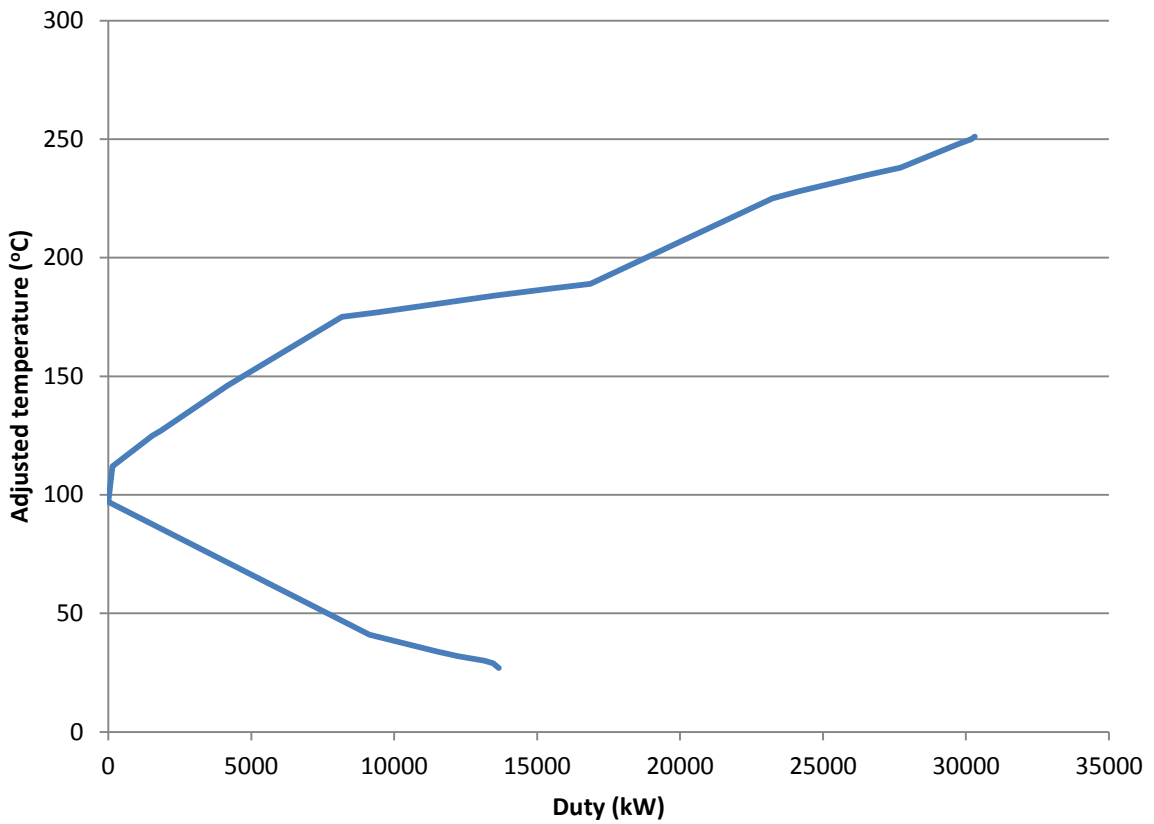


Figure 5.2: First example – grand composite curve.

5 Illustrative Examples

For the Case 1 scenario, an MP steam level with a saturation temperature of 195°C was selected based on the guidelines noted by Harrel (1996). Sizing the steam turbine for these steam levels and the shaft work target, the fixed flowrate of the MP steam level is found to be 3.243 kg/s. The cooling tower packing was chosen to have a cross sectional area of 50 m² and a packing height of 3 m. In the discretisation of the cooling tower model, 60 slices were used with a step size of 0.05m.

5.1.2 Base Case

To establish a base case, the problem in Table 5.1 was solved using the method of Yee and Grossmann (1990), with the typical placement of the utilities on the periphery. Once the process-process heat exchanger network was determined, the streams that required utility heating/cooling were tabulated (Table 5.2).

Table 5.2: Hot and cold utility requirements.

	$T_{\text{supp}} (^{\circ}\text{C})$	$T_{\text{tar}} (^{\circ}\text{C})$	$CP \text{ (kW/K)}$
Hot streams requiring cooling			
2	59.63	34	213.7
3	59.58	37	42.4
4	63.61	35	128.9
6	59.58	35	15.2
7	63.61	32	100.1
Cold streams requiring heating			
1	177.02	233	171.0
2	175.82	246	124.3
3	176.81	245	98.0
5	173.04	184	485.9

For Case 1, if no pinch techniques are applied to the steam system and cooling water system, a total of 18.75 kg/s of HP steam is required. The minimum

5 Illustrative Examples

cooling water flowrate is 102.086 kg/s with a cooling tower effectiveness of 0.893.

If pinch techniques are applied to the steam system and cooling water system independently, then a total of 15.849 kg/s of HP steam is required, a reduction of 15%. The minimum cooling water flowrate is 101.156 kg/s, a reduction of just under 1%, with a slightly improved cooling tower effectiveness of 0.895. These reductions are to be expected as a result of employing pinch techniques in the utility systems.

For Case 2, if no pinch techniques are applied to the steam system and cooling water system, a total of 18.191 kg/s of HP steam is required. The optimum saturation temperature of the MP steam level was found to be 256.6°C, and the steam turbine flowrate is 18.191 kg/s, that is, HP steam is only supplied to the turbine, and the MP exhaust steam is supplied to the heat exchanger network. Note that the minimum steam flowrate in Case 2 is lower than that for Case 1, confirming the observation of Beangstrom (2014) that optimising the steam levels together with the heat exchanger network yields lower total steam flowrates.

For the cooling water system with no pinch technique applied, a cooling tower with a minimum cost of \$10 585 was designed. The packing has a cross sectional area of 41.06 m² and a height of 3.327 m. The cooling water flowrate was found to be 107.734 kg/s with a tower effectiveness of 0.842, both worse than for Case 1. By noting that the cost of the fixed tower design in Case 1 is \$12 481, it is clear that minimum flowrate (and maximum effectiveness) do not correspond with minimum cost. It is therefore important that the objective function is chosen to suite situation at hand. If the objective of minimum

5 Illustrative Examples

flowrate had been used for Case 2, a costly cooling tower design would have been obtained.

Still considering Case 2, if pinch techniques are applied to the steam system and cooling water system independently, then a total of 15.794 kg/s of HP steam is required, a reduction of 13%. A cooling tower with a minimum cost of \$10 546 is obtained, a reduction of under 0.5%. The tower packing has a cross sectional area of 40.898 m² and a height of 3.33 m.

5.1.3 New Model

Having developed the base case, the problem must now be solved using the new models developed in Chapter 4. In Figure 5.3, the streams are shown relative to each other in terms of their adjusted supply and target temperatures. The location of the pinch has been shown, indicating where the problem has been divided into the two sub-problems. Figure 5.3 also shows how the cold streams are divided between 5 intervals in the Above Pinch Model, and how the hot streams have been divided between 2 intervals in the Below Pinch Model.

As has been noted, the holistic treatment of the utility systems is analogous to graphical targeting on the grand composite curve, as opposed to targeting on the hot and cold composite curves. Although graphical targeting on the GCC cannot take into account the operation of the steam turbine or cooling tower, nor can it synthesise the necessary heat exchanger networks, the targets are still of interest. Figure 5.4 shows an attempt at graphically targeting the minimum steam and cooling water flowrate. From this a total steam target of 14.365 kg/s and a cooling water target of 105.895 kg/s are obtained. Although these targets were obtained with no consideration for the operation of the steam turbine or cooling tower, they are useful as indications of the region in which one might expect the results of the new models to be

5 Illustrative Examples

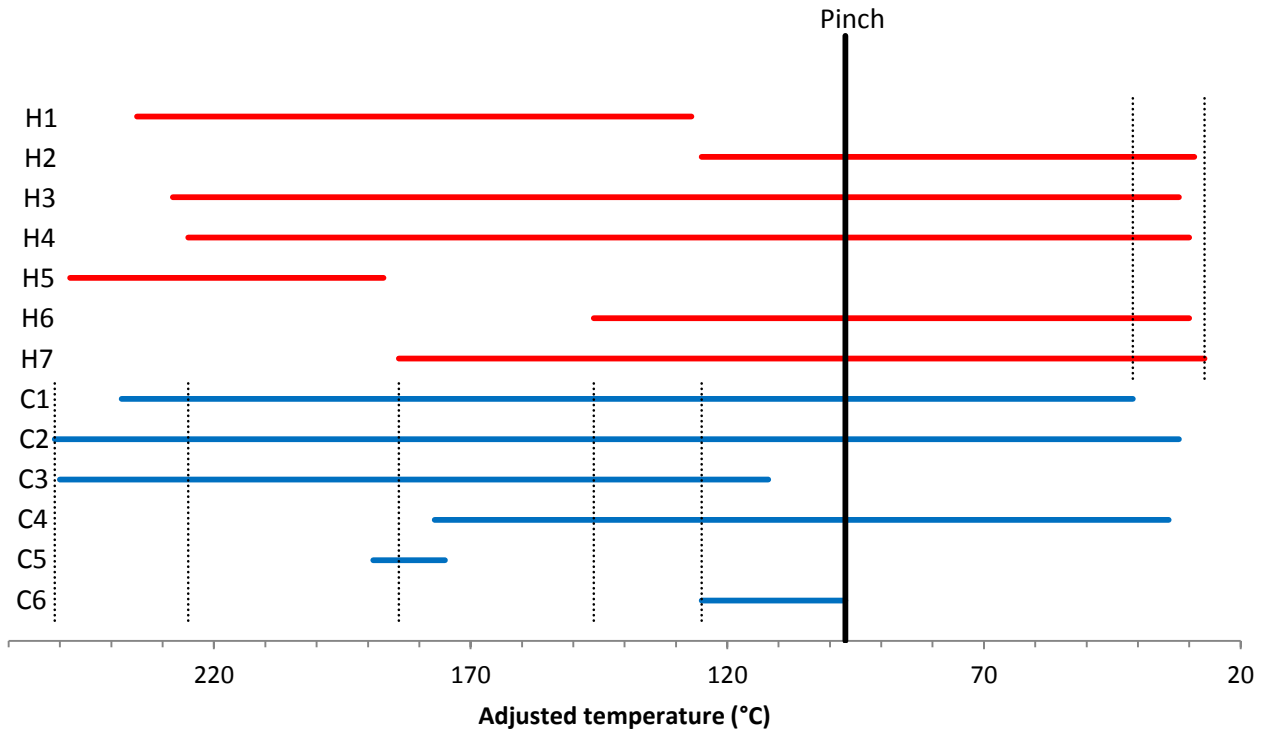


Figure 5.3: First example – relative stream positions and interval placement.

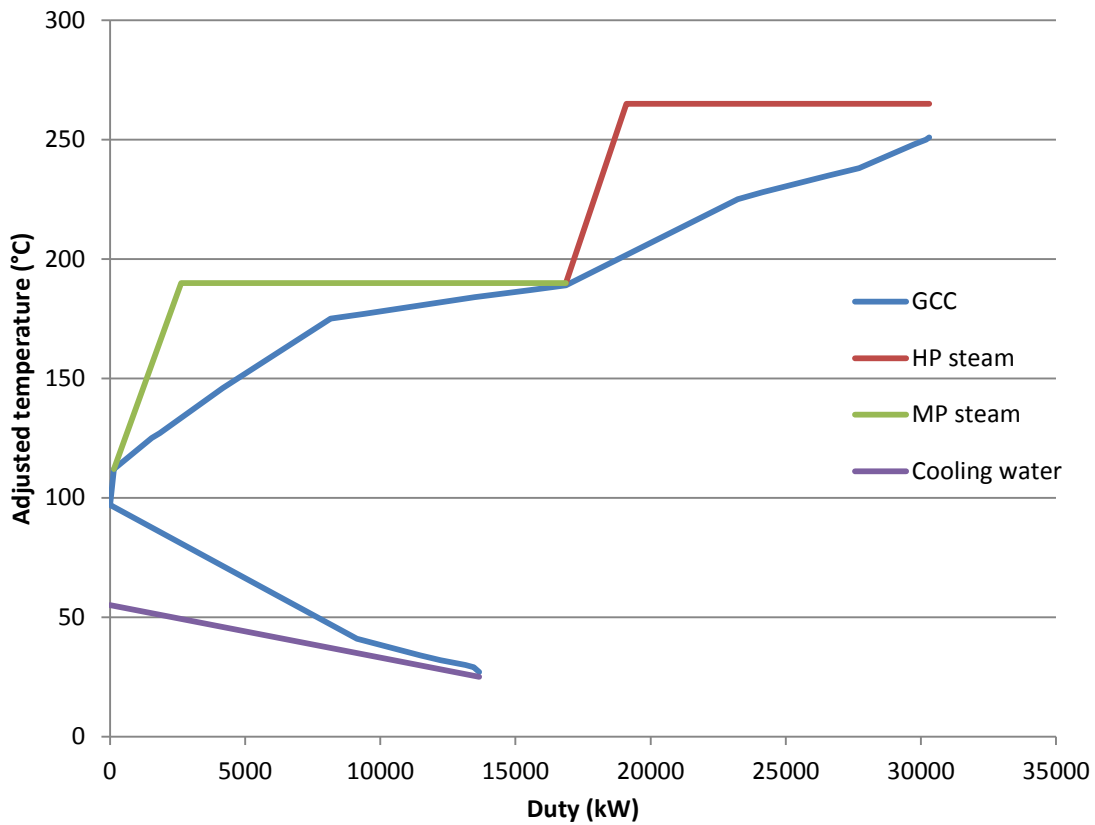


Figure 5.4: First example – graphical targeting.

5 Illustrative Examples

Turning to the new models developed in Chapter 4, for Case 1 the Above Pinch model obtained a minimum total steam flowrate of 13.682 kg/ s. This represents a 27% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and a 14% reduction compared to the base case where pinch techniques were applied to the three regions separately.

For Case 1, the Below Pinch Model obtained a minimum cooling water flowrate of 89.950 kg/s and an improved cooling tower effectiveness of 0.923. This represents a 12% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and an 11% reduction compared to the base case where pinch techniques were applied to the three regions separately. Note that these results are better than the targets obtained via graphical targeting on the GCC. It is concluded that graphical targeting on the GCC is not a suitable tool for holistically optimising the utility systems.

The heat exchanger networks obtained by the Above Pinch Model and Below Pinch Model for Case 1 are shown in Figure 5.5 and Figure 5.6 below. The duties exchanged between each match are given in Table 5.3 and Table 5.4 respectively. Note that these represent the solutions to two sub-problems. The final heat exchanger network comprises the two networks shown below joined at the pinch. Note also how the utility heat exchangers are not restricted to the periphery, but interact with the process-process heat exchangers throughout all of the intervals.

5 Illustrative Examples

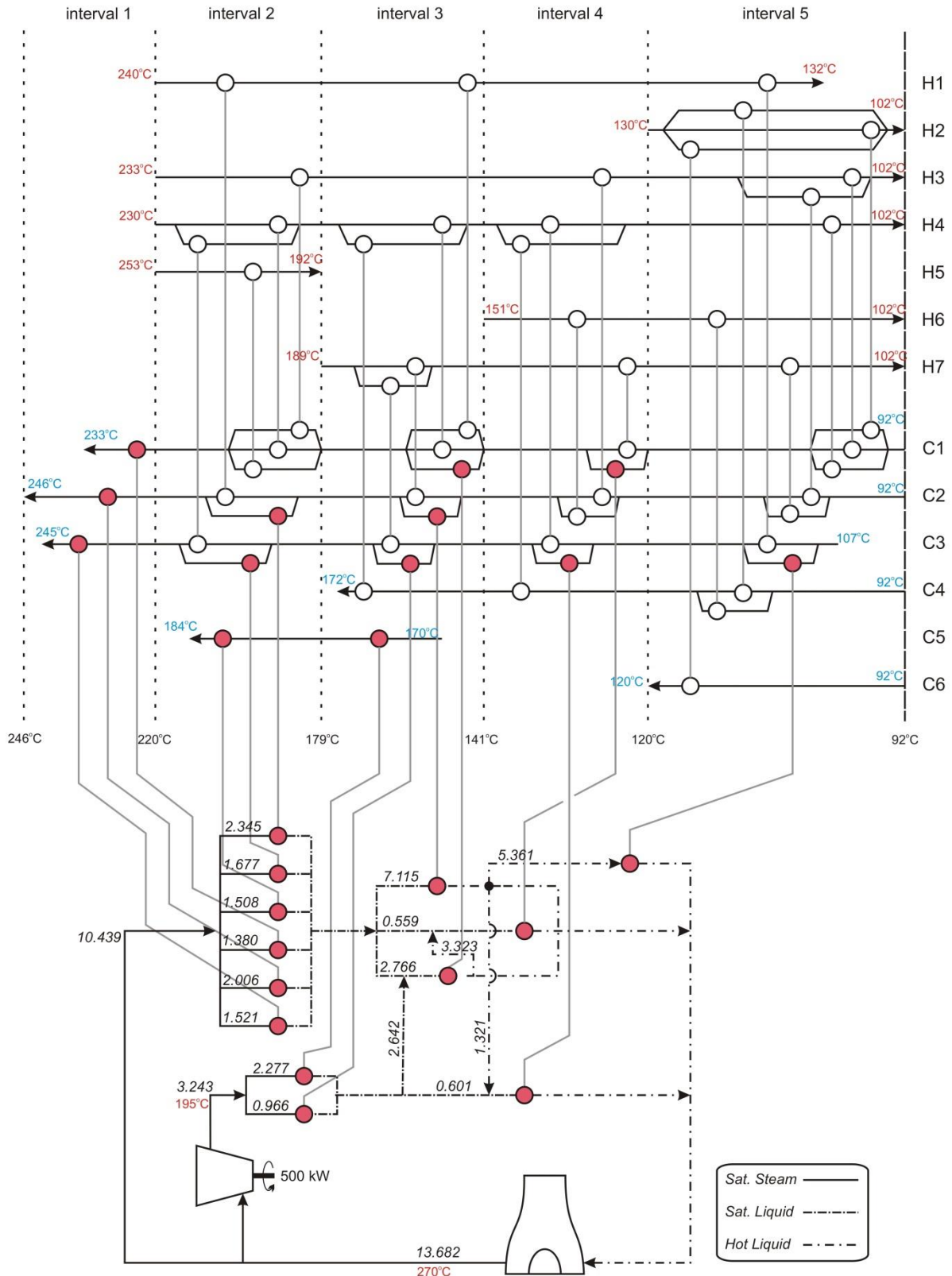


Figure 5.5: First example - above pinch HEN for Case 1.

5 Illustrative Examples

Table 5.3: Duties for Figure 5.5 in kW.

<u>Interval 1</u>			
C1 – Util	2223	C3 – Util	2450
C2 – Util	3231		
<u>Interval 2</u>			
C1 – H3	1866	C3 – H4	1317
C1 – H4	3968	C2 – Util	3781
C1 – H5	1177	C3 – Util	2701
C2 – H1	1316	C5 – Util	2430
<u>Interval 3</u>			
C1 – H1	980	C1 – Util	1915
C1 – H4	3602	C2 – Util	3641
C2 – H7	1083	C3 – Util	1856
C3 – H7	1868	C5 – Util	4373
C4 – H4	1296		
<u>Interval 4</u>			
C1 – H7	2955	C4 – H4	878
C2 – H3	2502	C1 – Util	636
C2 – H6	109	C3 – Util	287
C3 – H4	1771		
<u>Interval 5</u>			
C1 – H2	611	C3 – H1	490
C1 – H3	510	C4 – H2	534
C1 – H4	3668	C4 – H6	636
C2 – H3	678	C6 – H2	4838
C2 – H7	2803	C3 – Util	784

5 Illustrative Examples

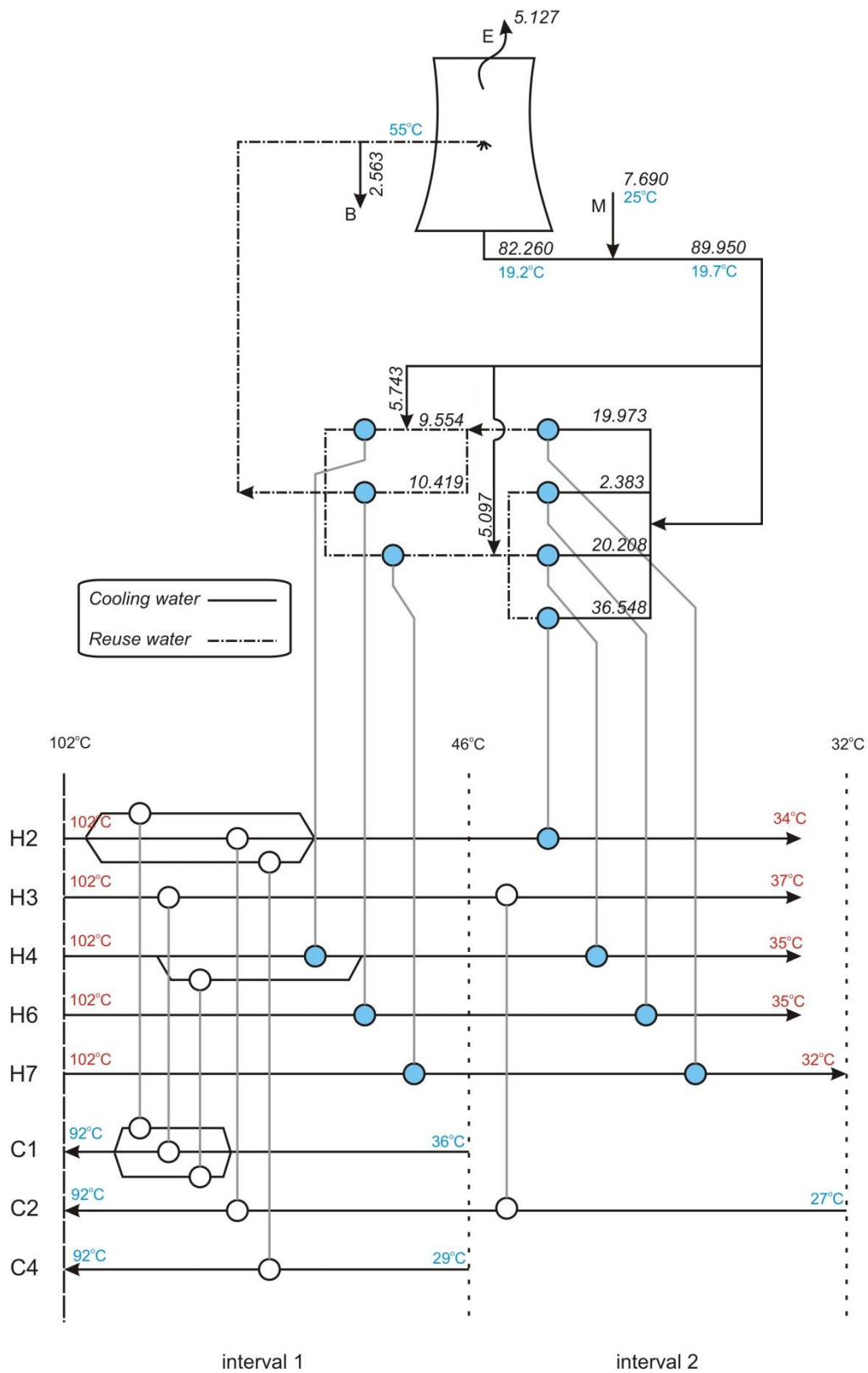


Figure 5.6: First example - below pinch HEN for Case 1.

5 Illustrative Examples

Table 5.4: Duties for Figure 5.6 in kW

<i>Interval 1</i>			
C1 – H2	1636	C4 – H2	2633
C1 – H3	2374	H4 – Util	1653
C1 – H4	5566	H6 – Util	851
C2 – H2	7698	H7 – Util	5606
<i>Interval 2</i>			
C2 – H3	382	H6 – Util	167
H2 – Util	2564	H7 – Util	1401
H4 – Util	1418		

5 Illustrative Examples

For Case 2, the Above Pinch Model obtained a minimum total steam flowrate of 13.490 kg/ s. This represents a 26% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and a 15% reduction compared to the base case where pinch techniques were applied to the three regions separately. The flowrate of steam supplied to the turbine was found to be 3.2 kg/s, resulting in an MP steam level with a saturation temperature of 194°C.

For Case 2, the Below Pinch Model obtained a minimum cooling tower cost of \$9 549. This represents a 10% reduction in cost compared to the base case with no pinch techniques applied to the utilities, and a 9% reduction compared to the base case where pinch techniques were applied to the three regions separately. The tower packing has a cross sectional area of 36.768 m² and a height of 3.403 m.

The heat exchanger networks obtained by the Above Pinch Model and Below Pinch Model for Case 2 are shown in Figure 5.7 and Figure 5.8 below. The duties transferred by each heat exchanger are given in Table 5.5 and Table 5.6 respectively. These two networks represent the solutions to the two sub-problems. The final heat exchanger network comprises the two networks shown below joined at the pinch.

It must be noted that in the above designs, the minimum energy targets for the utilities, as determined by the problem table, have been met. Therefore, the reductions in the flowrates have not come at the expense of higher energy consumption. Based on the above mentioned results, it is concluded that the holistic and unified approach to heat integration on chemical plants yields better results than the application of separate techniques in isolation of one another.

5 Illustrative Examples

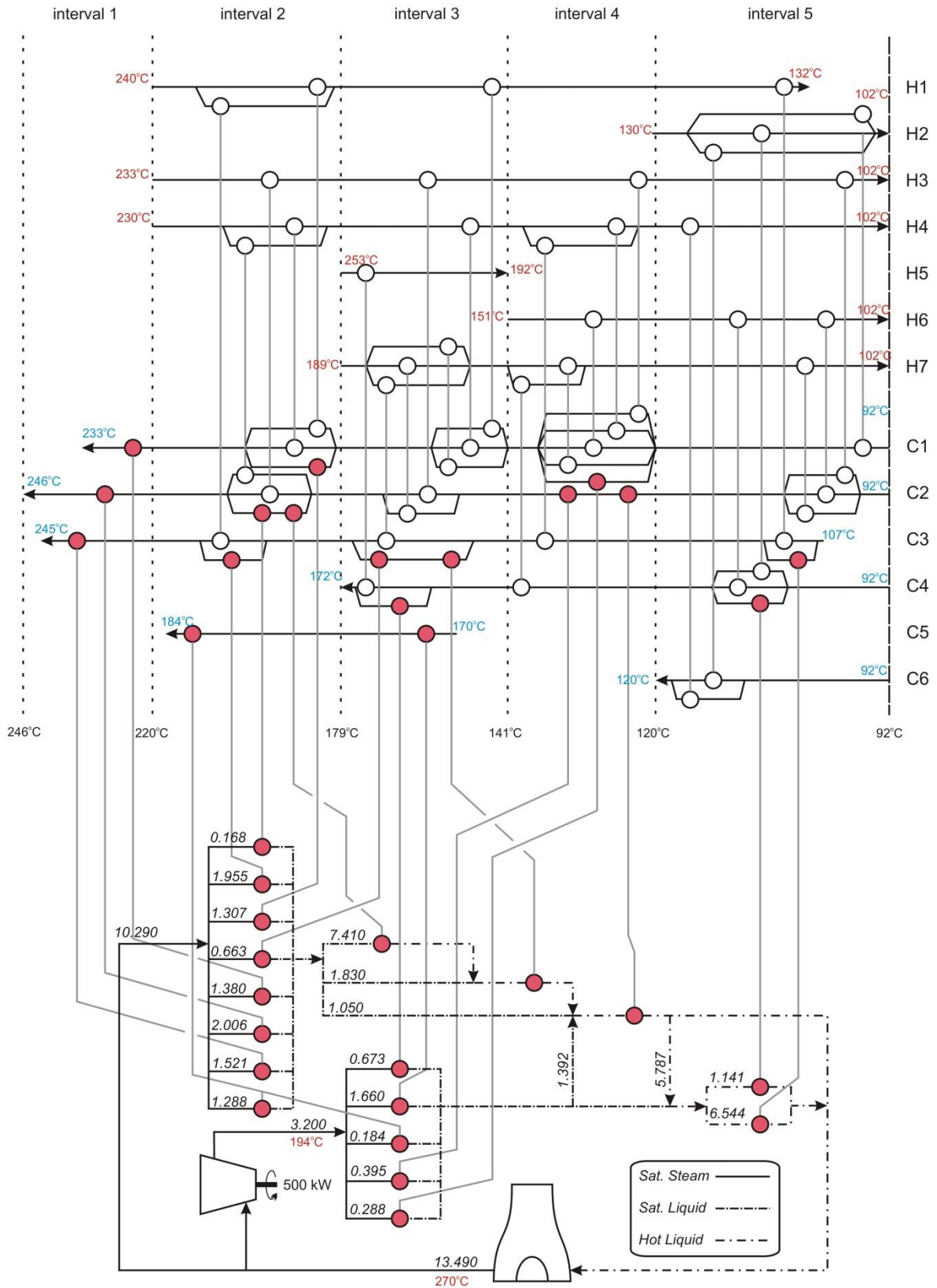


Figure 5.7: First example - above pinch HEN for Case 2.

5 Illustrative Examples

Table 5.5: Duties for Figure 5.7 in kW.

<u>Interval 1</u>			
C1 – Util	2223	C3 – Util	2450
C2 – Util	3231		
<u>Interval 2</u>			
C1 – H1	448	C1 – Util	2105
C1 – H4	4458	C2 – Util	2852
C2 – H3	1418	C3 – Util	3150
C2 – H4	826	C5 – Util	2430
C3 – H1	868		
<u>Interval 3</u>			
C1 – H1	448	C3 – H7	508
C1 – H4	4898	C5 – H5	1177
C1 – H7	619	C3 – Util	3216
C2 – H3	2047	C4 – Util	1296
C2 – H7	2676	C5 – Util	3196
<u>Interval 4</u>			
C1 – H3	902	C3 – H4	2058
C1 – H4	592	C4 – H7	878
C1 – H6	319	C1 – Util	554
C1 – H7	1224	C2 – Util	2610
<u>Interval 5</u>			
C1 – H2	4788	C4 – H3	935
C2 – H3	252	C6 – H2	1173
C2 – H6	426	C6 – H4	3665
C2 – H7	2803	C3 – Util	784
C3 – H1	490	C4 – Util	212
C4 – H2	23		

5 Illustrative Examples

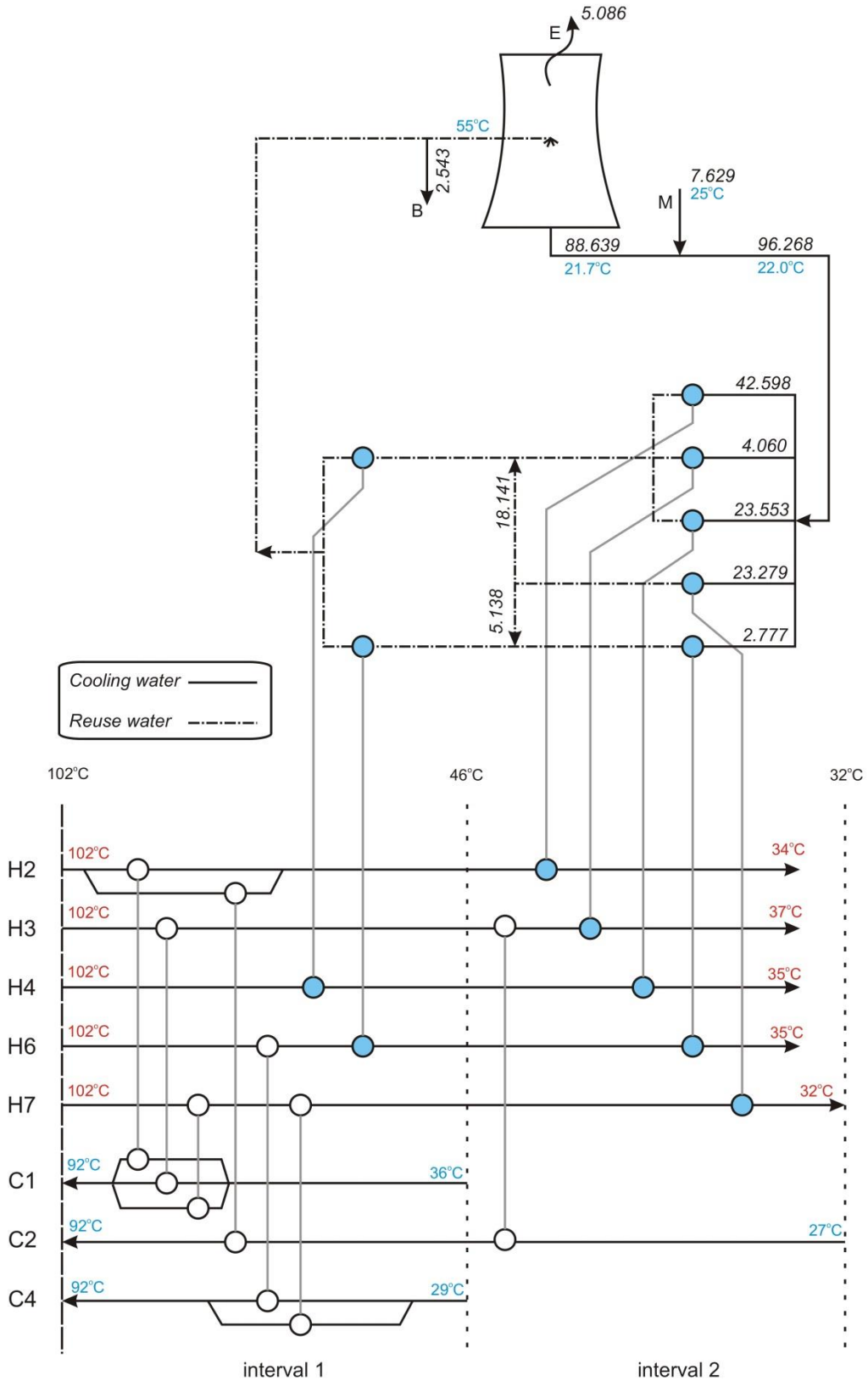


Figure 5.8: First example - below pinch HEN for Case 2.

5 Illustrative Examples

Table 5.6: Duties for Figure 5.8 in kW.

<i>Interval 1</i>			
C1 – H2	4025	C4 – H6	205
C1 – H3	2374	C4 – H7	2429
C1 – H7	3177	H4 – Util	7218
C2 – H2	7942	H6 – Util	647
<i>Interval 2</i>			
C2 – H3	137	H4 – Util	1418
H2 – Util	2564	H6 – Util	167
H3 – Util	244	H7 – Util	1401

5 Illustrative Examples

5.1.4 Summary

Table 5.7: Summary of first example, Case 1.

<u>Above pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	18.75		
Separate methods	15.85	15%	
New method	13.68	27%	14%
<u>Below Pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	102.09		
Separate methods	101.16	1%	
New method	89.95	12%	11%
<u>Model statistics</u>			
	Continuous variables	Binary variables	Solution time (s)
Above Pinch	1582	210	0.078
Below Pinch	1044	40	0.07

5 Illustrative Examples

Table 5.8: Summary of first example, Case 2.

<u>Above pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	18.19		
Separate methods	15.79	13%	
New method	13.49	26%	15%
<u>Below Pinch</u>			
	Cost (\$)	Reduction on Base Case	Reduction on separate methods
Base Case	10 585		
Separate methods	10 546	0.5%	
New method	9 549	10%	9%
<u>Model statistics</u>			
	Continuous variables	Binary variables	Solution time (s)
Above Pinch	1567	210	0.76
Below Pinch	1044	40	0.14

5 Illustrative Examples

5.2 Second Example

5.2.1 Problem description

The second example is taken from a study presented by Egeberg (1998). In this problem, there are 11 hot streams that require cooling, and 10 cold streams that require heating. The stream data are given in Table 5.9.

Table 5.9: Stream data for second example

	T_{supp} (°C)	T_{tar} (°C)	CP (kW/K)	Q (MW)
Hot streams				
H1	207.9	30	177.6	3160
H2	207.9	30	177.6	31.60
H3	62	22.5	652.3	25.77
H4	62	40.6	850.8	18.21
H5	40.6	22.5	416.7	7.54
H6	-0.2	-10.6	1073.0	11.05
H7	35	30.1	6165.3	30.21
H8	30.4	-45	81.5	6.15
H9	38.3	21.6	1812.8	30.27
H10	21.9	8	20.9	0.29
H11	51.4	8	36.2	1.57
Cold streams				
C1	2	75.2	241.1	17.65
C2	75.2	120.4	416.9	18.84
C3	2	75.2	241.1	17.65
C4	75.2	120.4	416.9	18.84
C5	206.1	226	1435.7	28.57
C6	206.1	226.2	1421.4	28.57
C7	87	88.7	13216.5	22.47
C8	-10.7	50	7.1	0.43
C9	82.9	82.94	579275	23.17
C10	51	51.2	135995	27.20

5 Illustrative Examples

In the original problem, high pressure steam is available with a saturation pressure of 240°C. Refrigerant is used exclusively as the cold utility. The refrigerant is available at a temperature of -55°C and must be returned to the compressor at no more than -50°C. For the purposes of this work, cooling water will be added as an alternative cold utility, to be used preferentially over refrigerant wherever possible.

Using the problem table algorithm and a ΔT_{\min} value of 10 °C (as used by Egeberg, 1998), it was found that the hot and cold pinch temperatures are 61 °C and 51 °C respectively, while the minimum heating and cooling duties are 125.653 MW and 116.507 MW respectively. These results are identical to those obtained by Egeberg (1998). Figure 5.9 and Figure 5.10 show the composite curves and the grand composite curve, respectively, for the second example.

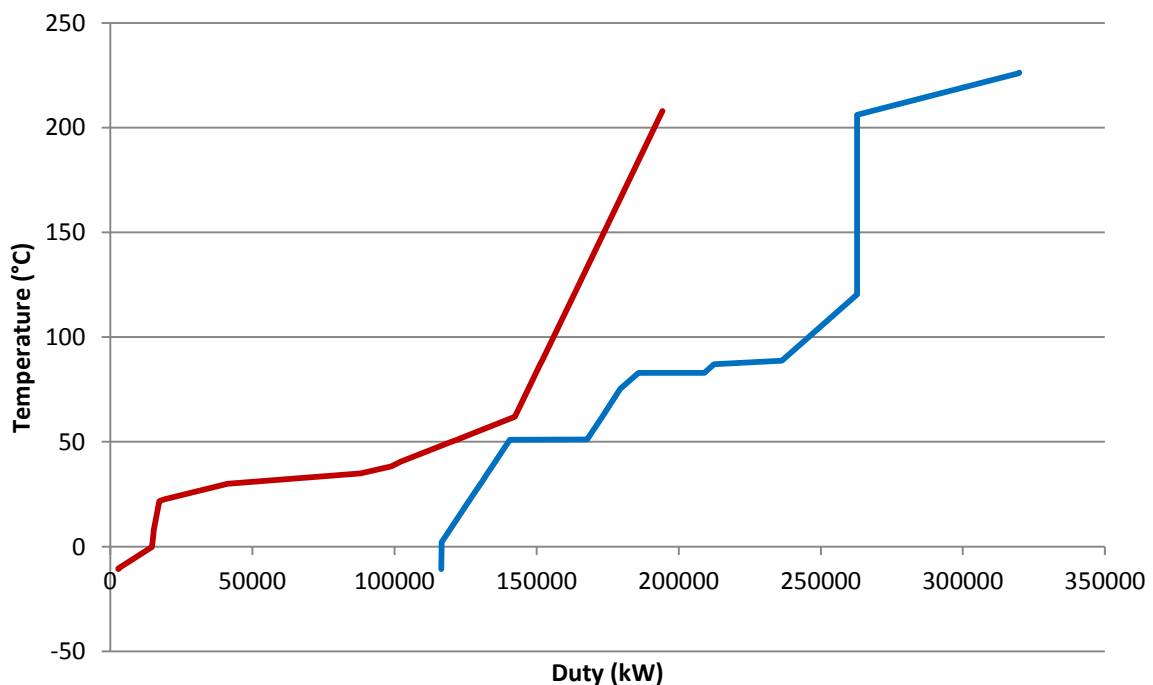


Figure 5.9: Second example - composite curve.

5 Illustrative Examples

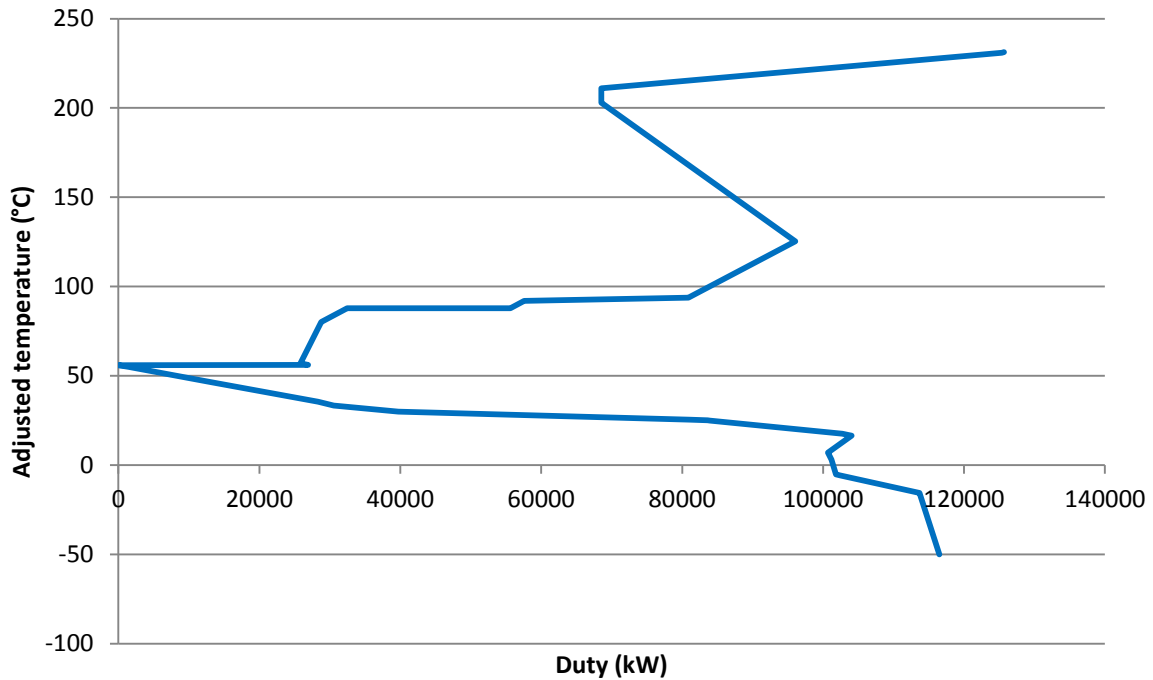


Figure 5.10: Second example - grand composite curve.

The presence of hot streams with very low target temperatures presents a special challenge in that cooling water alone cannot provide the necessary cooling. A combination of refrigerant and cooling water will have to be used. Since a refrigeration unit involves high operating costs, as little refrigerant as possible should be used. For this reason, the below pinch region will be further subdivided into two regions utilizing cooling water and refrigerant respectively.

Seider, Seader and Lewin (2004), in a heuristic for process design, recommend that it be assumed that cooling water is available at 90°F (32°C). This is perhaps a bit high, especially for a well operated cooling tower, so in this problem a value of 25°C will be used. Making allowances for ΔT_{\min} , hot streams will be cooled to 35°C using cooling water, and there after using refrigerant. The minimum cooling requirement of 116.507 MW is therefore made up of 39.746 MW from cooling water and 76.761MW from refrigerant.

5 Illustrative Examples

For this problem, a shaft work target of 3.5 MW is imposed on the steam turbine. Furthermore, the cooling water return temperature is limited to an upper value of 55 °C for tower fill considerations.

Furthermore, for Case 1 scenarios, an MP steam level with a saturation temperature of 200°C was selected. Sizing the steam turbine for these steam levels and the shaft work target, the fixed flowrate of the MP steam level is found to be 31.306 kg/s. The cooling tower packing was chosen to have a cross sectional area of 250 m² and a packing height of 3 m. In the discretisation of the cooling tower model, 60 slices were used with a step size of 0.05m.

5.2.2 Base Case

To establish a base case, the problem in Table 5.9 was solved using the method of Yee and Grossmann (1990), with the typical placement of the utilities on the periphery. Once the process-process heat exchanger network was determined, the streams that required utility heating/cooling were tabulated (Table 5.10).

For Case 1, if no pinch techniques are applied to the steam system and cooling water system, a total of 69.361 kg/s of HP steam is required. The minimum cooling water flowrate is 513.171 kg/s with a cooling tower effectiveness of 0.846.

If pinch techniques are applied to the steam system and cooling water system independently, then a total of 62.402 kg/s of HP steam is required, a reduction of 10%. The minimum cooling water flowrate is 355.508 kg/s, a reduction 30%, with an improved cooling tower effectiveness of 0.947. These reductions are to be expected as a result of employing heat integration techniques in the utility systems.

5 Illustrative Examples

Table 5.10: Hot and cold utility requirements.

	T_{supp} (°C)	T_{tar} (°C)	CP (kW/K)
Hot streams requiring cooling			
H1	54.2	35	177.6
H2	54.2	35	177.6
H3	54.1	35	652.3
H4	54.1	40.6	850.8
H5	40.6	35	416.7
H9	38.3	35	1812.8
H11	51.4	35	36.2
Cold streams requiring heating			
C2	86.2	120.4	416.9
C4	86.2	120.4	416.9
C5	206.1	226	1435.7
C6	206.1	226.2	1421.4
C7	87	88.7	13216.5
C9	82.9	82.94	579275

For Case 2, if no pinch techniques are applied to the steam system and cooling water system, a total of 69.361kg/s of HP steam is still required. The optimum saturation temperature of the MP steam level was found to be 205.6°C, and the steam turbine flowrate is 36.423 kg/s.

For the cooling water system with no pinch techniques applied, a cooling tower with a minimum cost of \$51 175 was designed. The packing has a cross sectional area of 227.585m² and a height of 2.01 m. The cooling water flowrate was found to be 840.449 kg/s with a tower effectiveness of 0.568, both worse than for Case 1. Again, this shows that minimum flowrate and maximum

5 Illustrative Examples

effectiveness do not correspond with minimum cost, and that the objective function must be carefully selected to suit the case.

Still considering Case 2, if pinch techniques are applied to the steam system and cooling water system independently, then a total of 53.104 kg/s of HP steam is required, a reduction of 23%. A cooling tower with a minimum cost of \$38 137 is obtained, a reduction of 25%. The tower packing has a cross sectional area of 153.072 m² and a height of 2.981 m.

5.2.3 New Model

Having developed the base case, the problem must now be solved using the new models developed in Chapter 4. In Figure 5.11, the streams are shown relative to each other in terms of their adjusted supply and target temperatures. The location of the pinch has been shown, along with the separation between the use of cooling water and refrigerant. Figure 5.11 also shows how the cold streams are divided between 3 intervals in the Above Pinch Model and how the hot streams have been divided between 2 intervals in the Below Pinch Model.

Similar to the first example, graphical targets for minimum utility flowrate will be determined using the GCC. Although graphical targeting on the GCC cannot take into account the functioning of the steam turbine or cooling tower, nor can it synthesise the necessary HENs, these targets give a fair indication of the flowrates that can be expected from the new model. Figure 5.12 shows the graphical targets on the GCC. From this a total steam target of 58.714 kg/s and a cooling water target of 298.170 kg/s are obtained.

5 Illustrative Examples

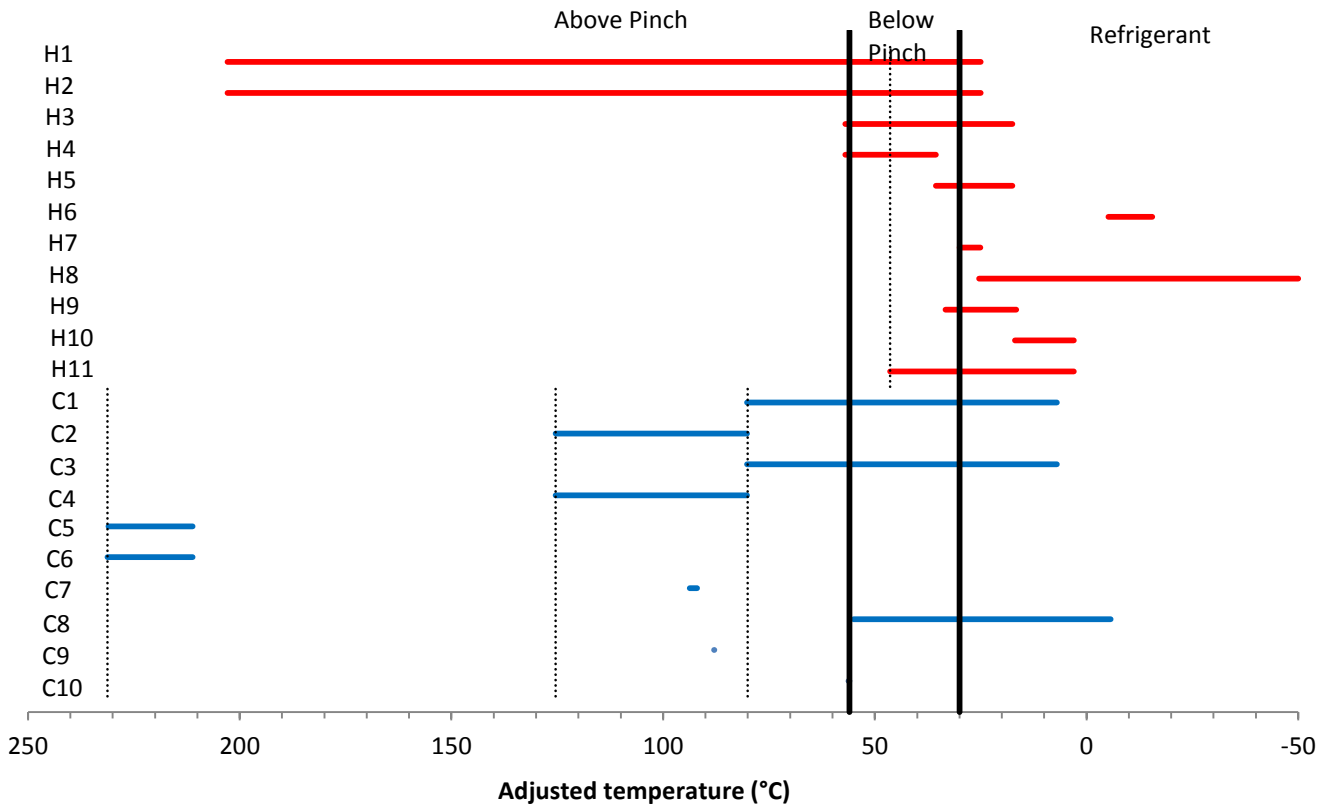


Figure 5.11: Second example – relative stream positions and interval placement.

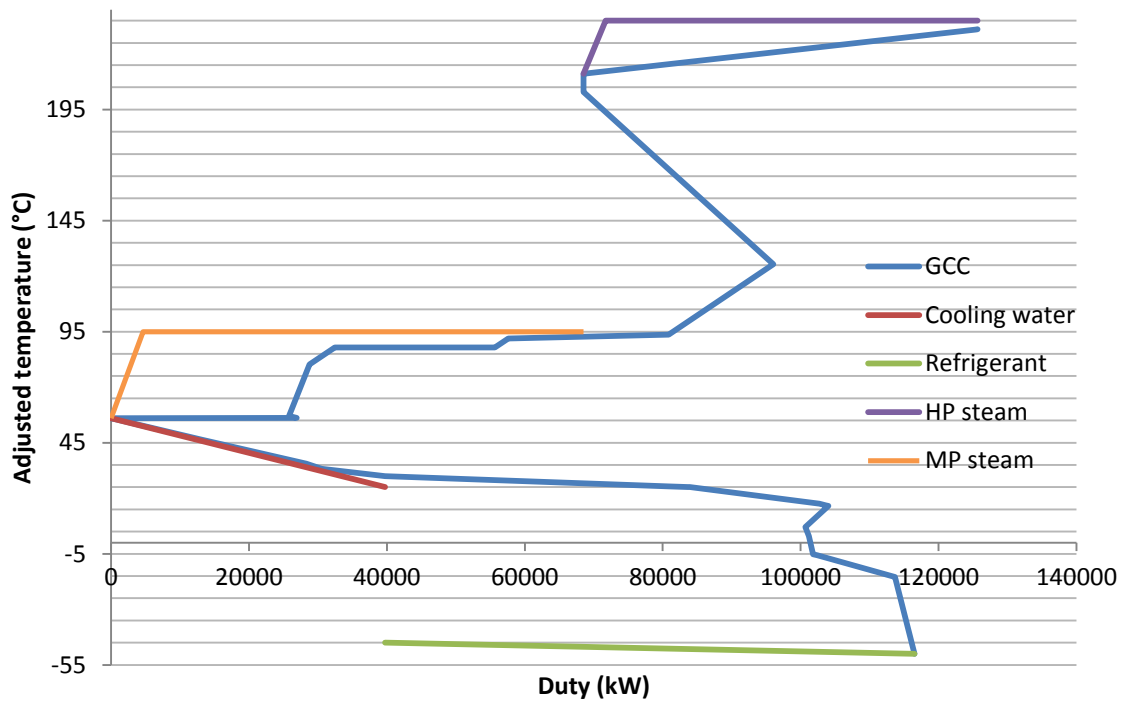


Figure 5.12: Second example – graphical targeting.

5 Illustrative Examples

Turning to the new models developed in Chapter 4, for Case 1 the Above Pinch model obtained a minimum total steam flowrate of 56.140 kg/s. This represents a 19% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and a 10% reduction compared to the base case where pinch techniques were applied to the three regions separately.

For Case 1, the Below Pinch Model obtained a minimum cooling water flowrate of 276.388 kg/s and an improved cooling tower effectiveness of 0.981. This represents a 46% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and a 22% reduction compared to the base case where pinch techniques were applied to the three regions separately. Note that these results are better than the targets obtained via graphical targeting on the GCC. It is concluded that graphical targeting on the GCC is not a suitable tool for holistically optimising the utility systems.

The heat exchanger networks obtained by the Above Pinch Model and Below Pinch Model for Case 1 are shown in Figure 5.13 and Figure 5.14 below. The duties transferred by each heat exchanger are given in Table 5.11 and Table 5.12 respectively. Note that these represent the solutions to two sub-problems. The section of the problem in which the temperatures are too low for cooling water, and which was dealt with using refrigerant as in the original problem is shown in Figure 5.15. The final heat exchanger network comprises the three networks shown below joined at the pinches. Note also how the utility heat exchangers are not restricted to the periphery, but interact with the process-process heat exchangers throughout all of the intervals.

5 Illustrative Examples

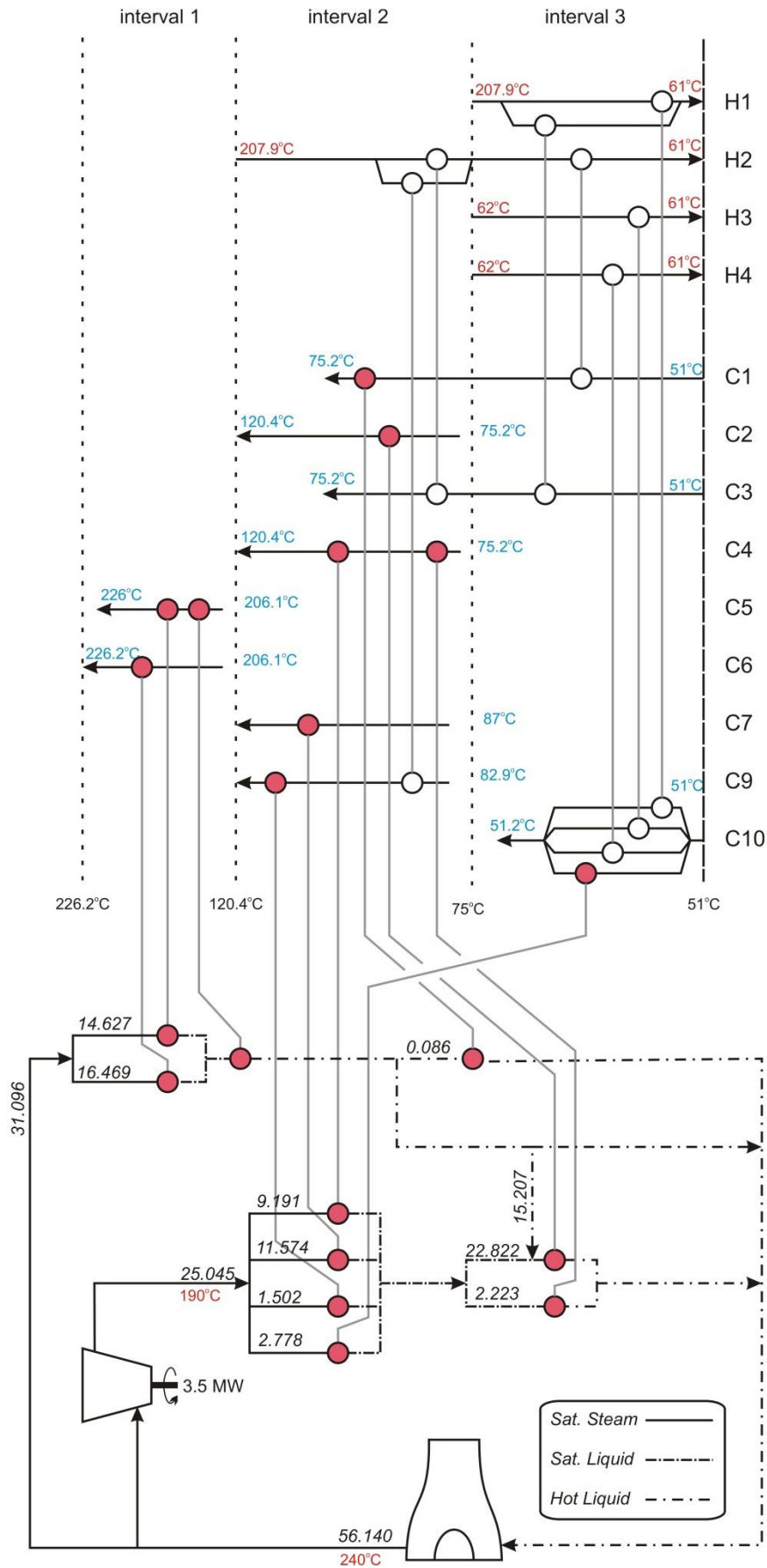


Figure 5.13: Second example - above pinch HEN for Case 1.

5 Illustrative Examples

Table 5.11: Duties for Figure 5.13 in kW.

<u>Interval 1</u>			
C5 – Util	28570	C6 – Util	28570
<u>Interval 2</u>			
C3 – H2	48	C4 – Util	18844
C9 – H2	20255	C7 – Util	22468
C1 – Util	48	C8 – Util	2916
C2 – Util	18844		
<u>Interval 3</u>			
C1 – H2	5786	C10 – H3	652
C2 – H1	5786	C10 – H4	851
C10 – H1	20303	C10 – Util	5393

5 Illustrative Examples

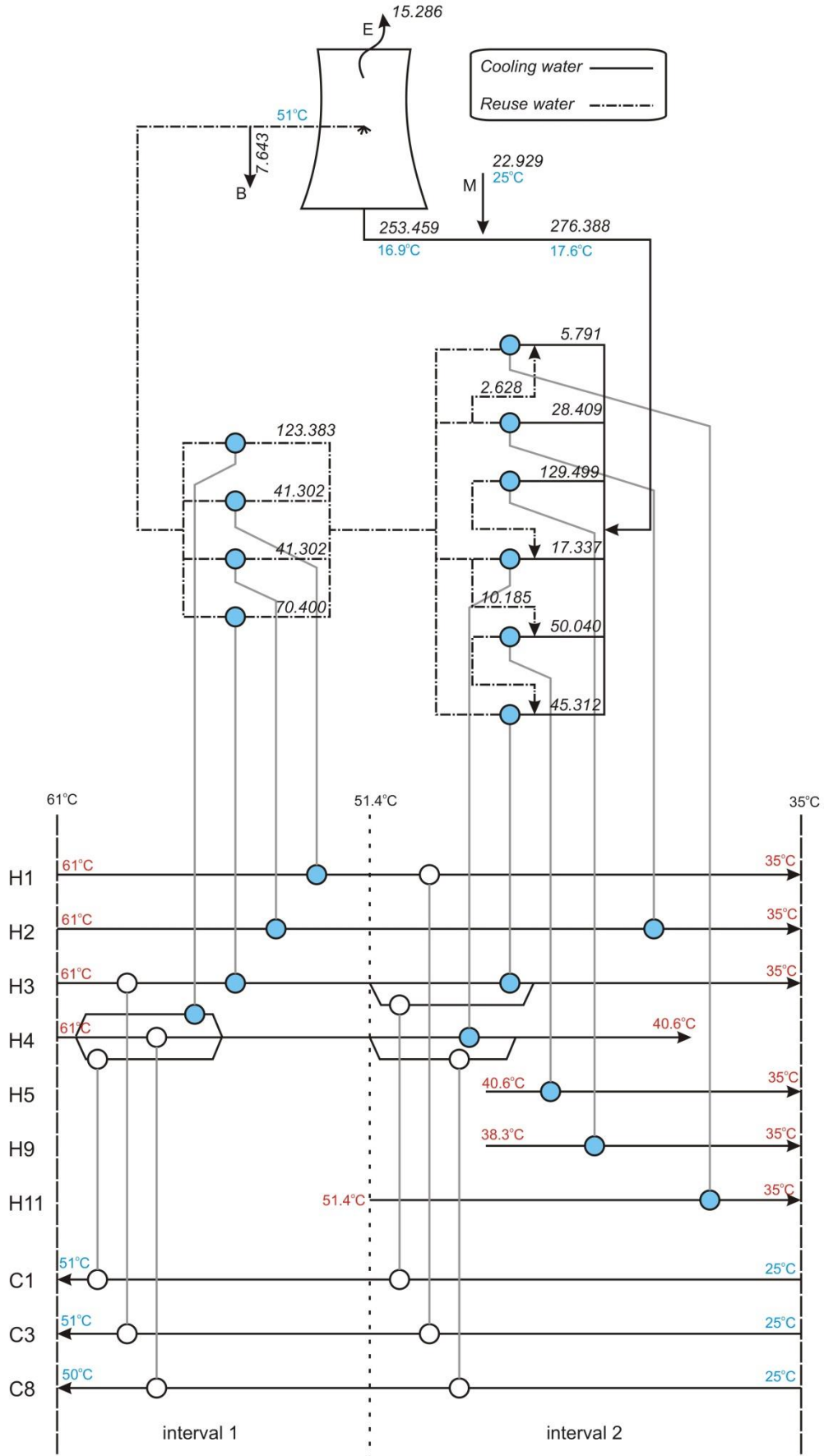


Figure 5.14: Second example - below pinch HEN for Case 1.

5 Illustrative Examples

Table 5.12: Duties for Figure 5.14 in kW.

<u>Interval 1</u>			
C1 – H4	3013	H2 – Util	1705
C3 – H3	3356	H3 – Util	2906
C8 – H4	61	H4 – Util	5093
H1 – Util	1705		
<u>Interval 2</u>			
C1 – H3	3255	H4 – Util	9072
C3 – H1	2913	H5 – Util	2334
C8 – H4	116	H9 – Util	5982
H2 – Util	2913	H11 – Util	594
H3 – Util	7442		

5 Illustrative Examples

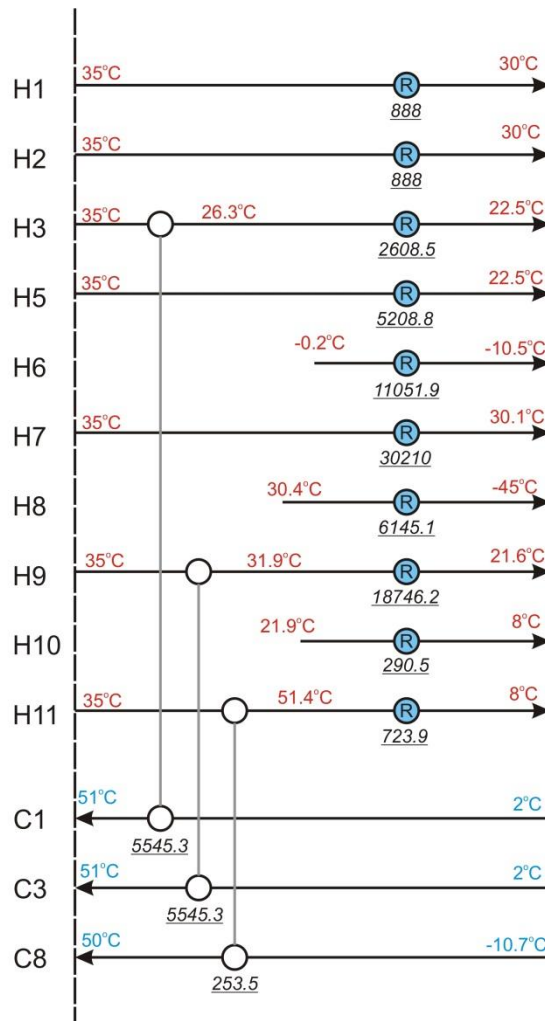


Figure 5.15: Second example - HEN for refrigerated section.

5 Illustrative Examples

For Case 2, the Above Pinch Model obtained a minimum total steam flowrate of 50.256 kg/s. This represents a 27% reduction in flowrate compared to the base case with no pinch techniques applied to the utilities, and a 5% reduction compared to the base case where pinch techniques were applied to the three regions separately. The flowrate of steam supplied to the turbine was found to be 12.522 kg/s, resulting in an MP steam level with a saturation temperature of 140°C.

For Case 2, the Below Pinch Model obtained a minimum cooling tower cost of \$33 050. This represents a 35% reduction in cost compared to the base case with no pinch techniques applied to the utilities, and a 13% reduction compared to the base case where pinch techniques were applied to the three regions separately. The tower packing has a cross sectional area of 130.204 m² and a height of 3.168 m.

The heat exchanger networks obtained by the Above Pinch Model and Below Pinch Model for Case 2 are shown in Figure 5.16 and Figure 5.17 below. The duties transferred by each heat exchanger are given in Table 5.13 and Table 5.14 respectively. The section of the problem in which the temperatures are too low for cooling water, and which was dealt with using refrigerant is same for Case 1, shown in Figure 5.15 above.

It must be noted that in the above designs, the minimum energy targets for the utilities, as determined by the problem table, have been met. Therefore, the reductions in the flowrates have not come at the expense of higher energy consumption. Based on the above mentioned results, it is concluded that the holistic and unified approach to heat integration on chemical plants yields better results than the application of separate techniques in isolation.

5 Illustrative Examples

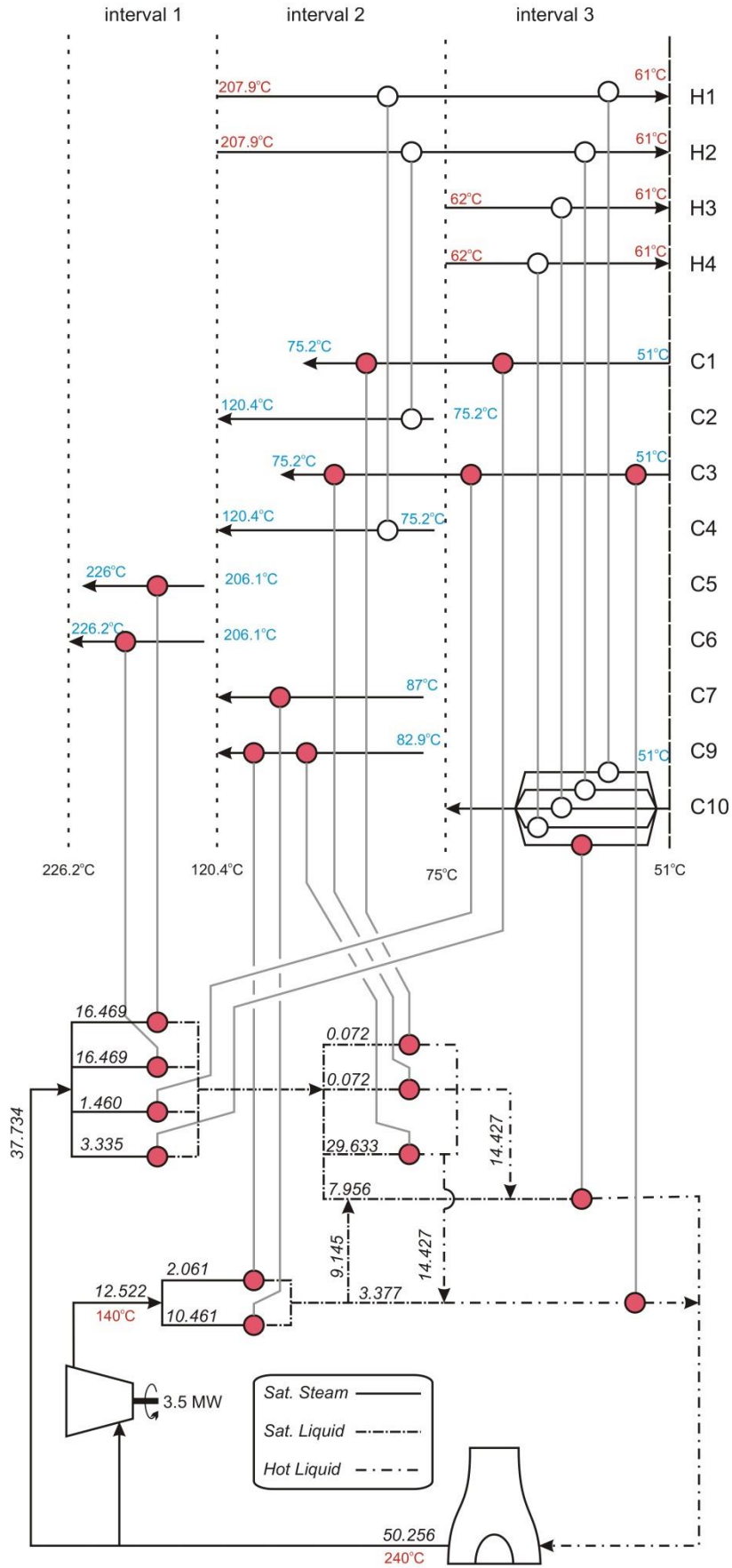


Figure 5.16: Second example - above pinch HEN for Case 2.

5 Illustrative Examples

Table 5.13: Duties for Figure 5.16 in kW.

<u>Interval 1</u>			
C5 – Util	28570	C6 – Util	28570
<u>Interval 2</u>			
C2 – H2	18844	C3 – Util	48
C4 – H1	18844	C7 – Util	22468
C1 – Util	48	C9 – Util	23171
<u>Interval 3</u>			
C10 – H1	7246	C1 – Util	5786
C10 – H2	7246	C2 – Util	5786
C10 – H3	652	C10 – Util	11205
C10 – H4	851		

5 Illustrative Examples

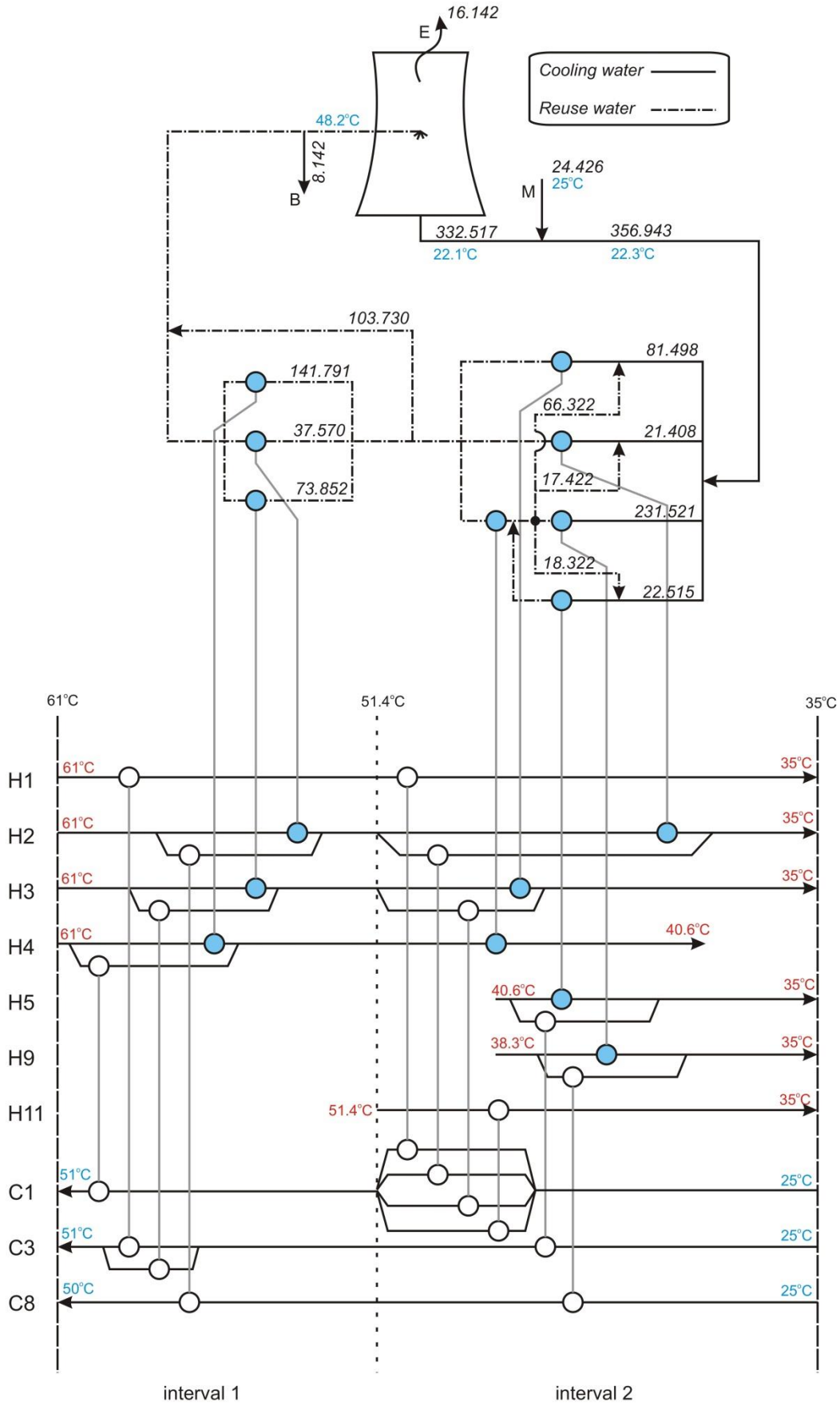


Figure 5.17: Second example - below pinch HEN for Case 2.

5 Illustrative Examples

Table 5.14: Duties for Figure 5.17 in kW.

<u>Interval 1</u>			
C1 – H4	2315	H2 – Util	1551
C3 – H1	1705	H3 – Util	3049
C3 – H3	3213	H4 – Util	5853
C8 – H2	154		
<u>Interval 2</u>			
C1 – H1	2913	H2 – Util	2738
C1 – H2	174	H3 – Util	10424
C1 – H3	273	H4 – Util	9189
C1 – H11	594	H5 – Util	983
C3 – H5	1350	H9 – Util	5959
C8 – H9	23		

5 Illustrative Examples

5.2.4 Summary

Table 5.15: summary of second example, Case 1.

<u>Above pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	69.36		
Separate methods	62.40	10%	
New method	56.14	19%	10%
<u>Below Pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	513.17		
Separate methods	355.51	30%	
New method	276.39	46%	22%
<u>Model statistics</u>			
	Continuous variables	Binary variables	Solution time (s)
Above Pinch	1715	77	0.078
Below Pinch	1121	44	0.83

5 Illustrative Examples

Table 5.16: Summary of second example, Case 2.

<u>Above pinch</u>			
	Flow (kg/s)	Reduction on Base Case	Reduction on separate methods
Base Case	69.36		
Separate methods	53.11	23%	
New method	50.26	27%	5%
<u>Below Pinch</u>			
	Cost (\$)	Reduction on Base Case	Reduction on separate methods
Base Case	51 175		
Separate methods	38 137	25%	
New method	33 050	35%	13%
<u>Model statistics</u>			
	Continuous variables	Binary variables	Solution time (s)
Above Pinch	1721	77	0.125
Below Pinch	1214	44	3.25

5.3 References

- Beangstrom SG (2013). *Steam system network analysis, synthesis and optimisation*. Master's thesis, Department of Chemical Engineering, University of Pretoria, South Africa.
- Egeberg LE (1998). *Efficient MILP models for design of heat exchanger networks*. Master's thesis, Department of Energy and Process Engineering, Norwegian University of Science and Technology, Norway.
- Gololo KV & Majazi T (2011). On synthesis and optimization of cooling water systems with multiple cooling towers. *Ind. Eng. Chem. Res.*, 50, 3775-3787.
- Harrel G (1996). *Steam system survey guide*. ORNL/TM-2001/263: Oak Ridge National Laboratory.
- Seider WD, Seader JD, & Lewin DR (2004). *Product & Process Design Principles*. USA: John Wiley & Sons.
- Yee F & Grossmann IE (1990). Simultaneous optimization models for heat integration - II. Heat exchanger network synthesis. *Comp. Chem. Eng.*, 14(10), 1165-1184.

Chapter 6

Conclusions and Recommendations

In this work, a unified approach to heat integration on chemical plants has been presented. The heat exchange between hot and cold streams, together with the cooling water system, the steam system, and the associated utilities have been treated in a holistic fashion. This addresses the shortcomings of previous methods in which the various regions of heat integration have been treated in isolation. Through this unified approach, greater improvements in the utility sections of a plant can be achieved, compared to when the various regions of heat integration are optimised independently.

In conventional practice, process-process heat integration is used to minimise the amount of hot and cold utilities by transferring heat from hot streams to cold streams, with hot and cold utilities placed on the periphery. Less conventional are pinch techniques applied to these utilities. In cooling water systems, the reuse of cooling water results in improved cooling due to reduced circulating flowrate and increased return temperature. In steam systems, reduced steam flowrate through hot condensate reuse results in smaller and cheaper boilers. In both cases, the reduction of utility flowrate can be used to debottleneck existing processes.

6 Conclusions and Recommendations

The shortcoming of current published methods is that the different systems are treated separately from one another. Since process-process heat integration, cooling water system design, and steam system design all form part of the larger energy system of a chemical plant, it is expected that these three regions all interact, and with their associated utilities behave as one system. By optimising the different sections independently, suboptimal results are obtained.

In this work, the energy system is treated as a single entity, creating a comprehensive utility system design. In this way, all of the interactions within the energy system can be accounted for. A new method is proposed in which the processes-process network, the cooling water system and the steam system are simultaneously synthesised. In addition, provision is made to include the operation of steam turbines and cooling towers. In doing so, the operation of the plant energy system and its accompanying unit operations can be accurately modelled, allowing optimisation procedures to fully explore all potential design options.

The objective of this work was to provide a holistic method of designing the process-process heat exchanger network, while simultaneously designing and optimising both the cooling water system and the steam system and their accompanying utility operations. Since the “Golden Rules” of heat integration make it possible to separate a design at the pinch point, two MINLP models were developed; an Above Pinch Model, and a Below Pinch Model. In the first, the steam system and half of the process-process heat exchanger network are synthesised simultaneously. In the second, the cooling water system and the other half of the process-process heat exchanger network are synthesised simultaneously. In keeping with the objectives of the investigation, the two utilities are optimised without compromising the minimum energy requirements of the process.

6 Conclusions and Recommendations

The two models are capable of being applied to two cases. First, in the case of existing utility systems, the model can be applied to make the optimum use of the existing utilities while minimising the utility flowrates. In doing so, the system will be debottlenecked, allowing the plant to be enlarged without expanding the utility system. Furthermore, since the new unified approach performs better than the previous approach of isolated application, the new method can be used to further debottleneck processes that have already been debottlenecked using old procedures. The second case concerns the grass roots design of a plant, in which the heat exchanger networks and the accompanying utility unit operations are optimised simultaneously.

The new models were applied to two illustrative examples to demonstrate their function. The same examples were also solved using no utility heat integration, and isolated application of utility heat integration to provide a basis on which to compare the results. The results are listed below. In all cases, the minimum energy requirements of the process were not compromised.

First example:

- For the case of existing utility systems
 - Steam flowrate was reduced by 27% compared to no application of steam system pinch techniques, and 14% compared to the separate treatment of heat integration regions.
 - Cooling water flowrate was reduced by 12% compared to no application of cooling water system pinch techniques, and 11% compared to the separate treatment of the heat integration regions.

6 Conclusions and Recommendations

- For the case of grass roots design
 - Steam flowrate was reduced by 26% compared to no application of steam system pinch techniques, and 15% compared to the separate treatment of heat integration regions.
 - Cooling tower capital cost was reduced by 10% compared to no application of cooling water system pinch techniques, and 9% compared to the separate treatment of the heat integration regions.

Second example:

- For the case of existing utility systems
 - Steam flowrate was reduced by 19% compared to no application of steam system pinch techniques, and 10% compared to the separate treatment of heat integration regions.
 - Cooling water flowrate was reduced by 46% compared to no application of cooling water system pinch techniques, and 22% compared to the separate treatment of the heat integration regions.
- For the case of grass roots design
 - Steam flowrate was reduced by 27% compared to no application of steam system pinch techniques, and 5% compared to the separate treatment of heat integration regions.
 - Cooling tower capital cost was reduced by 35% compared to no application of cooling water system pinch techniques, and 13% compared to the separate treatment of the heat integration regions.

From the above results, it is concluded that the comprehensive coverage of a plant's energy system provides greater reductions in utility flowrates than when heat integration is applied separately to the various regions of interest. It is concluded that the new unified approach to heat integration is a feasible method, superior to existing alternatives. The objective of developing a model

6 Conclusions and Recommendations

for the unified treatment of heat integration on chemical plants has been met. This model successfully addresses the shortcomings of the current practice of dealing with separate regions in isolation.

As process integration methods develop, and the unit operations on a plant interact to ever greater degrees, the issue of disturbance propagation becomes of concern. Highly integrated systems are harder to control, raising concerns regarding the meeting of product specifications, and safety. This is especially true when the utility systems, which serve to control temperatures on a plant, become more interactive. For this reason, it is recommended that the controllability of these systems be studied. Where these systems display poor controllability, new methods will have to be developed that will achieve similar savings within a more controllable frame work. Not only will this result in smoother plant operation, but will make such methods more attractive to potential investors.

Appendices

Appendix A: Steam levels and hot liquid reuse

In this work, it was stated that when hot liquid reuse is employed as a strategy for steam flowrate reduction, only two steam levels should be used. Here a brief justification is given, taken from an analysis performed by Beangstrom (2013). 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 A1) with minimum inlet and outlet temperatures of T_{in} and T_{out} respectively.

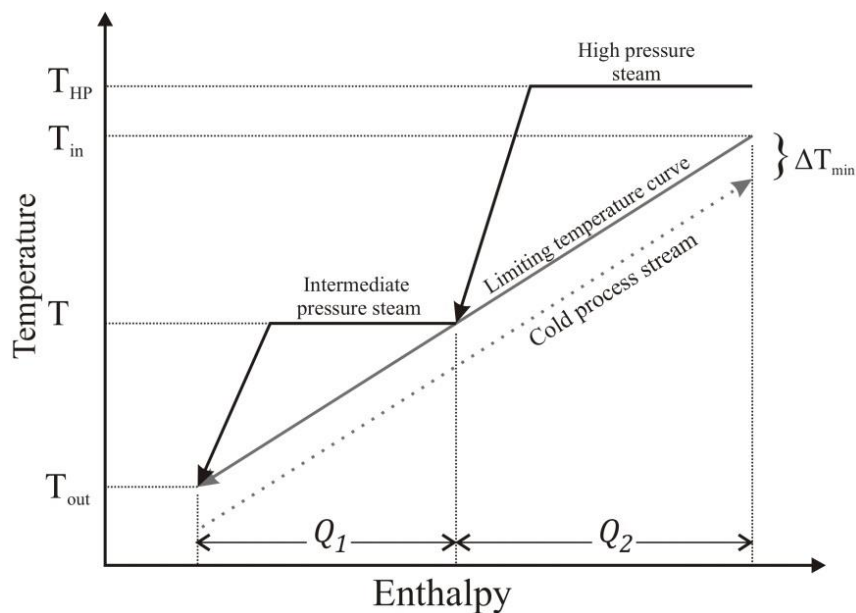


Figure A1: An arbitrary process heated using latent and sensible heat from two steam levels.

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. Here, T_{HP} must be fixed at any temperature greater than or equal to T_{in} to ensure heating is always possible. The second steam level considered is an intermediate pressure steam level with an arbitrarily chosen saturation temperature T . This steam level is the variable factor for this analysis.

The system depicted in Figure A1 represents the minimum steam flowrate for the given steam level saturation temperatures. The duties provided by both steam levels are calculated using similar triangles (Equations A1 and A2). 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 A3 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 A4 gives this function, with Equation A5 representing λ .

$$Q_1 = \frac{(T - T_{out})}{(T_{in} - T_{out})} Q \quad (A1)$$

$$Q_2 = \frac{(T_{in} - T)}{(T_{in} - T_{out})} Q \quad (A2)$$

$$\dot{m} = \frac{Q}{\lambda + c_p(T_{sat} - T)} \quad (A3)$$

$$\dot{m}(T) = \frac{(T - T_{out})Q}{(T_{in} - T_{out})(c_p(T - T_{out}) + \lambda)} + \frac{(T_{in} - T)Q}{(T_{in} - T_{out})(c_p(T_{HP} - T) + \lambda_{HP})} \quad (A4)$$

$$\lambda(T) = a - bT \quad (A5)$$

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 A4 with respect to T . Equation A6 gives this first derivative, after simplification.

$$\frac{d\dot{m}}{dT} = \frac{Q\lambda_{out}}{(T_{in} - T_{out})(c_p(T - T_{out}) + \lambda)^2} - \frac{Q\lambda_{HP}}{(T_{in} - T_{out})(c_p(T_{HP} - T) + \lambda_{HP})^2} \quad (A6)$$

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 A7, with the values expressed in Equations A8 and A9 used to reduce the overall length of Equation A7. It is noted that only the positive root leads to a sensible stationary point in the context of this investigation.

$$T^* = \frac{(\lambda_{out}c_p)T_{in} - (\theta - a\gamma)\lambda_{HP} \pm \{\theta - \gamma\lambda_{HP} - \gamma c_p T_{in}\}\sqrt{\lambda_{out}\lambda_{HP}}}{\lambda_{out}c_p^2 - \gamma^2\lambda_{HP}} \quad (A7)$$

$$\gamma = (c_p - b) \quad (A8)$$

$$\theta = (T_{out}c_p^2 - ac_p) \quad (A9)$$

To test whether this stationary point is a maximum or a minimum, the second derivative of Equation A6 with respect to T must be used. This second derivative, evaluated at the stationary point, is given in Equation A10.

$$\left. \frac{d^2 \dot{m}}{dT^2} \right|_{T^*} = \frac{-2Q(c_p - b)\lambda_{out}}{(T_{in} - T_{out})(c_p(T^* - T_{out}) + \lambda^*)^3} - \frac{2Qc_p\lambda_{HP}}{(T_{in} - T_{out})(c_p(T_{HP} - T^*) + \lambda_{HP})^3} \quad (A10)$$

It can be 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 A10 are positive. Since b has a value of 4.13 between 100°C and 300°C and because the heat capacity of water between these limits is greater than 4.13 in value (Cooper & Le Fevre, 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. The lowest flowrate is achieved when T is set to a value of either T_{out} or T_{HP} . In either case, this implies that for minimum steam flowrate, only the HP steam level should be used. Since having additional steam levels is unavoidable when turbines are present and supplying exhaust steam, the next best situation is to only have one large turbine and two steam levels, as confirmed by the results obtained by Beangstrom (2013).

Reference

Beangstrom SG (2013). *Steam system network analysis, synthesis and optimisation*. Master's thesis, Department of Chemical Engineering, University of Pretoria, South Africa.

Appendix B: GAMS codes

B.1 First case – Above Pinch Model

sets

h set of hot streams /h1*h7/

c set of cold streams /c1*c6/

k interval /k1*k6/

l steam level /HP, MP/;

Alias (c,cp);

Alias (k,kp);

parameters

TsupH(h) supply temperature of hot stream

/h1 240

h2 130

h3 233

h4 230

h5 253

h6 151

h7 189/

TtarH(h) target temperature of hot stream

/h1 132

h2 102

h3 102

h4 102

h5 192

h6 102

h7 102/

TsupC(c) supply temperature of cold stream

/c1 92

Appendices

c2 92
 c3 107
 c4 92
 c5 170
 c6 92/

TtarC(c) target temperature of cold stream

/c1 233
 c2 246
 c3 245
 c4 172
 c5 184
 c6 120/

CPH(h) heat capacity flow hot streams

/h1 25.8
 h2 213.7
 h3 42.4
 h4 128.9
 h5 19.3
 h6 15.2
 h7 100.1/

CPC(c) heat capacity flow cold streams

/c1 171
 c2 124.3
 c3 98
 c4 41.8
 c5 485.9
 c6 172.8/

tInt(k) interval temperature boundaries

/k1 246
 k2 220
 k3 179
 k4 141
 k5 120
 k6 92/

Tsat(l)

/HP 270
 MP 195/

tC(c,k) cold stream temperatures at interval boundaries

QH(h) heat from hot streams

QC(c) heat to cold streams

HLup(c,k) liquid upper flowrate

SSup(c,k) steam upper flowrate

Exist(c,k) stream c exists in interval k

Lam(l) latent heat

Appendices

DelH isentropic enthalpy change
 TUS Turbine supply;

$QH(h) = CPH(h) * (TsupH(h) - TtarH(h));$
 $QC(c) = CPC(c) * (TtarC(c) - TsupC(c));$
 $Lam(l) = 2726 - 4.13 * Tsat(l);$

loop((c,k)\$ord(k) lt card(k)),

 if((TtarC(c) > tInt(k+1)) and (TsupC(c) < tInt(k)),
 Exist(c,k) = 1);

loop((c,k)\$ord(k) lt card(k)),

 If((exist(c,k)) and (TtarC(c) < tInt(k)),
 tC(c,k) = TtarC(c);
 Elseif (exist(c,k)) and (TtarC(c) >= tInt(k)),
 tC(c,k) = tInt(k));

 If((exist(c,k)) and (TsupC(c) >= tInt(k+1)),
 tC(c,k+1) = TsupC(c));

Scalar

DelT minimum temperature difference /10/
 Gamma large number /500/
 CpW heat capacity of water /4.3/
 ShWork shaft work required (MW) /0.5/;

Positive variables

PPQ(c,h,k) process-process heat
 HUQ(c,k) heat from hot utility
 tH(h,k) temp of cold stream at k

RT Total liquid return
 ST(l) total saturated steam
 SS(c,k,l) Supply of steam to c in k
 HLin(c,k) total liquid flow in
 HOut(c,k) total liquid flow out
 FR(c,k) saturated boiler return
 SL(c,k,l) saturated liquid
 SLR(l) Saturated liquid return
 FRR(c,k,c,k) hot liquid from cp_in_kp to c_in_k
 SSQ(c,k,l) saturated steam duty
 HLQ(c,k) hot liquid duty;

$HLup(c,k) * exist(c,k) = CPC(c) / CpW;$
 $SSup(c,k) * exist(c,k) = CPC(c) * (tC(c,k) - tC(c,k+1)) / (2726 - 4.13 * 300);$

Appendices

scalar

A,B;

$$A = -0.131 + 0.00117 * \text{Tsat}('HP');$$

$$B = 0.989 + 0.00152 * \text{Tsat}('HP');$$

$$\text{DelH} = (\text{Tsat}('HP') - \text{Tsat}('MP')) / (391.8 + 2.215 * \text{Tsat}('HP'));$$

$$\text{TUS} = (A + B * \text{ShWork}) / (\text{DelH} * 3.6);$$

binary variable

pp(c,h,k) Process-process exists

x(c,k,l) Uses steam

y(c,k) Uses hot liquid;

Variable

Ob;

*===== Process-Process heat integration =====

Equations

p1,p2,p3,p4,p5,p6,p7,p8,p9,p10;

*overall stream heat balances

$$p1(h).. \quad QH(h) = e = \text{sum}((c,k), \text{PPQ}(c,h,k) \$ (\text{exist}(c,k)));$$

$$p2(c).. \quad QC(c) = e = \text{sum}((h,k), \text{PPQ}(c,h,k) \$ (\text{exist}(c,k))) + \text{sum}(k, \text{HUQ}(c,k) \$ (\text{exist}(c,k)));$$

*Stage heat balances

$$p3(h,k) \$ (\text{ord}(k) \text{ lt card}(k)).. \quad (tH(h,k) - tH(h,k+1)) * \text{CPH}(h) = e = \text{sum}(c, \text{PPQ}(c,h,k) \$ (\text{exist}(c,k)));$$

$$p4(c,k) \$ (\text{exist}(c,k)).. \quad (tC(c,k) - tC(c,k+1)) * \text{CPC}(c) = e = \text{sum}(h, \text{PPQ}(c,h,k)) + \text{HUQ}(c,k);$$

*Hot steam endpoints

$$p5(h).. \quad tH(h, 'k1') = e = \text{TsupH}(h);$$

$$p6(h).. \quad tH(h, 'k6') = e = \text{TtarH}(h);$$

*monotonically decreasing temperatures

$$p7(h,k) \$ (\text{ord}(k) \text{ lt card}(k)).. \quad tH(h,k) = g = tH(h,k+1);$$

*delta T min

$$p8(c,h,k) \$ (\text{exist}(c,k)).. \quad tH(h,k) - tC(c,k) + \text{Gamma} * (1 - \text{pp}(c,h,k)) = g = \text{DelT};$$

$$p9(c,h,k) \$ (\text{exist}(c,k)).. \quad tH(h,k+1) - tC(c,k+1) + \text{Gamma} * (1 - \text{pp}(c,h,k)) = g = \text{DelT};$$

*Binary variables

$$p10(c,h,k) \$ (\text{exist}(c,k)).. \quad \text{PPQ}(c,h,k) = l = \text{pp}(c,h,k) * (\text{CPC}(c) * (tC(c,k) - tC(c,k+1)));$$

*===== Steam system heat integration =====

Equations

s1,s2,s3,s4,s5,s6,s7,s8,s10,s11,s12,s13,s14,s15,s16,s17,s18,s19,t1,obj;

*material balances

$$s1(l).. \quad \text{ST}(l) = e = \text{sum}((c,k), \text{SS}(c,k,l) \$ (\text{exist}(c,k)));$$

Appendices

$$\begin{aligned} s2.. & RT = e = \text{sum}((c,k), FR(c,k) \$(\text{exist}(c,k))) + \text{sum}(l, SLR(l)); \\ s3.. & \text{sum}(l, ST(l)) = e = RT; \\ s4(l).. & \text{sum}((c,k), SL(c,k,l) \$(\text{exist}(c,k))) + SLR(l) = e = ST(l); \end{aligned}$$

$$\begin{aligned} s5(c,k) \$(\text{exist}(c,k)).. & HLin(c,k) = e = \text{sum}(l, SL(c,k,l)) + \text{sum}((cp, kp), \\ & FRR(cp, kp, c, k) \$(\text{exist}(cp, kp))); \\ s6(c,k) \$(\text{exist}(c,k)).. & HLout(c,k) = e = \text{sum}((cp, kp), FRR(c, k, cp, kp) \$(\text{exist}(cp, kp))) + FR(c, k); \\ s7(c,k) \$(\text{exist}(c,k)).. & HLin(c,k) = e = HLout(c,k); \\ \\ s8(c,k) \$(\text{exist}(c,k)).. & HLin(c,k) = l = y(c,k) * HLup(c,k); \\ s10(c,k,l) \$(\text{exist}(c,k)).. & SS(c,k,l) = l = x(c,k,l) * SSup(c,k); \\ s11(c,k) \$(\text{exist}(c,k)).. & FRR(c, k, c, k) = e = 0; \end{aligned}$$

*energy balances

$$\begin{aligned} s12(c,k) \$(\text{exist}(c,k)).. & HUQ(c,k) = e = \text{sum}(l, SSQ(c,k,l)) + HLQ(c,k); \\ s13(c,k,l) \$(\text{exist}(c,k)).. & SSQ(c,k,l) = e = Lam(l) * SS(c,k,l); \\ s14(c,k) \$(\text{exist}(c,k)).. & HLQ(c,k) = e = CpW * \text{sum}(l, (SL(c,k,l) * Tsat(l))) + \\ & CpW * \text{sum}((cp, kp), (FRR(cp, kp, c, k) * (tC(cp, kp+1) + DelT)) \$(\text{exist}(cp, kp))) - \\ & CpW * HLout(c,k) * (tC(c,k+1) + DelT); \\ s15(c,k,l) \$(\text{exist}(c,k)).. & (tC(c,k) + DelT) * x(c,k,l) = l = Tsat(l); \\ s16(c,k) \$(\text{exist}(c,k)).. & HUQ(c,k) = g = HLin(c,k) * CpW * (tC(c,k) - tC(c,k+1)); \\ \\ s17(c,k) \$(\text{exist}(c,k)).. & (tC(c,k) + DelT) * HLin(c,k) = l = \text{sum}(l, SL(c,k,l) * Tsat(l)) + \\ & \text{sum}((cp, kp), (FRR(cp, kp, c, k) * (tC(cp, kp+1) - DelT)) \$(\text{exist}(cp, kp))); \\ s18(cp, kp, c, k) \$(tC(cp, kp+1) <= tC(c, k+1)).. & FRR(cp, kp, c, k) = e = 0; \\ s19(c,k) \$(\text{exist}(c,k)).. & \text{sum}(l, x(c,k,l)) + y(c,k) = l = 1; \end{aligned}$$

*turbine equations

$$\begin{aligned} t1.. & ST('MP') = l = TUS; \\ \\ obj.. & Ob = e = ST('HP') + TUS; \end{aligned}$$

model SteamLinear /all/;
 solve SteamLinear using MIP minimizing Ob;

B.2 First case – Below Pinch Model

sets
 h set of hot streams /h2,h3,h4,h6,h7/
 c set of cold streams /c1,c2,c4/
 k interval /k1*k3/
 z /z0*z60/
 item /Tw, Ima, W, Liq/
 prop /Imasw, Psatw, Wsat, hdaf/;

Alias (h, hp);
 Alias (k, kp);

parameters
 TsupH(h) supply temperature of hot stream
 /h2 102

Appendices

h3 102
 h4 102
 h6 102
 h7 102/

TtarH(h) target temperature of hot stream

/h2 34
 h3 37
 h4 35
 h6 35
 h7 32/

TsupC(c) supply temperature of cold stream

/c1 36
 c2 27
 c4 29/

TtarC(c) target temperature of cold stream

/c1 92
 c2 92
 c4 92/

CPH(h) heat capacity flow hot streams

/h2 213.7
 h3 42.4
 h4 128.9
 h6 15.2
 h7 100.1/

CPC(c) heat capacity flow cold streams

/c1 171
 c2 124.3
 c4 41.8/

tInt(k) temperatures at interval boundaries

/k1 102
 k2 46
 k3 32/

tH(h,k) hot stream temps at interval boundaries

QH(h) heat from hot streams

QC(c) heat to cold streams

Lup(h,k) upper limit on water

exist(h,k) h exists in interval k

Tup(h,k) maximum outlet temperature of h in k;

$$QH(h) = CPH(h) * (TsupH(h) - TtarH(h));$$

$$QC(c) = CPC(c) * (TtarC(c) - TsupC(c));$$

loop((h,k)\$ord(k) lt card(k)),

Appendices

If((TsupH(h) > tInt(k+1)) and (TtarH(h) < tInt(k)),
 exist(h,k) = 1));

loop((h,k)\$ord(k) lt card(k),

If((exist(h,k))and(TsupH(h) < tInt(k)),
 tH(h,k) = TsupH(h);
 Elseif (exist(h,k))and(TsupH(h) >= tInt(k)),
 tH(h,k) = tInt(k));

If((exist(h,k))and(TtarH(h) >= tInt(k+1)),
 tH(h,k+1) = TtarH(h));

Scalar

DelT minimum temperature difference /10/
 Gamma large number /500/
 CpW heat capacity of water /4.3/
 CpA heat capacity of water /1/
 CpV heat capacity of water vapour /1.9/
 Tlimit Limiting return temperature /55/
 Tcw cooling water temperature guess /20/
 step numerical method step size /0.05/
 G air flowrate per m² /2/
 A base are of packing /50/
 Lambda latent heat at 0degC /2501.7/
 Patm atmospheric pressure /86000/
 coef1
 coef2
 coef3;

Tup(h,k)\$exist(h,k) = min((tH(h,k)-DelT),Tlimit);

Lup(h,k)\$exist(h,k) = CPH(h)*(tH(h,k)-tH(h,k+1))/(CpW*(Tup(h,k)-(tH(h,k+1)-DelT)));

Positive variables

PPQ(c,h,k) process-process heat
 CUQ(h,k) heat to cold utility

CW total cooling water
 TR total return
 WS(h,k) supply of water to h in k
 WR(h,k) return to tower
 Fin(h,k) total flow in
 Fout(h,k) total flow out
 RR(h,k,h,k) reuse stream from hp_in_kp to h_in_k
 tC(c,k) temp of cold stream at k
 Tret return temperature
 Tcool cooling water temperature

tower(z,item) Tower variables
 dtower(z,item) derivative terms
 param(z,prop) Calculated values

Appendices

E evapourative losses
 B blowdown
 M makeup;

binary variable

pp(c,h,k) Process-process exists
 y(h,k) uses cooling water;

Variables

Ob,ob3;

*===== Process-Process heat integration =====

Equations

p1,p2,p3,p4,p5,p6,p7,p8,p9,p10;

*overall stream heat balances

p1(h).. $QH(h) = e = \sum((c,k), PPQ(c,h,k) \$(exist(h,k))) + \sum(k, CUQ(h,k) \$(exist(h,k)))$;
 p2(c).. $QC(c) = e = \sum((h,k), PPQ(c,h,k) \$(exist(h,k)))$;

*Stage heat balances

p3(h,k)\$(exist(h,k)).. $(tH(h,k) - tH(h,k+1)) * CPH(h) = e = \sum(c, PPQ(c,h,k)) + CUQ(h,k)$;
 p4(c,k)\$(ord(k) lt card(k)).. $(tC(c,k) - tC(c,k+1)) * CPC(c) = e = \sum(h, PPQ(c,h,k) \$(exist(h,k)))$;

*Hot steam endpoints

p5(c).. $tC(c, 'k1') = e = TtarC(c)$;
 p6(c).. $tC(c, 'k3') = e = TsupC(c)$;

*monotonically decreasing temperatures

p7(c,k)\$(ord(k) lt card(k)).. $tC(c,k) = g = tC(c,k+1)$;

*delta T min

p8(c,h,k)\$(exist(h,k)).. $tH(h,k) - tC(c,k) + \text{Gamma} * (1 - pp(c,h,k)) = g = \text{DelT}$;
 p9(c,h,k)\$(exist(h,k)).. $tH(h,k+1) - tC(c,k+1) + \text{Gamma} * (1 - pp(c,h,k)) = g = \text{DelT}$;

*Binary variables

p10(c,h,k)\$(exist(h,k)).. $PPQ(c,h,k) = l = pp(c,h,k) * (CPH(h) * (tH(h,k) - tH(h,k+1)))$;;

*===== network synthesis =====

Equations

s1,s2,s3,s4,s5,s6,s7,s8,s9,s9a,s10,s10a,s11,s12,obj;

*Material balances

s1.. $CW = e = \sum((h,k), WS(h,k) \$(exist(h,k)))$;
 s2.. $TR = e = \sum((h,k), WR(h,k) \$(exist(h,k)))$;
 s3.. $CW = e = TR$;

s4(h,k)\$(exist(h,k)).. $Fin(h,k) = e = WS(h,k) + \sum((hp,kp), RR(hp,kp,h,k) \$(exist(hp,kp)))$;
 s5(h,k)\$(exist(h,k)).. $Fout(h,k) = e = \sum((hp,kp), RR(h,k,hp,kp) \$(exist(hp,kp))) + WR(h,k)$;
 s6(h,k)\$(exist(h,k)).. $Fin(h,k) = e = Fout(h,k)$;
 s7(h,k)\$(exist(h,k)).. $RR(h,k,h,k) = e = 0$;

Appendices

$$\begin{aligned}
 s8(h,k) \$(exist(h,k)).. \quad & Fin(h,k) = l = y(h,k) * Lup(h,k); \\
 s9(h,k) \$(exist(h,k)).. \quad & (tH(h,k+1) - DelT) * Fin(h,k) = g = \text{sum}((hp, kp), \\
 & (RR(hp, kp, h, k) * Tup(hp, kp)) \$(exist(hp, kp))) + WS(h, k) * Tcool; \\
 s9a(h,k) \$(exist(h,k)).. \quad & (tH(h,k+1) - DelT) * Fin(h,k) = g = \text{sum}((hp, kp), \\
 & (RR(hp, kp, h, k) * Tup(hp, kp)) \$(exist(hp, kp))) + WS(h, k) * Tcw;
 \end{aligned}$$

*energy balances

$$\begin{aligned}
 s10(h,k) \$(exist(h,k)).. \quad & CUQ(h,k) = e = CpW * Fout(h,k) * Tup(h,k) - \\
 & CpW * \text{sum}((hp, kp), (RR(hp, kp, h, k) * Tup(hp, kp)) \$(exist(hp, kp))) - CpW * WS(h, k) * Tcool; \\
 s10a(h,k) \$(exist(h,k)).. \quad & CUQ(h,k) = e = CpW * Fout(h,k) * Tup(h,k) - \\
 & CpW * \text{sum}((hp, kp), (RR(hp, kp, h, k) * Tup(hp, kp)) \$(exist(hp, kp))) - CpW * WS(h, k) * Tcw;
 \end{aligned}$$

$$\begin{aligned}
 s11.. \quad & \text{sum}((h, k), (WR(h, k) * (Tup(h, k))) \$(exist(h, k))) = e = TR * Tret; \\
 s12(hp, kp, h, k) \$(ord(kp) <= ord(k)).. \quad & RR(hp, kp, h, k) = e = 0;
 \end{aligned}$$

$$obj.. \quad Ob = e = CW;$$

*===== cooling tower =====

Equations

ct1, ct2, ct3, ct4, ct5, ct6, ct7, ct8, ct9a, ct9b, ct10a, ct10b, ct11, ct12, ct13, ct13a, ct14, ct15, ct16, ct17, ct18, obj3;

$$\begin{aligned}
 ct1(z).. \quad & CW * dtower(z, 'Tw') = e = (G * A) * (dtower(z, 'Ima') / CpW - \\
 & tower(z, 'Tw') * dtower(z, 'W')); \\
 ct2(z).. \quad & dtower(z, 'Ima') = e = (\text{param}(z, 'hdaf') / G) * (\text{param}(z, 'Imasw') - tower(z, 'Ima')); \\
 ct3(z).. \quad & dtower(z, 'W') = e = (\text{param}(z, 'hdaf') / G) * (\text{param}(z, 'Wsat') - tower(z, 'W')); \\
 ct4(z).. \quad & dtower(z, 'Liq') = e = G * dtower(z, 'W'); \\
 ct5(z).. \quad & \text{param}(z, 'Imasw') = e = CpA * tower(z, 'Tw') + \text{param}(z, 'Wsat') * (\text{Lambda} + \\
 & CpV * tower(z, 'Tw')); \\
 ct6(z).. \quad & \text{param}(z, 'Psatw') = e = \exp(23.7093 - 4111 / (237.7 + tower(z, 'Tw'))); \\
 ct7(z).. \quad & \text{param}(z, 'Wsat') = e = (18 / 29) * \text{param}(z, 'Psatw') / (\text{Patm} - \text{param}(z, 'Psatw')); \\
 ct8(z).. \quad & \text{param}(z, 'hdaf') = e = \text{coef1} + \text{coef2} * (tower(z, 'Liq') - \text{coef3});
 \end{aligned}$$

$$ct9a(z, item) \$((ord(z) > 1) \text{and} (ord(z) < 5)).. \quad tower(z, item) = e = tower(z-1, item) + step * dtower(z-1, item);$$

$$ct9b(z, item) \$(ord(z) > 4).. \quad tower(z, item) = e = tower(z-1, item) + step * (55 * dtower(z-1, item) - 59 * dtower(z-2, item) + 37 * dtower(z-3, item) - 9 * dtower(z-4, item)) / 24;$$

$$\begin{aligned}
 ct10a.. \quad & tower('z60', 'Tw') = e = Tret.l; \\
 ct10b.. \quad & tower('z60', 'Tw') = e = Tret; \\
 ct11.. \quad & tower('z0', 'Ima') = e = 49.19; \\
 ct12.. \quad & tower('z0', 'W') = e = 0.00949; \\
 ct13.. \quad & tower('z60', 'Liq') = e = (CW - B) / A; \\
 ct13a.. \quad & tower('z60', 'Liq') = e = (CW.l - B.l) / A; \\
 ct15.. \quad & E = e = A * (tower('z60', 'Liq') - tower('z0', 'Liq')); \\
 ct16.. \quad & B = e = 0.5 * E; \\
 ct17.. \quad & M = e = B + E; \\
 ct18.. \quad & Tcool * CW = e = 25 * M + tower('z0', 'Tw') * (CW - M);
 \end{aligned}$$

$$obj3.. \quad ob3 = e = tower('z0', 'Tw');$$

Appendices

*=====

```
model ColdSideLinear /p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s9a,s10a,s12,obj/;
solve ColdSideLinear using MIP minimizing Ob;
```

```
Tret.l = sum((h,k),(WR.l(h,k)*Tup(h,k))$(exist(h,k)))/TR.l;
E.l = 0.0016*CW.l*(Tret.l - Tcw);
B.l = 0.5*E.l;
M.l = B.l + E.l;
Tcool.l = (25*M.l + Tcw*(CW.l-M.l))/CW.l;
coef3 = (CW.l-B.l)/A;
coef1 = 1.88095*(G**0.48)*(coef3**0.52);
coef2 = 1.88095*0.52*(G**0.48)/(coef3**0.48);
```

```
model cooltower /ct1,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9a,ct9b,ct10a,ct11,ct12,ct13a,obj3/
solve cooltower using NLP minimising ob3;
```

```
model ColdNetwork
/p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s9,s10,s11,s12,ct1,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9a,c
t9b,ct10b,ct11,ct12,ct13,ct15,ct16,ct17,ct18,obj/
solve ColdNetwork using MINLP minimising Ob;
```

B.3 Second case – Above Pinch Model

sets

h set of hot streams /h1*h7/

c set of cold streams /c1*c6/

k interval /k1*k6/

l steam level /HP, MP/;

Alias (c,cp);

Alias (k,kp);

parameters

TsupH(h) supply temperature of hot stream

/h1 240

h2 130

h3 233

h4 230

h5 253

Appendices

h6 151
h7 189/

TtarH(h) target temperature of hot stream

/h1 132
h2 102
h3 102
h4 102
h5 192
h6 102
h7 102/

TsupC(c) supply temperature of cold stream

/c1 92
c2 92
c3 107
c4 92
c5 170
c6 92/

TtarC(c) target temperature of cold stream

/c1 233
c2 246
c3 245
c4 172
c5 184
c6 120/

CPH(h) heat capacity flow hot streams

/h1 25.8
h2 213.7
h3 42.4
h4 128.9
h5 19.3
h6 15.2
h7 100.1/

CPC(c) heat capacity flow cold streams

/c1 171
c2 124.3

Appendices

c3 98
 c4 41.8
 c5 485.9
 c6 172.8/

tInt(k) interval temperature boundaries\

/k1 246
 k2 220
 k3 179
 k4 141
 k5 120
 k6 92/

tC(c,k) cold stream temperatures at interval boundaries

QH(h) heat from hot streams

QC(c) heat to cold streams

HLup(c,k) liquid upper flowrate

SSup(c,k) steam upper flowrate

Exist(c,k) stream c exists in interval k;

$$QH(h) = CPH(h) * (TsupH(h) - TtarH(h));$$

$$QC(c) = CPC(c) * (TtarC(c) - TsupC(c));$$

loop((c,k)\$(ord(k) lt card(k)),

if((TtarC(c) > tInt(k+1)) and (TsupC(c) < tInt(k)),
 Exist(c,k) = 1));

loop((c,k)\$(ord(k) lt card(k)),

If((exist(c,k))and(TtarC(c) < tInt(k)),

tC(c,k) = TtarC(c);

Elseif (exist(c,k))and(TtarC(c) >= tInt(k)),

tC(c,k) = tInt(k));

If((exist(c,k)) and (TsupC(c) >= tInt(k+1)),

tC(c,k+1) = TsupC(c));

Appendices

Scalar

DelT	minimum temperature difference /10/
Gamma	large number /500/
CpW	heat capacity of water /4.3/
ShWork	shaft work required (MW) /0.5/
Thp	HP steam saturation temp guess /270/
Tmp	HP steam saturation temp guess /220/;

Positive variables

PPQ(c,h,k)	process-process heat
HUQ(c,k)	heat from hot utility
tH(h,k)	temp of cold stream at k

RT	Total liquid return
ST(l)	total saturated steam
SS(c,k,l)	Supply of steam to c in k
HLin(c,k)	total liquid flow in
HLout(c,k)	total liquid flow out
FR(c,k)	saturated boiler return
SL(c,k,l)	saturated liquid
SLR(l)	Saturated liquid return
FRR(c,k,c,k)	hot liquid from cp_in_kp to c_in_k
SSQ(c,k,l)	saturated steam duty
HLQ(c,k)	hot liquid duty

Tsat(l)	saturation temperature
Lam(l)	latent heat
DelH	isentropic enthalpy change
TUS	Turbine supply;

$$Tsat.l('HP') = Thp;$$

$$Tsat.l('MP') = Tmp;$$

$$Lam.l(l) = 2726 - 4.13 * Tsat.l(l);$$

$$HLup(c,k) \$(exist(c,k)) = CPC(c) / CpW;$$

$$SSup(c,k) \$(exist(c,k)) = CPC(c) * (tC(c,k) - tC(c,k+1)) / (2726 - 4.13 * 300);$$

scalar

A,B;

Appendices

$$A = -0.131 + 0.00117 * T_{\text{sat.l}}('HP');$$

$$B = 0.989 + 0.00152 * T_{\text{sat.l}}('HP');$$

$$\text{DelH.l} = (T_{\text{sat.l}}('HP') - T_{\text{sat.l}}('MP')) / (391.8 + 2.215 * T_{\text{sat.l}}('HP'));$$

$$\text{TUS.l} = (A + B * \text{ShWork}) / (\text{DelH.l} * 3.6);$$

binary variable

pp(c,h,k) Process-process exists

x(c,k,l) Uses steam

y(c,k) Uses hot liquid;

Variable

Ob;

*===== Process-Process heat integration =====

Equations

p1,p2,p2b,p3,p4,p4b,p5,p6,p7,p8,p9,p10;

*overall stream heat balances

$$p1(h).. \quad QH(h) = e = \sum((c,k), PPQ(c,h,k) \$(exist(c,k)));$$

$$p2(c).. \quad QC(c) = e = \sum((h,k), PPQ(c,h,k) \$(exist(c,k))) + \sum(k, HUQ(c,k) \$(exist(c,k)));$$

$$p2b(c).. \quad QC(c) = e = \sum((h,k), PPQ(c,h,k) \$(exist(c,k))) + \sum(k, HUQ.l(c,k) \$(exist(c,k)));$$

*Stage heat balances

$$p3(h,k) \$(ord(k) \text{ lt } card(k)).. \quad (tH(h,k) - tH(h,k+1)) * CPH(h) = e = \sum(c, PPQ(c,h,k) \$(exist(c,k)));$$

$$p4(c,k) \$(exist(c,k)).. \quad (tC(c,k) - tC(c,k+1)) * CPC(c) = e = \sum(h, PPQ(c,h,k)) + HUQ(c,k);$$

$$p4b(c,k) \$(exist(c,k)).. \quad (tC(c,k) - tC(c,k+1)) * CPC(c) = e = \sum(h, PPQ(c,h,k)) + HUQ.l(c,k);$$

*Hot steam endpoints

$$p5(h).. \quad tH(h, 'k1') = e = T_{\text{supH}}(h);$$

$$p6(h).. \quad tH(h, 'k6') = e = T_{\text{tarH}}(h);$$

*monotonically decreasing temperatures

$$p7(h,k) \$(ord(k) \text{ lt } card(k)).. \quad tH(h,k) = g = tH(h,k+1);$$

*delta T min

$$p8(c,h,k) \$(exist(c,k)).. \quad tH(h,k) - tC(c,k) + \text{Gamma} * (1 - pp(c,h,k)) = g = \text{DelT};$$

Appendices

$$p9(c,h,k)\$(exist(c,k)).. \quad tH(h,k+1) - tC(c,k+1) + \text{Gamma}*(1-pp(c,h,k)) =g= \text{DelT};$$

*Binary variables

$$p10(c,h,k)\$(exist(c,k)).. \quad \text{PPQ}(c,h,k) =l= pp(c,h,k)*(CPC(c)*(tC(c,k)-tC(c,k+1)));$$

*===== Steam system heat integration =====

Equations

s1,s2,s3,s4,s5,s6,s7,s8,s9,s10,s11,s12a,s13a,s14a,s15a,s16a,s12b,s13b,s14b,s15b,s16b,s17a,s17b,s18,s19,t
1a,t1b,t2,t3,t4,t5,t6,objA,objB;

*material balances

$$s1(l).. \quad \text{ST}(l) =e= \text{sum}((c,k),SS(c,k,l)\$(exist(c,k)));$$

$$s2.. \quad \text{RT} =e= \text{sum}((c,k),FR(c,k)\$(exist(c,k))) + \text{sum}(l,SLR(l));$$

$$s3.. \quad \text{sum}(l,ST(l)) =e= \text{RT};$$

$$s4(l).. \quad \text{sum}((c,k),SL(c,k,l)\$(exist(c,k))) + \text{SLR}(l) =e= \text{ST}(l);$$

$$s5(c,k)\$(exist(c,k)).. \quad \text{HLin}(c,k) =e= \text{sum}(l,SL(c,k,l)) + \text{sum}((cp,kp), \\ \text{FRR}(cp,kp,c,k)\$(exist(cp,kp)));$$

$$s6(c,k)\$(exist(c,k)).. \quad \text{HLout}(c,k) =e= \text{sum}((cp,kp),\text{FRR}(c,k,cp,kp)\$(exist(cp,kp))) + \text{FR}(c,k);$$

$$s7(c,k)\$(exist(c,k)).. \quad \text{HLin}(c,k) =e= \text{HLout}(c,k);$$

$$s8(c,k)\$(exist(c,k)).. \quad \text{HLin}(c,k) =l= y(c,k)*\text{HLup}(c,k);$$

$$s9(c,k,l)\$(exist(c,k)).. \quad \text{SL}(c,k,l) =l= x(c,k,l)*\text{HLup}(c,k);$$

$$s10(c,k,l)\$(exist(c,k)).. \quad \text{SS}(c,k,l) =l= x(c,k,l)*\text{SSup}(c,k);$$

$$s11(c,k)\$(exist(c,k)).. \quad \text{FRR}(c,k,c,k) =e= 0;$$

*energy balances

$$s12a(c,k)\$(exist(c,k)).. \quad \text{HUQ}(c,k) =e= \text{sum}(l,SSQ(c,k,l)) + \text{HLQ}(c,k);$$

$$s13a(c,k,l)\$(exist(c,k)).. \quad \text{SSQ}(c,k,l) =e= \text{Lam.l}(l)*\text{SS}(c,k,l);$$

$$s14a(c,k)\$(exist(c,k)).. \quad \text{HLQ}(c,k) =e= \text{CpW}*\text{sum}(l,(\text{SL}(c,k,l)*\text{Tsat.l}(l))) + \\ \text{CpW}*\text{sum}((cp,kp),(\text{FRR}(cp,kp,c,k)*(tC(cp,kp+1)+\text{DelT}))\$(exist(cp,kp))) - \\ \text{CpW}*\text{HLout}(c,k)*(tC(c,k+1)+\text{DelT});$$

$$s15a(c,k,l)\$(exist(c,k)).. \quad (tC(c,k)+\text{DelT})*x(c,k,l) =l= \text{Tsat.l}(l);$$

$$s16a(c,k)\$(exist(c,k)).. \quad \text{HUQ}(c,k) =g= \text{HLin}(c,k)*\text{CpW}*(tC(c,k)-tC(c,k+1));$$

$$s12b(c,k)\$(exist(c,k)).. \quad \text{HUQ.l}(c,k) =e= \text{sum}(l,SSQ(c,k,l)) + \text{HLQ}(c,k);$$

$$s13b(c,k,l)\$(exist(c,k)).. \quad \text{SSQ}(c,k,l) =e= \text{Lam}(l)*\text{SS}(c,k,l);$$

$$s14b(c,k)\$(exist(c,k)).. \quad \text{HLQ}(c,k) =e= \text{CpW}*\text{sum}(l,(\text{SL}(c,k,l)*\text{Tsat}(l))) + \\ \text{CpW}*\text{sum}((cp,kp),(\text{FRR}(cp,kp,c,k)*(tC(cp,kp+1)+\text{DelT}))\$(exist(cp,kp))) - \\ \text{CpW}*\text{HLout}(c,k)*(tC(c,k+1)+\text{DelT});$$

Appendices

$$s15b(c,k,l)\$(exist(c,k)).. \quad (tC(c,k)+DelT)*x(c,k,l) =l= Tsat(l);$$

$$s16b(c,k)\$(exist(c,k)).. \quad H U Q.l(c,k) =g= H L i n(c,k)*C p W*(tC(c,k)-tC(c,k+1));$$

$$s17a(c,k)\$(exist(c,k)).. \quad (tC(c,k)+DelT)*H L i n(c,k) =l= \sum(l, S L(c,k,l)*Tsat.l(l)) +$$

$$\sum((c p, k p), (F R R(c p, k p, c, k)*(tC(c p, k p+1)-DelT))\$(exist(c p, k p))));$$

$$s17b(c,k)\$(exist(c,k)).. \quad (tC(c,k)+DelT)*H L i n(c,k) =l= \sum(l, S L(c,k,l)*Tsat(l)) +$$

$$\sum((c p, k p), (F R R(c p, k p, c, k)*(tC(c p, k p+1)-DelT))\$(exist(c p, k p))));$$

$$s18(c p, k p, c, k)\$(tC(c p, k p+1) <= tC(c, k+1)).. \quad F R R(c p, k p, c, k) =e= 0;$$

$$s19(c,k)\$(exist(c,k)).. \quad \sum(l, x(c,k,l))+y(c,k) =l= 1;$$

*turbine equations

$$t1a.. \quad S T('M P') =l= T U S.l;$$

$$t1b.. \quad S T('M P') =l= T U S;$$

$$t2.. \quad D e l H =e= (Tsat('H P') - Tsat('M P'))/(391.8 + 2.215*Tsat('H P'));$$

$$t3.. \quad S h W o r k =e= (D e l H*3.6*T U S - A)/B;$$

$$t4.. \quad T s a t('H P') =e= T h p;$$

$$t5.. \quad T s a t('M P') =g= 100;$$

$$t6(l).. \quad L a m(l) =e= 2726 - 4.13*Tsat(l);$$

$$o b j A.. \quad O b =e= S T('H P');$$

$$o b j B.. \quad O b =e= S T('H P') + T U S;$$

model DoubleSteamLinear

/p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s10,s11,s12a,s13a,s14a,s15a,s16a,s17a,s18,s19,t1
a,objA/;

model DoubleSteamexact

/p1,p2b,p3,p4b,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s10,s11,s12b,s13b,s14b,s15b,s16b,s17b,s18,t1
b,t2,t3,t4,t5,t6,objB/;

solve DoubleSteamLinear using MIP minimizing Ob;

solve DoubleSteamExact using MINLP minimizing Ob;

B.4 Second case – Below Pinch Model

sets

h set of hot streams /h2,h3,h4,h6,h7/

c set of cold streams /c1,c2,c4/

k interval /k1*k3/

z /z0*z60/

item /Tw, Ima, W, Liq/

prop /Imasw, Psatw, Wsat, hdaf/;

Alias (h,hp);

Alias (k,kp);

parameters

TsupH(h) supply temperature of hot stream

/h2 102

h3 102

h4 102

h6 102

h7 102/

TtarH(h) target temperature of hot stream

/h2 34

h3 37

h4 35

h6 35

h7 32/

TsupC(c) supply temperature of cold stream

/c1 36

c2 27

c4 29/

TtarC(c) target temperature of cold stream

/c1 92

c2 92

c4 92/

CPH(h) heat capacity flow hot streams

/h2 213.7

Appendices

h3 42.4
 h4 128.9
 h6 15.2
 h7 100.1/

CPC(c) heat capacity flow cold streams

/c1 171
 c2 124.3
 c4 41.8/

tInt(k) temperatures at interval boundaries

/k1 102
 k2 46
 k3 32/

tH(h,k) hot stream temps at interval boundaries

QH(h) heat from hot streams

QC(c) heat to cold streams

Lup(h,k) upper limit on water

exist(h,k) h exists in interval k

Tup(h,k) maximum outlet temperature of h in k;

$$QH(h) = CPH(h) * (TsupH(h) - TtarH(h));$$

$$QC(c) = CPC(c) * (TtarC(c) - TsupC(c));$$

loop((h,k)\$ord(k) lt card(k)),

If((TsupH(h) > tInt(k+1)) and (TtarH(h) < tInt(k)),
 exist(h,k) = 1));

loop((h,k)\$ord(k) lt card(k)),

If((exist(h,k)) and (TsupH(h) < tInt(k)),

tH(h,k) = TsupH(h);

Elseif (exist(h,k)) and (TsupH(h) >= tInt(k)),

tH(h,k) = tInt(k);

If((exist(h,k)) and (TtarH(h) >= tInt(k+1)),

tH(h,k+1) = TtarH(h));

Appendices

Scalar

DelT minimum temperature difference /10/

Gamma large number /500/

CpW heat capacity of water /4.3/

CpA heat capacity of water /1/

CpV heat capacity of water vapour /1.9/

Tlimit Limiting return temperature /55/

Tcw cooling water temperaturee guess /20/

step numerical method step size /0.05/

G air flowrate per m² /2/

A base are of packing /50/

Lambda latent heat at 0degC /2501.7/

Patm atmospheric pressure /86000/

coef1

coef2

coef3;

$Tup(h,k) \text{ exist}(h,k) = \min((tH(h,k) - DelT), Tlimit);$

$Lup(h,k) \text{ exist}(h,k) = CPH(h) * (tH(h,k) - tH(h,k+1)) / (CpW * (Tup(h,k) - (tH(h,k+1) - DelT)));$

Positive variables

PPQ(c,h,k) process-process heat

CUQ(h,k) heat to cold utility

CW total cooling water

TR total return

WS(h,k) supply of water to h in k

WR(h,k) return to tower

Fin(h,k) total flow in

Fout(h,k) total flow out

RR(h,k,h,k) reuse stream from hp_in_kp to h_in_k

tC(c,k) temp of cold stream at k

Tret return temperature

Tcool cooling water temperature

tower(z,item) Tower variables

dtower(z,item) derivative terms

param(z,prop) Calculated values

E evaporative losses

B blowdown

Appendices

M makeup

area

st;

area.l = A;

st.l = step;

binary variable

pp(c,h,k) Process-process exists

y(h,k) uses cooling water;

Variables

Ob,ob2,ob3;

*===== Process-Process heat integration =====

Equations

p1,p2,p3,p4,p5,p6,p7,p8,p9,p10;

*overall stream heat balances

p1(h).. QH(h) =e= sum((c,k),PPQ(c,h,k)\$exist(h,k))) + sum(k,
CUQ(h,k)\$exist(h,k));

p2(c).. QC(c) =e= sum((h,k),PPQ(c,h,k)\$exist(h,k));

*Stage heat balances

p3(h,k)\$exist(h,k).. (tH(h,k)-tH(h,k+1))*CPH(h) =e= sum(c, PPQ(c,h,k)) + CUQ(h,k);

p4(c,k)\$ord(k) lt card(k).. (tC(c,k)-tC(c,k+1))*CPC(c) =e= sum(h, PPQ(c,h,k)\$exist(h,k));

*Hot steam endpoints

p5(c).. tC(c,'k1') =e= TtarC(c);

p6(c).. tC(c,'k3') =e= TsupC(c);

*monotonically decreasing temperatures

p7(c,k)\$ord(k) lt card(k).. tC(c,k) =g= tC(c,k+1);

*delta T min

p8(c,h,k)\$exist(h,k).. tH(h,k) - tC(c,k) + Gamma*(1-pp(c,h,k)) =g= DelT;

p9(c,h,k)\$exist(h,k).. tH(h,k+1) - tC(c,k+1) + Gamma*(1-pp(c,h,k)) =g= DelT;

*Binary variables

Appendices

$$p10(c,h,k)\$(exist(h,k)).. \quad PPQ(c,h,k) = 1 - pp(c,h,k) * (CPH(h) * (tH(h,k) - tH(h,k+1)));;$$

*===== network synthesis =====

Equations

s1,s2,s3,s4,s5,s6,s7,s8,s9,s9a,s10,s10a,s11,s12,obj;

*Material balances

$$s1.. \quad CW = e = \text{sum}((h,k), WS(h,k)\$(exist(h,k)));$$

$$s2.. \quad TR = e = \text{sum}((h,k), WR(h,k)\$(exist(h,k)));$$

$$s3.. \quad CW = e = TR;$$

$$s4(h,k)\$(exist(h,k)).. \quad Fin(h,k) = e = WS(h,k) + \text{sum}((hp, kp), RR(hp, kp, h, k)\$(exist(hp, kp)));$$

$$s5(h,k)\$(exist(h,k)).. \quad Fout(h,k) = e = \text{sum}((hp, kp), RR(h, k, hp, kp)\$(exist(hp, kp))) + WR(h, k);$$

$$s6(h,k)\$(exist(h,k)).. \quad Fin(h,k) = e = Fout(h,k);$$

$$s7(h,k)\$(exist(h,k)).. \quad RR(h, k, h, k) = e = 0;$$

$$s8(h,k)\$(exist(h,k)).. \quad Fin(h,k) = 1 = y(h,k) * Lup(h,k);$$

$$s9(h,k)\$(exist(h,k)).. \quad (tH(h,k+1) - \Delta T) * Fin(h,k) = g = \text{sum}((hp, kp), \\ (RR(hp, kp, h, k) * Tup(hp, kp))\$(exist(hp, kp))) + WS(h,k) * Tcool;$$

$$s9a(h,k)\$(exist(h,k)).. \quad (tH(h,k+1) - \Delta T) * Fin(h,k) = g = \text{sum}((hp, kp), \\ (RR(hp, kp, h, k) * Tup(hp, kp))\$(exist(hp, kp))) + WS(h,k) * Tcw;$$

*energy balances

$$s10(h,k)\$(exist(h,k)).. \quad CUQ(h,k) = e = CpW * Fout(h,k) * Tup(h,k) - \\ CpW * \text{sum}((hp, kp), (RR(hp, kp, h, k) * Tup(hp, kp))\$(exist(hp, kp))) - CpW * WS(h,k) * Tcool;$$

$$s10a(h,k)\$(exist(h,k)).. \quad CUQ(h,k) = e = CpW * Fout(h,k) * Tup(h,k) - \\ CpW * \text{sum}((hp, kp), (RR(hp, kp, h, k) * Tup(hp, kp))\$(exist(hp, kp))) - CpW * WS(h,k) * Tcw;$$

$$s11.. \quad \text{sum}((h,k), (WR(h,k) * (Tup(h,k)))\$(exist(h,k))) = e = TR * Tret;$$

$$s12(hp, kp, h, k)\$(ord(kp) <= ord(k)).. \quad RR(hp, kp, h, k) = e = 0;$$

$$obj.. \quad Ob = e = CW;$$

*===== cooling tower =====

Equations

ct1,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9a,ct9b,ct10a,ct10b,ct11,ct12,ct13,ct13b,ct14,ct15,ct16,ct17,ct18,obj3
ct1a,ct9c,ct9d,ct13a,ct15a,obj2;

$$ct1(z).. \quad CW * dtower(z, 'Tw') = e = (G * A) * (dtower(z, 'Ima') / CpW - \\ tower(z, 'Tw') * dtower(z, 'W'));$$

Appendices

- ct1a(z).. $CW*dtower(z,'Tw') = e = (G*Area)*(dtower(z,'Ima')/CpW - tower(z,'Tw')*dtower(z,'W'));$
- ct2(z).. $dtower(z,'Ima') = e = (param(z,'hdaf')/G)*(param(z,'Imasw') - tower(z,'Ima'));$
- ct3(z).. $dtower(z,'W') = e = (param(z,'hdaf')/G)*(param(z,'Wsat') - tower(z,'W'));$
- ct4(z).. $dtower(z,'Liq') = e = G*dtower(z,'W');$
- ct5(z).. $param(z,'Imasw') = e = CpA*tower(z,'Tw') + param(z,'Wsat')*(Lambda + CpV*tower(z,'Tw'));$
- ct6(z).. $param(z,'Psatw') = e = \exp(23.7093 - 4111/(237.7+tower(z,'Tw')));$
- ct7(z).. $param(z,'Wsat') = e = (18/29)*param(z,'Psatw')/(Patm-param(z,'Psatw'));$
- ct8(z).. $param(z,'hdaf') = e = coef1 + coef2*(tower(z,'Liq')-coef3);$
- ct9a(z,item)\$((ord(z) gt 1)and(ord(z) lt 5)).. $tower(z,item) = e = tower(z-1,item) + step*dtower(z-1,item);$
- ct9b(z,item)\$ord(z) gt 4).. $tower(z,item) = e = tower(z-1,item) + step*(55*dtower(z-1,item)-59*dtower(z-2,item)+37*dtower(z-3,item)-9*dtower(z-4,item))/24;$
- ct9c(z,item)\$((ord(z) gt 1)and(ord(z) lt 5)).. $tower(z,item) = e = tower(z-1,item) + st*dtower(z-1,item);$
- ct9d(z,item)\$ord(z) gt 4).. $tower(z,item) = e = tower(z-1,item) + st*(55*dtower(z-1,item)-59*dtower(z-2,item)+37*dtower(z-3,item)-9*dtower(z-4,item))/24;$
- ct10a.. $tower('z60','Tw') = e = Tret.l;$
- ct10b.. $tower('z60','Tw') = e = Tret;$
- ct11.. $tower('z0','Ima') = e = 49.19;$
- ct12.. $tower('z0','W') = e = 0.00949;$
- ct13.. $tower('z60','Liq') = e = (CW-B)/A;$
- ct13a.. $tower('z60','Liq') = e = (CW-B)/Area;$
- ct13b.. $tower('z60','Liq') = e = (CW.l-B.l)/A;$
- ct15.. $E = e = A*(tower('z60','Liq') - tower('z0','Liq'));$
- ct15a.. $E = e = Area*(tower('z60','Liq') - tower('z0','Liq'));$
- ct16.. $B = e = 0.5*E;$
- ct17.. $M = e = B + E;$
- ct18.. $Tcool*CW = e = 25*M + tower('z0','Tw')*(CW-M);$
- obj3.. $obj3 = e = tower('z0','Tw');$
- obj2.. $Obj2 = e = 200*0.2*13.715*Area/pi + 25*Area*st*60;$

*=====

Appendices

```
model ColdSideLinear /p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s9a,s10a,s12,obj/;
solve ColdSideLinear using MIP minimizing Ob;
```

```
Tret.l = sum((h,k),(WR.l(h,k)*Tup(h,k))$(exist(h,k)))/TR.l;
E.l = 0.0016*CW.l*(Tret.l - Tcw);
B.l = 0.5*E.l;
M.l = B.l + E.l;
Tcool.l = (25*M.l + Tcw*(CW.l-M.l))/CW.l;
coef3 = (CW.l-B.l)/A;
coef1 = 1.88095*(G**0.48)*(coef3**0.52);
coef2 = 1.88095*0.52*(G**0.48)/(coef3**0.48);
```

```
model cooltower /ct1,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9a,ct9b,ct10a,ct11,ct12,ct13b,obj3/
solve cooltower using NLP minimising ob3;
```

```
model ColdNetwork
/p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s9,s10,s11,s12,ct1,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9a,c
t9b,ct10b,ct11,ct12,ct13,ct15,ct16,ct17,ct18,obj/
solve ColdNetwork using MINLP minimising Ob;
```

```
model design
/p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,s1,s2,s3,s4,s5,s6,s7,s8,s9,s10,s11,s12,ct1a,ct2,ct3,ct4,ct5,ct6,ct7,ct8,ct9c,
ct9d,ct10a,ct11,ct12,ct13a,ct15a,ct16,ct17,ct18,obj2/
solve design using MINLP minimising Ob2;
```