Steam System Heat Exchanger Network Optimisation Using Degenerate Solutions: A focus on Pressure Drop and Boiler Efficiency

by

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Synopsis

This work presents a revised methodology to minimise pressure drop through a steam system heat exchanger network (HEN). This is based on previous work where network pressure drop is minimised after utility flow through the network has been reduced to its minimum. With the minimum utility flow as a parameter, the proposed methodology enlarges the solution space of the problem in an attempt to find a better pressure drop solution. The resulting minimum pressure drop found using this method is an improvement of 1.1 % and 7.4%, in two case studies respectively, on the current HEN minimisation problem formulation. The method is then extended to maintain boiler efficiency with the same minimum steam flowrate. Due to the simpler nature of the problem of maintaining boiler efficiency the proposed methodology did not yield improvements to the steam flowrate however a wider variety of network configurations was found.

The steam flowrate to a HEN can be substantially reduced with the application of process integration. Reducing the steam flowrate to the HEN involves creating series heat exchanger connections, which ultimately increase the pressure drop to the system. The reduced steam flowrate also compromises the return condensate temperature and consequently reduces the efficiency of the steam boiler.

A HEN optimisation and design methodology exists whereby the minimum steam flowrate to a heating utility system can be found and the pressure drop through the HEN can be minimised. This methodology does not however incorporate the full solution space of potential network configurations. This is as a result of network conditions of optimality which fix the outlet temperature of condensate streams leaving heat exchangers in order to achieve a globally optimal minimum steam flowrate.

The minimum steam flowrate can still be achieved by relaxing the optimality conditions and allowing for variable heat exchanger outlet temperatures. Solutions of this nature are referred to as degenerate and are formulated with bilinear terms forming part of the energy balance constraints. The presence of

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bilinear terms results in a nonlinear, nonconvex mixed integer nonlinear programming (MINLP) problem. The bilinear terms are catered for in the methodology by the reformulation and linearisation technique of Quesada and Grossmann (1995) as well as the transformation and convexification technique of Pörn et al (2008). The reformulation and linearisation approach proved to be the most successful for the proposed problem.

By utilising the larger solution space created by incorporating degenerate solutions into the HEN design process, many HEN design variables can potentially be further optimised once a minimum steam flowrate has been achieved.

Consequently, this thesis concerns the optimisation of a steam system HEN by finding the minimum steam flowrate to the system and using it as a parameter while relaxing the conditions of network optimality to create solutions which can be degenerate. The complexities of MINLPs in the degenerate solutions are explored and a methodology to further optimise network pressure drop through heating networks is proposed. The methodology was also used to maintain boiler efficiency with a reduced steam flowrate which was achieved, but not improved upon from previous methodologies.

While this methodology does not guarantee an improved HEN pressure drop, solutions adhering to the conditions of network optimality also fall within the solution space of the proposed methodology, therefore solutions achieved with current techniques from literature will not be compromised.

Declaration

I, Tim Price, with student number 04359968, declare that:

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1. Introduction

The optimisation of utility systems is beneficial to both grassroots process designs as well as existing processes. Lower utility consumption reduces costs through energy consumption, environmental impact and can have process benefits such as removing bottlenecks to expansion. Two key utilities in process plants are steam and cooling water. The reduction in the consumption of either of these has been shown to greatly reduce operational costs or capital costs for grassroots design. Reuse and recycle is very effective at reducing the consumption of fresh utilities in process networks. The key to reuse networks is to allow series heat exchanger connections as opposed to traditional parallel network designs. This is effectively shown for cooling systems by Kim and Smith (2001) and for heating systems by Coetzee and Majozi (2008).

These processes do however become more complex as the utility flows are reduced and care must be taken to ensure that the systems are not adversely affected by such reductions. The consideration of holistic systems has been shown to yield great utility flow savings while not adversely affecting other factors of heating and cooling circuits such as the steam boiler or cooling towers. Focus can now be directed to other design variables in the heat exchanger networks (HENs) themselves.

This chapter discusses the background, objectives, scope and layout of this thesis.

1.1. Background

Reuse and recycle of a heating or cooling utility involves using the utility stream leaving a heat exchanger to further heat or cool an additional process stream. This series type connection has been proposed to reduce utility consumption when used in place of traditional parallel networks which see the utility return to its source directly, typically a steam boiler or cooling tower. This has been accomplished successfully for cooling systems by Kim and Smith (2001) and for heating systems by Coetzee and Majozi (2008).

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A consequence of series connections is a greater pressure drop of the utility flow through the network. Increased pressure drop could lead to the requirement of additional fluid movers in retrofit designs and additional capital expenditure in grassroots designs. Reusing process utilities can also have adverse effects on the utility source, namely cooling towers and steam boilers. In this work steam systems are investigated. Reusing hot process utilities also reduces steam condensate return temperature to the steam boiler which can adversely affect the boiler efficiency. Pressure drop and boiler efficiency have thus been incorporated into many HEN design philosophies.

A condition of network optimality developed by Savelski and Bagajewicz (2001) exists which can guarantee a minimum utility flowrate. An infinite number of network layouts can achieve the optimality conditions of Savelski and Bagajewicz (2001). Therefore it is possible to optimise additional design aspects of the network. This concept was used to optimise pressure drop in HENs for cooling system by Kim and Smith (2003) as well as Gololo and Majozi (2013) and in heating systems by Price and Majozi (2010c).

A minimum utility flow can however also be achieved without all of the conditions of network optimality being adhered to. Savelski and Bagajewicz (2001) refer to such solutions as degenerate and utilise these to optimise internal network features such as the number of connections. The authors first use the conditions of optimality to target for the minimum utility flowrate and then optimise the network structure in a manual and iterative procedure. In heating systems, by allowing for degenerate solutions the utility stream temperature leaving heat exchangers becomes a variable and creates bilinear terms with the mass flowrate of steam in the energy balance constraints. These bilinear terms cause difficulty for MINLP solvers as they are both nonlinear and nonconvex.

1.2. Basis and Objectives

By relaxing the optimality condition of Savelski and Bagajewicz (2001) additional flow and network arrangement opportunities can be found. HEN arrangements of this type are referred to as degenerate solutions. These arrangements may give greater

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flexibility to the steam HEN arrangements so as to find an improved minimum pressure drop as well as result in better steam system alterations to maintain boiler efficiency while still achieving the minimum steam flowrate of the system.

MINLP solvers are adept at handling complex problems, however nonconvex terms can cause difficulties. A number of techniques in literature have attempted to aid the solution of MINLP problems. Quesada and Grossmann (1995) utilise a technique of relaxation and linearisation to overcome bilinear terms. This technique was also adopted by Price and Majozi (2010a). Pörn et al. (2008) describe transformation techniques to transform nonconvex terms in model formulations into convex terms. The network pressure drop minimisation model can be formulated with nonlinear pressure drop terms, however the inclusion of degenerate solutions creates bilinear terms. The bilinear terms are nonconvex and will be treated with appropriate techniques.

Degenerate solutions directly affect the HEN and therefore the focus of this work is on finding an improved steam system HEN pressure drop with the inclusion of degenerate solutions. This work attempts to formalise an approach to utilising degenerate solutions in HEN optimisation while also closing the loop on the steam system HEN pressure drop work initiated by Price and Majozi (2010c). Degenerate solutions are also incorporated into the boiler efficiency optimisation problem with retrofit steam flowrate minimisation.

1.2.1. Problem Statement

The steam flowrate to a steam system HEN can be minimised by the reuse and recycle of hot condensate to provide additional heat to process streams. Reuse and recycle requires series connections in the HEN. A consequence of these series connections is an increase in the utility pressure drop through the HEN. Another consequence of the reuse and recycle of hot condensate is the lowering of the boiler condensate return temperature. This, in addition to the reduced flowrate, can have detrimental effects on the steam boiler efficiency.

A means to guarantee a minimum steam flowrate is to implement the network condition of optimality which involves fixing utility stream heat exchanger outlet temperatures to their lower limits which reduces the solution space of feasible HEN layouts.

The problem statement can, therefore, be formally stated as follows,

Given:

- a steam system comprising a set of heat exchangers linked to a boiler with limiting temperatures and fixed duties; and
- a predetermined minimum steam flowrate for the HEN

determine the minimum network pressure drop while relaxing the network condition of optimality used to find the minimum steam flowrate for the system while maintaining the minimum steam flowrate. In addition determine whether the steam boiler efficiency can be maintained in an improved manner.

1.3. Thesis Scope

The scope of this research is to investigate the effects of relaxing the conditions of network optimality on HEN pressure drop as well as maintaining boiler efficiency while still achieving a minimised steam flowrate for the system.

Relaxing the conditions of network optimality involves allowing the outlet temperatures of utility streams leaving heat exchangers to vary.

A mathematical programming approach is proposed to solve the HEN pressure drop minimisation problem using degenerate solutions. The mathematical techniques created to incorporate degenerate solutions into the HEN are then applied to maintain the boiler efficiency with a dedicated heat exchanger with variable duty after retrofit steam flowrate minimisation.

1.4. Thesis Layout

This thesis is divided into the following chapters:

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- Chapter 1 introduces the thesis and provides relevant background to the work. The objectives and scope of the work are presented and a description of the thesis layout also given;
- Chapter 2 provides a literature review of research in the fields of HEN optimisation, wastewater, cooling water and steam utility optimisation as well as techniques from literature to aid the solution of MINLP problems;
- Chapter 3 shows a motivation for the study. Here previous work is deconstructed and a basis for the consideration of degenerate solutions for HEN pressure drop minimisation as well as boiler efficiency is given. The solution of MINLP problems is also discussed;
- Chapter 4 includes the formal model formulation. Flow minimisation constraints are provided as well as network pressure drop constraints. Solution techniques to aid the solution of problems with bilinear terms are introduced and adapted for the HEN pressure drop minimisation model. The chapter is concluded by incorporating the steam system alterations and constraints required to maintain the boiler efficiency with a reduced steam flowrate;
- Chapter 5 provides a case study where the original steam system pressure drop minimisation model of Price and Majozi (2010c) is given and solved using the techniques described in the thesis. The optimal pressure drop minimisation layout using degenerate solutions is also provided and the solution is compared to the results of the Price and Majozi (2010c) model. Similarly, the case study presented by Price and Majozi (2010a) is utilised with the allowance for degenerate solutions and this is then compared to the boiler efficiency problem of Price and Majozi (2010a); and
- Chapter 6 discusses conclusions of the work and evaluates the success of the methods described. A discussion of the results and suggestions for areas of further research and improvement conclude the chapter.

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2. Literature Review

This section is intended to discuss the relevant literature in various areas related to this field of research. These areas include heat exchanger network optimisation, heat exchanger network pressure drop optimization, MINLP solvers, as well as model manipulations which further improve their performance.

2.1. HEN Optimisation

The HEN of a process is intended to provide heating and cooling to process streams. In a process where there are both hot and cold streams, there exists an opportunity to exchange heat between the process streams themselves and reduce the amount of utilities that would ordinarily have been used to heat or cool the relevant process streams. In the context of this work, the reduction of utilities using improvements to the arrangement of the HEN will be referred to as HEN optimisation.

Improvements to other aspects of HEN design can also lead to reduced costs, such as area optimisation and improved heat exchanger design. These are, however, capital expenses that can often be overshadowed by operating expenses, such as utilities, in the life of a plant. This, coupled with the tendency for utility prices to increase, makes utility reduction and the study of HEN optimisation of paramount importance in process plant design.

Arguably the most common hot and cold utilities in process plants are steam and cooling water, respectively. The utility consumption can be reduced by process changes or improvements, but also HEN optimisation. Improvements can be made to maximize the amount of process to process heat exchange, or maximize the efficiency at which the utilities are used.

2.1.1. Early HEN Synthesis, Design and Optimisation

Several concepts have been developed to aid in the field of HEN optimisation. A prominent concept is pinch analysis which can be used to find the minimum utility requirement of a process. Pinch analysis can be carried out using graphical

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techniques, which can give a designer insight into the process and its constraints. Mathematical programming techniques are also prevalent in literature. While these appear as a more black box approach, the extent of application of mathematical programming makes it an excellent approach to HEN synthesis, design and optimisation.

Graphical techniques were first utilised by Hohmann (1971), who optimised a trade off between utilities and heat exchange area. This work laid the foundation for the formation of the Temperature-Duty (T-Q) diagram of Huang and Elshout (1976), which is used to represent process heating and cooling utility requirements in the form of a composite curve. The utilities can also be represented on the T-Q diagram and can be used to find the pinch point in the system, as shown by Umeda, Handa and Shiroko (1979). The pinch point is denoted where the process composite curve meets the utility supply curve. This technique was successfully used to target for a minimum utility flowrate.

Alternatively, Linnhoff and Flower (1978) developed the Problem Table Algorithm to both target minimum utilities and help design HENs. The results of this systematic technique were then used by the authors to construct a further graphical aid, the Grand Composite Curve. Whereas the T-Q diagram allowed a single utility to be targeted, the grand composite curve combines hot and cold utilities to target the minimum utility usage for the system.

Early work on HEN design by Linnhoff et al. (1979) showed how complicated this process was. This work led to a comprehensive understanding and subsequent design philosophy for HENs presented by Linnhoff and Hindmarsh (1982). This design methodology focussed on the pinch principle and has been the cornerstone in HEN design.

Asante and Zhu (1997) optimized HEN retrofit designs by not only considering the maximization of heat recovery with promising topological matches but also the minimisation of cost of additional heat exchange area. The complexities of HENs and the effect of network layout and topography is illustrated while an automated and interactive method utilising practical engineering is proposed to optimise the design. This work laid the foundation for further network optimisation where layout and topography were taken into account.

2.1.2. Other Applications of Pinch Analysis

Other utility systems also stand to benefit from pinch technology. Most common of these is arguably mass transfer in wastewater treatment. Other mass transfer applications are the likes of hydrogen pinch and water pinch in certain processes. Mass transfer, like heat transfer, relies on a driving force. Much work has been done in understanding and utilising concentration driving forces in mass transfer, while similarly temperature serves as the key driving force in heat transfer. Key research in both fields will be discussed in later chapters.

2.1.3. Early Mathematical Programming

Papoulias and Grossmann (1983a, 1983b and 1983c) set about to create a more systematic plant design methodology than the simple thermodynamic and heuristic techniques commonly used at the time. This method utilised Mixed Integer Linear Programming (MILP) models of plants at various discrete operating conditions, which required large amounts of background work. This work did, however, show the flexibility of mathematical programming in plant design and the importance of fully understanding the bounds of the optimisation problem.

The authors were able to explore many different arrangements of the systems through an effective and comprehensive superstructure. This superstructure was largely designed using thermodynamic and heuristic techniques. The power of the mathematical programming approach is then to find the optimal arrangement which is sometimes not obvious for even simple systems.

Early work in process to process HEN optimisation and mathematical programming laid a platform to further optimise the utility systems. The following sections examine optimisation of both cooling and heating systems.

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2.2. Water Utility Optimisation

As described in Section 2.1.2, similarity exists in heat and mass transfer in that a driving force is needed to transfer energy or material from streams of a high temperature or concentration to those with a low temperature or concentration. In process plants water is used as a key medium for both. Cooling systems frequently employ cooling water circuits to provide a cooling utility for hot process streams while cleaning water can be used to remove contaminants and unwanted material from process vessels. This section discusses certain key areas of research in wastewater and cooling water system optimisation.

2.2.1. Wastewater Optimisation

Takama et al. (1980) present the water allocation problem (WAP) for petroleum refineries. These authors utilise the concepts of the reuse and regeneration of wastewater within process wastewater circuits by generating a superstructure of all possible connections and then eliminating features which are not economic.

El-Halwagi and Manousiouthakis (1989) expanded the pinch design method based on that of heat exchangers developed by Linnhoff and Hindmarsh (1982) for mass exchange networks. They created a more general approach for mass exchange between streams of high and low concentration. The approach was only applicable to simple systems due to the heuristic nature of the design method, however El-Halwagi and Manousiouthakis (1990) developed a simple mathematical programming approach which overcomes this design shortfall.

Wang and Smith (1994) presented a conceptual approach to the WAP. The authors allowed for individual process constraints to be considered by defining the minimum and maximum contaminant concentrations for the limiting water profile. These profiles for various streams could then be combined into a limiting composite curve where minimum targets could be set. Targets were initially set to maximise reuse while regeneration was also considered. With a minimum wastewater target set the authors designed the network according to two methods with differing objectives while still achieving the target set in the initial phase. They subdivided the limiting composite curve into mass load intervals and utilised the network design grid diagram of Linnhoff and Flower (1978) to complete the design.

This procedure was thorough and allowed many network and process aspects to be considered, however it was also time consuming. Alternatively, mathematical solutions to network design were considered complex. Olesen and Polley (1996) identified the complexities of the design procedure proposed by Wang and Smith (1994) and proposed a much simplified procedure for single contaminants. Due to the inspection type solution procedure, this process was found to be restricted to smaller numbers of operations.

The complications involving numerical techniques, or mathematical programming, were found to be primarily due to the nonlinear nature of problems containing bilinear terms, which lead to infeasible solutions with conventional mathematical solvers at the time. Doyle and Smith (1997) proposed an iterative procedure to account for the bilinearity, while Alva-Argaez et al. (1998) attempted a two phase solution procedure for their MINLP version of the problem. Huang et al. (1999) also presented a mathematical programming solution for the problem of water allocation as well as treatment. The work of the authors listed above showed a gap in the water allocation problem, where network design was concerned. The time consuming nature of heuristic techniques as well as the complexity of mathematical programming with bilinear terms lead to the need to develop a more robust network design procedure.

Savelski and Bagajewicz (2000a) attempted to solve the WAP by designing a water utilisation system. The authors focused their attention on defining conditions of flow optimality for wastewater circuits with a single contaminant. The authors defined a condition of monotonicity, which is a net increase in concentration of water leaving an intermediate water provider as compared to all of the streams entering it. They proved mathematically that if a solution to the WAP is optimal, i.e. results in a minimum wastewater flowrate, the solution must display monotonicity and that the solution will result in the outlet concentration of the single contaminant reaching its maximum.

This work has definite impact on the design of wastewater systems. Up until the work of Savelski and Bagajewicz (2000a), optimal wastewater flowrates could be solved for, however network design procedures were either manual and time consuming or mathematical and the nonlinear, nonconvex nature of the problems were difficult to solve. The conditions of flow optimality allow for the outlet concentration of streams leaving units to be set to their maximum and guarantee that this system would achieve a minimum flowrate. This then eliminates the bilinear terms in the system mass balances and allows the problem to be solved as an LP or MILP problem, where optimisation algorithms were far more successful. Savelski and Bagajewicz (2000b) then formally introduced the conditions of optimality for water use networks associated with the WAP. The authors also described what they termed degenerate solutions to the WAP. These are solutions that do not show maximum outlet concentration but do result in the minimum water flowrate.

Savelski and Bagajewicz (2001) presented both LP and MILP models for the solution of the WAP using the conditions of optimality defined in their previous work. The authors maintained the scope to only limited contaminants, however this does still have wide application in industry. The formalised design procedure also allows for regeneration systems to remove contaminants in the system. The authors then also expanded on degenerate solutions and the conditions under which they can occur. A manual and iterative approach is presented to utilise these degenerate solutions to further optimise the number of connections in the system.

This work formalised the initial breakthrough conditions of optimality to systematically design wastewater systems, which show the minimum freshwater use.

Savelski and Bagajewicz (2003) then extended the conditions of monotonicity and optimality to systems which have multiple contaminants. They identified what they termed a key component, and for this component the same outlet concentration conditions can apply for optimum networks. A design procedure for the networks was also presented, as was done for single contaminant systems. The authors effectively closed the gap in the network design for the WAP.

2.2.2. Cooling Water System Optimisation

Kim and Smith (2001) continued the work involving the reuse of utilities from that completed by Kuo and Smith (1998) and applied these concepts to cooling water system design. At the time typical cooling systems consisted of a parallel HEN connected to the remainder of the cooling system, consisting of cooling towers, pumps, filters, etc. Due to the parallel nature of the HEN, each heat exchanger received cooling water directly from the cooling tower source. The heat exchanger outlet was then collected and returned to the cooling towers.

As Kuo and Smith (1998) and Savelski and Bagajewicz (2001) had done with mass transfer networks, increasing the concentration of the returning stream, in this case represented by an increased return temperature, Kim and Smith (2001) were able to reduce the amount of cooling water required for the system. The key to this increase in return temperature was the rearrangement of the HEN and the reuse of cooling water where possible.

The authors utilised the same pinch concept as was used by Kuo and Smith (1998) and represented the cooling system on a T-Q diagram. The cooling water supply was in turn represented by a single straight line. The intersection of the supply line and the composite curve represented the pinch point and the minimum cooling water flowrate could be calculated from this pinch point.

The authors then considered the subsequent effects of reducing the cooling water flowrate on the entire cooling system. By examining each element of the cooling system in a holistic manner the authors found that the two areas that stood to be most affected by a decrease in cooling water flowrate and an increase in cooling water return temperature were the fouling in heat exchangers and pipes as well as the performance of the cooling towers. Fouling can be catered for by a more comprehensive chemical treatment programme. The effects on cooling towers were reviewed based on cooling tower research performed by Bernier (1994). The Bernier (1994) model was used to simulate the effects of simultaneously decreasing the cooling water flowrate and increasing the cooling water return temperature. It was found that these changes increased the performance of the cooling tower and it was therefore concluded that rearranging the previously parallel HEN and resulting reuse of cooling water would be beneficial to the process plants as it would reduce the amount of cooling water required, along with all the benefits this brought about such as reduced makeup water and reduced capital cost for grassroots designs.

The HEN was then designed using the mains technique first developed by Wang and Smith (1994) for wastewater systems. This technique gives the designer a hands on

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approach to the HEN and allows many key design aspects such as forbidden matches and topological restrictions to be considered.

The techniques utilised by Kim and Smith (2001) showed that utility reuse is a powerful means in reducing the utility consumption of processes. The techniques used by both Wang and Smith (1994) and Kim and Smith (2001) are based on graphical targeting techniques which gives a designer insight into the intricacies of the system in question, but are somewhat time consuming. The inclusion of mathematical programming techniques have been shown to drastically reduce the time required to perform utility HEN optimisation and design tasks. The holistic approach of Kim and Smith (2001) showed the value in considering the entire utility network in the design process. For cooling systems, a reduction in the cooling water flowrate was found to be beneficial for the cooling tower performance but also found to increase the expected rate of fouling of the process equipment. These additional aspects could be instrumental to the practical success of process cooling water optimisation exercises.

Majozi and Moodley (2008) furthered the holistic approach to cooling system optimisation by considering reuse of cooling water from multiple cooling towers. Additional cooling towers complicate the optimisation problem such that a graphical technique becomes ineffective, unless the cooling towers behave in an identical fashion. The authors chose to represent the optimisation problem as a mathematical programme which allowed targeting and HEN design in the same mathematical model.

The authors developed a novel superstructure from which the necessary constraints were determined. From this superstructure four cases were developed relating to various assumptions and depictions of the cooling water return conditions. The resulting models contained a number of nonlinear constraints and as a result of bilinear terms created by flow and temperature variables. The flow optimality conditions of Savelski and Bagajewicz (2000b) were employed to fix the outlet temperatures of the cooling streams to their limits, thus linearising the energy balance constraints of the model. Several other nonlinear terms exist based on the representation of the cooling tower operation and these were linearised using a technique of reformulation and linearisation described by Quesada and Grossmann

(1995). This technique utilises convex outer approximation envelopes described by McCormick (1976) and first utilised in process optimisation by Sherali and Alameddine (1992). This technique will be discussed in more detail in later chapters. This technique serves to create a linearised version of the nonlinear model which is solved and used as a starting point for the exact nonlinear model.

Majozi and Moodley (2008) show how mathematical programming can be used to both target for minimum utility flows as well as design a HEN. The authors made considerations for the entire cooling system including return temperature and topological restrictions. This allowed a more realistic problem to be optimised. The authors did not however consider the complex workings of the cooling tower. It was alluded to by Kim and Smith (2001) that higher return temperatures favoured cooling tower performance, but this had not been developed into any model superstructure at that time.

Gololo and Majozi (2011) continued work in cooling systems by creating a grassroots cooling system design methodology which considers cooling water flowrate reduction by reuse as well as a cooling tower model used to investigate the subsequent effects of cooling water reuse on the cooling tower. The HEN is designed based on a superstructure allowing for series connections and reuse. The outlet conditions are fed to the cooling tower model which caters for multiple cooling towers and serves to calculate the effects of the HEN rearrangement on the cooling tower performance. The results are then iteratively fed back to HEN model until a stable system is formed. The authors developed both a NLP and MINLP formulation, both of which were solved for case studies.

The authors successfully incorporated two complex elements of a cooling water system into an iterative process which is used to optimise the system for cooling water flowrate. The authors show the benefits of a holistic approach but also the complications brought about by doing so. Further aspects of the cooling system can still be optimised, such as heat transfer area and network pressure drop.

2.2.3. Network Pressure Drop

Reuse and recycle of utilities is very effective at reducing the consumption of fresh utilities in a system. The nature of reuse networks is series exchanger connections. A

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consequence of these series connections is a greater pressure drop of the utility flow stream through the network. Increased pressure drop could lead to the requirement of additional fluid movers in retrofit designs and additional capital expenditure in grassroots designs. Pressure drop has thus been incorporated into many HEN design philosophies.

A number of heat transfer design variables are closely linked (Sinnot, 2005). Jegede (1990) and Jegede and Polley (1992) attempted to optimise the heat transfer coefficient, or h-value, and then calculated the subsequent pressure drop based on this value. These early attempts at heat exchanger optimisation did not focus solely on pressure drop, but did consider pressure drop as a key design variable. The authors then went on to develop a pressure drop correlation that was less dependent on the network geometry to reduce the complexity of the problem. Their technique was similar to that of Ahmed and Smith (1989) who optimised the heat exchange area and number of shells required for individual process streams.

Nie and Zhu (1999) realised the need to consider network pressure drop in retrofit designs brought about by process change or plant expansion. The authors found that pressure drop was not only dependant on process streams but also the network topography or layout. The authors separated the problem into two parts, the first being to find the optimal number of heat exchangers that required additional heat exchange area, the second to find the shell arrangement that best suited the network pressure drop. These two areas were initially incorporated into the same optimisation superstructure, however this proved to be extremely complex and impractical. The resulting mathematical models are based on pressure drop correlations derived in the work of Nie (1998).

The complex nature of network pressure drop is highlighted in this work. The authors also utilised pressure drop correlations as functions of the various fluid flows which allow them to be easily incorporated into a flow superstructure. The retrofit nature of the work examined and the sole focus on pressure drop do limit the scope of this work, however this did lay a solid platform for further network pressure drop optimisation research.

Nie and Zhu (2002) used the approach of Jegede and Polley (1992), along with a block decomposition technique described by Zhu et al. (1995), to develop linear pressure drop constraints by fixing the heat exchanger approach temperature ΔT_{LM}. This allowed utility flow, heat transfer area and pressure drop to be considered in the same optimisation exercise.

This work is based upon a complex superstructure where the complex nature of pressure drop as a function of individual heat exchanger pressure drop as well as the network structure is touched upon. The authors decouple the network aspect of pressure drop so true network pressure drop minimisation is not achieved. The correlations developed in this work are however invaluable in simplifying pressure drop through process units.

Following on from their work on cooling systems, Kim and Smith (2003) examined the effects of cooling water reuse on network pressure drop. The rearrangement of the HEN from a parallel to a series layout was found to increase the pressure drop over the HEN. The authors then found a systematic means to represent network pressure drop and then minimised it.

The authors' previous work on reducing the cooling water flowrate through a HEN utilised graphical means to determine the minimal flowrate as well as heuristic techniques to design the network. The complex relationship of pressure drop to both the network topology as well as the pressure drop over the individual process units makes a heuristic design approach much more complex and potentially time consuming. The authors therefore attempted to use mathematical programming to represent the pressure drop over the HEN. The authors used the pressure drop correlations of Nie and Zhu (1999) to form pressure drop constraints over process units. Series connections are likely to require additional piping and the authors catered for piping pressure drop using design heuristics of Peters and Timmerhaus (1991) to greatly simplify many of the piping design variables. The authors used the above sources to form simple but accurate correlations of pressure drop through heat exchanger tubes and shells as well as piping pressure drop as functions of mass flowrate through the units.

A key insight from the authors was not to create a mathematical model that optimised both flowrate and pressure drop, but to first optimise the mass flowrate and thermal performance of the cooling towers and then use that optimum mass flowrate to design a HEN which exhibited minimum pressure drop. If the subsequent pressure drop was found to be above certain limits the minimum flowrate could then be adjusted.

The intensive nature of network pressure drop was approached by the authors by creating a node representation of the system. Heat exchangers were fed by mixers, joining streams entering a particular heat exchanger. The streams leaving heat exchanger pass through splitters which distributed the cooling water to various locations. These mixers and splitters were defined as the nodes of the system. Pressure was then subsequently lost through the various elements separating the nodes in the network, namely heat exchangers and utility piping. All utility streams originated from the source node or cooling water supply and returned to the sink node or cooling tower return. The authors employed the longest or critical path concept described by Gass (1985) so as to find the greatest pressure drop over the system. This pressure drop was then minimised. As in other mathematical programming approaches, a superstructure was used to derive the constraints of the system. As certain connections in a superstructure system may or may not exist, binary variables had to be included in the formulation. The authors also encouraged heuristic design choices such as impractical node pairings to be removed so as to reduce the size of the problem.

The combination of nonlinear pressure drop correlations and energy balances coupled with the binary variables from the node superstructure lad to an MINLP model. The authors utilised limiting outlet conditions for the heat exchangers to linearise the energy balance constraints, as was proposed by Savelski and Bagajewicz (2001). The pressure drop correlations for heat exchangers were found to be close to linear in the flowrate ranges investigated, while piecewise linear approximations were employed for piping pressure drops. These linearisations then created an MILP problem. The authors also discuss the use of removing bilinear terms with the technique of Quesada and Grossmann (1995). The solution to this relaxed problem gives a starting point for the exact nonlinear problem.

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Kim and Smith (2003) addressed a large concern in network structure rearrangement in the minimisation of network pressure drop. The authors first optimised the mass flowrate of the cooling system in a holistic manner and then used this flowrate as a constraint in the pressure drop minimisation exercise. This allowed for a much simplified approach as compared to a multi objective minimisation problem. The authors did however utilise many simplifications and linearisations to solve the pressure drop minimisation problem, as well as restricted a degree of freedom, namely the heat exchanger outlet temperature, to simplify the solution of the problem.

Gololo and Majozi (2013) extended their work on multiple source cooling water systems to include the allowance for network pressure drop. The authors recognised the effects of rearranging parallel networks to reduce the cooling water flowrate and maximise cooling tower efficiency. As with the work done by Majozi and Moodley (2007), the network rearrangement led to increased pressure drop in the system. This was addressed by Kim and Smith (2003) and Gololo and Majozi (2013) who utilised a similar technique to capture the intricacies of pressure drop in their formulation. They included the provision for the cooling tower optimisation as was done in the iterative approach of Gololo and Majozi (2011). The inclusion of the pressure drop constraints created an MINLP in the network portion of the optimisation model. The authors utilised the relaxation and linearisation technique of Sherali and Alameddine (1992) to linearise the bilinear terms in the cooling water network portion of the model as well as piecewise linear approximation to create a linearised model. This is then used to create a starting point for the nonlinear model which was used to find a solution.

The authors showed the importance of considering pressure drop in any network rearrangement exercises and successfully incorporated the complicated network pressure drop into their iterative procedure using sophisticated solution techniques.

2.3. Heating Utility Optimisation

A very common heating utility for chemical plants is steam. Steam systems typically consist of a steam boiler which generates steam at a required temperature and pressure. Steam can be produced at a superheated state where it can be utilised in turbines, or at a saturated state for process heating. Steam can store a tremendous amount of energy as latent heat and transfer this heat to process streams in condensers. As with cooling systems where cooling water is returned to the cooling towers, steam condensate is collected and returned to steam boilers via a condensate tank. Boiler feed pumps require condensate to be sufficiently subcooled and away from saturated conditions to prevent cavitation and pump damage. The optimisation of steam systems has often focussed around designing optimal steam levels and optimising equipment in the steam system. Research in cooling systems has however shown the benefit of considering the entire system holistically when optimising utilities.

Shang and Kokossis (2004) attempted to optimise steam levels and satisfy the entire heating demand in grassroots plant design. The authors took into consideration the performance of the steam boiler by using their boiler hardware model (BHM) as well as that of steam turbines with their turbine hardware model (THM). With these models a better understanding of the cogeneration potential of a steam system and the effect of utility levels was investigated.

The BHM was developed from a thermodynamic approach considering all aspects of the boiler operation. Correlations for both heat loss and boiler capacity were derived from a study by Pattison and Sharma (1980) on behalf of British Gas. These correlations allowed the authors to link boiler efficiency and capacity to the mass flowrate and return temperature to the boiler. The THM was utilised from the work of Mavromatic and Kokossis (1998). This model was concluded to effectively predict efficiency trends based on turbine load and operating conditions.

The authors combined the BHM and THM and successfully integrated the operation of a HEN into their steam level optimisation model. They then solved their MILP to optimality and effectively found a means to optimise steam operating levels for process plants. The approach of the authors was however orientated towards grassroots design. While the authors considered the HEN in the framework of their model, the optimisation of this key part of the steam system is not addressed.

Coetzee and Majozi (2008) drew from work in cooling systems by Kim and Smith (2001) and Majozi and Moodley (2007) to minimise the steam flowrate required for a heating system. The authors employed the concept of recycle and reuse of hot steam condensate to heat certain process streams. The authors presented a graphical targeting technique to accommodate both latent and sensible heat as well as formulate a mathematical programming approach to design the HEN with the minimum steam flowrate. The authors also expanded the mathematical programming approach to include the steam flowrate minimisation and network design steps as a single model.

As with the work of Kim and Smith (2001), the key to utility stream minimisation is the recycle and reuse of the utility where possible. Coetzee and Majozi (2008) utilised hot condensate leaving condensers as a further heating source for the HEN. The saturated condensate then transferred sensible heat through conventional heat exchangers. The targeting of minimum cooling water flowrate had been accomplished by Kim and Smith (2001) using a T-Q diagram. A T-Q diagram plots the limiting temperatures and duty of a process stream. The plots of a number of process streams can then be combined to form a curve representing the energy and temperature demands of the process streams requiring utility heating. This is often referred to as a composite curve. An example of such a T-Q diagram is shown in **Figure 2-1**.

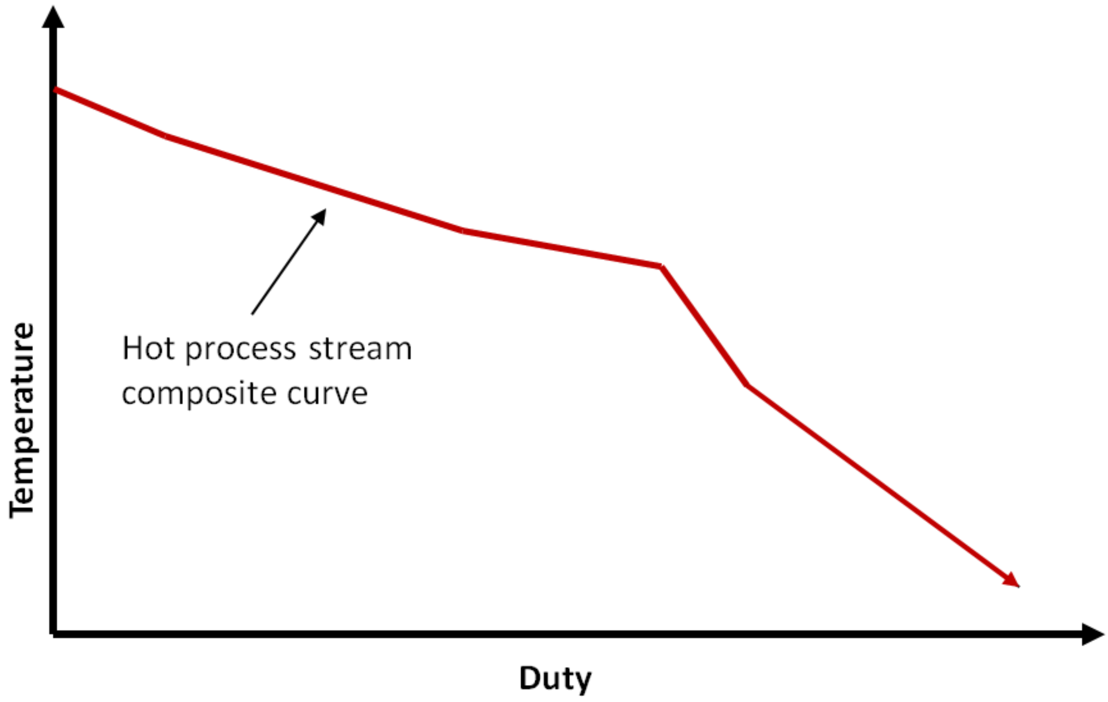

Figure 2-1: Example of Process Stream Hot Utility Demand Composite Curve

The hot process stream composite curve can then be offset by the minimum approach temperature, commonly referred to as the ΔT_{Min}, of the various heat exchangers providing energy to the process stream. This utility composite curve can then be used to target a minimum hot utility flowrate. If the minimum approach temperature is assumed equal for all heat exchangers, the process stream heating demand curve can take the same shape as the hot process stream composite curve.

Coetzee and Majozi (2008) represented their targeting technique on a T-Q diagram but needed to accommodate the latent energy from the steam. This latent energy is represented as a horizontal line on a T-Q diagram. By finding the various possible pinch points in the utility supply curve, the authors tested each possible pinch point on the diagram to determine which one did not violate the supply curve. The true pinch point then represented the minimum steam flowrate to the system. An example of a minimum steam flowrate targeting exercise is shown in **Figure 2-2**.

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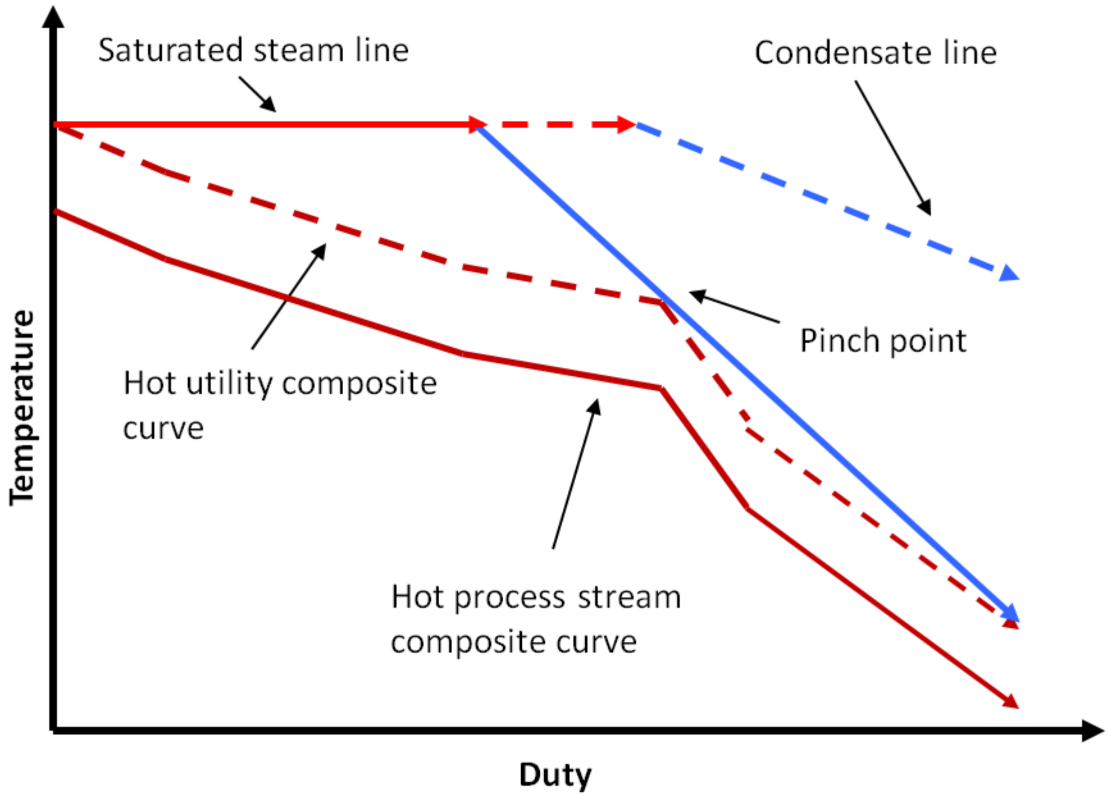

Figure 2-2: Example of Targeting a Minimum Steam Flowrate

The authors then designed the HEN using the minimum steam flowrate with a mathematical programming model. The steam condenser portion of the HEN would remain a parallel connection while the sensible heat transfer exchanger network was designed using an LP model. This model took advantage of the flow optimality conditions described by Savelski and Bagajewicz (2001) and utilised by Majozi and Moodley (2007). The authors also described that the true minimum steam flowrate may require a stream split, which is a process stream heated by a latent heat condenser as well as a sensible heat exchanger. The authors also expanded the model to incorporate the steam flowrate minimisation procedure. A model superstructure was developed to derive all heat and mass transfer constraints. The superstructure did however require the use of binary variables in the model formulation constraints. These binary variables, along with the nonlinear energy balance constraint resulted in a MINLP model. The authors then used the same optimality condition as before to reduce the model to a MILP which was solved.

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Coetzee and Majozi (2008) extended the very effective utility optimisation techniques developed for cooling systems to steam systems. They successfully accounted for the latent energy of steam and reduced the steam flowrate using both graphical and mathematical programming techniques. The authors however only focused on the HEN itself, without investigating the effects on the steam boiler or even system pressure drop.

2.3.1. Boiler Efficiency

Price and Majozi (2010a) followed on the work of Coetzee and Majozi (2008) and included a provision for a steam boiler in the steam flowrate minimisation model. The authors investigated the effects of a reduced steam flowrate and lower return temperature on the operation of the steam boiler. The authors studied the effects using the BHM derived by Shang and Kokossis (2004). The authors found that reducing the steam flowrate and the subsequent reduction of the condensate return temperature negatively affected the efficiency of the steam boiler. The authors then attempted to reduce the steam flowrate to the HEN while maintaining the boiler efficiency by more effectively pre-heating the boiler feed water stream.

When comparing a reduction in the steam flowrate and the subsequent condensate return temperature increase required to maintain the boiler efficiency a number of promising factors can be found. **Figure 2-3** shows an isoline of constant boiler efficiency for varying fractions of steam flowrate returns, sown on the x-axis, as well the required increase in boiler return temperature required to maintain the boiler efficiency, shown on the y-axis. In the figure it can be seen that in the region of interest of the study, where the fractional flowrate reduction is in the region of 30% and subsequent return flowrate in the region of 70%, the fractional increase in the return temperature required to maintain the boiler efficiency is in the region of 5%. This then allows an opportunity for a substantial steam flowrate reduction if a means can be found to preheat the boiler return temperature.

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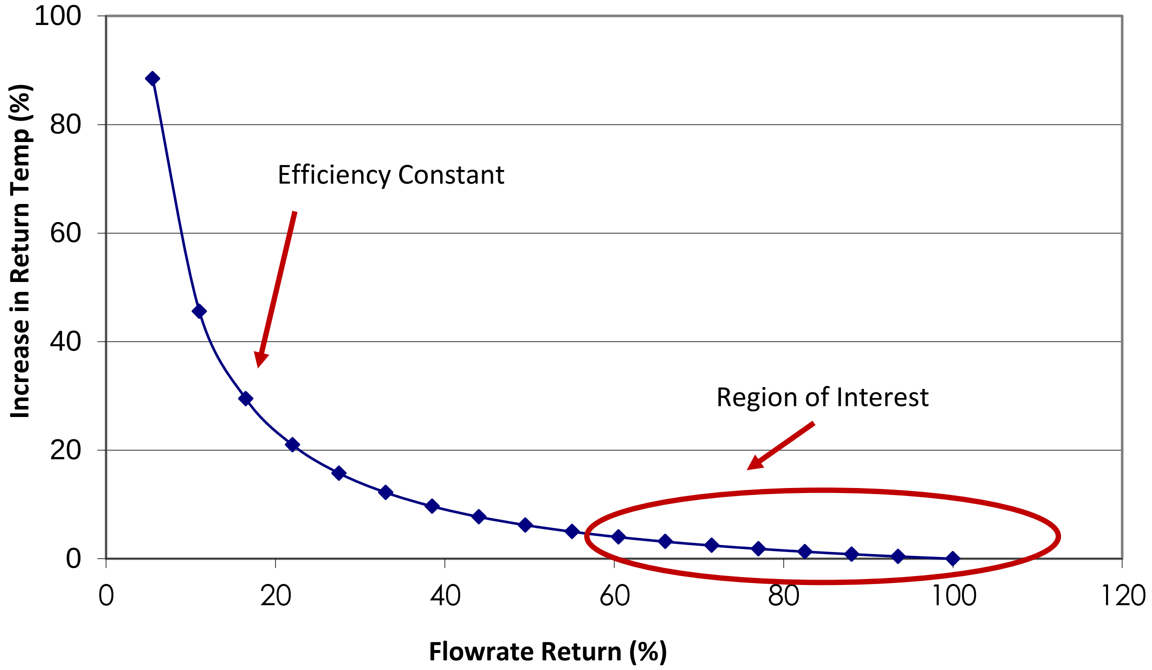

Figure 2-3: Sensitivity of Boiler Efficiency to Return Temperature and Flowrate

The authors then proposed several improvements to steam systems which provided for the additional heating requirements needed to retain the original boiler efficiency while reducing the steam flowrate. The first proposal was to utilise let down energy typically lost in expansion valves. Steam systems utilising steam for heating typically require steam as close to the allowable saturated steam temperature as possible, while adhering to the limiting temperatures of the heat exchangers. This is as a result of a property of steam that the latent energy available is higher at lower temperatures, as shown in **Figure 2-4**. The latent energy is plotted at saturated conditions against temperature in **Figure 2-5** and pressure in **Figure 2-6** to more clearly show this phenomenon. From the figure it can be seen that the latent energy of steam has a tendency to decrease as the saturated temperature and pressure of steam increases. As typical steam systems utilise only the latent heat of steam, there is an incentive to extract the maximum amount of energy from the steam as possible. The only limiting factor is then the approach temperatures required by the actual heat exchangers.

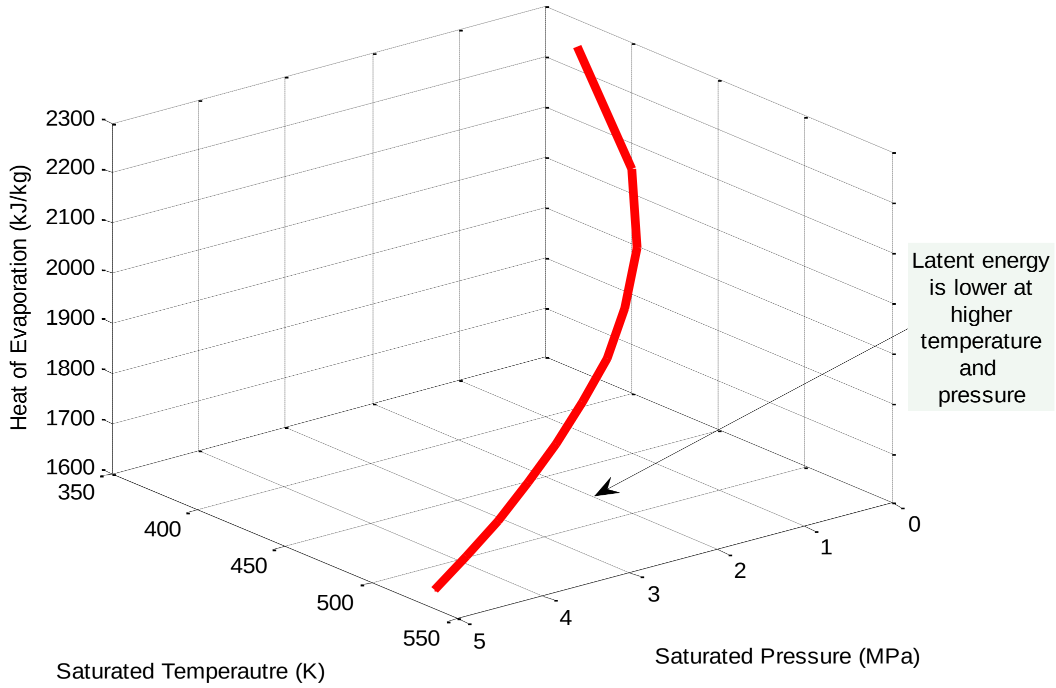

Figure 2-4: Latent Heat of Steam at Various Conditions

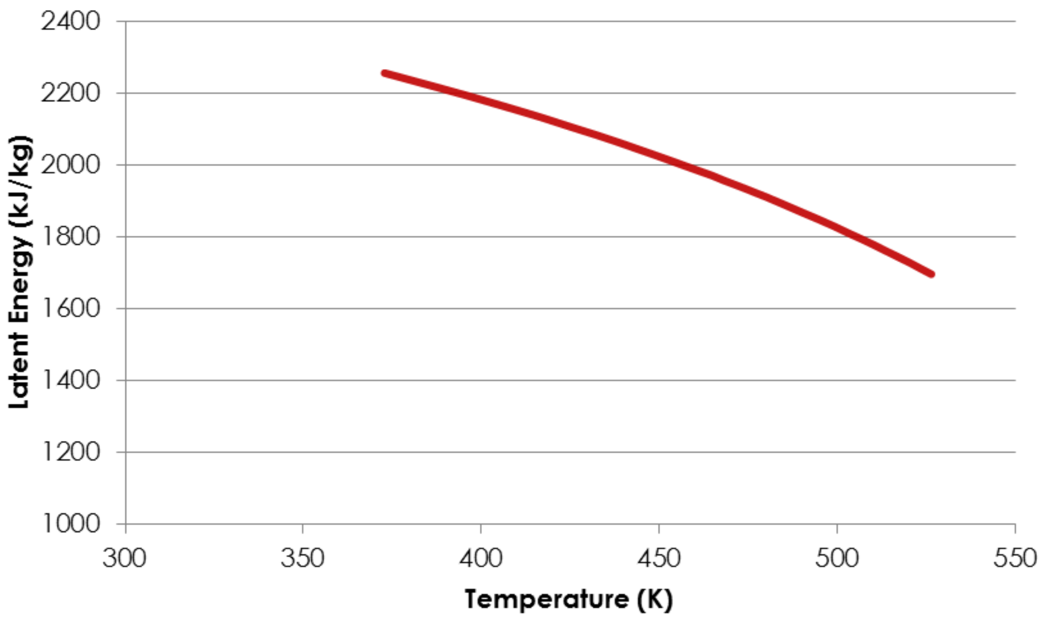

Figure 2-5: Latent Heat of Steam at Varying Saturated Steam Temperatures

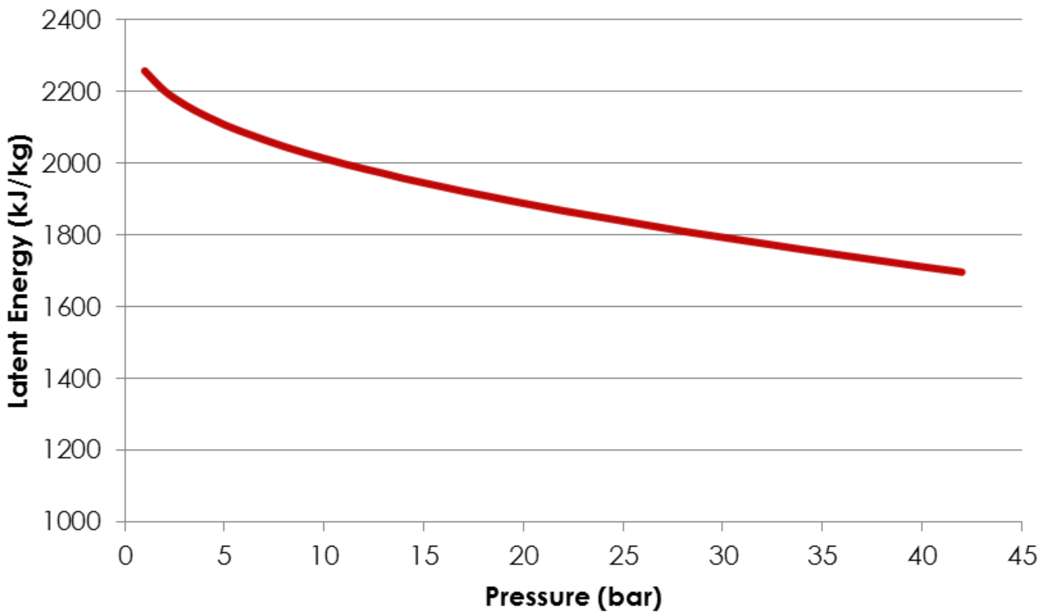

Figure 2-6: Latent Heat of Steam at Varying Saturated Steam Pressures

Steam systems often utilise expansion valves to reduce the pressure and temperature of steam to take advantage of the higher latent heat, as well as for safety and heat loss reasons. The energy lost through a let down valve could be harnessed to preheat the boiler return condensate such that the boiler efficiency could be maintained, even with a reduction in the steam flowrate.

The authors also proposed an additional heat exchanger in the system which had a dedicated function of preheating the boiler return condensate. This dedicated heat exchanger would then utilise a portion of the system steam so as to maintain the boiler efficiency.

The authors tested both techniques on a case study problem used by Coetzee and Majozi (2008) and it was found that the boiler efficiency could indeed be maintained with the minimum steam flowrate found by Coetzee and Majozi(2008). This was done by utilising the energy available from the steam let down in the system. In the event of no energy being available from let down, the dedicated heat exchanger was found to be able to maintain the boiler efficiency while still achieving a reduction in the steam flowrate.

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Due to the presence of bilinear terms in the formulation, the models were solved as MINLPs. The solution technique however utilised both the flow optimality conditions of Savelski and Bagajewicz (2001) as well as the relaxation and linearisation technique of Quesada and Grossmann (1995). These techniques allowed a linear model to be solved and used as a starting point for the exact model.

The authors successfully incorporated more aspects of the steam system into an optimisation framework. This holistic approach showed a pitfall in direct steam flowrate reduction in the reduced efficiency of the steam boiler. The authors then proposed a solution to maintain the boiler efficiency while still achieving the minimum or at least a reduced steam flowrate. The authors did not however consider other key aspects of HEN design, especially those related to rearranging the HEN, such as network pressure drop. The work also focussed on a single system steam level which does not encompass a large number of processes which utilise multiple steam levels.

Price and Majozi (2010b) expanded on the author's preceding work by incorporating multiple pressure levels into the optimisation framework. These steam levels are common in process plants and can originate from turbine exhaust. The authors employed the same reuse and recycle flowrate minimisation approach as well as the same techniques to maintain the boiler efficiency. The authors found that by maximizing the use of the steam leaving the turbines, which was assumed to be fixed, as well as the use of steam condensate for heating, the primary steam flowrate to the HEN could be reduced while the boiler efficiency could also be maintained.

A key factor in minimising steam flowrate in heating utility systems is the utilisation of hot condensate to heat process streams that do not require high heating temperatures. The rearrangement of the HEN as well as series nature of the retrofit HEN are likely to lead to additional pressure drop in the steam utility network.

2.3.2. HEN Pressure Drop

Price and Majozi (2010c) then investigated the pressure drop effects of rearranging the HEN from a parallel to a series based system. The authors followed a similar approach to that of Kim and Smith (2003) whereby the HEN minimum flowrate was

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first solved for and then used as a parameter in the pressure drop minimisation problem. The steam flowrate minimisation model solved by Coetzee and Majozi (2008) resulted in one of many HEN layouts which would lead to the minimum steam flowrate. This meant that the network structure could then be further optimised for an additional design variable such as pressure drop.

The authors constructed a node superstructure in a similar fashion to that of Kim and Smith (2003). Additional nodes were included to account for the steam condensers. The authors then formulated the pressure drop problem to minimise the maximum pressure drop of the system using the critical path algorithm of Gass (1985).

Due to the nature of both the pressure drop as well as the heat and mass balance superstructures binary variables were used to represent the existence of connections and heat exchangers in the system. The energy balance constraints were linearised using the optimality flow conditions of Savelski and Bagajewicz (2001). The pressure drop correlations utilised by Kim and Smith (2003) were adapted for steam systems and a condenser pressure drop correlation was added utilising approximations from Frank (1978) and Kern (1950). The resulting binary variables and nonlinear constraints meant the model was formulated as an MINLP.

The authors were successful in solving the model as an MINLP, however no indication of the optimality of the result could be concluded. The solution procedure was based on significant experience from Price and Majozi (2010c) where the authors attempted to solve the heating system pressure drop minimisation problem in a number of ways.

The authors attempted to solve the model by linearising the nonlinear pressure drop correlations using piecewise linear approximations, which resulted in an MILP model. Furthermore the authors attempted to solve the problem using the MILP problem as the starting point for the exact model. The authors then also solved the model as an MINLP directly. A comparison of the results showed the solution to the MINLP to be more consistent among the various other design variables and to have a better minimum pressure drop.

Price and Majozi (2010c) also encountered difficulties in solving the MINLP model due to singularities in the nonlinear terms. The authors overcame these difficulties by

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slightly relaxing the minimum steam flowrate and were able to solve the MINLP model.

The authors Price and Majozi (2010c) were successful in formulating a pressure drop minimisation model for steam systems which included the consideration of the steam condensing units. The authors were able to find the minimum network pressure drop while achieving a slightly higher steam flowrate than was shown by Coetzee and Majozi (2008). The authors did not however adequately overcome the singularities found in the solution of the MINLP and instead slightly relaxed the minimum steam flowrate. The authors also did not fully explore the bounds of the HEN solution space as the optimal flow conditions of Savelski and Bagajewicz (2001) fixed the heat exchanger outlet temperatures to their minimum.

The series of papers by Price and Majozi (2010a, 2010b and 2010c) investigated the holistic optimisation of heating systems and addressed a number of concerns with steam flowrate reduction. Of these focus areas the optimisation of steam system pressure drop was the least developed.

2.4. Conditions of Network Optimality

The conditions of optimality described in Savelski and Bagajewicz (2000a) play an important role in network design with the intention of minimising the total water intake. This work will be examined in slightly more detail and the scope of the conditions, as well as degenerate solutions will be discussed. The application to HEN design will also be mentioned.

The authors presented four theorems which were proven to hold when the solution to a WAP was found to be optimal. The first was a condition of concentration monotonicity, which stated that the concentration of a contaminant leaving a unit cannot be lower than the combined concentration of all streams leading to that unit. This essentially implied a net increase in concentration. The second required that a unit that received only fresh water had an outlet concentration equal to its maximum. This implied that the minimum fresh water is sent to these units. The third required that units which received wastewater from certain units and then in turn provided water to other units must have a maximum outlet concentration. Finally, units that are fed by wastewater and return their wastewater to treatment should have maximum outlet concentrations.

These theorems were then used to create a solution algorithm for designing a network. Savelski and Bagajewicz (2001) then produced linear models to solve the WAP problem which utilised the conditions of optimality. The key difference to their approach as compared to previous attempts to use mathematical programming to solve the problems was the condition stating that at least one optimal solution existed where the outlet concentrations of all units were at their maximum. This allowed the outlet concentration of the units to be fixed in the formulation, eliminating bilinear terms which caused difficulties in the solution of previous models.

The authors first used the linearised models, formulated as LP or MILP problems depending on the objective function, to solve for the minimum flowrate. The authors then utilised the existence of multiple networks which exhibited the minimum flowrate to further optimise the network. If the conditions of optimality were also applied, the minimum flowrate could be added to the model as a constraint and the model, now with a new objective function, could still be solved as an LP or MILP. Aspects such as the minimum number of interconnections or minimum fixed cost were some examples of objectives searched for with success. The authors also built into their model the option to consider regeneration and what positive effects this can have on the system.

One area briefly explored by the authors was degenerate solutions. The authors stated that solutions can exist where the minimum freshwater intake is realised, however the maximum outlet concentrations of units are not met. These solutions are termed degenerate and the authors utilised these to further reduce the number of connections in the system. The method used was fairly ad hoc and could potentially be time consuming. It involved systematically increasing and decreasing the freshwater utilised by certain key units and observing the resulting effects. The authors stated that this could be done once the LP model is solved and the minimum flowrate found as an additional means to further optimise an additional variable. A disadvantage mentioned is an increased internal water flowrate. The authors made mention of the fact that the degenerate solutions are infinite in

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number and as such enumeration was futile. They further stated that no mathematical model could make their proposed solution procedure more efficient.

The authors did allude to the fact that the conditions of optimality and their resulting benefits would only hold if the relevant assumptions were true. As such, the authors stated that the relationship between the outlet concentration and the wastewater unit load should be investigated. The work presented was however an excellent starting point for all investigations into the reduction of fresh water in wastewater systems. The conditions of optimality also have implications in other network optimisation fields such as HEN design. As such it was successfully utilised by Coetzee and Majozi (2008) to reduce the steam mass flowrate to a HEN.

The authors did elaborate on the use of degenerate solutions, as well as the benefits and shortcomings of such investigations. They presented an iterative approach to investigating degenerate solutions however these solutions were not directly incorporated into the optimisation framework and were rather considered once the freshwater intake had been minimised. There is the possibility that degenerate solutions can be utilised to further optimise utility networks, however the existence of bilinear terms in the mathematical formulation of such problems is likely to be an obstacle.

2.5. Some Mathematical Techniques for Nonlinear, Nonconvex Constraints

Bilinear terms are frequently found in chemical engineering applications where mass flowrates are combined with a further variable to create the transfer of a medium such as contaminant mass as well as utilities such as heat or materials such as hydrogen. These bilinear terms are both nonlinear and nonconvex, making their solution using NLP solvers difficult. This, combined with the superstructure type arrangement prevalent in mathematical programming type network optimisation frequently requires the use of binary variables to denote the existence or non-existence of certain nodes and therefore problems are often formulated as MINLPs. This section explores two techniques which have been formulated to simplify the use of bilinear terms in literature as well as several notes on MINLP solvers.

2.5.1. Relaxation and Linearisation

Sherali and Alameddine (1992) approached the problem of bilinear terms by utilising a relaxation and linearisation technique to simplify the nonconvex bilinear term into a single variable. This variable was the product of the various bounds of the variables constituting the original bilinear term. This approach was based on the convex and concave envelopes used by McCormick (1976) to create over and under estimators for bilinear terms in an attempt to simplify them. The approach by Sherali and Alameddine (1992) was not a direct linearisation technique and as such this programming approach does not always result in a feasible solution. The approach did however propose an effective and simple linearisation for bilinear terms.

Quesada and Grossmann (1995) expanded on the work of Sherali and Alameddine (1992) in their work with process networks. The authors attempted to optimise network systems with multi-component flows where bilinear terms arose from mass balance constraints. The networks in question consisted of a series of mixers, splitters as well as linear process networks. The authors used the convex and concave envelopes created by the variable bounds to replace the bilinear terms with a single variable encapsulating the limits of the variable within its bounds. This linearised solution was then solved and formed a lower bound on the optimisation problem. This lower bound was then used as a starting point for the exact, nonlinear model. Any feasible solution to the nonlinear model then formed an upper bound of the current solution. The relaxed solution was then embedded within a branch and bound procedure to obtain a solution.

The authors presented an algorithm which first defined effective bounds for the variables making up the bilinear terms, then solved the relaxed model to form a lower bound of the solution within the problem bounds and finally solved the exact model within the same bounds. Due to the lower bound solution of the relaxed problem, this algorithm was guaranteed to result in a globally optimal solution, within a set tolerance, as stated by Sherali and Alameddine (1992).

Although the authors identified a limitation in the direct lack of application of the algorithm to binary variable systems, the relaxation and linearisation formulation can be extended to various sub-regions of the total solution space, allowing for the

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application to systems which do contain binary variables. This work provided a systematic means to optimise process networks, even with multi-component flows. The authors utilised a relaxation and linearisation technique to reformulate bilinear terms which held a large scope of application in many facets of network optimisation. The algorithm presented by the authors was, in this form, limited to processes with linear process units. The ability of the algorithm to find a tight lower bound and effective starting point for the exact problem made this algorithm applicable to many network type optimisation problems. This technique was used successfully used by Majozi and Moodley (2007), Gololo and Majozi (2011) and Gololo and Majozi (2013) to overcome bilinear terms in cooling network optimisation.

2.5.2. Transformation and Convexification

Bilinear terms are problematic to solve due to the nonconvex nature of the constraints that contain them. Conventional NLP solvers typically utilise gradient based methods to find an optimal solution, however nonconvex functions can lead to local optimum results. Westerlund et.al. (1994) tried to formulate a pump configuration as an MINLP problem. The authors utilised a variable number of pumps in either a series or parallel configuration. The objective function for the formulation caused complexity as it was nonlinear and nonconvex. The other constraints in the problem were both equality and inequality constraints that were linear and nonlinear. The authors propose an extended cutting plane (ECP) technique combined with a general linear branch and bound technique to solve the resulting MINLP. This work highlighted the complexity of proposing optimisation problems as MINLP problems. The authors did however begin to consider techniques to simplify the formulation and compare their proposed ECP technique to that of DICOPT + + of Viswanathan and Grossmann (1990).

Westerlund and Petterssen (1995) furthered the development of the ECP method to solve convex MINLP problems. The authors developed their own technique based on NLP optimisation integer cuts first proposed by Kelley (1960). The binary variable elements of the problem were handled using branch and bound techniques (Land and Doig, 1960) or other mixed integer or mixed binary variable type solution techniques by authors such as Van Roy and Wolsey (1987) or Crowder et al. (1983). This method would be further developed by the authors, however a key limitation

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was the restriction of the technique to solve problems with only convex nonlinear constraints. Westerlund et al. (1998) presented a nonconvex MINLP problem solution methods based on the ECP method. This method showed global optimum convergence for pseudo convex problems, i.e. problems that contain nonconvex terms, however in the operating region of the problem the terms are in fact found to be convex. The method proposed by the authors sought to solve MINLP problems with an iterative approach utilising the solution of MILP subproblems. This was quite different from the conventional outer approximation solvers which employed MILP master problems along with NLP subproblems.

Harjunkoski et al. (1997) explored the convexification of bilinear integer functions in optimisation problems. The authors explored various mathematical transformations to aid the optimisation of trim loss problems in the paper industry. The authors recognised the existence of nonlinear, nonconvex terms in the mathematical representation of the trim loss problem. The authors attempted to linearise or transform bilinear terms containing discrete variables appearing in the formulation into convex terms. The authors proposed four different linearisation approaches which allowed the problem to be solved as a MILP or LP problem, however consequently the number of variables and equations in the formulation increase dramatically. The authors also proposed a convexification technique based on transformations to exponential or square root functions, both of which are convex. The problem was then solved using convex MINLP solvers such as the ECP. The authors took an interesting approach to bilinear terms, opting to transform the terms as oppose to replacing them.

Harjunkoski, Westerlund and Pörn (1999) formalised the transformation and convexification of the bilinear terms in the trim loss problem and extended their research into limiting the combinatorial space and reducing the size of the problem. The authors also focussed on the benefits of carefully selecting an objective function which not only minimised trimmed paper waste but also energy along with other environmentally impacting variables. The authors discovered the benefit of keeping several variables as part of the objective function. The authors also recognised certain limitations to the heuristic approach of reducing the combinatorial solution space and conceded that this area of work required specific attention. The authors showed effective means of transforming bilinear terms into convex terms and building these techniques into a solution procedure. Many MINLP solvers were effective at solving convex problems and as such an effective convexification technique could reduce difficult problems with bilinear terms to solvable problems, perhaps even yielding globally optimum solutions.

Harjunkoski, Pörn and Westerlund (1999) continued to investigate the convexification techniques for bilinear problems. The authors extend the application to several example problems. They focused on the application of convex transformations over linearisations and concluded that in certain cases convex transformations could lead to the addition of fewer variables and constraints. Further, the authors explored which of the transformations investigated led to tighter bounds, fewer variables and better solution processes.

Following successful work with convex transformations, Pörn et al. (1999) discussed general convexification techniques of bilinear terms consisting of discrete and integer variables and in some cases continuous variables. They broached the subject of posynomials, or products of variables to various powers, and stated the prevalence of these variables in chemical engineering type optimisation problems. They showed how discrete variables could be represented as integer variables, for which more rigorous optimisation techniques exist such as the Glover transform (Glover, 1975). The authors also showed that certain continuous functions were convex, specifically exponential functions if the function was positive and posynomial functions if the product of the powers was less than 1 and the term was negative. Using appropriate inverse transformations, the authors could transform nonconvex terms into convex terms and applied these to certain test problems. The authors began to refer to these transforms as exponential transforms for positive terms and potential transforms for negative terms. This work solidified the previous advancements in this field by the authors and showed how problems could be mathematically simplified. These simplifications could allow conventional solvers to overcome numerical difficulties and possibly provide better solutions which are globally optimal.

Pörn and Westerlund (2000) continued to develop the extended cutting plane MINLP optimisation algorithm. The authors showed and proved the algorithm to

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optimise pseudo-convex functions and this was demonstrated through further example problems. The ECP MINLP solver was compared to other branch and bound type MINLP solvers such as DICOPT (Viswanathan and Grossmann, 1990) by Björk and Westerlund (2002) in their adaptation of the Synheat model of Yee and Grossmann (1990). The authors utilised previously derived convexification techniques to allow non-isothermal mixing of streams and as such allowed the already comprehensive superstructure of Yee and Grossmann (1990) to allow for a larger solution space and possibly a more optimal solution. The Synheat model of Yee and Grossmann (1990) used this comprehensive HEN superstructure to attempt to optimise cost by considering utilities, number of heat exchangers and heat exchange area. This work showed the application of the convexification techniques with already developed models. The uses of other optimisation algorithms such as DICOPT were shown to be compatible and effective with convexification techniques.

Björk et al. (2003) extended their research onto more comprehensive convexifications. The authors attempted to create convex transformations of signomial terms. Signomial terms are similar to polynomial terms, only with exponents taking values of any real number. The authors showed how the choice of transformation functions was essential in creating effective subproblems from the transformed terms. The authors extended the exponential and potential transformation techniques as well as showed how the concept of power convex functions can be utilised to test the quality of the convexifications. The authors made an important step in the work on convexification techniques by including signomial terms which constituted exceptionally complex terms, as well as bilinear terms.

Pörn et al. (2008) then presented a global optimisation strategy for optimisation problems with signomial parts. The authors presented a unified methodology to transform signomial parts of constraints into convex terms on a term by term basis, allowing already convex parts of the formulation to be unaffected. The transformations were intended to create a convex lower bound of the problem which could be solved by conventional methods. The transformations employed were the exponential transform (ET) or the inverse transform (IT) for positively signed terms as well as the potential transform (PT) for negatively signed terms. The transformations did create nonconvex constraints which were discretised using a piecewise linear approximation. The authors tested the transformations on a number of test problems with promising results. The accuracy of the ET and IT were also compared in this work and the ET was found to produce tighter lower bounds. The authors stated that when problems were solved without a predefined starting point the MINLP solution process could be expensive. This work did however provide a formalised convexification tool to allow individual nonconvex terms of signomial nature to be individually convexified. This had considerable potential to not only make solution processes more efficient but also guarantee global optimality with certain solvers such as aECP, DICOPT and BARON.

The transformation techniques themselves continued to be investigated. Lundell and Westerlund (2009a) introduced a power transformation for positively signed signomial terms and this was compared to the exponential transform. In more detailed comparisons by Lundell and Westerlund (2009b) it was found that the power transform only gave tighter lower bounds than the exponential transforms for signomial terms of more than one variable in certain areas of the domain. Lundell and Westerlund (2009c) then proposed a technique to find the optimal transformations in nonconvex optimisation problems with signomial terms. The authors developed an MILP method to optimally transform signomial terms as a pre-processing step.

Lundell et al.(2013) then included the so called aBB-underestimator technique to cater for the convexification of non-signomial functions which were twice differentiable. Regular signomial terms are convexified using techniques already described. The authors used the convexified formulation to create an underestimation of the problem. This piecewise convex reformulation allowed the entire problem to be solved using conventional MINLP solvers. This work further solidified the advances of convexification strategies set out by Westerlund and his co-workers.

The convexification of nonconvex terms is an important area of research as nonconvex optimisation is abundant in the realistic modelling of systems. The complexities caused by nonconvex terms therefore hamper the true optimisation of such systems, however convexification strategies allow these problems to be solved with a sense of the globally optimal nature of the solution. The use of piecewise approximation in the ET, IT and PT transformations does require an iterative type approach, however this will be discussed in later chapters of this work.

2.5.3. Notes on MINLP Solvers

A large number of commercial solvers have been created to solve MINLP problems. Certain solvers are more suited to various applications due to internal heuristics. Many successful solvers employ a two phase type optimisation approach utilising a master problem in addition to subproblems. The MINLP problem is then split to create NLP or relaxed LP problems combined with an MILP master problem. Such solvers include the ECP type solvers of Westerlund and co-workers, DICOPT of Viswanathan and Grossmann (1990) and BARON of Sahindis and Tawarmalani (2005).

The ECP methodologies evolved from early work with convex MINLP optimisation based on work with integer cuts to solve nonlinear problems by Kelley (1960). The methodology evolved to include the global optimisation of pseudo-convex functions with the aECP solver (Pörn and Westerlund, 2000) which was updated and introduced into the general algebraic modelling software (GAMS) optimisation package with the title GAMS/AlphaECP. A comparison of this algorithm to other MINLP solvers is found in Lastusilta et al. (2009) where it was found that the solver did not solve as many NLP test problems as the best solver.

Baron is a relatively new addition to GAMS as compared to other solvers such as DICOPT. Experience at the University of Pretoria is related to DICOPT with many publications (Majozi and Moodley, 2008, Price and Majozi, 2010, Gololo and Majozi, 2013, and many others) having made use of the solver. DICOPT is an outer approximation (OA) type solver, based on original work of Duran and Grossmann (1986a), Duran and Grossmann (1986b) and Duran (1984). The solver essentially deconstructs a MINLP problem into an MILP master problem by linearising the nonlinear elements of the MINLP. An outer shell of the solution space is created using these linearisations and the optimal solution is underestimated. The relaxed, linearised master MILP problem is then solved. The resulting binary variables from this solution are then fixed and the problem is solved as an NLP for that particular arrangement of the binary variables. This process is repeated until a certain

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tolerance is reached between the best underestimating master MILP solution and that of an NLP solution. A large number of integer cuts are made to remove infeasible solutions and to reduce the linearised solution space.

Before implementation in GAMS, DICOPT was further evolved by Kocis and Grossmann (1987) where an equality-relaxation variation was added to the OA formulation. Kocis and Grossmann (1988) then approached nonconvex MINLP problems. The authors found that the MILP master problem could, on occasion, remove the most optimal solution during linearisations when nonconvexities were present in the nonlinear portion of the MINLP formulations. The authors proposed a two phase approach to identify potentially nonconvex areas and where applicable alter the MILP master problem. While the technique did not guarantee a globally optimal solution, this strategy did focus attention on the key aspects of nonconvexity in MINLP formulations. Kocis and Grossmann (1989a) discussed computational experience with DICOPT for a large number of test problems. The authors noted a key area of using DICOPT as the existence of nonconvexities in the model formulations. Two areas of concern for the authors were the existence of local optimal results in the NLP subproblems as well as sub optimal lower bounds in the MILP master problem. The authors showed the flexibility of DICOPT but also pointed out a key feature which should be addressed in model formulation. Kocis and Grossmann (1989b) then presented a modelling and decomposition strategy for process flowsheets so as to maximise the efficiency of DICOPT. The authors used certain heuristics to replace nonconvex splitter representations with linear models in choice areas. NLP subproblems were also limited to the particular flowsheet as opposed to the entire superstructure. The size of the master problem was also reduced using a lagrangian based decomposition scheme. The authors then demonstrated these additional procedures using nonconvex test problems. The authors recognised the aspects of nonconvexity as being potentially problematic for DICOPT, however steps could be implemented to cater for these nonconvexities and utilise the robust and effective solution procedure employed by DICOPT. A key feature was recognising areas of potential difficulty and making modelling alterations to cater for these situations. DICOPT forms part of the GAMS suite of MINLP solvers (Viswanathan and Grossmann, 1990).

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The intricacies of MINLP problems are the binary or discrete nature coupled with nonlinearity. MINLP solvers need to efficiently tackle both. Key modelling changes can greatly affect the solution of problems and diligent pre-processing should always be conducted before utilising MINLP solvers. Nonconvexity has also been pointed out as a key area, however advances in relaxation and linearisation strategies such as that of Quesada and Grossmann (1995) or convexification techniques such as that of Pörn et al. (2008) can be used to aid in the optimisation of MINLP type problems.

2.6. Conclusion

This literature review has considered areas of HEN optimisation and the development of techniques to optimise HEN in terms of utility flowrate as well as design aspects such as network arrangement and the effects these have on aspects such as pressure drop. It has been found that holistic approaches to systems yield the most optimal results.

Flow networks are complicated systems to model as they often include bilinear terms which are nonlinear and nonconvex. Conditions of optimality can allow optimal networks to be designed from a flowrate minimisation perspective and bypass the difficulty of bilinear terms. These conditions may however stifle attempts to further optimise networks by limiting a key design variable and minimising the problem solution space. Degenerate solutions have been shown to yield optimal utility flowrates while also facilitating the optimisation of further design variables.

Degenerate solutions do however pose optimisation difficulties as bilinear terms must be addressed. Techniques in literature have been developed to aid MINLP solvers in the solution of problems with nonconvex terms.

In this work degenerate solutions will be exploited to further optimise HEN pressure drop while utilising relaxation or convexification techniques to overcome bilinear terms. The solution technique will then be applied to the entire steam system in an attempt to maintain boiler efficiency with a reduced steam flowrate in a more optimal way.

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3. Motivation for Study

This chapter discusses the general background to the work presented in this thesis. The topics include previous work, heat exchanger network pressure drop, boiler efficiency, degenerate solutions of flow networks and the general principals of some MINLP solvers.

3.1. Background

This section is intended to give a background and motivation for further investigation of heat exchanger network pressure drop. Techniques developed in this work will then also be applied to other aspects of steam system HEN optimisation such as boiler efficiency.

3.1.1. Previous Work

Utility system optimisation has been explored by Majozi and co-workers for both batch and continuous systems. The focus of this thesis is specifically continuous steam system optimisation.

Coetzee and Majozi (2008) minimised the steam flowrate required for HENs by utilising sensible heat from steam condensate to heat process streams along with the latent heat from the steam. The subsequent effects on the steam boiler efficiency were addressed by Price and Majozi (2010a) while the pressure drop effects of adding series connections to utilise condensate to the HEN were investigated by Price and Majozi (2010c).

Price and Majozi (2010c) formulated the pressure drop model using a novel superstructure to develop flow and pressure drop constraints. The resulting formulation was presented as an MINLP. The authors attempted to simplify the formulation to create an MILP using various techniques. These included those employed by Glover (1975) to cater for bilinear terms involving binary variables as well as that of Quesada and Grossmann (1995). The resulting techniques were found to be ineffective and the best solution to the pressure drop formulation came from

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solving the problem as an MINLP. Slight flow relaxations were required in order for a feasible solution to be found. The MINLP used to represent the HEN pressure drop problem is complex due to binary variables present in the formulation as well as the nonconvex nature of the bilinear terms making up formulation.

The authors identified the need to further explore the steam system HEN pressure drop problem. The key aspect of solving the pressure minimisation problem is to do so while still achieving the minimum steam flowrate for the system. In this way two or more design variables, steam flowrate as well as an additional variable such as network pressure drop, can be minimised in order to reduce the cost of grassroots designs or debottleneck existing steam systems. Any techniques developed will then also be applied to other aspects of HEN optimisation such as pressure drop.

This work is intended to build from the experience of and Price and Majozi (2010c). The model formulation will be deconstructed in an attempt to solve the pressure drop problem with the exact minimum steam flowrate as described by the method of Coetzee and Majozi (2008). The assumptions and simplifications utilised by preceding authors to this work such as Coetzee and Majozi (2008) will also be examined in an attempt to find a better minimum pressure drop solution.

Certain formulations developed by Price and Majozi (2010a) used to maintain boiler efficiency also exhibit bilinear terms in the MINLP formulation. Therefore any techniques developed to aid the HEN pressure drop minimisation problem will also be applied to those complex MINLP formulations intended to maintain boiler efficiency.

3.1.2. Modelling Experience

Majozi and co-workers have large amounts of network optimisation experience. Certain features of flow networks make optimisation of such systems difficult to solve, the most prevalent of which are bilinear terms. Bilinear terms exhibit nonconvex, nonlinear properties which cause difficulties for most MINLP solvers. An additional complexity for some systems is the batch nature of the operations which have an additional time component which adds an additional number of complicated constraints when optimising batch systems.

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A number of simplification and optimisation techniques are used by Majozi and his co-workers. These include simplifying systems using the relaxation and linearisation technique of Quesada and Grossmann (1995), formerly of Sherali and Alameddine (1992). This technique allows bilinear terms to be linearised and models to be solved as MILPs. This technique has been used by many researchers to optimise a number of networks involved in heat exchange and wastewater minimisation. Glover transforms allow bilinear terms formed from a single continuous and a single binary term to be considered as a single variable in the formulation. Optimal mass exchange unit outlet conditions as described by Savelski and Bagajewicz (2000) have been proved to yield optimal flow conditions in mass exchange networks and this was successfully used to optimise heat exchange networks by Coetzee and Majozi (2008) as certain principles of mass and heat transfer are interchangeable.

While techniques are available in literature to handle a number of complex constraints encountered by Majozi and co-workers, a number of alternative techniques can be used to overcome these difficulties. Further understanding of network flow models as well as alternative constraint formulation can also be used to optimise these problems.

3.2. System of Interest

The steam system in the context of this investigation is shown in **Figure 3-1**. The boiler unit produces superheated high pressure steam, shown as stream 1. This steam can then proceed to a let down valve as stream 2 or can proceed to a high pressure steam turbine as stream 3. Stream 1 is superheated high pressure steam, however the heating utility for processes is typically saturated steam. This is due to the parallel configuration typically seen in HENs. Each heat exchanger receives saturated steam and latent energy is used to heat the appropriate process stream. A let down valve provides a means to reduce the pressure of stream 2 such that it becomes saturated steam as in stream 4.

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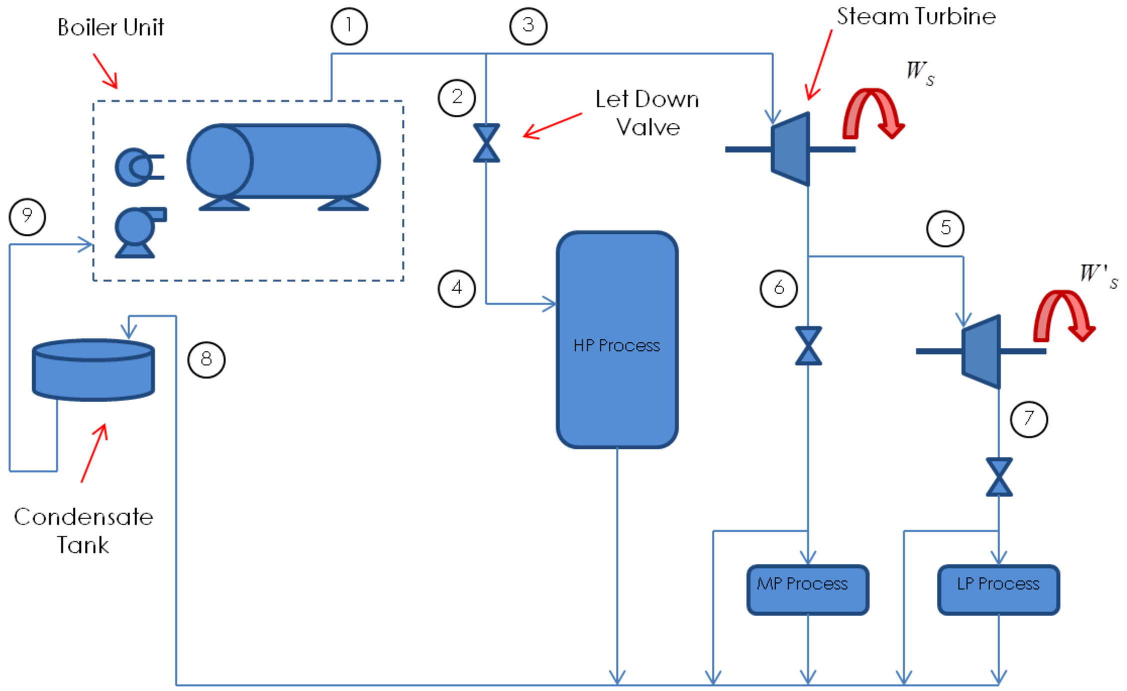

Figure 3-1: Steam System in the Context of this Investigation

Stream 3 passes through the turbine where energy is recovered in the form of shaft work W_S, which is typically used to drive other process equipment or generate electricity. The exhaust from the high pressure turbine is generally at medium pressure. This steam then either passes through a medium pressure turbine as stream 5 where shaft work W'_S is recovered or passes through a let down valve and proceeds to a process as a heating utility, shown as stream 6. The purpose of this let down valve is the same as that mentioned above. The exhaust of the medium pressure turbine is at low pressure and proceeds as a further heating utility to background processes as stream 7. A let down valve is indicated in stream 7 however low pressure steam is extremely close to saturation and as such this valve may not be necessary. The bypass streams around the MP Process and LP Process have been included for completeness.

The heating utility outlet streams from the various HENs are typically saturated condensate. These streams then combine to form stream 8 and proceed to a condensate tank. The condensate then either passes through a condenser or is subject to a large increase in pressure due to liquid head which is often achieved by elevating the condensate tank. This is to ensure the condensate is sufficiently far away from the saturation temperature so as to prevent the risk of cavitation during pumping to the steam boiler. The risk of cavitation is mostly associated with centrifugal pumps which are the most prevalent in boiler systems. Make up water is also typically added in this region although this has been omitted for simplicity. The stream proceeding to the boiler feed water pump is shown as stream 9. After being pumped the return stream to the boiler passes through a pre heater or economiser to heat the boiler feed. The economiser is often found as part of a commercial boiler package.

The steam lost during let down is typically collected in flash drums which have been excluded from **Figure 3-1** for simplicity. Typically the supply temperature of steam to a HEN is designed as close to the highest limiting utility supply temperature of the HEN. This is due to the property of steam where latent energy per unit mass of steam decreases as the temperature and pressure of the steam increases. Thus the steam leaving the let down valve as stream 4 is at a lower pressure than stream 2. This is referred to as the process pressure from here onwards.

HEN pressure drop will be explored within the individual HEN processes, whereas boiler efficiency will include all elements of **Figure 3-1**.

3.3. HEN Pressure Drop

This section is intended to explore some of the complexities of pressure drop in a flow network.

3.3.1. Background to HEN Pressure Drop

The steam flowrate to a heating utility heat exchange network can be considerably reduced if energy is further harnessed from the saturated and sub cooled

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condensate leaving condensers. This is achieved by recycling and reusing condensate where possible. A technique to systematically achieve the minimum steam flowrate is presented in Coetzee and Majozi (2008). One concern with the recycle and reuse of condensate is the effect on the steam boiler. A means to achieve the minimum steam flowrate while maintaining boiler efficiency was presented by Price and Majozi (2010a). Price and Majozi (2010b) then reduced the steam required for HENs where multiple steam levels are available and presented a means of still maintaining the required boiler efficiency.

A further concern for recycle and reuse in HENs is the aspect of increased pressure drop within the network. With recycling hot condensate, utility streams have to pass through multiple heat exchangers in series which greatly increase the pressure drop of the system. Kim and Smith (2003) identified the need to minimise pressure drop in such networks from their work in cooling systems. From the work of Savelski and Bagajewicz (2000), Coetzee and Majozi(2008) found that multiple networks could be found for the same minimum flowrate due to the linear nature of the network design model. Thus a further objective function could be applied to these optimum flow networks. Additional objectives could include cost or pressure drop. Following a similar approach to Kim and Smith (2003), pressure drop was minimised for a HEN in steam systems by Price and Majozi (2010c).

In HENs pressure can be lost through pipes, condensate heat exchangers and condensers. The mixing and splitting junctions that redirect flow can be considered as part of the piping network. Pressure drop correlations are therefore needed in the form of constraints so as to incorporate this into an optimisation framework.

Many correlations exist in literature, however those used by Kim and Smith (2003) are the most appropriate as they are readily integrated with flowrate which is a variable typically used in heat and mass exchange network optimisation problems. The correlations are derived from the work of Nie (1998). These derivations will be summarised for heat exchangers, condensers and pipework. The author represents pressure drop through conventional shell and tube heat exchangers. Thus it will be assumed that these heat exchangers are used in the investigation

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Heat Exchanger and Condenser Pressure Drop

The tube side pressure drop for a heat exchanger is much more easily determined than the shell side pressure drop as determined by Nie (1998). As such it will be assumed that steam and condensate pass through the tube side of the heat exchanger.

The pressure drop function presented by Kim and Smith (2003) is shown in Constraint (3-1).

$$\Delta P_t = N_{t1} V_t^{1.8} + N_{t2} V_t^2 \qquad (3\text{-}1)$$

In this constraint the tube side pressure drop is calculated with respect to the tube side fluid velocity. Kim and Smith (2003) then convert this velocity constraint to one with respect to volumetric flowrate, as seen in Constraint (3-1). According to Nie (1998) the two terms account for the pressure drop as a result of the friction loss in the tubes and the loss as a result of sudden contractions, expansions and flow reversals. The two factors N_{t1} and N_{t2} are shown in Constraints (3-2) and (3-3) below.

$$N_{t1} = \frac{1.115567}{\pi^{2.8}} \frac{\rho^{0.8} \mu^{0.8} n_{tp}^{2.8} A}{N_t^{2.8} d_o d_i^{4.8}} \qquad (3\text{-}2)$$

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

In Constraints (3-1), (3-2) and (3-3), ΔP_t is the tube side pressure drop, V_t is the tube side volumetric flowrate, ρ is the fluid density, μ is the fluid viscosity, n_{tp} is the number of tube passes, *A* is the heat transfer area, N_t is the number of tubes, d_o is the outside tube diameter and d_i is the inside tube diameter.

Kim and Smith (2003) utilise certain industrial design guidelines to help approximate realistic heat exchanger parameters such as heat exchange area, tube number and tube diameter. Many of these terms in these constraints such as the heat transfer area, the number of tubes and the tube dimensions are very much interrelated in heat exchanger design. These guidelines, as well as those used for this work, are discussed in Appendix A.

The pressure drop for condensers must also be catered for as they also appear in HENs utilising steam as a heating medium. According to Sinnot (2005), the pressure drop through condensers where total condensation occurs can be approximated by calculating the pressure drop in the conventional fashion using the inlet vapour conditions and multiplying this by a factor. Two factors are put forward, the first by Kern (1950) who suggests a 50% factor and the second by Frank (1978) who suggests 40%. The more conservative approximation of 50% will be utilised for this work. The condenser pressure drop will therefore be approximated by Constraint (3-4).

$$\Delta P_{t,c} = 0.5\left(N_{t1}V_t^{1.8} + N_{t2}V_t^{2}\right) \qquad (3\text{-}4)$$

In Constraint (3-4) N_{t1} and N_{t2} are equivalent to those for Constraint (3-1).

Piping Pressure Drop

Kim and Smith (2003) define the piping pressure drop according to Constraint (3-5). Piping pressure drop can be approximated using commonly used correlations as well as a friction factor by Hewit et al. (1994) to approximate the fanning friction factor. This was utilised by Kim and Smith (2003) to define piping pressure drop and this derivation is shown in Constraint (3-5).

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$$\Delta P_P = N_P^{EX} V_P^{1.8} \qquad (3\text{-}5)$$

In Constraint (3-5), N_P^{EX} is a factor to relate fluid properties and the pipe structure. This has been expanded to demonstrate the relationship between the fluid and design variables for the piping system. The expanded term N_P^{EX} is shown in Constraint (3-6).

$$N_P^{EX} = \frac{1.11557}{\pi^{1.8}} \frac{\rho^{0.8} \mu^{0.2} L}{D_i^{4.8}} \qquad (3\text{-}6)$$

In Constraint (3-6) L is the pipe length and D_i is the pipe inside diameter. Since the diameter is a design choice Kim and Smith (2003) use an economic trade-off of the optimal pipe size suggested by Peters and Timmerhaus (1991) where the optimal pipe diameter is given as a function of volumetric flowrate and fluid density. Using this relation Constraints (3-5) and (3-6) are rewritten as Constraints (3-7) and (3-8) respectively.

$$\Delta P_P = N_P^{NW} \frac{1}{V_P^{0.36}} \qquad (3\text{-}7)$$

$$N_P^{NW} = \frac{188.318}{\pi^{1.8}} \rho^{0.176} \mu^{0.2} L \qquad (3\text{-}8)$$

Constraint (3-7) suggests that pressure drop is an inverse function to volumetric flowrate which appears counterintuitive. The relation by Peters and Timmerhaus

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(1991) however ensures that every fluid velocity has an optimal pipe diameter given standard pipe diameter sizes. This correlation is utilised from a cost saving perspective but does represent a reasonable design basis and shall be utilised in this study. Now the pressure drop through the pipes is only a function of the pipe length, the fluid properties and the volumetric flowrate.

Pressure Drop with respect to Mass Flowrate

The heat exchanger and piping pressure drops shown in Constraints (3-1), (3-2), (3-3), (3-4), (3-7) and (3-8) can be changed so that they can accommodate the fluid mass flowrate as used by the flowrate reduction models developed by Coetzee and Majozi (2008) and implemented in model development which is discussed in Chapter 4. Constraints (3-9), (3-10), (3-11) and (3-12) show these adjustments for the tube side heat exchanger correlations.

$$\Delta P_t = N_{t1}^* \dot{m}_t^{1.8} + N_{t2}^* \dot{m}_t^2 \qquad (3\text{-}9)$$

$$N_{t1}^* = \frac{1.115567}{\pi^{2.8}} \frac{\rho^{-1} \mu^{0.8} n_{tp}^{2.8} A}{N_t^{2.8} d_o d_i^{4.8}} \qquad (3\text{-}10)$$

$$N_{t2}^* = \frac{20}{\pi^2} \frac{n_{tp}^3 \rho^{-1}}{N_t^2 d_i^4} \qquad (3\text{-}11)$$

$$\Delta P_{t,c} = 0.5\left(N_{t1}^* \dot{m}_t^{1.8} + N_{t2}^* \dot{m}_t^2\right) \qquad (3\text{-}12)$$

Constraints (3-13) and (3-14) show the adjustment for the piping correlations.

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$$\Delta P_P = N_P^{NW*} \frac{1}{\dot{m}_P^{0.36}} \quad (3\text{-}13)$$

$$N_P^{EX*} = \frac{188.318}{\pi^{1.8}} \rho^{0.536} \mu^{0.2} L \quad (3\text{-}14)$$

These correlations will be used for pressure drop through equipment in this work.

Heat Exchanger Network Pressure Drop

It has been established that pressure drop in HENs is not only dependent on stream variables such as flowrate, but also on the network layout (Nie and Zhu, 2002). To account for the network layout Kim and Smith (2003) utilise the concept of the longest, or critical, path as described in Gass (1985). This critical path represents the maximum distance between points, or in the context of this work, the maximum network pressure drop. These can be calculated using the Critical Path Algorithm (CPA) which is prevalent in mathematical programming. The total pressure drop of the network is essentially represented by the largest pressure drop of a connection of streams. This critical path should then be minimised in order to minimise the total pressure drop of the system. Kim and Smith (2003) used a node superstructure as a framework to establish the critical path model. The nodes represent mixers that combine streams before heat exchangers as well as splitters that redirect streams after heat exchangers. Each of these nodes has a pressure associated with it. Pressure is then lost between nodes, for example in the heat exchanger between mixers and splitters or in the pipes between the mixers and splitters of different heat exchangers. The mixers are linked to a source node and the splitters to a sink node. The source node represents the maximum pressure of the system, usually the outlet pressure of the utility source, i.e. the cooling water circulation pumps or the steam boiler. The sink node represents the minimum pressure of the system, i.e. the stream returning to the utility source. The objective of the model is then to find the maximum pressure drop through the network and then minimise this pressure drop using mathematical programming.

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3.3.2. Steam System HEN Pressure Drop Problem

The steam system heat exchanger network pressure drop problem was solved by Price and Majozi (2010c). The authors utilised the MILP steam minimisation formulation of Coetzee and Majozi (2008) as the heat exchange basis for the pressure drop formulation. This is necessary as the heating requirements of the utility streams in the network must still be maintained. The pressure drop correlations alluded to in Section 3.3.1 and expanded on in Chapter 4 were then added to the formulation and the objective function was changed from steam flowrate minimisation to overall pressure drop minimisation. The minimum steam flowrate for the system is fixed and used as a parameter. The objective is then to exploit one of the multiple solutions which exhibit the minimum steam flowrate and optimise these systems for the minimum pressure drop (Price, 2010).

The steam flowrate minimisation model is initially formulated to contain a single nonlinear constraint. This constraint describes the sensible heat transfer from condensate to the process streams. This constraint is linearised using a condition of optimality described in Savelski and Bagajewicz (2000). The pressure drop correlations are however nonlinear with respect to the mass flowrate of steam and condensate, therefore the resulting formulation is an MINLP model. Price and Majozi (2010c) attempted several methods to solve the MINLP model. Firstly the author linearised the pressure drop correlations using piecewise linear approximations which resulted in an MILP model. Secondly the author used the linearised problem as a starting point for the exact nonlinear problem. Finally the author solved the problem as an MINLP. After comparing the results it was found that the simple nonlinear formulation was the most reliable and these results were presented by Price and Majozi (2010c). Several easing techniques were employed by the authors to achieve a feasible solution, such as slightly relaxing the minimum steam flowrate such that a feasible solution could be found. These techniques are further discussed in Chapter 5.

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3.4. Boiler Efficiency

This section is intended to show a derivation of the boiler efficiency used for this investigation.

3.4.1. Derivation

Boiler efficiency in its simplest form is a ratio of the energy content of the steam produced by the boiler to the energy content of fuel used to fire the boiler. This relationship is shown in Constraint (3-15). Since energy is lost in the process of transferring energy from the fuel to the steam, the energy of the fuel can often be expressed as the energy gained by the steam in addition to the energy lost by the boiler. This relationship is shown in Constraint (3-16). By substituting the energy of the fuel with that gained by the steam and the losses, Constraint (3-15) can be rewritten as Constraint (3-17).

$$\eta_b = \frac{Q_{steam}}{Q_{fuel}} \tag{3-15}$$

$$Q_{fuel} = Q_{steam} + Q_{loss} \tag{3-16}$$

$$\eta_b = \frac{Q_{steam}}{Q_{steam} + Q_{loss}} \tag{3-17}$$

In the constraints above, η_b is the boiler efficiency, Q_{steam} is the energy gained by the steam, Q_{fuel} is the energy contained in the fuel and Q_{loss} represents heat losses in the boiler. The energy gained by the steam can be broken down into latent and saturated parts as shown in Constraint (3-18).

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$$Q_{steam} = F\left(c_P \Delta T_{sat} + q\right) \qquad (3\text{-}18)$$

In Constraint (3-18) c_P is the specific heat capacity of the boiler feed water and ΔT_{sat} is the difference between the saturated temperature and the temperature of the boiler feed water. This along with the mass of steam raised by the boiler, F, constitutes the sensible portion of the energy gained by the steam up until the saturation point. The latent energy as well as the energy of superheat is represented by q along with the mass of steam raised F (Shang and Kokossis, 2004).

The Q_{loss} term originates in the most part from two areas namely the boiler surface losses and the flue gas losses. A study for British Gas was undertaken by Pattison and Sharma (1980) and from their data they were able to form a correlation relating heat losses to the steam load percentage of the boiler, F/F^U and the amount of energy gained by the steam, Q_{steam}, using two regression parameters, *a* and *b*. Constraint (3-19) shows this relationship.

$$Q_{loss} = Q_{steam}\left(a \frac{1}{F/F^U} + b\right) \qquad (3\text{-}19)$$

Using Constraints (3-18) and (3-19) in the expression for boiler efficiency, Constraint (3-20) can be formulated. Simplifying this constraint gives Constraint (3-21) which accounts for the variation of boiler efficiency with changing load and capacity. Shang and Kokossis (2004) then define the boiler efficiency η_b as the ratio of the heat load of the steam to the heat of fuel which is shown in Constraint (3-22).

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$$\eta_b = \frac{F(c_P \Delta T_{sat} + q)}{F(c_P \Delta T_{sat} + q) + F(c_P \Delta T_{sat} + q)\left(a \frac{1}{F/F^U} + b\right)} \quad (3\text{-}20)$$

$$\eta = \frac{F/F^U}{(1+b)(F/F^U) + a} \quad (3\text{-}21)$$

$$\eta_b = \frac{q(F/F^U)}{(c_P \Delta T_{sat} + q)[(1+b)(F/F^U) + a]} \quad (3\text{-}22)$$

While not a technically correct definition of boiler efficiency, Constraint (3-22) can be used to compare changes in boiler efficiency based on altered steam load F as well as the resultant change to the boiler feed water temperature shown within the term ΔT_{sat}. The ΔT_{sat} value is calculated by subtracting T_{ret} from T_{sat}.

3.4.2. Sensitivity

To examine the sensitivity of the boiler efficiency constraint to changes in return flowrate, F, a plot of boiler efficiency against fractional changes in return flowrate was made. This can be seen in **Figure 3-2**. For this plot the return temperature, represented by ΔT_{sat}, was kept constant. In this figure it can be seen that as return flowrate is decreased the comparative decrease in boiler efficiency is fairly minimal, however reducing the boiler return flowrate by 50% and more sees a more substantial decrease in boiler efficiency.

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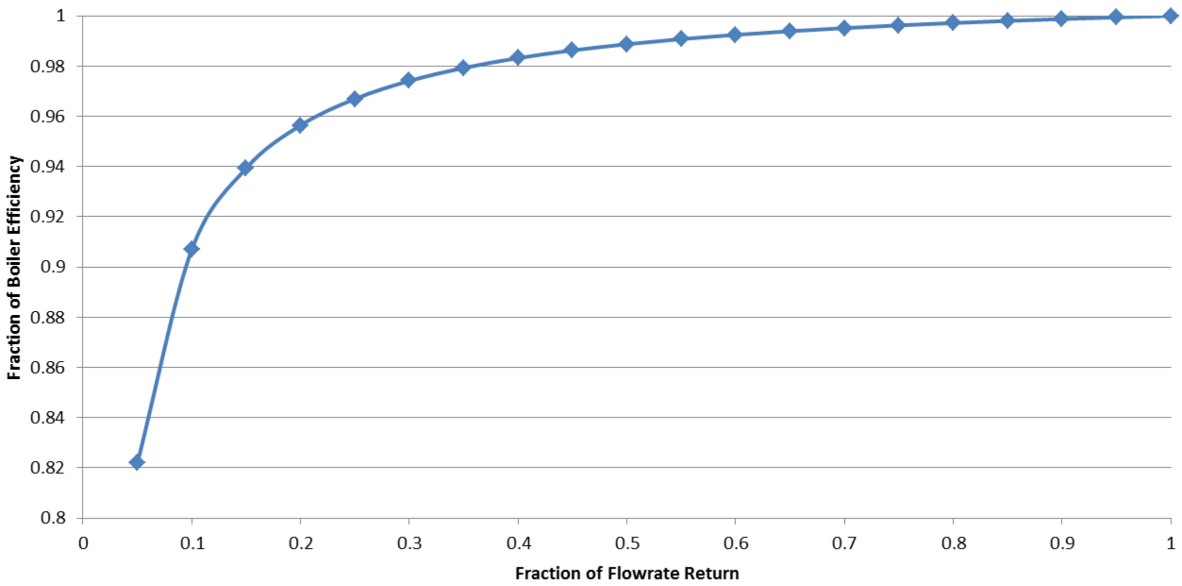

Figure 3-2: Fractional Change in Boiler Efficiency with Changing Return Flowrate

The effect of reducing the steam flowrate in the steam system will reduce F in Constraint (3-22). Minimising the steam flowrate also has the effect of reducing the condensate return temperature to the steam boiler. The sensitivity of the boiler efficiency to a decrease in return temperature is shown in **Figure 3-3**. From the figure it can be seen that the boiler efficiency decreases in a somewhat linear fashion as the return temperature decreases.

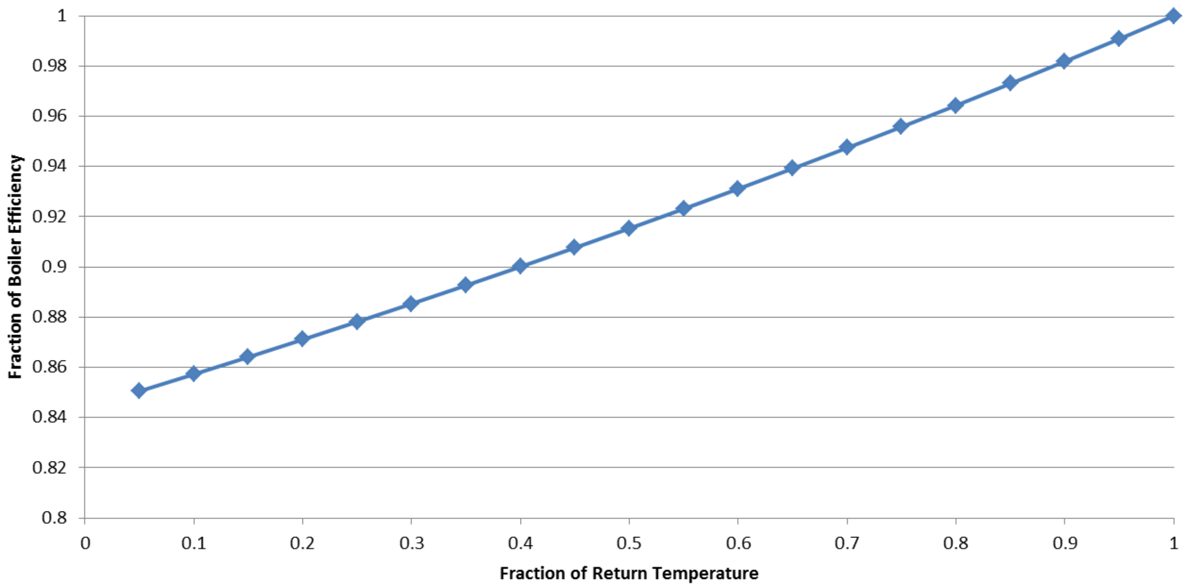

Figure 3-3: Fractional Change in Boiler Efficiency with Changing Return Temperature

The return flowrate and temperature are however related. To examine the relationship between the return flowrate to the boiler, F, and the boiler return temperature, represented by ΔT_{sat}, a plot of these variables at constant boiler efficiency was created and is shown in **Figure 3-4**. The effect of reducing the steam flowrate in the steam system will reduce *F* in Constraint (3-22). Minimising the steam flowrate also has the effect of reducing the condensate return temperature to the steam boiler and the individual effects of these changes are shown in **Figure 3-2** and **Figure 3-3**.

One means of maintaining the efficiency η_b is to increase the temperature of the stream returning to the boiler, which effectively reduces the value of ΔT_{sat}. **Figure 3-4** shows the percentage increase in return temperature necessary to retain the boiler efficiency for a specified decrease in the return mass flowrate. Typical values of the other parameters were used to create **Figure 3-4** and these are shown in **Table 3-1**. Typical temperatures are taken from the work of Harrel (1996) while the enthalpy change from enthalpy from saturated condensate to superheated steam taken from steam tables and the regression parameters from the work of Pattison and Sharma (1980).

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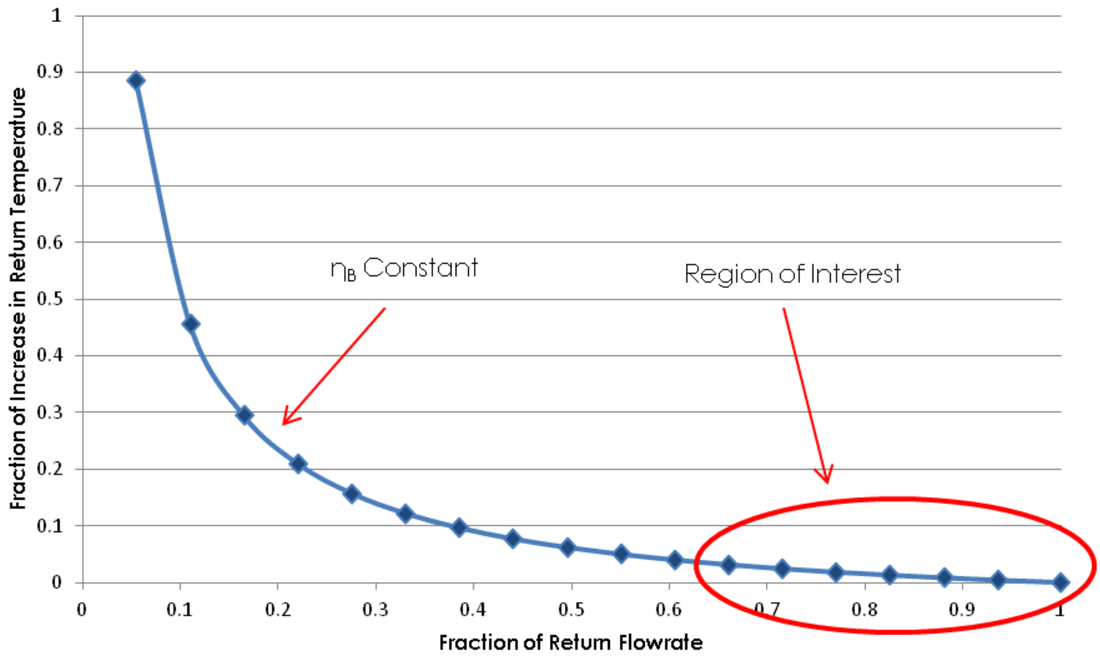

Figure 3-4: Sensitivity of Boiler Efficiency to Changes in Steam Return Flowrate and Return Temperature

Table 3-1: Steam System Data

Parameter	
q (sum of the latent and superheated energy)	2110 (kJ/kg)
F^U (maximum steam load of boiler)	20.19 (kg/s)
c_P (specific heat capacity of boiler feed water)	4.3 (kJ/kg.K)
a (regression parameter)	0.0126
b (regression parameter)	0.2156
T_{sat} (saturated steam temperature at boiler pressure)	253.20 (°C)
T_{boil} (initial return temperature to the boiler for 100% η_b calculation)	116.10 (°C)
F (initial return flowrate for 100% η_b calculation)	18.17 (kg/s)

The region of interest shown in **Figure 3-4** indicates the area where typical pinch based utility optimisation reduction fractions exist. These are typically between 10% and 30%. Within the region of interest it can be seen that for a fairly substantial

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decrease in return flowrate a relatively small increase in the return temperature is required to maintain the efficiency defined by Constraint (3-22).

Maintaining the boiler efficiency during a debottlenecking exercise remains a brownfields application as newer steam systems may be designed with heat integration considered.

3.5. Optimality of Flow Solutions in Network Optimisation Problems

The advent of pinch techniques in the design and optimisation of heat and mass exchange networks gave process designers a systematic tool to reduce utility consumption. Many of the techniques described by Linnhoff and Hindmarsh (1982) are still used as the basis of utility stream design and optimisation.

Heat and mass exchange networks, and the optimisation of these networks share several common features. These include, but are not limited to:

- The requirement for a driving force to transfer so called units of interest (heat or the mass of a particular component);
- The use of a medium to transfer units of interest; and
- The requirement to create products of the flow medium and the unit of interest so as to achieve the objective of interest (heating duty or mass load).

The last point brings with it the difficulty of variable product bilinear terms in optimisation. These terms are nonconvex and present difficulties for MINLP solvers.

In most heat and mass exchange network optimisation formulations the mass balance elements of the transfer medium are simple and are based around a superstructure. The constraints derived from this superstructure are typically linear. The inclusion of heat and mass transfer constraints are typically accompanied by bilinear terms as described above, making the formulation nonlinear. Formulations based around a generic superstructure also typically contain binary variables to denote the existence of streams and units and therefore the resulting heat or mass exchange optimisation problem is presented as an MINLP.

Savelski and Bagajewicz (2000) began investigating the nature of the concentration of streams leaving mass exchange units in wastewater minimisation problems. Initially with single contaminants, the authors derived a proof whereby if the outlet concentration of the stream leaving a mass exchange unit was set to its maximum, the minimum wastewater flowrate could be realised by the system. Also, as the outlet concentration limits are fixed values, their inclusion transformed the nonlinear mass exchange constraints of the formulation to linear constraints. The wastewater minimisation problem could therefore be presented as an MILP. The authors expanded this theorem to include multiple contaminants and presented the proofs and formulation in Savelski and Bagajewicz (2003).

A parallel to this work can be drawn to heat exchange networks and the minimisation of cooling water or steam. Coetzee and Majozi (2008) utilised this technique to minimise the steam flowrate to HENs by the recycle and reuse of hot condensate.

3.5.1. Degenerate Solutions

Savelski and Bagajewicz (2000) identify that multiple solution networks exist when solving wastewater minimisation problems using the condition of maximum outlet concentration. They further describe how optimal mass flowrate solutions can exist where the maximum outlet concentrations are not met. These network solutions are termed degenerate solutions by the authors, who describe manual iterative solution technique to find such solutions. The authors do however point out how the degenerate solutions can be used to optimise a further network variable, such as the number of flow connections, while still achieving the minimum fresh water intake.

The primary drawback to using degenerate solutions to further optimise flow networks is the bilinear terms which need to be solved. These bilinear terms are nonlinear and nonconvex, which, as will be shown in Section 3.6, present severe difficulties to MINLP solvers.

3.6. Branch and Bound MINLP Solvers

A wide variety of MINLP solvers have been developed in the last few decades. Those stemming from the work of Kelley (1960) tend to exhibit a linearisation step which is used to create an MILP master problem in conjunction with non linear sub problems. These solvers include BARON by Sahinidis and Tawamalani (2005), DICOPT by Grossmann et al. (2005) and alphaECP by Westerlund and Pettersson (1995). These solvers utilise an iterative search procedure which fixes binary variables and solves NLP sub problems and thereafter uses the solution to the NLP sub problem to create linearisations of nonlinear constraints to form an MILP master problem. The solvers vary in how the various NLP solutions and their linearised solutions, often referred to as integer cuts, are used. A very generic solution diagram is shown in **Figure 2-1**.

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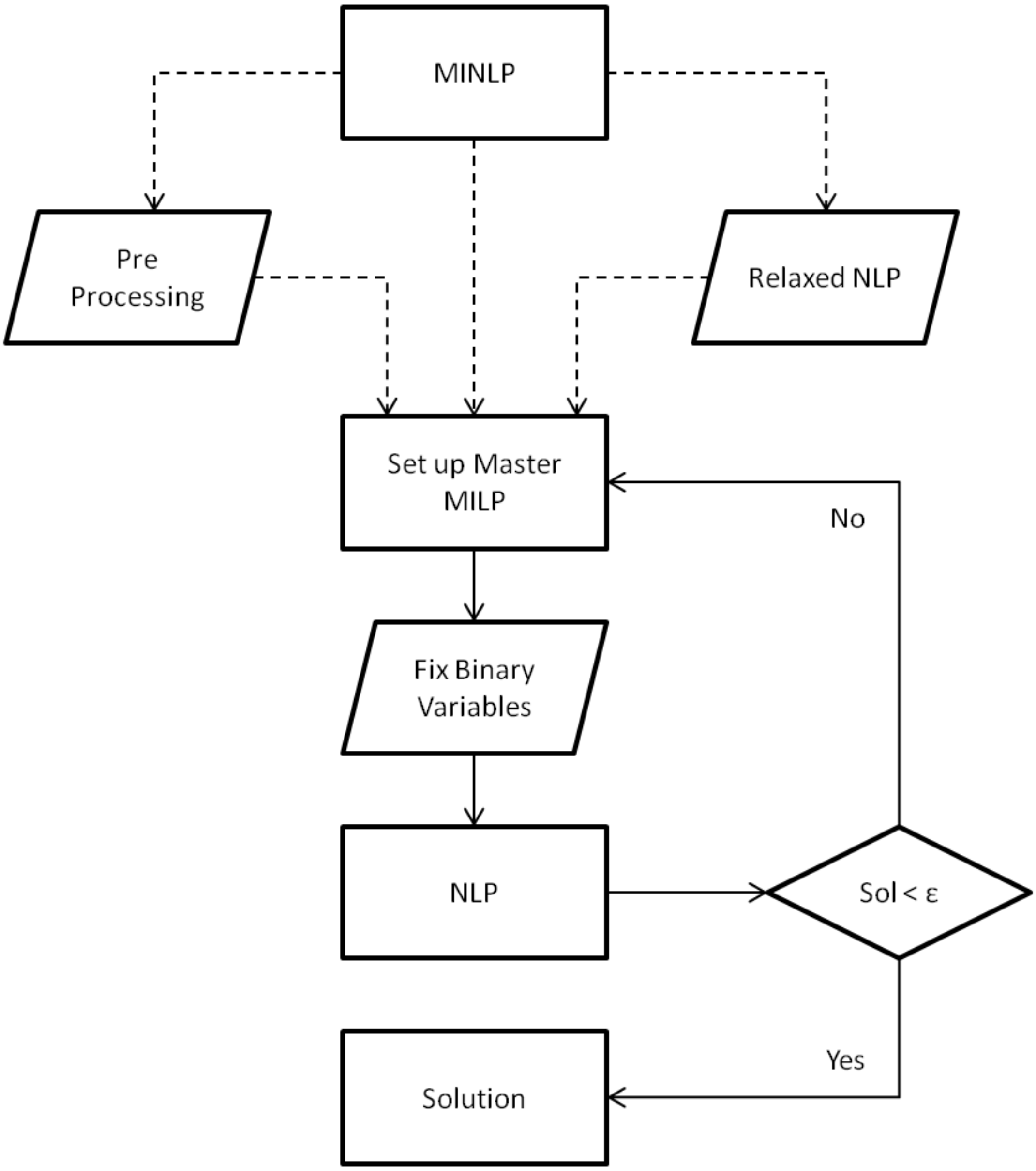

Figure 3-5: Generic flowchart for certain MINLP solvers

As these techniques have been refined, a common element concerning the convexity of the nonlinear elements of the MINLP has become apparent. The linear approximations of the NLP sub problem solutions can effectively approximate the nonlinear constraints and create an outer shell of the solution space. The linearisation of nonconvex constraints at particular points may not encompass the entire solution space presented by such constraints. This is demonstrated in **Figure 3-6**.

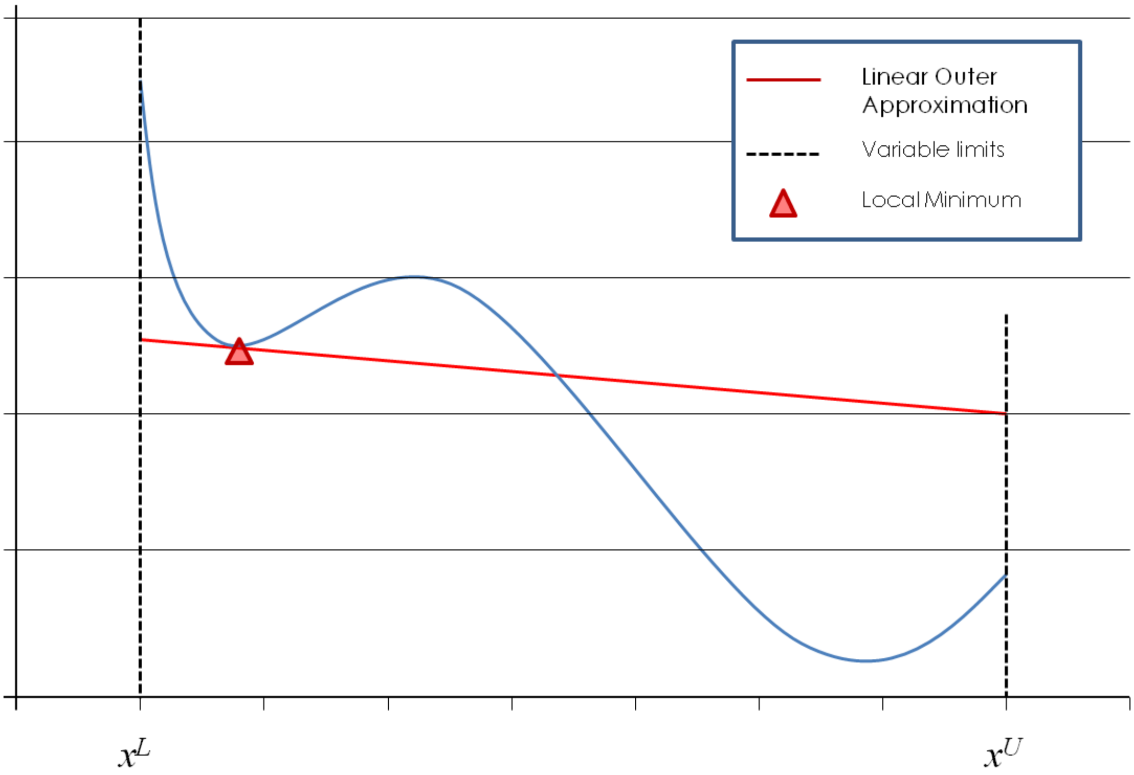

Figure 3-6: Outer approximation at locally optimum solution

The convex hull created by the approximations of convex constraints in minimisation problems serves to create a lower bound of the solution space and this hull is often used as an indicator of the accuracy of the current solution. The global optimality of solutions found by many of the solvers can be proven if the solution space is either convex or quasi-convex, which is convex within the operating bounds of the variables.

The issue of nonconvexity can be approached in a number of ways. The mathematical models of systems can be formulated so as to not contain nonconvex terms. This can be achieved using simplifying assumptions, however this is often not an ideal situation due to the loss of accuracy of the system. New solvers can be created where nonconvexity is overcome, however other issues could arise where the robustness of branch and bound solvers could be required. Another well researched area is the reformulation of the problem utilising techniques to overcome the nonconvexity once the problem has been formulated. This has proven effective at allowing the branch and bound solvers to overcome the problem. Some of these techniques are mentioned below.

3.6.1. Techniques to Overcome Bilinear Terms and Nonconvexity

To utilise the degenerate solutions described in Section 3.5.1 above, a means to deal with bilinear terms will be needed. A well established technique, which has been used to the predecessor of this work by Price and Majozi (2010a), is the relaxation and linearisation technique of Sherali and Alameddine (1992) which was utilised very successfully be Quesada and Grossmann (1995). A large amount of research has also been conducted into the convexification of nonconvex, nonlinear terms in order to find optimal solutions for difficult MINLP problems. This work culminated in a technique described by Pörn, et al. (2008), where transformations are used to alter the nonconvex polynomial terms. Bilinear terms are a special, simpler variety of polynomials. Therefore this technique shows great potential to deal with the bilinear terms formed by the degenerate solutions described by Savelski and Bagajewicz (2000).

Relaxation and Linearisation

Quesada and Grossmann (1995) investigate systems of mixers, splitters and process units where multi-component streams vary in flow and composition. The authors identify the complexity of bilinear terms created by products of wither the flow and concentration variables of the streams or the flow and composition fraction variables of the streams. The authors present an efficient global optimisation methodology termed reformulation and linearisation. This method is based on concave and convex envelopes formed from the bounds of the variables constituting the bilinear term. This method was first described by McCormick (1976) and first proposed for use of reformulation and linearisation by Sherali and Alameddine (1992). The authors utilise this technique to remove the nonlinear, nonconvex bilinear terms and replace them with single variables whose bounds are formulated from the bounds of the individual variables in the bilinear terms. This effectively linearises the composition and flow bilinear terms and helps prevent solutions becoming trapped in sub optimal solutions and convergence failures of NLP problems. The linearised model also creates an effective lower bound for the

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optimisation problem. The authors then develop a branch and bound technique to cater for binary terms often found in process stream optimisation problems. The technique is successfully demonstrated on a number of test problems.

Price and Majozi (2010a) utilised the reformulation and linearisation technique to eliminate bilinear terms in their work to reduce steam consumption in HENs and maintain boiler efficiency. The authors used this technique to create a linearised MILP model where the solution would be the starting point of an exact MINLP model. Global optimality can be proven if the solution to the exact model is equivalent to the solution to the relaxed model.

Transformation and Convexification

Westerlund and co-workers describe conditions of convexity and make large strides to transform various kinds of nonconvex, nonlinear terms into convex terms. The techniques developed focus on a transformation of the nonconvex terms into convex terms. The sign of the nonconvex terms dictate which transformation is utilised. Pörn et al.(1999)first describe the Exponential Transform (ET) or the Inverse Transform (IT) for positively signed terms as well as the Potential Transform (PT) for negatively signed terms.

The convexification principle is based on the fact that positive logarithmic and inverse functions are convex when positive while negative inverse power functions are convex in the positive variable space. A transformation variable is created for each convexification. This transformation variable is consequently also nonlinear and nonconvex, however this variable appears individually in constraints and can more easily be approximated with piecewise approximations. Pörn et al. (1999) discuss different convexification techniques for various classes of nonconvex posynomial functions. The authors present the Exponential Transform (ET) as well as the Potential Transform (PT) which are used to transform positively and negatively signed posynomial terms into convex terms respectively. The transformations take advantage of certain convex functions, exponential and power functions, and transform nonconvex functions such that the convex exponential and power functions may be used in the formulation. Pörn et al, (2008) present a more general transformation strategy for functions with signomial terms. The authors further suggest the use piecewise linear approximations to handle the nonconvex constraints resulting from the transformation of signomial terms. The authors present a systematic solution strategy for the convexification and optimisation of MINLP problems which contain nonconvex signomial terms.

This technique can be used to transform signomial terms into convex terms and if a solution is found it can be proved to be a globally optimal solution. This feature could make this technique favourable as bilinear terms frequently cause locally optimal solutions.

3.6.2. Application in Degenerate Flow Network Problems

If the flowrate minimisation model of Coetzee and Majozi (2008) is examined, a nonlinear, nonconvex constraint is identified as the energy constraint describing the sensible heat transfer from the condensate streams to the process streams. Coetzee and Majozi (2008) utilise the optimality conditions described by Savelski and Bagajewicz (2000) to overcome these nonlinearities and create an MILP formulation which is subsequently solved to optimality.

As the formulation of Coetzee and Majozi (2008) is linear, there are multiple network configurations which exhibit the minimum steam flowrate. These networks can therefore be optimised for another design variable while still achieving the minimum steam flowrate. Price and Majozi (2010c) use this methodology to minimise the network pressure drop for the system while maintaining the minimum steam flowrate. This work will be examined in Chapter 4.

As discussed in Section 3.5.1, if the optimality conditions of Savelski and Bagajewicz (2000) are removed from a network system, the minimum flowrate through the system can still be achieved. Therefore it follows that these degenerate solutions should be examined in an attempt to find better secondary objectives for the networks, such as a better minimum system pressure drop. The formulation of Price and Majozi (2010c) will be further examined for this purpose.

The sensible heat transfer constraint defined by Coetzee and Majozi (2008) and also used by Price and Majozi (2010c) contains three bilinear terms. The difficulty in finding the network which minimises system pressure drop as well as achieves the

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minimum steam flowrate through the system is in solving an MINLP formulation which contains bilinear as well as other nonlinear terms. In accordance with the conditions described by Westerlund et al. (2011) the bilinear terms are not only nonlinear but also nonconvex. The bilinear terms appear in the same constraint which is binding as the energy requirements of the process streams heated by the network need to be met.

In addition the formulation contains nonlinear terms to represent pressure drop as a function of the mass flowrate of steam and condensate. The formulation also contains binary variables which necessitate the use of an MINLP solver.

3.6.3. Solution Process

The solution process will therefore need to focus on handling the bilinear terms as well as being considerate of the workings of the MINLP solvers for complex problems. The relaxation and convexification techniques discussed in Section 3.6.1 show promise for handling the bilinear terms while a number of other techniques are advised by the authors of the MINLP solvers themselves.

Therefore the solution process performed by Price and Majozi (2010a) as well as Price and Majozi (2010c) will be reviewed and where possible improved upon, while a solution algorithm specific to further optimising network problems using degenerate flow solutions will be proposed.

Initially the solution process will focus on steam system heat exchanger network pressure drop, however the steam system boiler efficiency will also be examined.

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4. Model Formulation

This chapter is intended to present all models formulated for this thesis. The models are largely based on the flow minimisation model of Coetzee and Majozi (2008) as well as the steam system network pressure drop model of Price and Majozi (2010c) and the single supply steam pressure boiler efficiency optimisation model of Price and Majozi (2010a). These models will be presented first and then where necessary areas will be expanded upon.

The chapter will first investigate the basic flow minimisation model as well as some techniques used to simplify the formulation. The basic network pressure drop model which includes condensers will be presented next, followed by the alterations needed to solve the flow minimisation model for degenerate solutions as well as techniques used to simplify this formulation. Two solution techniques have been explored to solve the degenerate solution MINLP problem and these will be presented, along with any simplification techniques that are applicable. Lastly this chapter will apply the techniques discussed above to an additional area of HEN optimisation, namely boiler efficiency.

4.1. Flow Minimisation Constraints

This section shows the flow minimisation model as well as solution techniques directly associated with it.

4.1.1. Steam System Heat Exchanger Network Flow Minimisation Constraints

Figure 4-1 shows the superstructure used by Coetzee and Majozi (2008) to represent a system where steam and condensate are used to provide heat to a HEN. Referring to **Figure 4-1**, FS is the total flowrate of saturated steam from the boiler. Each heat exchanger, represented by i or j in the figure, can receive saturated steam or recycled/reused condensate, represented in the figure by SS and FRR respectively. The outlet from each heat exchanger can be saturated or subcooled condensate, depending on the nature of the inlet stream. The same outlet stream can return to the boiler in the form of FR or be recycled or reused to other heat exchangers as FRR. The total return to the boiler is then represented by FB. The indices in the constraints and in the figure show which heat exchanger the variables are associated with. If two indices appear, the first represents the source heat exchanger and the second the sink. In reality, each heat exchanger in the superstructure represents a process stream requiring heating, so these terms are used interchangeably. This fact becomes important when multiple heat exchangers are introduced to heat a single process stream.

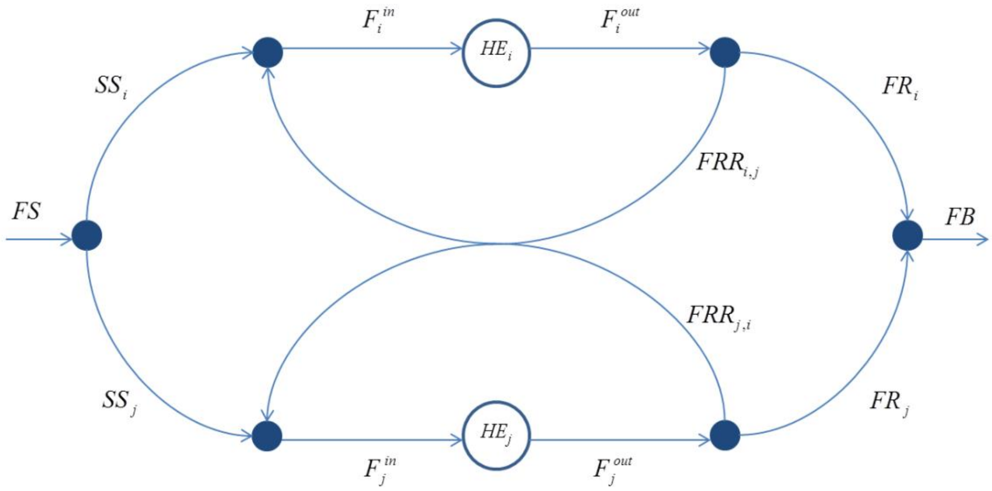

Figure 4-1: Superstructure representing the HEN at single pressure level

The first section of the model encompasses the mass balance constraints. Constraint (4-1) shows how FS is comprised of the sum of SS_i for all the heat exchangers i. Constraint (4-2) is the inlet mass balance for each heat exchanger i, while Constraint (4-3) shows the outlet mass balance. Constraint (4-4) is then the mirror of Constraint (4-1), showing the return stream to the boiler.

$$FS = \sum_{i \in I} SS_i \qquad (4\text{-}1)$$

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$$F_i^{in} = SS_i + \sum_{j \in I} FRR_{j,i} \qquad \forall i \in I \tag{4-2}$$

$$F_i^{out} = FR_i + \sum_{j \in I} FRR_{i,j} \qquad \forall i \in I \tag{4-3}$$

$$FB = \sum_{i \in I} FR_i \tag{4-4}$$

The two remaining mass balances simply state the conservation of mass for a single heat exchanger i, in the case of Constraint (4-5) and for the entire HEN in Constraint (4-6).

$$F_i^{in} = F_i^{out} \qquad \forall i \in I \tag{4-5}$$

$$FS = FB \tag{4-6}$$

The inlet stream for a heat exchanger cannot consist of both steam and condensate since this is impractical in reality. As such the inlet to a heat exchanger is controlled using binary variables. The variable controlling condensate is represented by x_i and the variable controlling steam is represented by y_i. Therefore if a heat exchanger receives saturated steam the binary variable y_i associated with that heat exchanger will take on a value of 1, whereas x_i for that heat exchanger will take on the value of 0.

Implementing these binary variables in the normal mass balance constraints would lead to a situation where the inlet flowrates SS_i and $FRR_{j,i}$ would be multiplied by the binary variables y_i and x_i respectively. This nonlinearity can be linearised by the Glover transformation Glover (1975). There is however a simpler means of employing the binary variables which requires the upper limits of steam and condensate to the heat exchanger. Constraints (4-7) and (4-8) show these limits.

$$SS_i^U = \frac{Q_i}{\lambda} \qquad \forall i \in I \qquad (4\text{-}7)$$

$$FRR_i^U = \frac{Q_i}{c_P\left(T_i^{in,L} - T_i^{out,L}\right)} \qquad \forall i \in I \qquad (4\text{-}8)$$

In Constraint (4-7), Q_i is the duty for heat exchanger i while λ is the latent energy of the saturated steam. In Constraint (4-8), $T_i^{in,L}$ and $T_i^{out,L}$ are the limiting temperature values for the heat exchanger while c_P is the specific heat capacity.

These limits are constant for each heat exchanger and as such the inequalities shown in Constraints (4-9) and (4-10) are linear.

$$SS_i \leq SS_i^U y_i \qquad \forall i \in I \qquad (4\text{-}9)$$

$$\sum_{j \in i} FRR_{j,i} \leq FRR_i^U x_i \qquad \forall i \in I \qquad (4\text{-}10)$$

Constraint (4-11) then ensures that each process stream, represented by the heat exchangers, is only heated by one heat exchanger. This constraint effectively ensures that steam and condensate will not enter the same heat exchanger.

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$$y_i + x_i = 1 \qquad \forall i \in I \qquad (4\text{-}11)$$

A situation may arise where the restriction of only one heat exchanger supplying heat to a process stream leads to a sub-optimal minimum flowrate. Thus an alternative to Constraint (4-11) is given. By allowing a certain number of process streams to be heated by two heat exchangers (implying one heat exchanger supplied with saturated steam, the other with condensate) an improved minimum flowrate may be found. Therefore the variable n is included in the upper limit of the sum for the binary variables, where n is the number of process streams that may be heated by both steam and condensate. The value for n is not known beforehand, but can take a maximum value of the number of heat exchangers and a minimum of zero. Thus it can be found by iteration or included in the model as a variable. Consequently, Constraints (4-12)and (4-13) can be used instead of Constraint (4-11).

$$\sum_{i \in I} y_i + \sum_{i \in I} x_i \geq |i| \qquad (4\text{-}12)$$

$$\sum_{i \in I} y_i + \sum_{i \in I} x_i \leq |i| + n \qquad (4\text{-}13)$$

The energy gained by saturated steam is shown in Constraint (4-14), while energy gained by condensate is shown in Constraint (4-15). The duty for each heat exchanger/process stream must be satisfied and Constraint (4-16) ensures this. The restrictions on the mass flowrates of steam and condensate will propagate through the energy balance constraints and as such there is no need for restrictions in the energy balances. Q_i^S and Q_i^L represent the actual amount of energy gained from steam and condensate in the following constraints respectively.

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$$Q_i^S = SS_i \lambda \qquad \forall i \in I \qquad (4\text{-}14)$$

$$Q_i^L = \sum_{j \in i} \left(c_P SL_{j,i} T^{sat} \right) + \sum_{j \in I} \left(c_P L_{j,i} T_j^{out} \right) - \sum_{j \in I} \left(c_P SL_{j,i} T_i^{out} \right) - \sum_{j \in I} \left(c_P L_{j,i} T_i^{out} \right) \qquad \forall i \in I \qquad (4\text{-}15)$$

$$Q_i = Q_i^S + Q_i^L \qquad \forall i \in I \qquad (4\text{-}16)$$

Several other constraints are required to complete the formulation. As previously mentioned the recycle/reuse variable $FRR_{j,i}$ can be saturated or subcooled condensate, represented by $SL_{j,i}$ and $L_{j,i}$ respectively. Constraint (4-17) is needed for this distinction.

$$FRR_{j,i} = SL_{j,i} + L_{j,i} \qquad \forall i, j \in I \qquad (4\text{-}17)$$

The return streams to the boiler from each heat exchanger i can be saturated or subcooled. Constraint (4-18) allows for this distinction, where FRS_i represents saturated condensate return flow to the boiler and FRL_i subcooled condensate return flow to the boiler.

$$FR_i = FRS_i + FRL_i \qquad \forall i \in I \qquad (4\text{-}18)$$

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The amount of saturated condensate recycled/reused or returned to the boiler is limited by the amount of saturated steam supplied to the heat exchanger which is illustrated in Constraint (4-19). Constraint (4-20) then shows the equivalent for subcooled condensate and subcooled return to the boiler. In this constraint j and j' represent any other heat exchangers.

$$SS_i = \sum_{j \in I} SL_{i,j} + FRS_i \qquad \forall i \in I \qquad (4\text{-}19)$$

$$\sum_{j' \in I} SL_{j',i} + \sum_{j' \in I} L_{j',i} = \sum_{j \in I} L_{i,j} + FRL_i \qquad \forall i \in I \qquad (4\text{-}20)$$

Local recycle of subcooled condensate is not common in industry, but mathematically possible with the current constraints. Constraint (4-21) is included in the formulation to prevent this.

$$L_{i,j} = 0 \qquad \forall i, j \in I, \qquad i = j \qquad (4\text{-}21)$$

A number of limiting constraints can be used to ensure flow and energy variables do not take values when that particular stream is inactive. These are controlled with binary variables as shown in Constraints (4-22) to (4-28).

$$Q_i^S \le Q_i y_i \qquad \forall i \in I \qquad (4\text{-}22)$$

$$Q_i^L \le Q_i x_i \qquad \forall i \in I \qquad (4\text{-}23)$$

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$$SS_i \le SS_i^U y_i \qquad \forall i, j \in I \qquad (4\text{-}24)$$

$$SL_{j,i} \le SL_{j,i}^U x_i \qquad \forall i, j \in I \qquad (4\text{-}25)$$

$$L_{j,i} \le L_{j,i}^U x_i \qquad \forall i, j \in I \qquad (4\text{-}26)$$

$$FRS_i \le FRS_i^U y_i \qquad \forall i \in I \qquad (4\text{-}27)$$

$$FRL_i \le FRL_i^U x_i \qquad \forall i \in I \qquad (4\text{-}28)$$

In Constraints (4-25) to (4-28) $SL_{j,i}^U$ is the upper limit of saturated condensate that can be transferred from heat exchanger j to heat exchanger i. This is also equivalent to the maximum steam flowrate to heat exchanger j, SS_j^U. $L_{j,i}^U$ is the upper limit of subcooled condensate that can flow from heat exchanger j to heat exchanger i. This limit could potentially be very high as all of the condensate in the HEN could theoretically proceed to one heat exchanger. FRS_i^U is the maximum saturated condensate that can be returned to the steam boiler. This is also equivalent to the maximum steam flowrate to heat exchanger i, SS_i^U. FRL_i^U is the maximum subcooled condensate return to the steam boiler. This limit could also potentially be high as all of the steam condensate could proceed back to the steam boiler through a single heat exchanger.

The final section of the MILP is the objective function. The overall steam flowrate to the HEN is to be minimised, which is shown in the objective function (4-29). In this constraint FS and FB can be used interchangeably as they are equal.

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$$MinZ = FS \qquad (4\text{-}29)$$

Constraints (4-1) to (4-28) along with the objective function (4-29) constitute the basic flowrate minimisation model. Constraint (4-15) is nonlinear. Therefore with the existence of binary variables x_i and y_i the formulation exists as an MINLP.

4.1.2. Conditions of Flow Optimality

Savelski and Bagajewicz (2000) proved that setting wastewater outlet concentrations to their limit would lead to minimum wastewater flowrates. Since an analogy can be made between concentration and temperature as driving forces in mass and heat transfer respectively, Constraint (4-15) can be linearised by setting the outlet temperature of each heat exchanger to its limiting value, which is constant. Therefore Constraint (4-30) can replace Constraint (4-15) in the formulation so as to make the flowrate minimisation model an MILP problem.

$$Q_i^L = \sum_{j \in i}\left(c_P SL_{j,i} T^{sat}\right) + \sum_{j \in I}\left(c_P L_{j,i} T_j^{out,L}\right) - \sum_{j \in i}\left(c_P SL_{j,i} T_i^{out,L}\right) - \sum_{j \in i}\left(c_P L_{j,i} T_i^{out,L}\right) \quad \forall i \in I \qquad (4\text{-}30)$$

In Constraint (4-30), $T_j^{out,L}$ and $T_i^{out,L}$ are the lower limit utility outlet temperatures based on the process conditions.

4.2. Pressure Drop Minimisation Constraints

This section demonstrates the constraints required to minimise pressure drop as well as formulation techniques appropriate for this section.

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4.2.1. Steam System Heat Exchanger Network Pressure Minimisation Constraints

Price and Majozi (2010c) minimised the pressure drop in steam system heat exchanger networks. Pressure drop on the utility side in these networks is characterised by a series pressure drop through condensers, condensate heat exchangers and pipework. The pressure drop through these elements was based on the work of Kim and Smith (2003). These derivations have been discussed in Section 3.3.1 however they are expanded below for convenience.

For heat exchangers it was assumed that the steam or condensate passed through the tube side of the heat exchanger such that the pressure drop could be fairly similar to that of pipes. The tube side pressure drop derived by Kim and Smith (2003) is shown in Constraint (4-31).

$$\Delta P_t = N_{t1} V_t^{1.8} + N_{t2} V_t^2 \qquad (4\text{-}31)$$

ΔP_t is the tube side pressure drop, V_t is the tube side volumetric flowrate and the two factors N_{t1} and N_{t2} are shown in Section 3.3.1.

The pressure drop for condensers must also be catered for as they also appear in the networks developed thus far. As discussed in Section 3.3.1 the condenser pressure drop will be approximated by Constraint (4-32).

$$\Delta P_{t,c} = 0.5\left(N_{t1} V_t^{1.8} + N_{t2} V_t^2\right) \qquad (4\text{-}32)$$

In Constraint (4-32), N_{t1} and N_{t2} are equivalent to those for Constraint (4-31).

Kim and Smith (2003) define the piping pressure drop according to Constraint (4-33). This is derived from commonly used pressure drop correlations, as well as a friction factor by Hewit et al. (1994) to approximate the fanning friction factor.

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$$\Delta P_P = N_P^{EX} V_P^{1.8} \qquad (4\text{-}33)$$

This is remarkably similar to the first term of the tube side pressure drop correlation shown before. In Constraint (4-33), N_P^{EX} is a factor to relate fluid properties and the pipe structure and is shown in Constraint (4-34)

$$N_P^{EX} = \frac{1.11557}{\pi^{1.8}} \frac{\rho^{0.8} \mu^{0.2} L}{D_i^{4.8}} \qquad (4\text{-}34)$$

In Constraint (4-34), L is the pipe length and D_i is the pipe inside diameter. Since the diameter is a design choice Kim and Smith (2003) use an economic trade-off of the optimal pipe size suggested by Peters and Timmerhaus (1991) where the optimal pipe diameter is given as a function of volumetric flowrate and fluid density. Using this relation Constraints (4-33) and (4-34) are rewritten as Constraints (4-35) and (4-36) respectively.

$$\Delta P_P = N_P^{NW} \frac{1}{V_P^{0.36}} \qquad (4\text{-}35)$$

$$N_P^{NW} = \frac{188.318}{\pi^{1.8}} \rho^{0.176} \mu^{0.2} L \qquad (4\text{-}36)$$

In Constraint (4-35) it can be seen that pressure drop is now an inverse function to volumetric flowrate which seems counterintuitive. The relation by Peters and Timmerhaus (1991) however ensures that every time a new velocity is chosen the

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optimal pipe diameter is used, giving the inverse relation. Now the pressure drop through the pipes is only a function of the pipe length, the fluid properties and the volumetric flowrate.

Price and Majozi (2010c) then derive the pressure drop correlations for condensate, condensers and pipework as functions of mass flowrate as shown in Constraints (4-37), (4-38) and (4-39) respectively:

$$\Delta P_t = N_{t1}^* \dot{m}_t^{1.8} + N_{t2}^* \dot{m}_t^2 \qquad (4\text{-}37)$$

$$\Delta P_{t,c} = 0.5\left(N_{t1}^* \dot{m}_t^{1.8} + N_{t2}^* \dot{m}_t^2\right) \qquad (4\text{-}38)$$

$$\Delta P_P = N_P^{NW*} \frac{1}{\dot{m}_P^{0.36}} \qquad (4\text{-}39)$$

The factors N_{t1}^*, N_{t2}^* and N_P^{NW*} are shown in Section 3.3.1. These correlations will be used for pressure drop through equipment in this work.

Price and Majozi (2010c) use the pressure drop correlations shown in Constraints (4-37), (4-38) and (4-39) to calculate pressure drop through individual elements in heat exchanger networks. Due to the series nature of the HENs derived in Coetzee and Majozi (2008) and Price and Majozi (2010a) the calculation of pressure drop through the network is not a simple task.

It has been widely established that pressure drop in HENs is not only dependent on stream variables such as flowrate, but also on the network layout. To account for the network layout Kim and Smith (2003) utilise the concept of longest or critical path, depicted in the Critical Path Algorithms (CPA) shown in Gass (1985) which is prevalent in mathematical programming. The total pressure drop of the network is essentially represented by the largest pressure drop of a connection of streams. This critical path should then be minimised to minimise the total pressure drop of the

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system. Kim and Smith (2003) used a node superstructure as a framework to establish the critical path model. The nodes represent mixers that combine streams before heat exchangers as well as splitters that redirect streams after heat exchangers. Each of these nodes has a pressure associated with it. Pressure is then lost between nodes, for example in the heat exchanger between mixers and splitters or in the pipes between the mixers and splitters of different heat exchangers. The mixers are linked to a source node and the splitters to a sink node. The source node represents the maximum pressure of the system, usually the outlet pressure of the utility source, i.e. the cooling tower or steam boiler. The sink node represents the minimum pressure of the system, i.e. the stream returning to the utility source. The objective of the model is then to find the maximum pressure drop through the network and then minimise this pressure drop using mathematical programming.

Price and Majozi (2010c) developed a superstructure that follows that of Kim and Smith (2003) for cooling networks with the exception that condensers are also accounted for. This is shown in **Figure 4-2**.

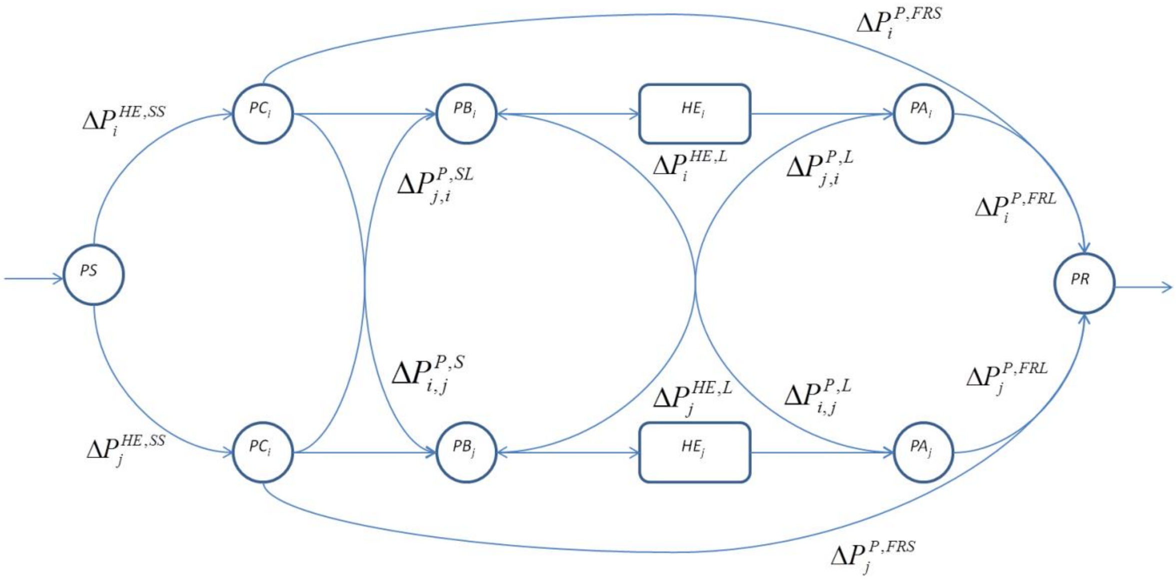

Figure 4-2: Node superstructure that accommodates phase change

In the figure it can be seen that the condensers are connected to the main source node at source pressure PS. Since it is assumed that steam does not lose pressure in pipes, $\Delta P^{HE,SS}$ is only as a result of the pressure drop in the condensers. The distributing or splitting node after the condensers then has pressure PC. This node is then connected to each condensate heat exchangers source node or mixer PB, as well as the final sink node for return to the boiler PR. Since saturated condensate exits the condensers, the pressure drop in the pipes between the PC and PB is a function of the saturated condensate flowrate and the pressure drop is designated $\Delta P^{P,SL}$. It must also be noted that condensate can be reused by the same process stream, and as such the $\Delta P_{i,i}^{P,SL}$ and $\Delta P_{j,j}^{P,SL}$ terms also exist. The direct return to the boiler is accomplished by the saturated return flowrate FRS, thus this pressure drop is designated $\Delta P^{P,FRS}$.

The mixer node for each heat exchanger can also receive condensate from the splitter nodes of other heat exchangers. This occurs in the form of subcooled liquid, designated L, with associated pressure drop $\Delta P^{P,L}$. The two condensate streams then combine and pass through the heat exchanger. The pressure drop for each heat exchanger is therefore a function of the sum of saturated and subcooled condensate entering it. This is shown as $\Delta P^{HE,L}$.

Finally each splitter node has the pressure PA. The return stream to the boiler, FRL, then proceeds to the return mixer with pressure PR. The pressure drop in the pipes of this return stream is thus a function of this flowrate and is subsequently labelled $\Delta P^{P,FRL}$.

The method used by Kim and Smith (2003) based on the CPA to determine the maximum pressure drop for the system is in the form of a difference in pressure between nodes and the pressure drop between the nodes. This is represented in a manner similar to Constraint (4-40) below.

$$PA - PB \geq \Delta P^{A,B} \qquad (4\text{-}40)$$

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In Constraint (4-40) it is understood that fluid flows from node A to node B. The pressure difference between the nodes is essentially a result of the piping pressure loss. Since the mixing nodes before a heat exchanger may receive fluid from multiple sources, this constraint will occur several times with different source splitter nodes and consequently different pressure drop values. The inequality in Constraint (4-40) ensures that the PB assumes the lowest pressure value that satisfies all of the constraints. In this way the node pressure is always at this low value when the model is solved.

This constraint, though simple, is very elegant and effective at finding the critical path, or in this case critical pressure drop for a given network. However, since it will occur in the network design stage a means of eliminating those nodes that do not exist must be made. Kim and Smith (2003) turned to binary variables to achieve this. They established a connection existence binary variable for each connection in the network. This binary variable takes the value of 1 if the connection exists and 0 if it does not. An additional term is then added to Constraint (4-40) to render it redundant for the cases where no connection exists. This is done by adding a large pressure term BP such that it is satisfied for these cases. The large pressure is represented by the term in Constraint (4-41).

$$PA - PB + BP\left(1 - y_{A,B}\right) \geq \Delta P^{A,B} \qquad (4\text{-}41)$$

The binary variables are created using the actual flow variables that are part of the network design model and that are used to calculate the various pressure drops in the model. The only nodes affected by this phenomenon are those that could possibly receive multiple inputs. These are the PB and PR nodes, the mixers before the condensate heat exchangers and the boiler return respectively. Only four flow variables are associated with these and they are the saturated liquid flowrate between heat exchangers $SL_{j,i}$, the subcooled liquid flowrate between streams $L_{j,i}$, the subcooled liquid flowrate to the boiler FRL_i and the saturated liquid return flowrate to the boiler FRS_i. Each of the binary variables requires two constraints as

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well as known upper and lower bounds for the flowrates. Constraints (4-42) and (4-43) are used to demonstrate this for the variable $SL_{j,i}$.

$$SL_{j,i} - SL_{j,i}^{U}\left(y^{SL}\right) \leq 0 \qquad (4\text{-}42)$$

$$SL_{j,i} - SL_{j,i}^{L}\left(y^{SL}\right) \geq 0 \qquad (4\text{-}43)$$

The binary variable will assume the correct value if the appropriate connection is active. In Constraints (4-42) and (4-43), $SL_{j,i}^{U}$ and $SL_{j,i}^{L}$ are the upper and lower limits respectively. Constraints (4-44) to (4-49) represent the longest path constraints that exist according to the superstructure in **Figure 4-2**.

$$PS - PC_i = \Delta P_i^{HE,SS} \qquad \forall i \in I \qquad (4\text{-}44)$$

$$PC_j - PB_i - BP\left(1 - y_{j,i}^{SL}\right) = \Delta P_{j,i}^{P,SL} \qquad \forall i, j \in I \qquad (4\text{-}45)$$

$$PA_j - PB_i - BP\left(1 - y_{j,i}^{L}\right) = \Delta P_{j,i}^{P,L} \qquad \forall i, j \in I \qquad (4\text{-}46)$$

$$PA_i - PR - BP\left(1 - y_i^{FRL}\right) = \Delta P_i^{P,FRL} \qquad \forall i \in I \qquad (4\text{-}47)$$

$$PC_i - PR - BP\left(1 - y_i^{FRS}\right) = \Delta P_i^{P,FRS} \qquad \forall i \in I \qquad (4\text{-}48)$$

$$PB_i - PA_i = \Delta P_i^{HE,L} \qquad \forall i \in I \tag{4-49}$$

The constraints shown above, as well as those showing the various pressure drops are combined to form the pressure drop model. All that remains is to state the objective function. Since the CPA finds the maximum pressure drop through the network, the objective function then simply minimises this pressure drop. The objective function is thus (4-50).

$$MinZ = PS - PR \tag{4-50}$$

A number of heuristic methods can be used to remove some of the constraints. Topological restrictions are common, but a constraint from the original network design model is also relevant for the pressure drop model. Local recycle cannot occur for thermodynamic reasons, but also due to the pressure gradient since the pressure for a given heat exchanger PA_i is less than or equal to PB_i according to Constraint (4-49).

The HEN model represents steam and condensate flowrates in terms of mass flowrate. To integrate the pressure drop constraints it will be appropriate to also represent them in terms of mass flowrate. In this way the HEN model can be used to rearrange the network so as to find the minimum network pressure drop using the pressure drop constraints. By linking the pressure drop correlations shown in Constraints (4-37), (4-38) and (4-39) to the appropriate terms of the RHS of Constraints (4-44) to (4-49) the pressure drop for the network can be minimised by rearranging the network structure and minimising the appropriate mass flowrates. Constraint (4-51) shows the pressure drop through a condenser associated with stream i.

$$\Delta P_i^{HE,SS} = 0.5\left(N_{t1}^{*} SS_i^{1.8} + N_{t2}^{*} SS_i^{2}\right) \qquad \forall i \in I \tag{4-51}$$

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Constraint (4-52) shows the pressure drop through a heat exchanger utilising condensate. This constraint must utilise all of the condensate flowing through a particular heat exchanger. The constants N_{t1}^{*} and N_{t2}^{*} were described above.

$$\Delta P_i^{HE,L} = N_{t1}^{*}\left(\sum_{j\in I} SL_{j,i} + \sum_{j\in I} L_{j,i}\right)^{1.8} + N_{t2}^{*}\left(\sum_{j\in I} SL_{j,i} + \sum_{j\in I} L_{j,i}\right)^{2} \quad \forall i \in I \tag{4-52}$$

The piping pressure drops are for the various piping connections. These include the steam flow from the boiler to condensers, the saturated condensate from the condensers to heat exchangers where no phase change occurs, the saturated condensate from condensers to the boiler, the recycle streams between heat exchangers and the subcooled condensate return flow to the boiler. The piping pressure drop relations for these flowrates will be shown below. The pressure drop for the steam flowing from the boiler to the condensers is considered negligible due to the low density of steam and the density dependence of Constraint (4-37). The pressure drop from saturated condensate flow from heat exchanger j to i is shown in Constraint (4-53). Similarly the pressure drop for subcooled condensate flow from heat exchanger j to i is shown in Constraint (4-54).

$$\Delta P_{j,i}^{P,SL} = N_P^{NW*}\frac{1}{\left(SL_{j,i}\right)^{0.36}} \qquad \forall i \in I \tag{4-53}$$

$$\Delta P_{j,i}^{P,L} = N_P^{NW*}\frac{1}{\left(L_{j,i}\right)^{0.36}} \qquad \forall i \in I \tag{4-54}$$

Constraint (4-55) shows the pressure drop through the pipe connecting the condenser outlet to the boiler return stream, while Constraint (4-56) shows the

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pressure drop through the pipe connecting the condensate heat exchanger outlet and the boiler return stream.

$$\Delta P_i^{P,FRS} = N_P^{NW*} \frac{1}{(FRS_i)^{0.36}} \qquad \forall i \in I \qquad (4\text{-}55)$$

$$\Delta P_i^{P,FRL} = N_P^{NW*} \frac{1}{(FRL_i)^{0.36}} \qquad \forall i \in I \qquad (4\text{-}56)$$

Constraints (4-51) to (4-56) show the various pressure drop correlations for the heat exchanger network. These will be incorporated into the overall network pressure drop scheme discussed below.

4.2.2. Pressure Drop Correlations

The network design portion of the model has already been linearised into an MILP using the maximum outlet conditions specified by Savelski and Bagajewicz (2000). The pressure drop correlations are highly nonlinear however, which creates an MINLP that is difficult to solve. Kim and Smith (2003) examined the individual constraints and determined that the pressure drop for heat exchangers was fairly linear in the design flowrate region. The piping pressure drop was more nonlinear, however they proposed a piecewise linear approximation.

The same approach is used for the steam system. The results from the case study shown previously are used to create the appropriate limits and variables to plot pressure drop against flowrate for the condensers, condensate heat exchangers and pipes. These are shown in the case study.

Price and Majozi (2010c) represented the pressure drop through heat exchangers and condensers as second order quadratic functions of mass flowrate of saturated and subcooled condensate as well as steam respectively. As compared to the correlations shown in Constraints (4-37) and (4-38) the second order quadratic functions show a correlation factor of greater than 0.99. The pipework pressure drop correlation shown in Constraint (4-39) was approximated with a cubic function with a correlation factor of greater than 0.99 in the operating region of the curve. The pressure drop through a heat exchanger i is shown in **Figure 4-3** as an example. The polynomial representing the curve is created using a simple second order approximation. For the example shown the residual is equivalent to 0.9999.

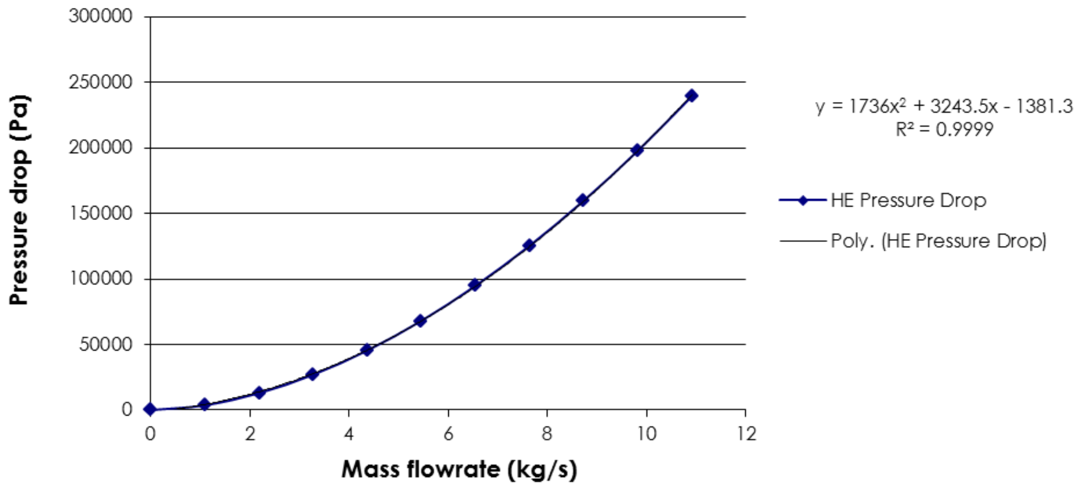

Figure 4-3: Heat exchanger pressure drop simplified to polynomial

The pressure drop through a heat exchanger as a function of the mass flowrate of condensate through the tubes is shown in Constraint (4-57) while through pipework between a condenser and a heat exchanger (represented by the flow $SL_{j,i}$) is shown in Constraint (4-58).

$$\Delta P_i^{HE,L} = k_i^{HE,2}\left(\sum_{j\in I} SL_{j,i} + \sum_{j\in I} L_{j,i}\right)^2 + k_i^{HE,1}\left(\sum_{j\in I} SL_{j,i} + \sum_{j\in I} L_{j,i}\right) + k_i^{HE,0}(x_i) \qquad \forall i \in I \qquad (4\text{-}57)$$

Where $k_i^{HE,2}$ is the first term constant associated with the square function of mass flowrate $\sum_{j\in I} SL_{j,i} + \sum_{j\in I} L_{j,i}$ derived from the pressure drop through the particular HE.

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For the HE in **Figure 4-3** this value is equivalent to 1 736. Similarly $k_i^{HE,1}$ and $k_i^{HE,0}$ are the constants for the second and third terms of Constraint (4-57). The third term is a constant multiplied by the binary variable representing the existence of the condensate heat exchanger i. If the heat exchanger doesn't exist in the optimisation structure the flowrate to the heat exchanger will be zero, eliminating the first two terms of Constraint (4-57) while the binary variable x_i will also take the value of zero, eliminating the third term. The flow through pipework is similarly represented, however with a cubic function as shown in Constraint (4-58).

$$\Delta P_{j,i}^{P,SL} = k_i^{P,3}\left(SL_{j,i}\right)^3 + k_i^{P,2}\left(SL_{j,i}\right)^2 + k_i^{P,1}\left(SL_{j,i}\right) + k_i^{P,0}\left(ySLp_{j,i}\right) \qquad \forall i \in I \qquad (4\text{-}58)$$

If the piping connection between heat exchanger j and i does not exist the mass flowrates will eliminate the first three terms of the RHS while the binary variable $ySLp_{j,i}$ will also take the value zero and eliminate the final term. The constants $k_i^{P,3}$, $k_i^{P,2}$, $k_i^{P,1}$ and $k_i^{P,0}$ are all derived in a similar fashion to those of heat exchangers using a third order polynomial approximation. For all piping systems the residual value was never less than 0.99. In order to simplify further calculations, the third order polynomial approximations for various piping pressure drops utilised by Price and Majozi (2010c) will be approximated instead with second order polynomials. Therefore constraints such as Constraint (4-58) can be simplified to Constraint (4-59).

$$\Delta P_{j,i}^{P,SL} = k_i^{P,2}\left(SL_{j,i}\right)^2 + k_i^{P,1}\left(SL_{j,i}\right) + k_i^{P,0}\left(ySLp_{j,i}\right) \qquad \forall i \in I \qquad (4\text{-}59)$$

The third order regression R^2 value was originally 0.99, while the second order R^2 value was found to be 0.97. Therefore this simplification did not influence the regression of the cubic function significantly and therefore any loss of accuracy was tolerable.

4.3. Basic Steam System Pressure Drop Minimisation Model

This section describes how the flowrate minimisation constraints from Section 4.1 as well as the pressure drop constraints from Section 4.2 are combined to minimise the overall pressure drop of a steam system heat exchanger network.

4.3.1. Combination of Basic Constraints

The nature of the CPA dictates that the overall network pressure drop constraint is made the sole objective function of the formulation. Therefore the minimum flowrate for the network is found first using the flowrate minimisation constraints represented by Constraints (4-1)to (4-29) with Constraint (4-30) replacing Constraint (4-15). The minimum steam flowrate isthen fixed for the entire pressure drop minimisation model. Constraint (4-60) fixes the steam flowrate to the network and is therefore added to the formulation.

$$FS = FS^{set} \quad (4\text{-}60)$$

Where FS^{set} is the fixed mass flowrate found using the flowrate minimisation constraints discussed above. As the heating duty for the process streams needs to be met, the bulk of the flowrate minimisation model must be satisfied for the pressure drop minimisation model. Therefore, excluding the objective function, Constraints (4-1) to (4-21) will appear in the pressure drop minimisation model. Once again Constraint (4-30) can replace Constraint (4-15) to make this section of the model an MILP problem.

The pressure drop minimisation model will consist of the flowrate activation Constraints (4-42) and (4-43) (expanded to include all relevant interconnecting mass flowrates SS_i, $L_{j,i}$, FRS_i and FRL_i), the node pressure drop equality and

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inequality Constraints (4-44) to (4-49) as well as the objective function Constraint (4-50). The pressure drop terms in Constraints (4-44) to (4-49) are then represented using polynomial approximations as shown in Constraints (4-57) and (4-59) for condensate heat exchangers and connections with $SL_{j,i}$ respectively. These must then be applied to condensing heat exchangers as well as connections with $L_{j,i}$, FRS_i and FRL_i. Connections for saturated steam, SS_i are not considered to contribute significantly to the overall system pressure drop as is discussed in Price and Majozi (2010c).

4.3.2. Problem Formulation

The basic network pressure drop minimisation constraints as well as those required to construct the network can be combined to form problem A as shown below.

$$
(A)\quad \begin{cases}
MIN & f^{OBJ}(x) \\
s.t. & f_e(x) = 0 \\
 & f_e(x) + f_e(x,y) \le 0 \\
 & f_e(x) + g_e(x) \le 0 \\
 & f_e(x) + h_e(x) \le 0 \\
 & Mx = m \\
 & x^L \le x \le x^U \\
 & y \in \{0,1\} \\
 & e \in \{1,2,\ldots,E\}
\end{cases}
$$

In Problem A, $f^{OBJ}(x)$ is the objective function, $f_e(x)$ are convex linear constraints which appear in both equality and inequality constraints, while $f_e(x,y)$ are similar with the exception that these contain binary variables. $g_e(x)$ are nonlinear convex constraints while $h_e(x)$ are nonlinear and nonconvex constraints. M is a matrix and m is a column vector of dimensions. The variables x are continuous and have bounds x^L and x^U. Binary variables are denoted by y. The number of constraints is denoted by e up to a maximum of E.

4.3.3. Singularities

All problems in this work are formulated and solved in the optimisation software package GAMS. In GAMS exponentiations such as square or cubic functions are calculated as $\exp[n.\ln(x)]$ where n is the exponent and x is the variable. The natural logarithm of zero is undefined in GAMS and causes errors in NLP solvers.

As the pressure drop minimisation variables are second order polynomial functions these constraints are nonlinear and run the risk of encountering singularities when the flow variables approach zero as these functions are evaluated in GAMS.

Singularities can also occur in the solution of any nonlinear optimisation problems where gradient based solution techniques are used. Singularities are formed whenever variables approach the value of zero. This is due to the fact that any derivative information about the constraints becomes extremely large or small near these areas.

A translation variable can be used to shift the operating area of the variables away from zero. This is possible for the flow variables in all of the formulations in this work as the flow variables are strictly positive. A translation of the flow variables will result in additional variables for the formulation. The translation will be demonstrated using the variable $SL_{j,i}$ in Constraint (4-61). The value of the translation is selected as 1 to demonstrate the technique, however this value can typically take on any positive value. Solver guides should be consulted as larger translation values could require scaling for gradient based nonlinear solvers.

$$SL_{j,i}^{trans} = (SL_{j,i} + 1)^2 \qquad \forall i, j \in I \qquad (4\text{-}61)$$

Where $SL_{j,i}^{trans}$ represents the translation variable to replace the square of the flow variable $SL_{j,i}$. Therefore the exponential variable $SL_{j,i}^2$ can be represented by the RHS of Constraint (4-62).

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$$SL_{j,i}^{2} = SL_{j,i}^{trans} - 2SL_{j,i} - 1 \qquad \forall i, j \in I \qquad (4\text{-}62)$$

These translations can be applied to all flow variables. The RHS of Constraint (4-62) will then replace the term $SL_{j,i}^{2}$ in piping connection pressure drop constraints such as Constraint (4-59).

4.3.4. Pressure Drop Approximation

By utilising Constraint (4-30) in place of Constraint (4-15) in the flowrate minimisation constraints this portion of the formulation can be linearised. In the entire pressure drop minimisation problem the only remaining nonlinear constraints are those representing the pressure drop of the heat exchangers and pipework connections, represented by Constraints (4-57)and (4-59) and further expansions as discussed in Section 4.3.1.

The constraints approximating pressure drop through heat exchangers and pipework have been simplified to second order polynomial functions. These nonlinear constraints can be simplified by a number of techniques as discussed below.

Piecewise Linear Approximation

Price and Majozi (2010c) attempted piecewise linear approximations to entirely represent pressure drop as a function of mass flowrate. This eliminated the nonlinear aspects of the pressure drop model. A more accurate approximation is to represent only the nonlinear elements in the pressure drop function using piecewise linear approximations. As stated above, all pressure drop constraints have been simplified to second order polynomial functions of mass flowrate. Therefore only the first term of these approximations will require a piecewise linear approximation to result in the constraint being linear.

The square terms in the pressure drop approximations are all positive. A square function $f(x) = x^2$ will be convex in the region where x is positive. Therefore the approximation of a square flowrate will always be convex in the area of operation.

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Therefore the piecewise approximation of these functions will lead to an overestimation of the function at all points with the exception of the break points at which the piecewise linear approximation will equal the function.

Using the steam flowrate variable $SL_{j,i}$ as an example, the above implies that the piecewise approximation is always greater than or equal to the actual function as shown in Constraint (4-63).

$$SL_{j,i}^{pl} \geq SL_{j,i}^{2} \qquad \forall i \in I, SS_i \in R^+ \qquad (4\text{-}63)$$

Where $SL_{j,i}^{pl}$ is the piecewise linear approximation of $SL_{j,i}^{2}$.

Since the term $SL_{j,i}^{2}$ appears with a positive sign in the all second order polynomial pressure drop approximations, the use of $SL_{j,i}^{pl}$ as a substitute for $SL_{j,i}^{2}$ will lead to an overestimation of the pressure drop itself. Therefore all solutions using a piecewise approximation of pressure drop will conservatively overestimate the pressure drop of the individual element.

Piecewise approximations can be formulated in a number of ways. The methodology employed in this work will be the same as that of Pörn et al. (2008). This method will be described below. **Figure 4-4** shows an example of the piecewise approximation of a convex function such as a square function x^2. Here binary variables are used to isolate a section of the linear approximation which can represent the function in that particular area and allow the function to be modelled linearly with a small degree of inaccuracy. The break points, represented by p_1 to p_4, represent the points where the piecewise approximations are equal to the function.

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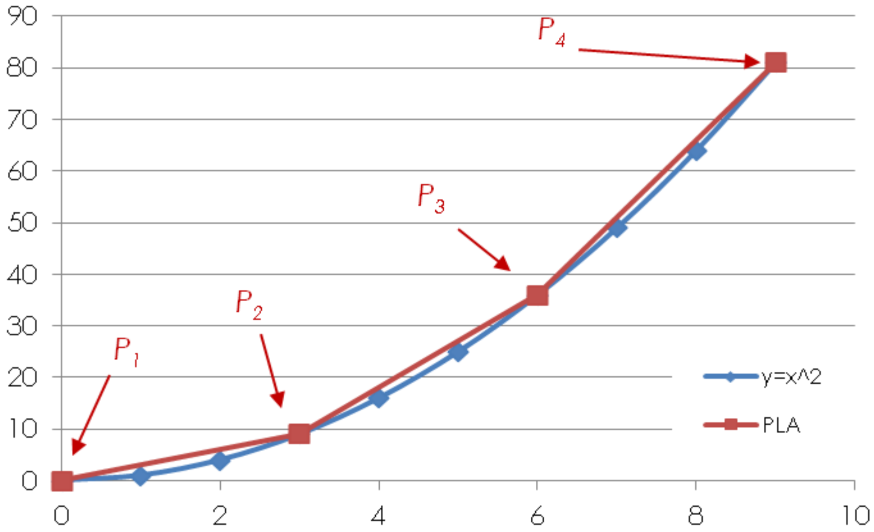

Figure 4-4: Piecewise approximation of a Convex Function

The individual linear sections are combined using binary variables. The piecewise approximation of the line $f(x)$ is represented as $PLA(x)$. if $x \in [p_1, p_n]$ where p_1 and p_n are the minimum and maximum values of x then for some k it can be stated $p_k \leq x \leq p_{k+1}$. Then for some real number $\lambda_k \in [0,1]$, x can be written as $x = \lambda_k p_k + (1-\lambda_k)p_{k+1}$. It follows similarly for the piecewise approximation that $PLA(x) = \lambda_k PLA(p_k) + (1-\lambda_k)PLA(p_{k+1})$. By associating a binary variable β_k for the interval $[p_k, p_{k+1}]$ the piecewise approximation can be represented by Constraints (4-64) to (4-68).

$$PLA(x) = \lambda_1 PLA(p_1) + \lambda_2 PLA(p_2) + \ldots + \lambda_n PLA(p_n) \qquad \forall \lambda \in [0,1] \qquad (4\text{-}64)$$

$$x = \lambda_1 p_i + \lambda_2 p_2 + \ldots + \lambda_n p_n \qquad \forall \lambda \in [0,1] \qquad (4\text{-}65)$$

$$\lambda_1 \leq \beta_1, \lambda_2 \leq \beta_1 + \beta_2, \ldots, \lambda_{n-1} \leq \beta_{n-2} + \beta_{n-1}, \lambda_n \leq \beta_{n-1} \qquad \forall \lambda \in [0,1], \beta \in \{0,1\} \qquad (4\text{-}66)$$

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$$\beta_1 + \beta_2 + ... + \beta_{n-1} = 1 \qquad \forall \beta \in \{0,1\} \qquad (4\text{-}67)$$

$$\lambda_1 + \lambda_2 + ... + \lambda_n = 1 \qquad \forall \lambda \in [0,1] \qquad (4\text{-}68)$$

Constraints (4-64) to (4-68) represent a type of ordered set of type 2, or SOS2. Several MILP solvers can accommodate SOS2 type sets, in which case the piecewise approximation can be made by excluding Constraint (4-67) but ensuring that at most two adjacent λ_k are non-zero.

Relaxation Linearisation

Quesada and Grossmann (1995) used a technique of relaxation and linearisation to reduce bilinear terms to a single variable. This variable is approximated using the limits of the two variables constituting the bilinear term. The resulting convex envelope was first proposed by McCormick (1976). This technique can also be used to approximate a square term. As the pressure drop constraints are represented as second order polynomials an opportunity exists to linearise the square term in the approximation with the over and under estimator technique employed by Quesada and Grossmann (1995). Using this technique a square term can be aproximated by a variable as shown in Constraint (4-69).

$$(SS_i)^2 \Rightarrow w_i \qquad \forall i \in I \qquad (4\text{-}69)$$

In this instance the square of the saturated steam flowrate to a condenser, SS_i, is approximated by w_i.

Relaxation linearisation is discussed in more detail in Section 4.5.

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Pressure Drop Approximation in Formulation

By linearising the nonlinear pressure drop terms in the minimum HEN pressure drop model formulation the constraints $g_e(x)$ from Problem A can be approximated by $g_e^{lin}(x)$ which has been linearised using either the piecewise linear approximation technique or a special instance of the relaxation and linearisation technique. This formulation is presented as problem B.

$$
(B) \quad \begin{cases} MIN & f^{OBJ}(x) \\ s.t. & f_e(x) = 0 \\ & f_e(x) + f_e(x,y) \leq 0 \\ & f_e(x) + g_e^{lin}(x) \leq 0 \\ & f_e(x) + h_e(x) \leq 0 \\ & Mx = m \\ & x^L \leq x \leq x^U \\ & y \in \{0,1\} \\ & e \in \{1,2,\ldots,E\} \end{cases}
$$

4.3.5. Piecewise Approximation with MINLP Solvers

The piecewise linear approximation methodology described above presents an interesting situation. The exact, nonlinear heat transfer terms require the problem be formulated as an MINLP. A large number of MINLP solvers utilise an iterative solution strategy of NLP sub problems along with an MILP master problem. These solvers are discussed in more detail in Section 3.6. The master problem is an outer approximation of the constraints and is considered to be a lower bound if it can be shown that the constraints are convex, or at least pseudo convex within the operating region of the variables. The different sub problems attempt to converge on the master problem solution within a certain degree of accuracy. The NLP sub problems are created by fixing binary variables and solving the subsequent nonlinear constraints. The solution values of the variables are then taken as points where linear approximations of the nonlinear constraints are made. This is done in

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order to establish, and in subsequent iterations, update the MILP master problem. Here new binary variables are found and fixed for the next NLP sub problems. The linear approximations used to establish the MILP master problem also create integer cuts for the master problem, reducing the solution space.

The MILP master problem fixes binary variables based on the solution to this problem. These fixed binary variables also include those established to isolate a portion of the piecewise approximation of a nonlinear function. Therefore when the branch and bound MINLP solver fixes binary variables after every master MILP iteration only a single tangent in the approximation over the entire variable range can be used for the NLP sub problem iteration. **Figure 4-5** demonstrates this phenomenon.

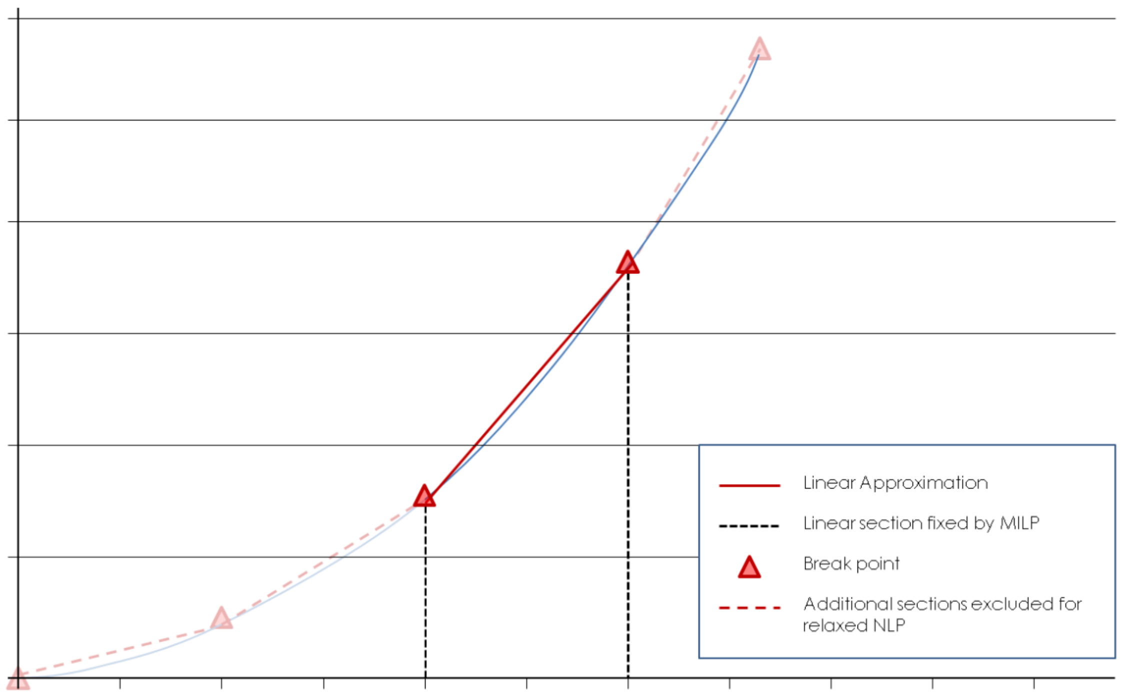

Figure 4-5 Segment of function isolated by MINLP solver for NLP sub problems

In **Figure 4-5** the MILP master problem isolates a single section of the entire piecewise linear approximation of the function, thus restricting the operating region of the optimisation problem.

The piecewise approximations here represent the square terms of the second order polynomial pressure drop approximations as described in Section 4.2.2. As these flowrates are likely to vary anywhere between their bounds, depending on the

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network configuration, the restriction to only a small number of sections of the available solution space for the NLP sub-problems not only greatly reduces the chances of finding an optimal solution, but from finding a feasible solution.

To overcome these phenomena, fewer linear segments can be used to approximate nonlinear functions, therefore giving larger solution spaces for NLP sub problems. The disadvantage of this technique is larger error values between the piecewise approximation function and the exact function. using more linear segments may in turn lead to longer solution times as more potentially MILP problems need to be solved to find a successful combination of variables to satisfy all constraints. Furthermore, solvers such as DICOPT utilise information from the individual NLP sub problems. If these sub problems cannot be solved due to an infeasible solution space provided by the MILP, the NLP sub problem will be infeasible and not provide any feedback information for the solver.

4.4. Degenerate Solutions

Degenerate solutions are discussed in Section 3.5.1. If degenerate solutions are allowed for in the formulation the number of feasible HENs that exhibit the minimum steam flowrate is larger. It is proposed that the additional networks can be examined to find a better minimum HEN pressure drop than when the optimality conditions of Savelski and Bagajewicz (2000) are applied to the system.

To utilise degenerate solutions, Constraint (4-15) is left as a nonlinear constraint. This constraint exhibits three bilinear terms. These terms will require further processing to find a feasible, and potentially improved optimal solution.

4.4.1. Temperature and Flow Limits

The outlet temperatures are not necessarily limited between the saturated liquid temperature and the minimum outlet temperature dictated by the process stream. The sum of the variations of the outlet temperatures with the minimum outlet temperatures can be utilised as a limit, just as a minimum mass flowrate limit can be found for these networks (as shown in Coetzee and Majozi, 2008).

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The sum of deviations of the outlet temperature can be calculated with Constraint (4-70). In the constraint $\Delta T^{out,Lim}$ is the sum of the variations while T_i^{out} is the outlet temperature from heat exchanger i.

$$\Delta T^{out,Lim} = \sum_{i \in I} \left(T_i^{out} - T_i^{out,L} \right) \qquad (4\text{-}70)$$

By calculating the minimum mass flowrate using the technique of Coetzee and Majozi (2008) the minimum mass flowrate of the system can be calculated. By fixing the mass flowrate the maximum deviation of the outlet temperatures can be found. As Constraint (4-15) this maximisation problem will be formulated as an MINLP. Constraint (4-71) can be used to set the minimum mass flowrate for the system while Constraint (4-72) can be used to replace Constraint (4-29) as the objective function. FS^{set} is the minimum mass flowrate calculated using a technique such as that of Coetzee and Majozi (2008).

$$FS \leq FS^{set} \qquad (4\text{-}71)$$

$$MinZ = \Delta T^{out,Lim} \qquad (4\text{-}72)$$

The maximum outlet temperature deviation can be used as a constraint in further formulations as well as being used as a limit for the individual outlet temperatures. These limits can be calculated by adding the maximum deviation to the minimum outlet temperature dictated by the process. This is done by applying Constraint (4-73) to each process stream. If the limit calculated by Constraint (4-73) is higher than the saturation temperature, the saturation temperature will become the upper limit of the outlet temperature.

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$$T_i^{out,U} = \begin{cases} T_i^{out,L} + \Delta T^{out,Lim} & \\ T^{sat} & T^{sat} \leq T_i^{out,L} + \Delta T^{out,Lim} \end{cases} \qquad \forall i \in I \tag{4-73}$$

4.5. Relaxation and Linearisation

Quesada and Grossmann (1995) used a technique of relaxation and reformulation to reduce bilinear terms to a single variable. This variable is approximated using the limits of the two variables constituting the bilinear term. The resulting convex envelope was first proposed by McCormick (1976) and later used successfully by Sherali and Alameddine (1992). This technique will be the first used to overcome the bilinear terms found in Constraint (4-15) while attempting to find a minimum pressure drop from a degenerate flow solution in a heating system. Appendix B describes this linearisation technique in more detail.

The method of using the relaxation and linearisation technique to solve MINLP problems with bilinear terms involves linearising the bilinear terms and solving the resulting model. The solution to this model is then used as a starting point for the exact model. If the relaxation and linearisation technique results in a linear model then the solution to this model can be used as a lower bound for a possible globally optimal solution of the exact model. If the solution to the resulting exact model is equivalent to the relaxed model then it can be concluded that the solution is globally optimal.

The pressure drop minimisation formulation described in Section 4.3 contains bilinear terms in Constraint (4-15). These terms are the products of the saturated and subcooled condensate flowrates between heat exchangers i and j with the outlet temperature of these heat exchangers. Using the liquid flowrate and outlet temperature from heat exchanger j to heat exchanger i as an example, the variable $d_{j,i}$ replaces the bilinear term as shown in Constraint (4-74).

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$$L_{j,i}T_j^{out} \Rightarrow d_{j,i} \quad \forall i, j \in I \tag{4-74}$$

The same procedure is used to create the linearisation variables $e_{j,i}$ and $f_{j,i}$ from the product of $SL_{j,i}$ and $Tout_i$ and the product of $L_{j,i}$ and T_i^{out} respectively.

4.5.1. Sensible Energy Constraint with Relaxation and Linearisation Technique

Constraint (4-15) can be reformulated using the relaxation and linearisation technique as demonstrated in Constraint (4-74). The resulting change can be seen in Constraint (4-75).

$$Q_i^L = \sum_{j \in i}\left(c_p SL_{j,i}T_{sat}\right) + \sum_{j \in I}\left(c_p d_{j,i}\right) - \sum_{j \in I}\left(c_p e_{j,i}\right) - \sum_{j \in I}\left(c_p f_{j,i}\right) \qquad \forall i \in I \tag{4-75}$$

The relaxation and linearisation technique creates a situation where all of the energy transfer constraints are linear. Along with the linearised pressure drop constraints discussed in Section 4.3.4

As the only bilinear terms in the formulation have been simplified, the nonlinear, nonconvex variables, depicted by $h_e(x)$ can be restated as $h_e^{lin}(x)$. Therefore Problem B can be restated as Problem C as follows.

$$(C)\quad\begin{cases} MIN & f^{OBJ}(x) \\ s.t. & f_e(x)=0 \\ & f_e(x)+f_e(x,y)\leq 0 \\ & f_e(x)+g_e^{lin}(x)\leq 0 \\ & f_e(x)+h_e^{lin}(x)\leq 0 \\ & Mx=m \\ & x^L\leq x\leq x^U \\ & y\in\{0,1\} \\ & e\in\{1,2,\ldots,E\} \end{cases}$$

With the pressure drop constraint linearisations discussed in Section 4.3.4 along with relaxation and linearisation alterations shown above, the entire pressure drop minimisation problem can now be solved as an MILP problem and used as a starting point for the exact model, as discussed in the methodology of Quesada and Grossmann (1995).

4.5.2. Initial MILP Problem

By linearising the bilinear terms of Constraint (4-15) the only remaining nonlinear terms are those in the pressure drop approximations. Section 4.3.4 describes a procedure to linearise the pressure drop approximations. Combining the formulation from Section 4.3.4 with Constraint (4-75) allows the pressure drop of the system to be solved for as an MILP problem, shown as Problem C.

This MILP problem is intended to be used as a starting point for an exact model, or at least a model with no relaxation and linearisation constraints. This is represented by Problem B. As such should be as tightly bound as possible. The relaxation and linearisation technique allows the linearisation variables to assume values that are bounded by the limits of the flowrate variables as well as the outlet temperature variables. Therefore these limits should be as tight as possible so as to allow the relaxed MILP formulation to be as accurate as possible.

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Limits for Flow Variables

Limits for the flow variable $SL_{j,i}$ can be found from Constraints (4-7) and (4-19). The maximum amount of saturated condensate available from the outlet of a heat exchanger is equivalent to the maximum steam flowrate that can flow to that heat exchanger. Therefore the upper limit of saturated condensate can be found with Constraint (4-76).

$$SL_j^U = \frac{Q_j}{\lambda} \qquad \forall j \in I \qquad (4\text{-}76)$$

Similarly the sum of all saturated condensate from heat exchanger j can be represented by Constraint (4-77).

$$\sum_{i \in I} SL_{j,i} \le SL_j^U \qquad \forall j, i \in I \qquad (4\text{-}77)$$

Constraint (4-19) shows that saturated condensate leaving a heat exchanger can either be circulated to another heat exchanger or returned to the boiler. Therefore the limits applying to the flow variable $SL_{j,i}$ also apply to the variable FRS_j as shown in Constraint (4-78).

$$FRS_j \le SL_j^U \qquad \forall j \in I \qquad (4\text{-}78)$$

The subcooled condensate flowrates are more flexible as the sum of all condensate in the steam system can be fed to heat a single process stream. Therefore the minimum steam flowrate for the system can be used as a limit for the subcooled

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condensate flowrate as well as the subcooled boiler return flowrate when optimising the system for pressure drop. The minimum steam flowrate is typically set as a constraint for the pressure drop model by using Constraint (4-60). In a similar way the limits for $L_{j,i}$ and FRL_j can be shown in Constraints (4-79)and (4-80).

$$\sum_{i \in j} L_{j,i} \leq FS^{set} \qquad \forall j \in I \qquad (4\text{-}79)$$

$$FRL_j \leq FS^{set} \qquad \forall j \in I \qquad (4\text{-}80)$$

The lower limits for all flow variables are zero.

Limits for Outlet Temperature Variables

Section 4.4 describes how the outlet temperatures in degenerate solutions can be limited. These limits will be applied for the relaxed MILP formulation. The limit for outlet temperatures T_i^{out} are shown in Constraint (4-73) and applied through Constraint (4-81)

$$T_i^{out} \leq T_i^{out,U} \qquad \forall i \in I \qquad (4\text{-}81)$$

The lower limits for all outlet temperatures are set by the process conditions and the allowable $\Delta T^{\min}$ of the heat exchangers.

4.5.3. Exact Problem

The exact problem is solved directly after the relaxed MILP using that solution as a starting point. The exact problem does not include the relaxation and linearisation of

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the bilinear terms of the formulation and must therefore be solved as an MINLP problem.

Two areas of the formulation have been linearised, namely the bilinear heat transfer terms of Constraint (4-15) as well as the square terms of the pressure drop correlations for pipework, condensers and heat exchangers. The primary intention of linearising the bilinear terms is to create a lower bound for optimisation as well as a feasible starting point for the exact formulation which was proved to be difficult to solve.

Problem A can represent an exact problem to be solved in this problem formulation. The exact model only requires thecontraints where bilinear terms have been relaxed and linearised to be returned to bilinear terms. The approximations used to estimate the pressure drop constraints can remain linearised as discussed in Section 4.3.4. Therefore Problem B can also be utilised as an exact problem in this context.

4.5.4. Solution Strategy for Relaxation and Linearisation Formulation

This section describes the steps necessary to solve the heat exchanger pressure drop minimisation problem using the relaxation and linearisation technique to handle bilinear terms.

The first part of the solution strategy to find the minimum network pressure drop for a HEN while maintaining the minimum steam flowrate is to establish the minimum steam flowrate. This can be achieved by applying the technique proposed by Coetzee and Majozi (2010).

With the minimum steam flowrate achieved a starting point minimum pressure drop is found by completely linearising problem A using the techniques discussed in Section 4.3.4 and 4.5.1. This produces the linearised problem C with $g_e^{lin}(x)$ and $h_e^{lin}(x)$ replacing $g_e(x)$ and $h_e(x)$ respectively.

This problem can then be used as a starting point for a problem with exact energy constraints. The exact problem contains bilinear terms and must therefore be solved as an MINLP.

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As problem C is a relaxed representation of the system, the solution of problem C may relax the energy demands shown by the sensible energy constraint. Therefore a potential concern with using the linearised problem C as a starting point for the exact model is that this starting point may not satisfy the energy constraints due to the over and under estimators (McCormick, 1976) applied during the reformulation and linearisation simplification of the sensible energy constraint. Therefore a slack variable for the sensible energy constraint, γ^{SE}, is added to the sensible energy constraint (4-15) such that a feasible starting point can be found. This adjustment is shown as constraint (4-82).

$$Q_i^L = \sum_{j\in i}\left(c_p SL_{j,i} T_{sat}\right) + \sum_{j\in I}\left(c_p L_{j,i} T_j^{out}\right) - \sum_{j\in I}\left(c_p SL_{j,i} T_i^{out}\right) - \sum_{j\in I}\left(c_p L_{j,i} T_i^{out}\right) + \gamma_i^{SE} \qquad \forall i \in I \tag{4-82}$$

In constraint (4-82) γ_i^{SE} represents a slack variable used to allow the problem to solve feasibly with the NLP sub problems of the MINLP solver required for the exact problem. This alters the nonlinear, nonconvex elements of the formulation and are represented as $h_e^{relax}\left(x, \gamma^{SE}\right)$. This slack variable is then minimised as part of the objective function as shown in constraint (4-83)

$$MinZ = P_S - P_R + \sum_i \left(\gamma_i^{SE}\right)\Omega \tag{4-83}$$

Where Ω is a penalty function factor. This is then represented as $f^{OBJ}\left(x, \gamma^{SE}\right)$ in the formulation. The value of Ω can be varied but should not compromise the scaling of the MINLP solver. The solver notes on penalty functions should be consulted for guidance in this area. This problem still utilises the linearised pressure drop approximations and can be formulated as problem D.

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$$(D)\quad\begin{cases} MIN & f^{OBJ}\left(x,\gamma^{SE}\right)\\ s.t. & f_e(x)=0\\ & f_e(x)+f_e(x,y)\le 0\\ & f_e(x)+g_e^{lin}(x)\le 0\\ & f_e(x)+h_e^{relax}\left(x,\gamma^{SE}\right)\le 0\\ & Mx=m\\ & x^L\le x\le x^U\\ & y\in\{0,1\}\\ & e\in\{1,2,\dots,E\}\\ & \gamma^{SE}\in R:\gamma^{SE}\ge 0 \end{cases}$$

A solution to problem D where the slack variable can be reduced to zero represents a viable solution for pressure drop minimisation as the energy demands of the HEN are met. By fixing the variable outlet temperatures T_i^{out} from the solution to problem D and using these fixed temperatures the pressure drop minimisation problem can be solved with exact pressure drop constraints from Section 4.2. For this the nonlinear, nonconvex sensible energy constraint (4-15) is simplified by fixing T_i^{out} which is represented as $T_i^{out,fix}$ in constraint (4-84).

$$Q_i^L=\sum_{j\in i}\left(c_pSL_{j,i}T_{sat}\right)+\sum_{j\in I}\left(c_pL_{j,i}T_j^{out,fixed}\right)-\sum_{j\in I}\left(c_pSL_{j,i}T_i^{out,fix}\right)-\sum_{j\in I}\left(c_pL_{j,i}T_i^{out,fix}\right)\qquad\forall i\in I \tag{4-84}$$

These constraints can be represented by $h_e^{fixed}(x)$ in the formulation. With this addition the exact pressure drop constraints can be utilised to find a minimum pressure drop for a system with the fixed outlet temperatures found by problem D. This is accomplished with problem E.

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$$
(E)\quad \begin{cases}
MIN & f^{OBJ}(x) \\
s.t. & f_e(x) = 0 \\
 & f_e(x) + f_e(x,y) \le 0 \\
 & f_e(x) + g_e(x) \le 0 \\
 & f_e(x) + h_e^{fixed}(x) \le 0 \\
 & Mx = m \\
 & x^L \le x \le x^U \\
 & y \in \{0,1\} \\
 & e \in \{1,2,\ldots,E\}
\end{cases}
$$

The solution procedure is shown in a flow chart in **Figure 4-6**

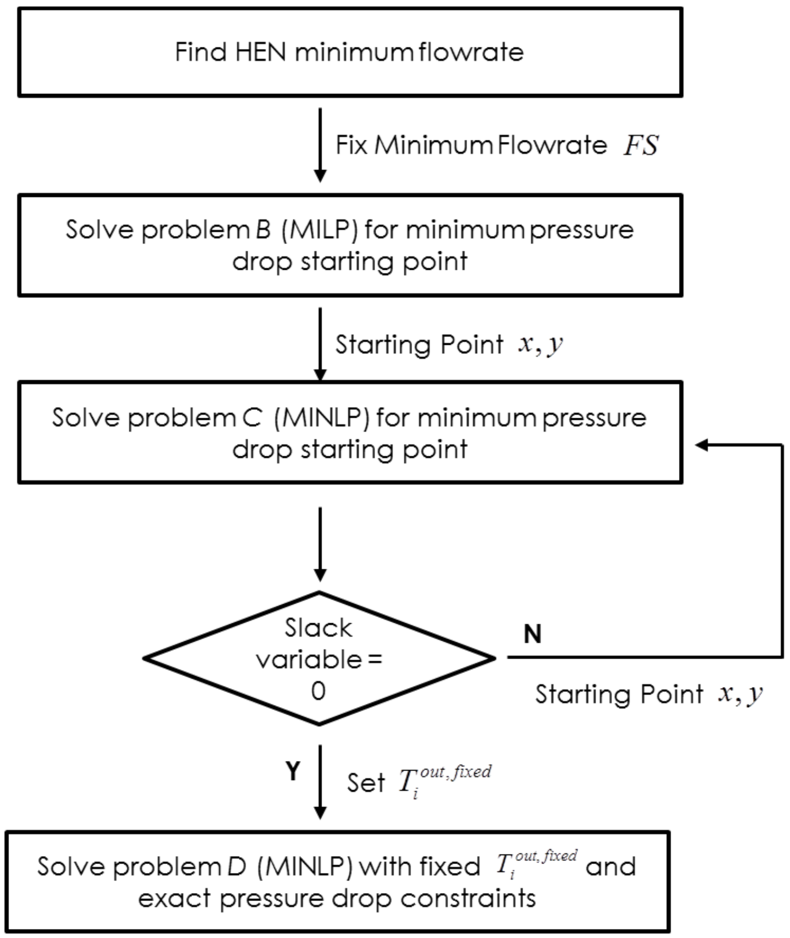

Figure 4-6: Flowchart showing relaxation linearisation solution procedure

4.6. Transformation and Convexification

Bilinear terms are a special kind of signomial function. The nonconvexity of bilinear terms is discussed in Section 3.6.1. Pörn et al. (2008) reformulate and transform signomial terms into convex terms such that they can be solved to optimality using certain MINLP solvers. The authors describe signomial expressions as a sum of terms as shown in Constraint (4-85):

$$a x_1^{r1} x_2^{r2} \ldots x_n^{rn} \qquad a, r_1, \ldots r_n \in R \tag{4-85}$$

The signomial term is nonconvex if the sum of the exponents $r_1,\ldots r_n$ is greater than 1 (Pörn et al. 1999). Pörn et al. (2008) and their preceding authors developed the following techniques to transform signomial terms into convex terms. The techniques are dependent on the sign of a in Constraint (4-85). When the sign of a is positive an Exponential Transform (ET) or an Inverse Transform (IT) is used. These are based on convex functions shown in Constraints (4-86) and

(4-87).

$$a e^{\{r_1 x_1 + r_2 x_2 + \ldots + r_n x_n\}} \text{ is convex on } R_+^n \text{ if } a \ge 0, r_i \in R \tag{4-86}$$

$$a \frac{e^{\{r_1 x_1 + r_2 x_2 + \ldots + r_n x_n\}}}{x_1^{s_1} x_2^{s_2} \ldots x_n^{s_n}} \text{ is convex on } R_+^n \text{ if } a, s_i \ge 0, r_i \in R \tag{4-87}$$

Constraint (4-86) is the basis of the exponential transform while Constraint

(4-87) is the basis of the inverse transform.

When the sign of a is negative a Potential Transform (PT) is used. Constraint (4-88) is the basis for the potential transform.

$$ax_1^{r_1}x_2^{r_2}...x_n^{r_n} \text{ is convex on } R_+^n \text{ if } a \le 0, r_i \ge 0 \text{ and } R = \sum_{i=1}^{n} r_i \le 1 \qquad (4\text{-}88)$$

The bilinear term $\sum_{j \in I}\left(c_p L_{j,i} T_j^{out}\right)$ is positively signed in Constraint (4-15) and will therefore be convexified by either the ET or IT. According to Pörn et al. (2008) the ET generates better lower bounds for the optimisation problem than the IT. Therefore the ET will be used for this term.

The terms $\sum_{j \in I}\left(c_p SL_{j,i} T_i^{out}\right)$ and $\sum_{j \in I}\left(c_p L_{j,i} T_i^{out}\right)$ are negatively signed in Constraint (4-15) and therefore the PT will be used to transform them into convex terms.

4.6.1. Exponential Transform

The exponential transform requires additional variables. $L_{j,i}^{ET}$ will be the transform of the variable $L_{j,i}$, while $T_j^{out,ET}$ will be the transform of T_j^{out}. The relationships between the ET variables and the original variables will be shown below. Since the flowrate variable $L_{j,i}$ could take the value of zero in the formulation it will be offset using a translation as described in Section 4.3.3. As the lower bound of the variable T_i^{out} is not zero, this variable will not need a translation. Constraints (4-89) to (4-92) constitute the ET for the positive bilinear term in Constraint (4-15).

$$L_{j,i}^{ET} = \ln(L_{j,i} + \phi_L^{ET}) \qquad \forall i, j \in I \qquad (4\text{-}89)$$

$$\left(L_{j,i} + \phi_L^{ET}\right) = \exp\left(L_{j,i}^{ET}\right) \qquad \forall i, j \in I \qquad (4\text{-}90)$$

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$$T_j^{out,ET} = \ln\left(T_j^{out}\right) \qquad \forall i \in I \tag{4-91}$$

$$T_j^{out} = \exp\left(T_j^{out,ET}\right) \qquad \forall i \in I \tag{4-92}$$

The translation constant shown in Constraint (4-89) is defined as ϕ_L^{ET} . Therefore the positively signed bilinear term in Constraint (4-15) can be replaced by

$$\sum_{j \in I}\left(c_p L_{j,i} T_j^{out}\right) = \sum_{j \in I}\left(c_P \left(\exp\left(L_{j,i}^{ET}\right) - \phi_L^{ET}\right)\left(\exp\left(T_j^{out,ET}\right)\right)\right) \tag{4-93}$$

Constraints (4-90) and (4-91) remain nonlinear and nonconvex, however these can more easily be approximated using a piecewise linear approximations, as advised by Pörn et al. (2008).

4.6.2. Potential Transform

The potential transform is very similar to the exponential transform in application. The flow variables $SL_{j,i}$ and $L_{j,i}$ will be offset using a translation. The outlet temperature T_i^{out} has a lower bound greater than zero and therefore may not require a translation, however modelling experience showed that it did and a translation variable has been added for T_i^{out}. Due to the nature of piecewise linear approximations that will be required, and discussed later, a translation can be used to ensure that all transformation variables take values that are positive and greater than zero.

The potential transforms require an exponential which is the sum of the exponents of the variables involved in each term. For bilinear terms the sum of the exponents is therefore two. The examples below will show the relationships between the variables $SL_{j,i}$ and T_i^{out} as well as their transforms, which will also be applied to the bilinear term of $L_{j,i}$ and T_i^{out}. Constraints (4-94) to (4-97) show these transformations.

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$$SL_{j,i}^{PT} = \left(SL_{j,i} + \phi_{SL}^{PT}\right)^2 \quad \forall i, j \in I \tag{4-94}$$

$$\left(SL_{j,i} + \phi_{SL}^{PT}\right) = \left(SL_{j,i}^{PT}\right)^{1/2} \quad \forall i, j \in I \tag{4-95}$$

$$T_i^{out,PT} = \left(T_i^{out} + \phi_{T^{out}}^{PT}\right)^2 \quad \forall i \in I \tag{4-96}$$

$$T_i^{out} + \phi_{T^{out}}^{PT} = \left(T_i^{out,PT}\right)^{1/2} \quad \forall i \in I \tag{4-97}$$

Therefore the first negatively signed term in Constraint (4-15)will be replaced by Constraint (4-98). The same transformation will then also be needed for the term $\sum_{j \in I}\left(c_p L_{j,i} T_i^{out}\right)$.

$$\sum_{j \in I}\left(c_p SL_{j,i} T_i^{out}\right) = \sum_{j \in I}\left(c_P\left(\left(SL_{j,i}^{PT}\right)^{1/2} - \phi_{SL}^{PT}\right)\left(\left(T_i^{out,PT}\right)^{1/2} - \phi_{T^{out}}^{PT}\right)\right) \quad \forall i \in I \tag{4-98}$$

4.6.3. Sensible Energy Constraint with Transformation and Convexification

Section 4.6.1 and Section 4.6.2 allow Constraint (4-15) to be rewritten as Constraint (4-99).

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$$Q_i^L = \sum_{j \in i} \left(c_p SL_{j,i} T_{sat} \right) + \sum_{j \in I} \left(c_P \left(\exp\left(L_{j,i}^{ET} \right) - \phi_L^{ET} \right) \left(\exp\left(T_j^{out,ET} \right) \right) \right) \; \forall i \in I \qquad (4\text{-}99)$$
$$- \sum_{j \in I} \left(c_P \left(\left(SL_{j,i}^{PT} \right)^{1/2} - \phi_{SL}^{PT} \right) \left(\left(T_i^{out,PT} \right)^{1/2} - \phi_{T^{out}}^{PT} \right) \right)$$
$$- \sum_{j \in I} \left(c_P \left(\left(L_{j,i}^{PT} \right)^{1/2} - \phi_L^{PT} \right) \left(\left(T_i^{out,PT} \right)^{1/2} - \phi_{T^{out}}^{PT} \right) \right)$$

Constraint (4-99) needs to be accompanied by the various transformation constraints for the ET and PT found in Section 4.6.1 and Section 4.6.2 respectively.

4.6.4. Approximation of Nonlinear ET and PT Terms

Pörn et al. (2008) discuss the nonlinear terms created by using the ET and PT. These terms are approximated by the authors using piecewise linear approximation. A similar analysis of the orientation of the approximation was done for the pressure drop approximations in Section 4.3.4 and this will be done for the ET and PT approximations. As before, all variables that can take a value of zero will be offset by a translation. The piecewise linearisation of the variable $L_{j,i}^{ET}$ in the ET is the natural logarithm of $(L_{j,i} + \phi_L^{ET})$. The natural logarithm is a concave function where $L_{j,i}$ is feasible. Therefore the ET of $L_{j,i}$ can be shown as in Constraint (4-100).

$$L_{j,i}^{ET,PL} <= L_{j,i}^{ET} = \ln\left(L_{j,i} + \phi_L^{ET} \right) \qquad \forall i, j \in I, L_{j,i} \in R^+ \qquad (4\text{-}100)$$

Where $L_{j,i}^{ET,PL}$ is the piecewise linear approximation of the natural logarithm of the flow variable $L_{j,i}$ with a translation of ϕ_L^{ET}. The exponent of the ET of a variable is used in Constraint (4-99) therefore the piecewise linear approximation of the ET will result in an underestimate of the original variable. This is shown in **Figure 4-7**. As this variable represents a positive term in Constraint (4-99), this transform underestimates the value of Q_i^L in Constraint (4-99). As the operating range of T_j^{out}

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is also positive, a similar underestimation will occur. Therefore the ET underestimates the energy gained from sensible heat, Q_i^L.

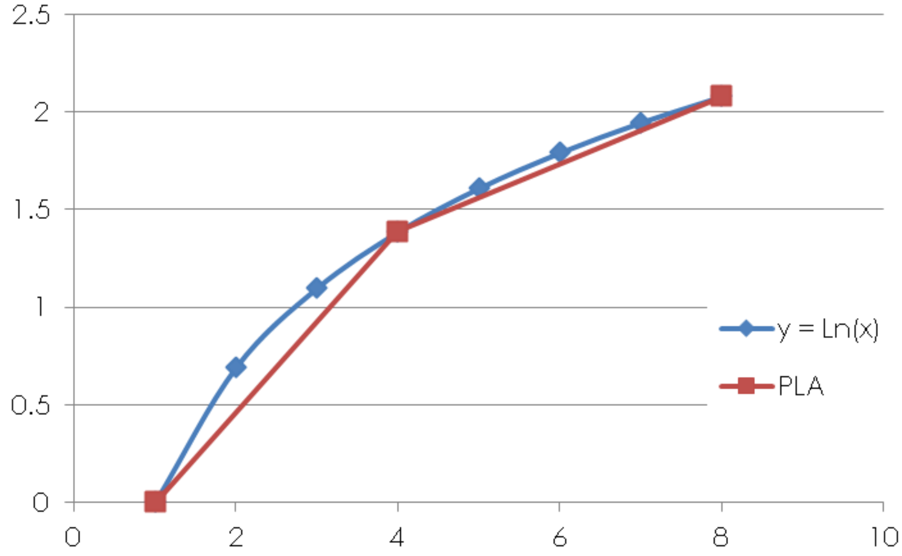

Figure 4-7: Underestimation of piecewise linear approximation of $\ln(x)$ function

The PT can be analysed in a similar way. The piecewise linearisation of the variable $SL_{j,i}^{PT}$ is the square of the flow variable $\left(SL_{j,i} + \phi_{SL}^{PT}\right)$. The square function is convex in the positive operating range of $\left(SL_{j,i} + \phi_{SL}^{PT}\right)$ and therefore the piecewise linear approximation of the PT will overestimate the transform as is shown in Constraint (4-101).

$$SL_{j,i}^{PT,PL} \geq SL_{j,i}^{PT} = \left(SL_{j,i} + \phi_{SL}^{PT}\right)^2 \qquad \forall i, j \in I, SL_{j,i} \in R^+ \qquad (4\text{-}101)$$

Where $SL_{j,i}^{PT,PL}$ is the piecewise linear approximation for the PT variable $SL_{j,i}^{PT}$. As the PT is of a bilinear term, the square root of the PT variable is used in Constraint (4-99). As the piecewise linear approximation of the PT is always larger than or equal to the PT variable, and the variables are always positive, the square root of $SL_{j,i}^{PT,PL}$ will

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always be larger than or equal to the square root of $SL_{j,i}^{PT}$. As the PT variables appear negatively in Constraint (4-99) the effect of the piecewise linear approximation on the PT is to further reduce the value of the energy gained from sensible heat, Q_i^L, in Constraint (4-99).

Some complexities arise when utilising the piecewise approximations of the ETs and PTs along with translations. The translations cause additional terms to be required in the ET and PT approximations of the bilinear terms. For the ET the flow variable $L_{j,i}$ and temperature variable T_j^{out} combine as is shown in Constraint (4-102).

$$\left(L_{j,i}\right)\left(T_j^{out}\right) = \exp\left(L_{j,i}^{ET} + T_j^{out,ET}\right) \qquad \forall i, j \in I, L_{j,i} \in R^+ \qquad (4\text{-}102)$$

Therefore using a translation to shift the operation range of the variable $L_{j,i}$ away from zero, the ET is rewritten as shown in Constraint (4-103). Constraint (4-102) can be rewritten as Constraint (4-104).

$$\left(L_{j,i}\right) = \exp\left(L_{j,i}^{ET}\right) - \phi_L^{ET} \qquad \forall i, j \in I, L_{j,i} \in R^+ \qquad (4\text{-}103)$$

$$\left(L_{j,i}\right)\left(T_j^{out}\right) = \left(\exp\left(L_{j,i}^{ET}\right) - \phi_L^{ET}\right)\exp\left(T_j^{out,ET}\right) \qquad \forall i, j \in I, L_{j,i} \in R^+ \qquad (4\text{-}104)$$

Therefore the piecewise linear transform appears as Constraint (4-105).

$$\left(L_{j,i}\right)\left(T_j^{out}\right) = \left(\exp\left(L_{j,i}^{ET,PL}\right) - \phi_L^{ET}\right)\exp\left(T_j^{out,ET,PL}\right) \qquad \forall i, j \in I, L_{j,i} \in R^+ \qquad (4\text{-}105)$$

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Considering the nature of the linearisation shown in **Figure 4-7** it can be concluded that the piecewise linear approximation of the ET for the bilinear term $(L_{j,i})(T_j^{out})$ always underestimates or is equal to the exact ET as shown in Constraint (4-106).

$$\left(\exp\left(L_{j,i}^{ET,PL}\right)-\phi_L^{ET}\right)\exp\left(T_j^{out,ET,PL}\right)\leq \left(\exp\left(L_{j,i}^{ET}\right)-\phi_L^{ET}\right)\exp\left(T_j^{out,ET}\right) \quad \forall i,j\in I, L_{j,i}\in R^+ \tag{4-106}$$

Similarly, it can be shown that the piecewise linear approximations to the PT formulations overestimate the exact PT variables as shown in Constraints (4-107) and (4-108) respectively.

$$\left(\left(SL_{j,i}^{PT,PL}\right)^{1/2}-\phi_{SL}^{PT}\right)\left(\left(T_i^{out,PT,PL}\right)^{1/2}-\phi_{T^{out}}^{PT}\right)\geq \left(\left(SL_{j,i}^{PT}\right)^{1/2}-\phi_{SL}^{PT}\right)\left(\left(T_i^{out,PT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) \quad \forall i,j\in I, SL_{j,i}\in R^+ \tag{4-107}$$

$$\left(\left(L_{j,i}^{PT,PL}\right)^{1/2}-\phi_{L}^{PT}\right)\left(\left(Tout_i^{PT,PL}\right)^{1/2}-\phi_{T^{out}}^{PT}\right)\geq \left(\left(L_{j,i}^{PT}\right)^{1/2}-\phi_{L}^{PT}\right)\left(\left(Tout_i^{PT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) \quad \forall i,j\in I, L_{j,i}\in R^+ \tag{4-108}$$

Considering that the approximations to the ET underestimate the exact transforms and those of the PT overestimate the transforms, the energy terms derived by the bilinear transforms using piecewise linear approximations underestimate the energy term in Constraint (4-99), unless all break points from the approximations match those of the appropriate variables.

This is of large concern as the energy constraints are binding. Therefore it is likely that infeasibilities will arise in the solving of problems with these formulations unless the energy term is dealt with specifically. The duty required for each process stream

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must be met, therefore the piecewise linear approximations can be changed so as to overestimate the ET and underestimate the PT. This can be done with a tangential linear approximation as shown in **Figure 4-8**. The method of tangential approximation will be described in a Section 4.6.5.

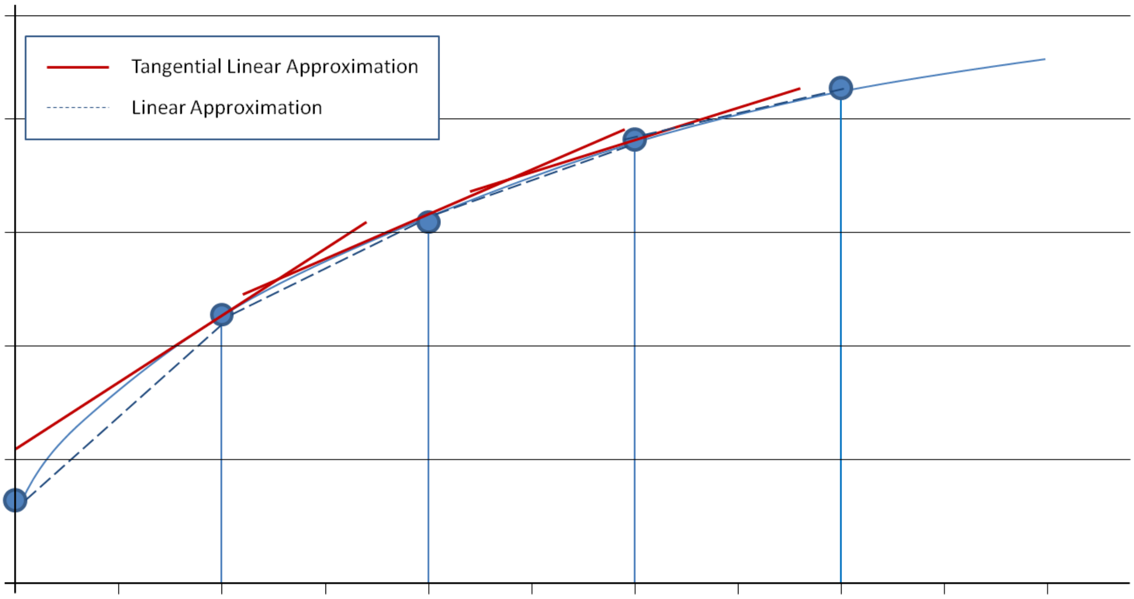

Figure 4-8: Tangential linear approximation

By tangentially approximating the ET variables as is shown in **Figure 4-8**, the energy derived by the bilinear ET function shown in Constraint (4-102) is overestimated. Therefore using the translation, the comparison of the tangential piecewise approximation of the ET to the exact transformation can be written as Constraint (4-109).

$$\left(\exp\left(L_{j,i}^{ET,PLT}\right)-\phi_L^{ET}\right)\exp\left(T_j^{out,ET,PLT}\right)\geq \left(\exp\left(L_{j,i}^{ET}\right)-\phi_L^{ET}\right)\exp\left(T_j^{out,ET}\right) \quad \forall i,j\in I, L_{j,i}\in R^{+} \tag{4-109}$$

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Where $L_{j,i}^{ET,PLT}$ and $T_{j}^{out,ET,PLT}$ are the tangential piecewise linear approximations of the ET variables.

Similarly, by using a tangential piecewise approximation, the PT can be underestimated. Constraints (4-110) and (4-111) ensuring that both PTs which appear negatively in Constraint (4-99) underestimate the exact PTs.

$$\left(\left(SL_{j,i}^{PT,PLT}\right)^{1/2}-\phi_{SL}^{PT}\right)\left(\left(T_{i}^{out,PT,PLT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right)\leq \left(\left(SL_{j,i}^{PT}\right)^{1/2}-\phi_{SL}^{PT}\right)\left(\left(T_{i}^{out,PT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) \quad \forall i,j\in I, SL_{j,i}\in R^{+} \tag{4-110}$$

$$\left(\left(L_{j,i}^{PT,PLT}\right)^{1/2}-\phi_{L}^{PT}\right)\left(\left(T_{i}^{out,PT,PLT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right)\leq \left(\left(L_{j,i}^{PT}\right)^{1/2}-\phi_{L}^{PT}\right)\left(\left(T_{i}^{out,PT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) \quad \forall i,j\in I, L_{j,i}\in R^{+} \tag{4-111}$$

Where $SL_{j,i}^{PT,PLT}$, $T_{i}^{out,PT,PLT}$, $L_{j,i}^{PT,PLT}$ and $T_{i}^{out,PT,PLT}$ are the tangential piecewise linear approximations for the PT variables.

By overestimating the ET variables and underestimating the PT variables, the energy terms in Constraint (4-99) will always be overestimated. The sensible energy constraint can now be rewritten as an inequality shown in Constraint (4-112).

$$QL_{i}\leq \sum_{j\in i}\left(c_{p}SL_{j,i}T_{sat}\right)+\sum_{j\in i}\left(\exp\left(L_{j,i}^{ET,PLT}\right)-\phi_{L}^{ET}\right)\exp\left(T_{j}^{out,ET,PLT}\right) - \sum_{j\in i}\left(\left(SL_{j,i}^{PT,PLT}\right)^{1/2}-\phi_{SL}^{PT}\right)\left(\left(T_{i}^{out,PT,PLT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) - \sum_{j\in i}\left(\left(L_{j,i}^{PT,PLT}\right)^{1/2}-\phi_{L}^{PT}\right)\left(\left(T_{i}^{out,PT,PLT}\right)^{1/2}-\phi_{T^{out}}^{PT}\right) \quad \forall i\in I \tag{4-112}$$

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By using Constraint (4-112) in the network design constraints the energy gained from sensible heat by each process stream will be able to be realised, even for the minimum flowrate which can be found for a heat exchanger network using the techniques of Coetzee and Majozi (2008).

While Constraint (4-112) can ensure that the ET and PTs can transform the sensible heat constraint into a convex term without compromising the other energy balance constraints, a danger exists that the piecewise linear approximations of the transforms, which are related to flow and temperature variables, will allow the these flow and temperature variables to take more favourable values to minimise pressure drop.

By allowing the sensible energy to take on a larger value due to the piecewise linear approximations, it is theoretically possible to acquire a lower minimum flowrate to the system, however this will be a false representation. Therefore when using the ET and PT in the sensible energy constraint, the minimum flowrate will be set as a constraint. This flowrate will be found using either the method of Coetzee and Majozi (2008) or the nonlinear method described in Section 4.1 to give a potential starting point with variable outlet temperatures.

The piecewise linear approximations also more closely match the exact ET and PT variables at the break points in the approximations. Therefore, to increase the accuracy of the optimisation process, an iterative approach is proposed. The break points will be updated in each step of the iterative process, while a penalty function will be used to ensure that the flow and temperature variables tend closer to the break points. The penalty functions will be linked directly to the objective function. Each iteration will see an update of the break points based on the previous flow and temperature variable level values.

4.6.5. Tangential Piecewise Linear Approximation

This section will demonstrate the method used to construct the tangential piecewise linear approximations to the ET and PT variables. The method will be similar to that employed by Pörn et al. (2008) for conventional piecewise approximation, however the break points will be used to find tangential intersection points and these will determine which section of the approximated curve is utilised.

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Tangents and Intersections

The equation representing a tangent is shown in Constraint (4-113) and demonstrated in **Figure 4-9**

$$f^{PL}(x) = f(a) + f'(a)(x - a) \qquad (4\text{-}113)$$

Where $f^{PL}(x)$ is the piecewise linear approximation at the point x, a is the x value at the tangent point, $f(a)$ is the function value at a and $f'(a)$ is the first derivative of the function at a.

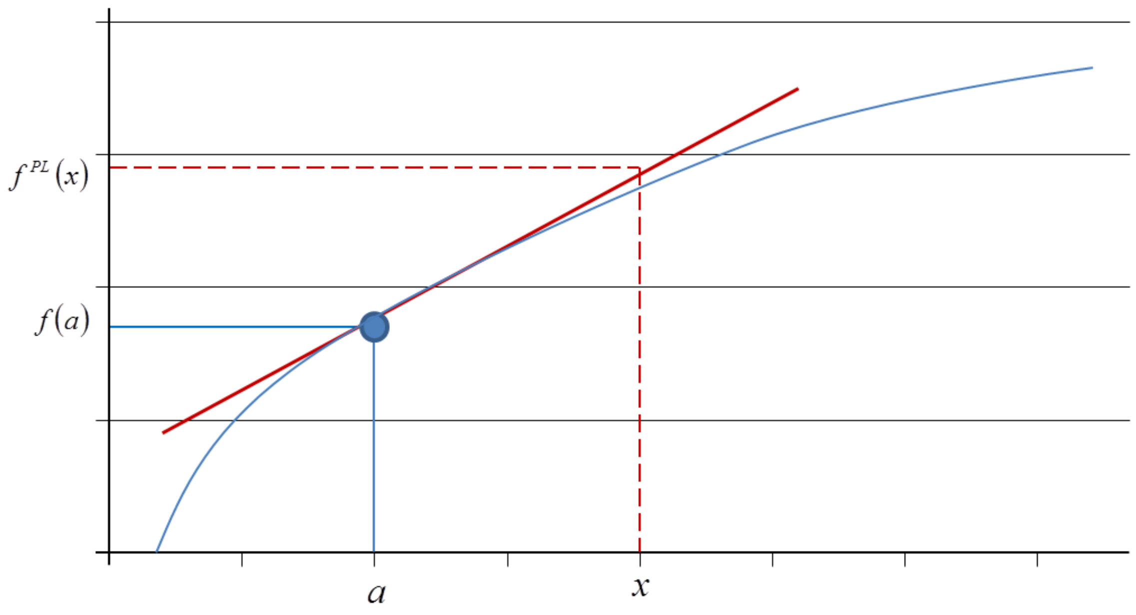

Figure 4-9: Formulae for the tangent to a curve

The intersection points of two tangents can be found simply by making the function values of two tangents equivalent to each other. **Figure 4-10** will be used to explain the process. In **Figure 4-10**, the variable break points are represented by $x_1^{BP}, x_2^{BP}, \ldots, x_{n-1}^{BP}, x_n^{BP}$.

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Therefore there will be n tangents, $n-1$ intersection points and $n+1$ tangent end points (represented by △ in **Figure 4-10**). The variable values of these end points, or intersection points, are shown as $x_1^{\text{int}}, x_2^{\text{int}}, x_3^{\text{int}},..., x_n^{\text{int}}, x_{n+1}^{\text{int}}$. The equivalent approximated function values are therefore denoted as $y_1^{\text{int}}, y_2^{\text{int}}, y_3^{\text{int}},..., y_n^{\text{int}}, y_{n+1}^{\text{int}}$ where the first and last intersection points, y_1^{int} and y_{n+1}^{int} are equivalent to the function values of the first and last intersection points, which are in turn the lower and upper bound of the variable x.

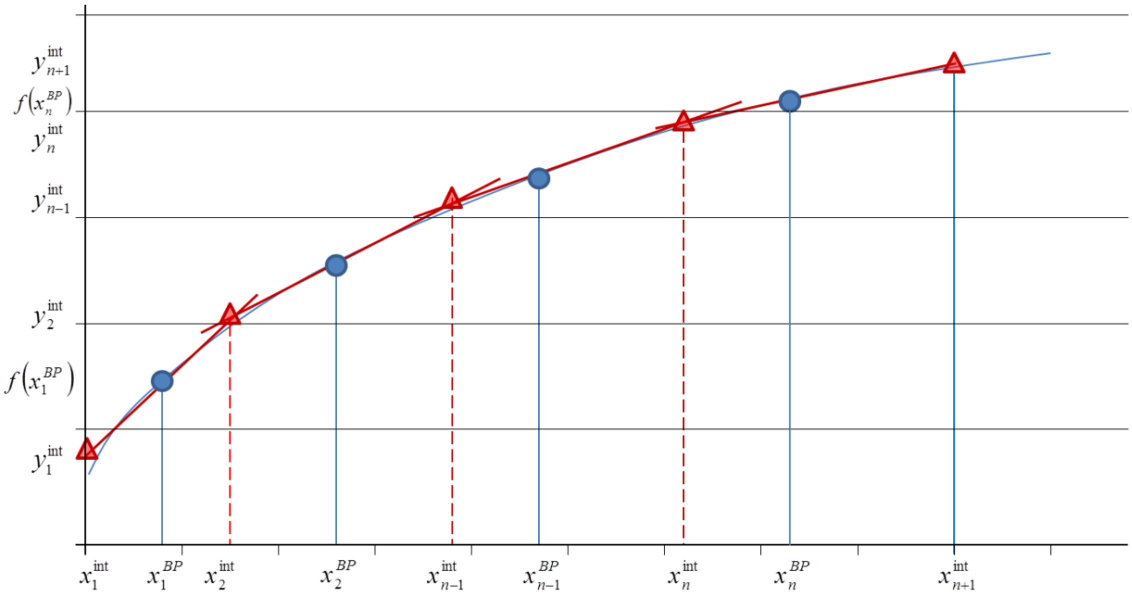

Figure 4-10: Method for Tangential linear approximation

By writing Constraint (4-113) with the variables defined in **Figure 4-10** and setting the function values of two tangents equal to one another, the intersection point of two tangents can be found using Constraint (4-114).

$$f\left(x_m^{BP}\right)+f'\left(x_m^{BP}\right)\left(x_{m+1}^{\text{int}}-x_m^{BP}\right)=f\left(x_{m+1}^{BP}\right)+f'\left(x_{m+1}^{BP}\right)\left(x_{m+1}^{\text{int}}-x_{m+1}^{BP}\right) \qquad (\text{4-114})$$

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Where m is a value from 1 to n in **Figure 4-10**. The intersection point x_{m+1}^{int} can then be solved for as all other values can be calculated from the function and the break points x_m^{BP} and x_{m+1}^{BP}.

Piecewise Approximation Using Multiple Tangents

The same combination of binary variables and fractions used by Pörn et al. (2008) will be described below, however as opposed to using break points of the piecewise linear approximations, the intersection points will be used. This formulation is used widely in literature; however it is not the only formulation and may not necessarily be the most appropriate.

As described in **Figure 4-10** as well as Constraints (4-113) and (4-114) the piecewise linear function will be represented by $f^{PL}(x)$ and break points by intersection points $x_1^{\text{int}}, x_2^{\text{int}}, x_3^{\text{int}}, ..., x_n^{\text{int}}, x_{n+1}^{\text{int}}$. Therefore if $x \in \left[x_1^{\text{int}}, x_{n+1}^{\text{int}}\right]$ then there exists a p where $x_p^{\text{int}} \leq x \leq x_{p+1}^{\text{int}}$. Then for a real number $\lambda \in [0,1]$, x can be represented as $x = \lambda_p x_p^{\text{int}} + (1-\lambda_p) x_{p+1}^{\text{int}}$. Therefore the function can be represented as $f^{PL}(x) = \lambda_p f^{PL}(x_p^{\text{int}}) + (1-\lambda_p) f^{PL}(x_{p+1}^{\text{int}})$. By utilising a binary variable β_p to represent each interval $\left[x_p^{\text{int}}, x_{p+1}^{\text{int}}\right]$, the tangential piecewise linear approximation of the ET and PT variables can be represented by the Constraints (4-115) to (4-119).

$$f^{PL}(x) = \lambda_1 f^{PL}(x_1^{\text{int}}) + \lambda_2 f^{PL}(x_2^{\text{int}}) + ... + \lambda_{k-1} f^{PL}(x_{k-1}^{\text{int}}) + \lambda_k f^{PL}(x_k^{\text{int}}) \quad (4\text{-}115)$$

$$x = \lambda_1 x_1^{\text{int}} + \lambda_2 x_2^{\text{int}} + ... \lambda_{k-1} x_{k-1}^{\text{int}} + \lambda_k x_k^{\text{int}} \quad (4\text{-}116)$$

$$\lambda_1 \leq \beta_1, \lambda_2 \leq \beta_1 + \beta_2, ... \lambda_{k-1} \leq \beta_{k-2} + \beta_{k-1}, \lambda_k \leq \beta_{k-1} \quad (4\text{-}117)$$

$$\beta_1 + \beta_2 + ... + \beta_{k-1} = 1 \qquad \forall \beta_p \quad \in \{0,1\} \tag{4-118}$$

$$\lambda_1 + \lambda_2 + ... + \lambda_{k-1} + \lambda_k = 1 \qquad \forall \lambda_p \in [0,1] \tag{4-119}$$

As was described in Section 4.3.4, if the particular MILP solver used for the optimisation is compatible with SOS2 variables then the binary component of the above formulation, Constraints (4-116) and (4-117), can be omitted as long as ensuring that at most two adjacent λ_p are non-zero.

All that remains is to define the function values $f^{PL}(x)$ for the ET and PT variables. The ET utilises a natural logarithm function, therefore for a break point or tangential point x_m^{BP} the function value can be written from Constraint (4-113) as Constraint (4-120).

$$f^{PL}(x) = \ln(a) + \frac{(x-a)}{a} \tag{4-120}$$

The PT utilises a square function, therefore for a break point or tangential point x_m^{BP} the function value can be written as Constraint (4-121).

$$f^{PL}(x) = (a)^2 + 2(a)(x-a) \tag{4-121}$$

In the interval formulation represented by Constraints (4-115) to (4-119), the interval function values are calculated using either Constraint (4-120) or Constraint (4-121) for the ET and PT variables respectively at the interval points x_m^{int} .

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These interval points can be calculated before using Constraint (4-114) and the pre-defined break points $x_1^{BP}, x_2^{BP}, ..., x_{n-1}^{BP}, x_n^{BP}$.

4.6.6. Tangential Piecewise Linear Approximation using Branch and Bound MINLP Algorithms

Section 4.3.5 describes the complexity of using piecewise linear approximation with branch and bound type MINLP solvers. This section shows this process for tangential piecewise linear approximation.

When the branch and bound MINLP solver fixes binary variables after every master MILP iteration, only a small portion of the available break points (as described in Section 4.6.5) are made available to the NLP solver. This can be seen in Constraint (4-116) where only two of the λ values will be available to solve the constraint. For the interval x_n^{int} to x_{n+1}^{int} there exists a single binary variable (either calculated as a dedicated variable as in Constraint (4-117) or calculated by the solver in the SOS2 process) which activates the fractions λ_n and λ_{n+1}. If the values of λ are limited to $\in [0,1]$ then if a value of x were to fall outside of the interval of x_n^{int} to x_{n+1}^{int} no combination of λ_n and λ_{n+1} would be able to satisfy Constraint (4-116). This is further illustrated in **Figure 4-11**. In the figure the binary variable β_n activates the fractions λ_n and λ_{n+1} allowing these to be solved for the interval between x_n^{int} to x_{n+1}^{int}, essentially limiting the solution space to this interval.

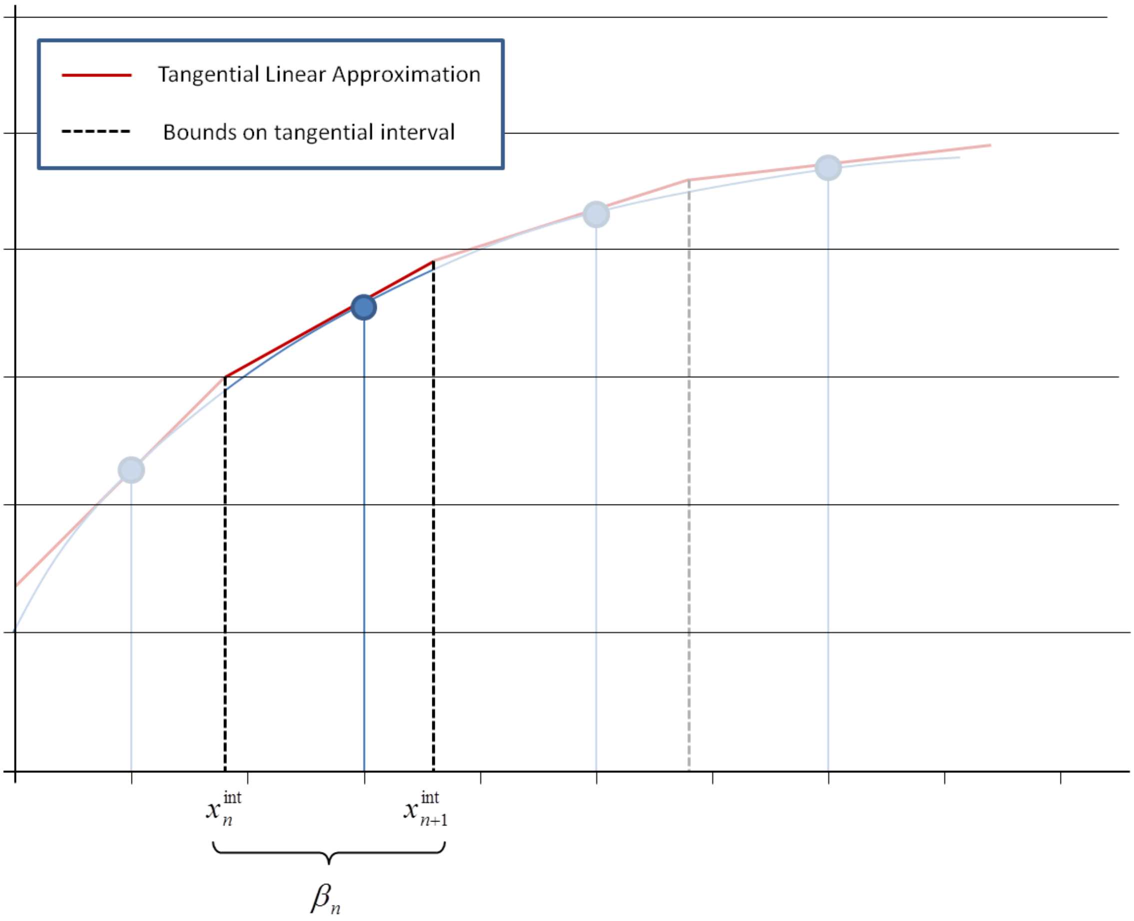

Figure 4-11: Single tangent and bounds as a result of branch and bound MINLP

The tangential bounds shown in **Figure 4-11** are calculated as the intercepts of neighbouring tangents. Ordinarily the NLP sub problems must find solutions in a space smaller than the MILP master problem, however over the entire range of the allowed variables. When piecewise linear approximation is used with branch and bound MINLP solvers, the NLP sub problems are required to find solutions in a much reduced solution space. As a result many of the NLP sub problems result in infeasible solutions due to various constraints not being able to be adhered to by the combination of variables allowed by the tangential segments provided by the MILP master problem. This is particularly evident in formulations which contain a large number of equality constraints which must be satisfied.

A potential solution discussed in Section 4.3.5 is to utilise larger and therefore fewer tangents. With fewer tangents the MINLP master problem only has a limited number of tangents to utilise and therefore the solution space or the following NLP sub problems will be larger. The consequence of using larger tangents is that the error created by approximating the variables using piecewise approximations is larger. An iterative approach can be used to update the tangential points, creating a more accurate approximation for the following iteration. Furthermore penalty functions can be utilised to force the solution points as close to any tangential point as possible so as to further minimise the error and ensure the error does not cause infeasibilities in future iterations.

This approach is demonstrated in **Figure 4-12**. In the figure two tangents are used to approximate the function of x. This figure represents the i^{th} iteration where this first tangent point is the solution of the previous iteration. Three interval limits are shown, x_1^{int} which is equivalent to the lower bound of the variable x, x_2^{int} which is the intercept of the two tangents and x_3^{int} which is equivalent to the upper limit of x. The second tangent can then be assigned a value based on any number of methodologies such as minimisation of the error between the tangent and the function value, half the distance between the previous solution and one of the limits, etc. This tangential arrangement is then used for the i^{th} iteration and the solution of this can be used for the following iteration.

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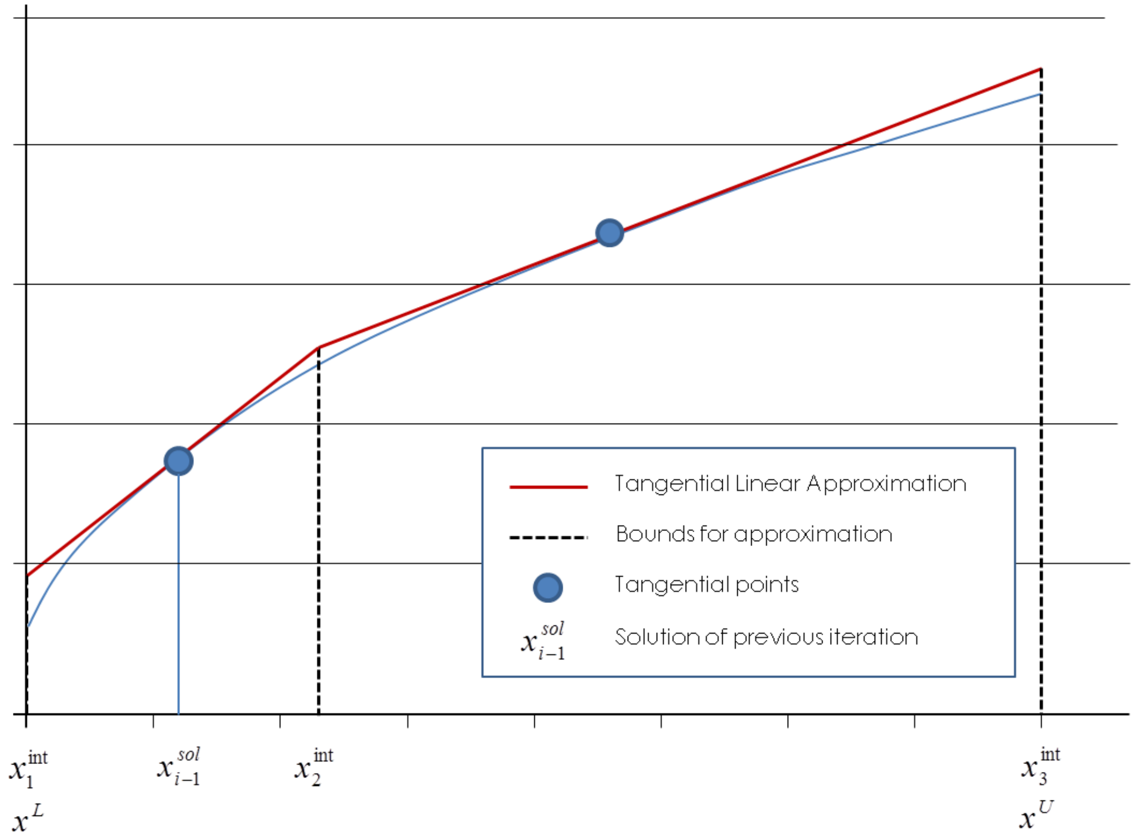

Figure 4-12: Example of approximation with two tangents

The objective of this technique is to allow the NLP sub problems to have a larger solution area so as to find possible solutions. As stated, a penalty function can be utilised to force the solutions close to one of the tangent points, thus minimising the error and creating a convergence around certain tangent points.

Penalty Functions for Transformations

Penalty functions will be used to ensure that the saturated and subcooled condensate flows as well as the outlet temperature variables remain close to the tangential points during optimisation. The objective of this is to discourage the model to deviate significantly from the exact bilinear terms created by the product of the flow and temperature variables. As the linear approximations overestimate the variables the model may favour solutions that are infeasible when reverted back to the exact bilinear terms.

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The method proposed to implement the penalty functions will be similar to that discussed in Section 4.5.4, however the variables affected will be the saturated and subcooled flow variables $SL_{j,i}$ and $L_{j,i}$ as well as the outlet temperature variables T_i^{out}. As multiple tangent points represent areas where the error between the piecewise approximation and the function value are zero, solution values near to any of these points are favourable. If the error was to be calculated between the variable, say $SL_{j,i}$, and a single tangent point then the error is simply the absolute value of the difference between the values. However with multiple tangents the nearest tangent will have to be selected to calculate the error. This can be achieved with binary variables, however the same complexity with MILP master problems isolating binary variables is likely to arise. Therefore it is proposed to instead apply penalty functions to the additional energy created from the product of the transformation variables in the sensible energy constraint, shown in Constraint (4-112).

A slack variable can be added to the constraint to represent the additional sensible energy created from the product of the transformation variables. This constraint is then reformulated as an equality constraint and shown as Constraint (4-122).

$$\begin{aligned} QL_i = {} & SL_{j,i}Tsat + \left(\exp\left(L_{j,i}^{ET,PLT}\right) - \phi_L^{ET}\right)\exp\left(T_j^{out,ET,PLT}\right) \\ & -\left(\left(SL_{j,i}^{PT,PLT}\right)^{1/2} - \phi_{SL}^{PT}\right)\left(\left(T_i^{out,PT,PLT}\right)^{1/2} - \phi_{T^{out}}^{PT}\right) \\ & -\left(\left(L_{j,i}^{PT,PLT}\right)^{1/2} - \phi_L^{PT}\right)\left(\left(T_i^{out,PT,PLT}\right)^{1/2} - \phi_{T^{out}}^{PT}\right) \\ & -\gamma_i^{SE} \qquad \forall i,j \in I \end{aligned} \tag{4-122}$$

In Constraint (4-122) γ_i^{SE} is the slack variable used to represent the excess energy created by the product of the transformation variables. This variable is then assigned a penalty function and added to the objective function as shown in Constraint (4-123).

$$MinZ = P_S - P_R + \left(\sum_i \gamma_i^{SE}\right)\Omega \tag{4-123}$$

Where Ω is some penalty function constant. The values of the penalty function coefficients will typically be lower than those used for the Relaxation and Linearisation formulation as the product of two variables is far greater than that of the individual variables. Also the intention is to typically allow the variables to deviate from the tangential points slightly if the resulting pressure drop is justified.

Selecting Penalty Coefficients

Several heuristics can be used to aid the selection of the penalty coefficients. The slack variables added to Constraint (4-122) allow the energy overestimation as a result of the linear approximation of the transformation variables to be added to the objective function and minimised. Essentially these terms in the objective function will force solution values closer to tangential points, where the linear approximations and the exact functions are equal. The selection of the coefficients is slightly complicated by the fact the energy approximation constraints are not directly related to pressure drop. Therefore a balance of duty feasibility and pressure drop should be found.

4.6.7. Pressure Drop Constraints in the Transformation and Convexification Formulation

As in the Relaxation and Linearisation formulation the pressure drop constraints can be represented exactly as in Problem A or as an approximation as in Problem B. The approximated pressure drop constraints from Problem B will create the simplest linear constraints. If the pressure drop constraints are linearised using piecewise approximation the same complexity as described in Section 4.3.5 will be encountered. An alternative is to use a single linearisation, which prevents the need for binary variables. This approach is however not as accurate as piecewise approximations. Due to the simplicity of the linear approximation for the nonlinear terms in the pressure drop correlations, these will be used initially to solve the model and where necessary these can be made into more accurate piecewise approximations or exact, nonlinear correlations.

4.6.8. Additional Model Considerations

This section describes further considerations for solving the pressure minimisation model which include stopping criteria for the model, the initial tangential points and how these are updated between iterations as well as limits for the transforms.

Stopping Criteria

As linear approximations are made for the energy constraints, it is proposed to test each solution against the linearised pressure drop model of Price and Majozi (2010c). Any additional energy gained by the Convexification and Transformation solution will be assigned to the model of Price and Majozi (2010c) and the resulting minimum pressure drop solutions will be compared.

It is further proposed that with superior processing power, very precise linear approximations can be made. This will enable insignificant additional energy to be made available to the model of Price and Majozi (2010c) and any resulting solutions could be compared to the reworked results of those authors, as described in Section 4.3.

Initial Tangential Point

The points where tangents are made to the natural logarithms of the ET and the square functions of the PT will typically be the solution values of the previous iteration. The first iteration will require starting tangent points.

One option is to use a solution of a simpler problem such as a flowrate minimisation problem or even utilise the linearised MILP from Section 4.5.2. These solutions can be used to find the initial tangents for the transformation and convexification solution strategy.

A further option is to select tangents such that the difference between the tangents and the curve is minimised. One means to find the minimum difference is to find the expression for the difference in area below the two curves and minimise this difference. For single tangents the difference is relatively simple to calculate,

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however for multiple tangents the difference and subsequent minimisation of the difference becomes more complex.

A further option is to divide the solution space into a number of intervals which is equivalent to the number of tangents. A tangent is assigned to the middle of each interval. The end points of the intervals are then based on the intercepts of the tangents as well as where the tangents cross the boundaries of the solution space.

Updating of Tangential Points

The initial tangential approximations, a_1^m will be selected based on any number of criteria. These include selecting the starting tangents based on solution values of another model and distributing the remaining tangents according to some method, minimisation of error between the tangents and the exact function simply to equally divide the solution space. Thereafter, where feasible, one tangential point will be set equivalent to the solution variable of the previous solution. Therefore $a_n^{x,m}$ is set equivalent to x_{n-1}^*. The other tangents are then distributed throughout the remaining solution space using any criteria, similar to assigning the initial tangential point.

Limits of Tangents for Potential Transforms

The PT requires square functions of the transformation variables. The linear approximations for concave square functions have the potential to lead to negative approximation variables, as demonstrated in **Figure 4-13**.

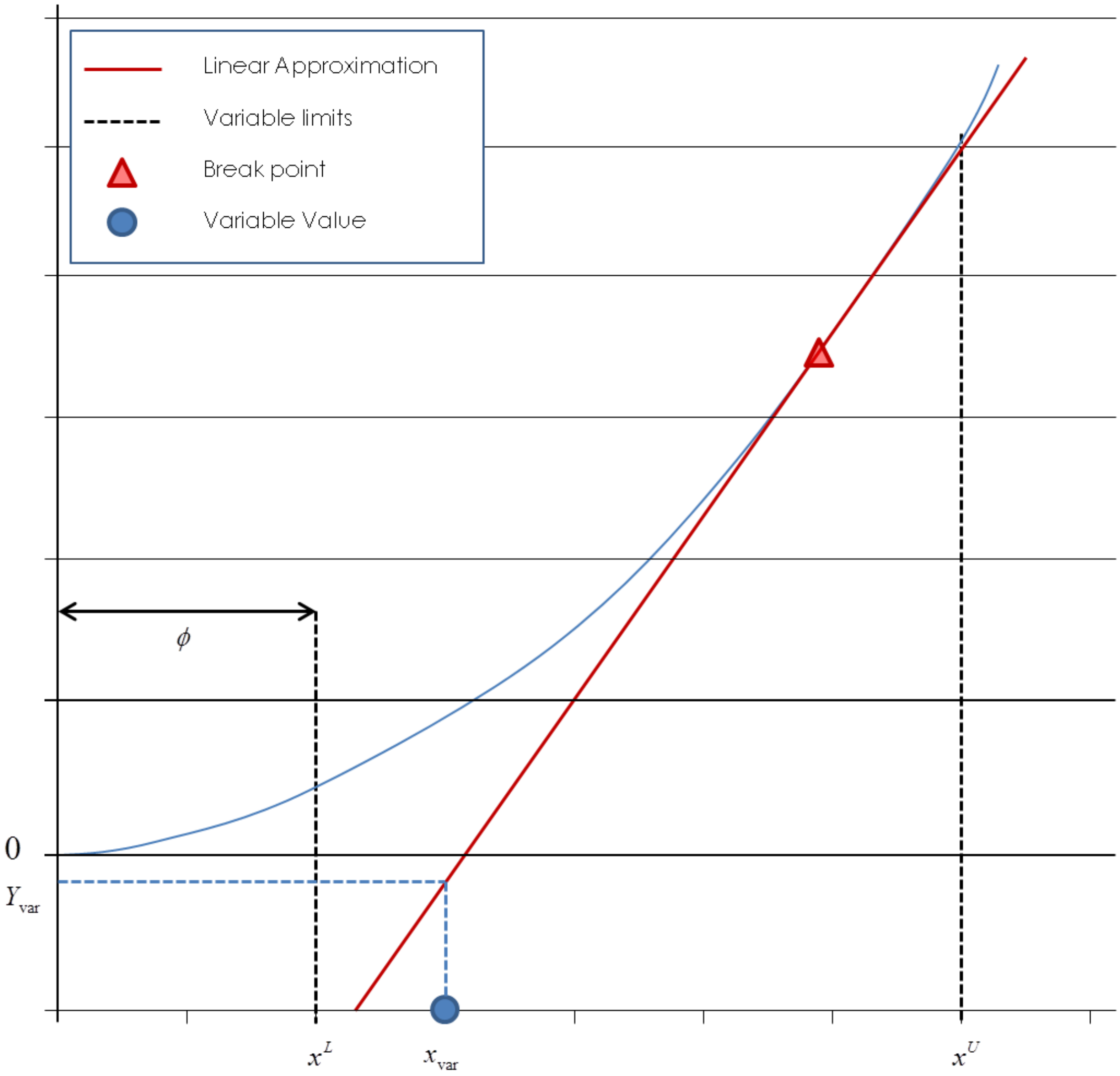

Figure 4-13: Tangential points for PT approximations can lead to negative approximations

In **Figure 4-13** the linear approximation creates negative values of the approximated value Y_{var}. In the figure the translation value is represented by the x-axis value ϕ while the limits are shown by dashed lines as indicated in the key.

The negative approximated value Y_{var} leads to singularities when used in the PT approximation as shown in Constraint (4-95). These singularities can occur in any of the PT linear approximations. As x value of the tangential point increases, the y value of the approximations approach zero. Therefore there exists some translation value ϕ that can shift the operating region far enough away from zero such that

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any value of x will lead to a corresponding positive y value. This translation value is dependent on the number of sub divisions for the solution space, $divs$ as well as the limit values of the variable x^L and x^U. Constraint (4-124) shows the appropriate translation so as to make the tangential points always lead to positive y value between the limits x^L and x^U. Constraint (4-124) can apply to any of the variables affected by the PT, namely SL, L and T^{out}.

$$\phi = \frac{\left(x^U - x^L\right)}{divs} - x^L \qquad (4\text{-}124)$$

4.6.9. Solution strategy for Transformation and Convexification Formulation

A solution strategy will be presented for the linear approximation pressure drop constraints of Problem B. This strategy will involve an iterative approach where the tangential points are updated using the most recent solution. Penalty functions are used to draw the solution variables closer to the tangential points, reducing the energy over-approximations.

The number of tangents, a_n^m, can be varied. Section 4.6.6 describes how a larger number of tangents create smaller individual solution spaces when branch and bound MINLP solvers are used. More tangents do however create more accurate solutions. Therefore a balance between accuracy and efficiency should be found. The number of tangents is represented by m, while the number of iterations is represented by n.

The basic formulation is presented in Section 4.3.4. The Transformation and Convexification technique alters Problem B from Section 4.3.4 as by changing $h_e(x)$ into $h_e^{Conv}(x,\tilde{x})$ which are now also a function of transformation variables $\tilde{x}$ which are linked to the exact variables x through the linear approximations denoted by $L[x,\tilde{x}]^T = l$. These are shown as Problem F.

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$$(F)\quad \begin{cases} MIN & f^{OBJ}\left(x,\gamma^{SE}\right) \\ s.t. & f_e(x)=0 \\ & f_e(x)+f_e(x,y)\leq 0 \\ & f_e(x)+g_e^{Lin}(x)\leq 0 \\ & f_e(x)+h_e^{Conv}(x,\tilde{x})\leq 0 \\ & L[x,\tilde{x}]^T=l \\ & Mx=m \\ & x^L\leq x\leq x^U \\ & y\in\{0,1\} \\ & e\in\{1,2,\ldots,E\} \end{cases}$$

Problem F is solved as an MINLP.

Solution stopping criteria

A number of different stopping criteria were attempted so as to arrive at a solution. These included iterations until a solution was found that was sufficiently close to tangential points. This condition was however not controlled and there was no guarantee that a solution sufficiently close to tangential points could be found.

The stopping criteria decided upon was that of a comparison between the solution found by the transformation and convexification technique, represented by problem F in Section 4.6.9 and that of a solution found by utilising the stream outlet conditions of Savelski and Bagajewicz (2000) but including any overestimations of energy which came about from solving problem F. This will be referred to as the test problem shown as G below.

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$$(G)\quad \begin{cases} MIN & f^{OBJ}(x) \\ s.t. & f_e(x) = 0 \\ & f_e(x) + f_e(x,y) \leq 0 \\ & f_e(x) + g_e^{Lin}(x) \leq 0 \\ & Mx = m \\ & x^L \leq x \leq x^U \\ & y \in \{0,1\} \\ & e \in \{1,2,\ldots,E\} \end{cases}$$

In problem G the nonlinear constraint from problem F is linearised by utilising fixed outlet temperatures.

Therefore the solution from problem F will be processed and the actual energy transferred will be calculated. Any additional energy made available by the piecewise approximations or slack variables will also be calculated. This additional energy will then be made available to problem G.

Both models utilised the fixed minimum steam flowrate as found by Coetzee and Majozi (2008). Problem G will then find a minimum pressure drop to be compared to the result of problem F. Any results from any iterations where the solution from problem F is an improvement to problem G will be recorded.

The iterative solution scheme to update the tangential points is shown in the problem flow diagram in **Figure 4-14**. In the figure the model result of problem F is represented as x_i^* while the result of the test model utilising the additional energy is represented as x_i^{*test} which is found by problem G. These values are compared and the model is stopped if the model result is favourable compared to the test model.

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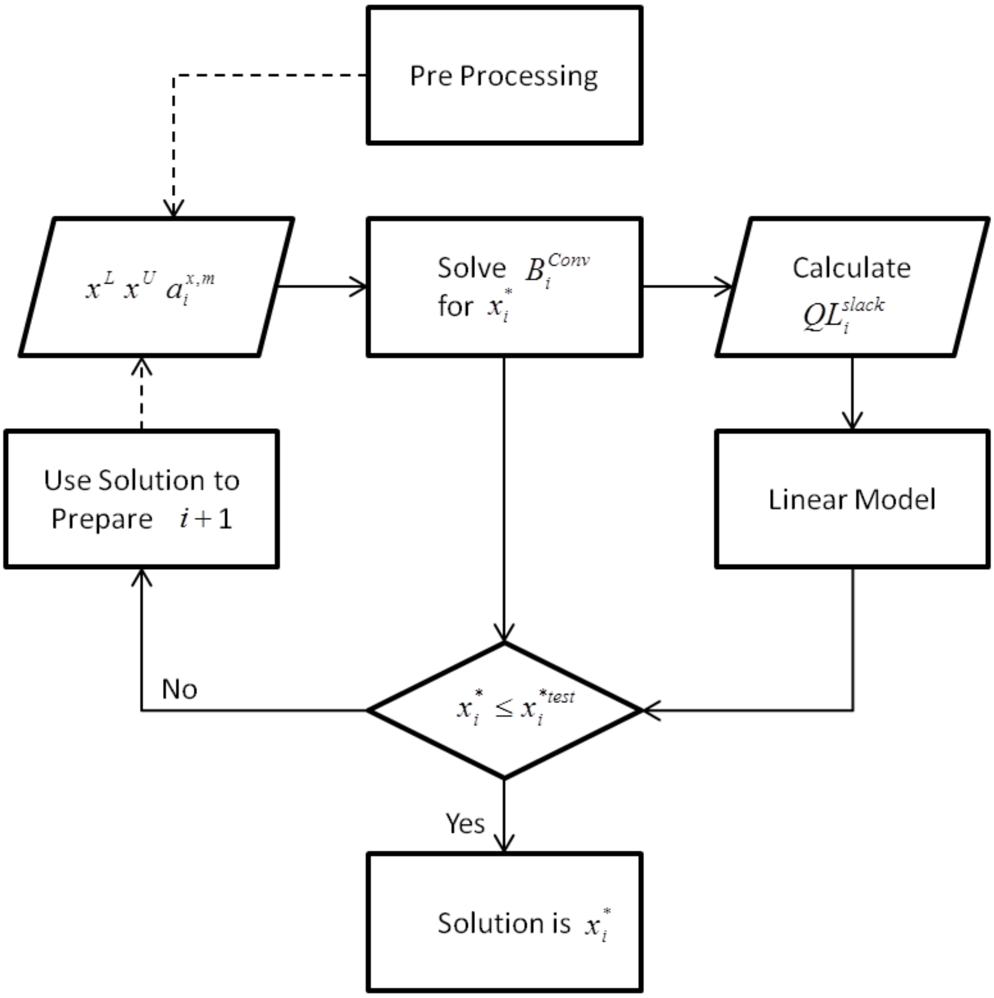

Figure 4-14: Flow diagram for the solution of the convexification and transformation formulation

A larger number of tangential points will lead to tighter energy solutions thus reducing the value of γ_i^{SE}. The only drawback of using larger numbers of tangents is the complication described in Section 4.3.5. The subsequent rise in solution times as well as possible loss of accuracy was addressed to an extent in this work but was not the focus of the study. These results are discussed in Chapter 5.

4.7. Additional Solver Techniques

The removal of binary variables from functions involving other variables can also improve the solution procedure of DICOPT Kocis and Grossmann (1989). Continuous

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variables can be used to replace binary variables and then set equivalent to binary variables in separate constraints. Therefore constraints such as Constraints (4-42) and (4-43) will be replaced by Constraints (4-125) and (4-126).

$$SL - SL^U\left(Cy^{SL}\right) \leq 0 \qquad (4\text{-}125)$$

$$SL - SL^L\left(Cy^{SL}\right) \geq 0 \qquad (4\text{-}126)$$

Cy^{SL} is a continuous variable and is made equivalent to the original binary variable y^{SL} as shown in Constraint (4-127).

$$y^{SL} = Cy^{SL} \qquad (4\text{-}127)$$

4.8. Consideration for Steam System Boiler Efficiency

This section is intended to incorporate the various techniques presented above to aspects of steam system boiler efficiency.

Boiler efficiency is negatively affected by reducing the steam flowrate of a steam system. Boiler efficiency is further negatively affected by a reduced condensate return temperature to the boiler. These phenomena are discussed in Price and Majozi (2010a). Therefore reducing the steam flowrate to a HEN as suggested by Coetzee and Majozi (2008) is likely to have negative effects on the boiler efficiency.

A sensitivity analysis of the relationship between return condensate flowrate and temperature shown in Section 3.4 reveals how if the steam flowrate to a HEN is reduced the boiler efficiency can be maintained by increasing the condensate return temperature.

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Price and Majozi (2010a) propose two methods to maintain the boiler efficiency of a system where the steam flowrate has been reduced. These methods include utilising the energy lost during let down of the steam to the most appropriate steam pressure or to include a dedicated heat exchanger in the HEN that will preheat the return stream to the steam boiler and therefore maintain the boiler efficiency. This heat exchanger will form part of the normal process optimisation problem.

Of the two methods described, the latter resulted in the more complex MINLP found in Price and Majozi (2010a). This is due to the variable duty and limiting temperatures found in this formulation. Therefore it is this MINLP that will be adapted using the relaxation and linearisation MINLP optimisation technique discussed in Section 4.5 as well as the transformation and convexification technique discussed in Section 4.6.

4.8.1. Calculation of Boiler Efficiency

The method for the reduction of steam flowrate to a HEN was developed by Coetzee and Majozi (2008). Section 3.4 showed how reducing the steam flowrate to a HEN had the effect of reducing the boiler efficiency as a result of the lower flowrate, as did the lower return temperature to the boiler. The HEN constraints for single steam pressure level systems shown in Section 4.1 can be used to effectively find the minimum steam flowrate for a particular HEN. Using this flowrate the new boiler efficiency for the steam system can be calculated. Several intermediate flow and temperature variables are required so as to calculate the boiler efficiency. **Figure 4-15** is a reproduction of **Figure 3.1** which has been included to show the origin of certain variables as they relate to the steam system. Additional variables have been created in amongst the boiler feed water pump and the economiser. These were not distinguished in **Figure 3.1** as they typical form part of a boiler package.

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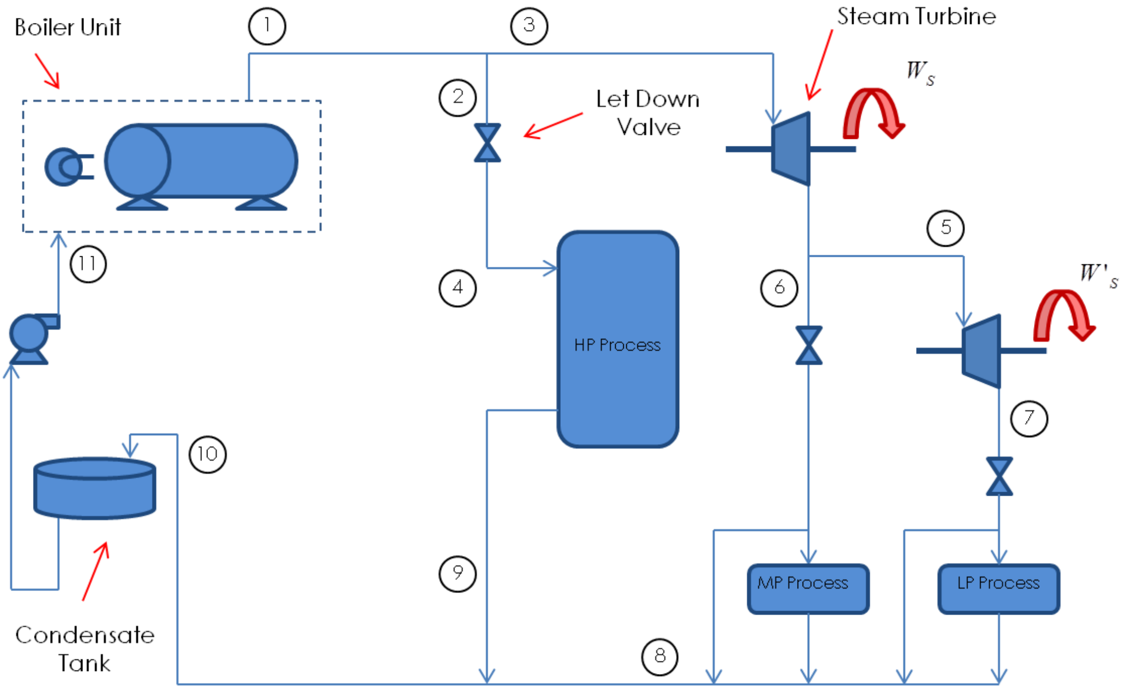

Figure 4-15: Steam System Showing Key Variables to Calculate Boiler Efficiency

The constraint used to calculate the boiler efficiency requires the return flowrate and temperature to the boiler. The flowrate to the boiler is seen as stream 11 in **Figure 4-15**. Stream 9 is the outlet stream from the process that has undergone heat integration while the combined outlet of the two turbine background process, streams 6 and 7 combine into stream 8. These streams then combine to form stream 10 which returns condensate to the condensate tank. Thus the mass flowrate and outlet temperature of streams 8 and 9 must be known so as to calculate the return temperature and flowrate to the boiler, if it is assumed that minimal losses occur at the condensate tank due to sufficient insulation. The mass flowrate of stream 9 is simply the steam flowrate through the HEN, calculated as *FS* in the HEN model. The temperature of stream 9 is determined by the return streams of all the heat exchangers in the HEN. This is calculated as T^{proc} and is shown in Constraint (4-128).

$$T^{proc} = \frac{\sum_{i \in I} FRS_i T^{sat} + \sum_{i \in I} FRL_i T_i^{out}}{FS} \qquad (4\text{-}128)$$

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T^{proc} represents the return temperature of the process while *FS* is the mass flowrate. Stream 9 then combines with stream 8 to form stream 10. If it is assumed that the mass flowrate to the turbines is constant and that the outlet temperature of the background processes is also known then the temperature and flowrate of stream 8 will be known and can be assumed constant. These will be referred to as T^{turb} and F^{turb} in the following constraints respectively. The flowrate of stream 10 is thus simply the sum of FS and F^{turb}, whereas the temperature is calculated by Constraint (4-129).

$$T^{coll} = \frac{\left(T^{proc}FS\right) + \left(T^{turb}F^{turb}\right)}{\left(FS + F^{turb}\right)} \qquad (4\text{-}129)$$

The temperature of Stream 10 is referred to as the collection temperature and is thus labelled as T^{coll}. Stream 10 then enters the condensate tank. Realistically some heat losses will occur in this area as well as the addition of makeup water to account for losses from steam traps and blowdown. These factors will be excluded for the purposes of this investigation but could easily be added as terms to Constraint (4-129). This stream then proceeds to the boiler feed water pump.

Stream 10 passes through the pre heater or economiser, where any additional heat is represented by $Q_{preheat}$. Stream 11 then represents the return stream to the boiler at flowrate $FS + F^{turb}$ and temperature T^{boil}, calculated in Constraint (4-130).

$$T^{boil} = T^{coll} + \frac{Q_{preheat}}{c_p\left(FS + F^{turb}\right)} \qquad (4\text{-}130)$$

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Substituting these variables into the constraint for boiler efficiency produces Constraint (4-131) for single steam pressure levels.

$$\eta_b = \frac{q\left(\left(FS + F^{turb}\right)/F^U\right)}{\left(c_p\left(T^{sat} - T^{boil}\right) + q\right)\left[\left(1+b\right)\left(\left(FS + F^{turb}\right)/F^U\right) + a\right]} \qquad (4\text{-}131)$$

4.8.2. Sensitivity of Boiler Efficiency

Section 3.4 discusses the relationship between the boiler efficiency and changes in the condensate flowrate return to the boiler as well as the condensate return temperature. As either variable is decreased they negatively affect the boiler efficiency. A means of maintaining the boiler efficiency in the event of a decrease in return flowrate is to increase the return temperature. This relationship is shown in Section 3.4 and is reproduced in **Figure 4-16** for convenience.

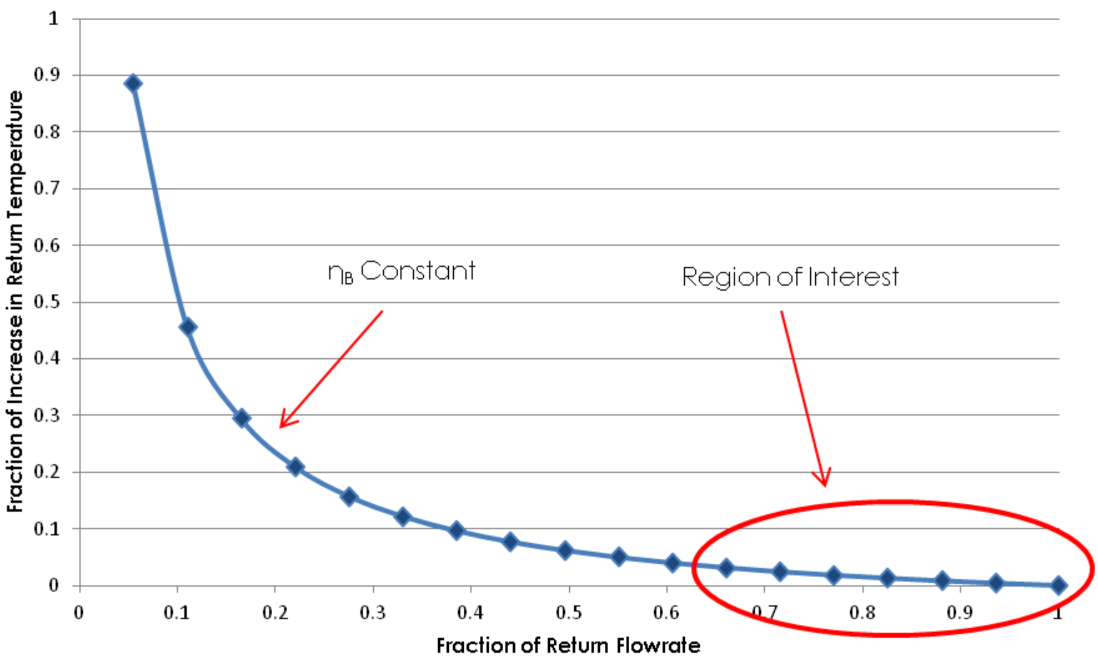

Figure 4-16: Sensitivity of Boiler Efficiency to Changes in Steam Return Flowrate and Return Temperature

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It can be seen that boiler efficiency is a function of both the return flowrate to the boiler as well as the return temperature. In the region of interest in **Figure 4-16** it can be seen that for a reasonably large reduction in steam flowrate the boiler efficiency can be maintained by a slight increase in return temperature. The steam flowrate reduction achieved by Coetzee and Majozi (2008) was 29.6%. For this reduction an increase in return temperature of 2.6% would be required to maintain the efficiency of the boiler with the characteristics discussed in Section 3.4.

By considering the steam system layout shown in **Figure 4-15**, the boiler feed water temperature is dependent on the return temperature to the condensate tank as well as any additional energy added by the pre heater. The pre heater in the system typically utilises the heat from stack gases in the boiler and is often referred to as an economiser. This pre heater may not have the capacity to increase the boiler return temperature to a point where the boiler efficiency can be maintained. Therefore an additional heat exchanger is proposed that will form part of the HP Process network with the sole purpose of preheating the boiler feed water so as to maintain the boiler efficiency in the event of a reduction in steam flowrate from a heat integration process such as that described by Coetzee and Majozi (2008).

4.8.3. Dedicated Pre heater to Maintain Boiler Efficiency

By reducing the steam flowrate required to heat process streams in a HEN using heat integration the resulting return flowrate as well as return temperature to the steam boiler. A reduction in either variable negatively affects the boiler efficiency. However a sensitivity analysis of the boiler efficiency against both return flowrate and return temperature revealed that the boiler efficiency can be maintained for a reduced steam flowrate if the return temperature can be increased. For steam flowrate reductions in the region of up to 30% the associated increase in return temperature required to maintain the boiler efficiency is typically less than 5%. Therefore an opportunity exists to significantly reduce the steam flowrate through a HEN and maintain the boiler efficiency by pre heating the boiler feed.

One means to achieve the desired level of pre heating is to pass the boiler feed water through a pre heater utilising the energy generally lost during steam let down.

This pre heater would have to ensure the correct steam conditions for the utility systems while still achieving the required level of pre heat for the boiler feed water such that the boiler efficiency is maintained. This concept is explored in detail in Coetzee and Majozi (2008).

Another means to preheat the boiler feed water so as to maintain the boiler efficiency is to include an additional heat exchanger in the conventional HEN. The proposed steam system setup to incorporate this additional heat exchanger is shown in **Figure 4-17**.

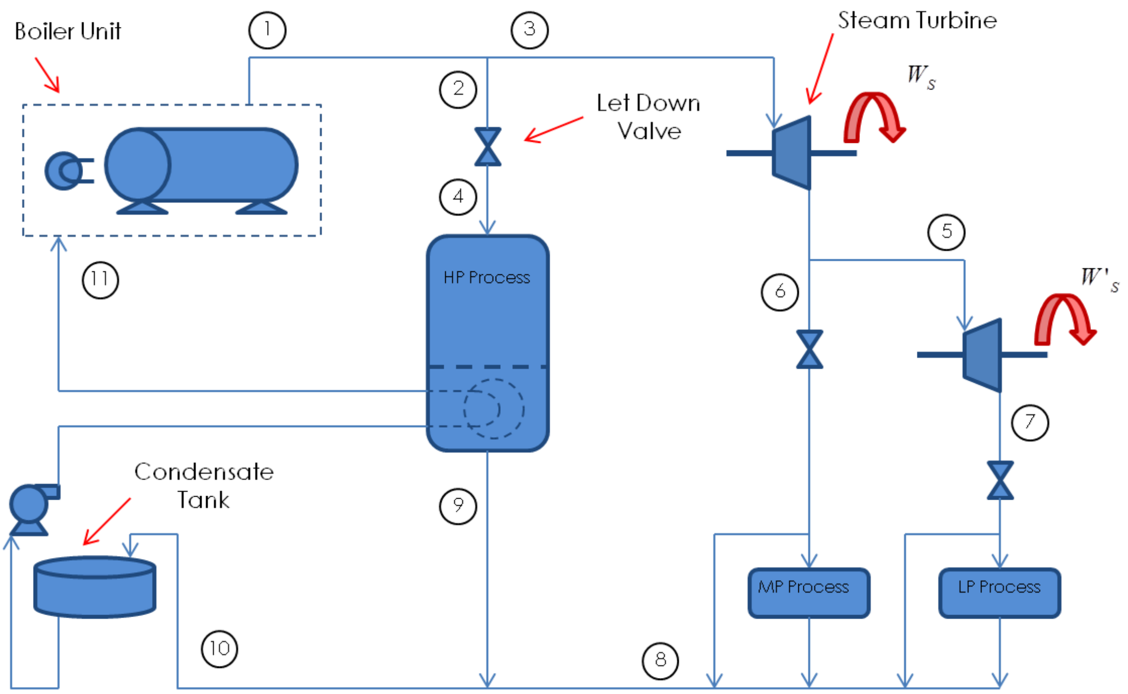

Figure 4-17: Additional Pre Heater Included in the HEN

The boiler feed water pump is removed from the boiler unit to show the path of the feed to the boiler as it passes through an additional heat exchanger in the main HEN. The temperature of stream 10 is therefore increased using the pre heater to give stream 11 the correct temperature for the reduced steam flowrate such that the boiler efficiency is maintained.

The conventional process streams requiring heating in the HP Process in **Figure 4-17** would typically have fixed limiting temperatures and a known heating duty. These parameters make the modelling of such heat exchangers simpler. The additional heat exchanger has a variable flowrate and varying limiting temperatures. Depending on the minimum steam flowrate the heating duty will also be unknown initially. These variables create an additional complication to modelling the new steam system.

The flow minimisation constraints presented in Section 4.1 will be utilised as the base and augmented where necessary. Constraints (4-1) to (4-29) will remain the same, however the number of current heat exchangers, $|i|$, will be increased by one so as to capture the additional heat exchanger. The additional heat exchanger will be designated as $i*$ to identify it in the formulation. The $i*$ heat exchanger behaves as all others in the model, it is able to receive steam from the boiler as well as saturated or subcooled condensate from other heat exchangers. It can then discharge saturated or subcooled condensate to any other heat exchanger or return these streams to the boiler. The limiting temperatures and the duty of the $i*$ heat exchanger will however be variables in the formulation as these can change depending on the arrangement of the HEN.

The inlet to the $i*$ heat exchanger is stream 10, as can be seen in **Figure 4-17**. Using the terminology defined in Section 4.8.1 the temperature of the inlet stream to the pre heater was designated as T^{coll}. The outlet of the $i*$ heat exchanger is stream 11 with a designated temperature of T^{boil}. These temperatures are essentially the process stream temperatures and limiting temperatures for the $i*$ heat exchanger can be developed by augmenting T^{coll} and T^{boil} with the global $\Delta T^{\min}$. The limiting temperatures of the additional heat exchanger are shown in Constraints (4-132) and (4-133). The duty of the $i*$ heat exchanger can be seen in Constraint (4-134).

$$T_{i*}^{in,L} = T^{coll} + \Delta T^{\min} \qquad \forall i* \in I \qquad (4\text{-}132)$$

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$$T_{i*}^{out,L} = T^{boil} + \Delta T^{\min} \qquad \forall i* \in I \qquad (4\text{-}133)$$

$$Q_{i*} = SS_{i*}\lambda + \sum_{j \in I}\left(c_P SL_{j,i*} T^{sat}\right) + \sum_{j \in I}\left(c_P L_{j,i*} T_j^{out}\right) - \left(c_P F_{i*}^{out}\left(T^{boil} + \Delta T^{\min}\right)\right) \qquad \forall i* \in I \qquad (4\text{-}134)$$

The temperature of the stream returning to the boiler, T^{boil}, was calculated in Constraint (4-130) by adding energy gained by the pre heater to the stream leaving the condensate tank, T^{coll}. This is now shown by the energy added to stream 10 as being the duty of the $i*$ heat exchanger. This is represented in Constraint (4-135).

$$T^{boil} = T^{coll} + \frac{Q_{i^*}}{c_P\left(FS + F^{turb}\right)} \qquad (4\text{-}135)$$

The basic boiler efficiency constraints are shown in Section 4.8.1. Therefore Constraints (4-128) to (4-131) with Constraint (4-135) replacing Constraint (4-130) will complete the formulation. It remains to specify an objective function for this formulation. The objective is, as in the work of Coetzee and Majozi (2008) to minimise the steam flowrate to the HEN. The boiler efficiency is therefore set as a parameter in the formulation and the objective function is to reduce the steam flowrate as far as possible.

Without considering the boiler efficiency the minimum steam flowrate for the HEN can be found using the technique of Coetzee and Majozi (2008) shown in Section 4.1. The result of this process is a minimum steam flowrate FS. This solution can be used as a starting point for the next objective of maintaining the boiler efficiency. As additional steam will be required to pre heat the boiler return, an additional slack variable is added to the minimum steam flowrate FS. The objective will therefore be to minimise this slack variable. The addition of the slack variable will be shown in the appropriate boiler efficiency constraints below as well as the new objective function. Constraints (4-136) to (4-139) will allow the boiler efficiency to be accounted for. η_B in Constraint (4-139) will be set as a constant equivalent to that of the steam system before heat integration. Constraint (4-140) then represents the objective function. The slack variable for boiler efficiency problems is represented by γ^{BE} .

$$T^{proc} = \frac{\sum_{i \in I} FRS_i T^{sat} + \sum_{i \in I} FRL_i T_i^{out}}{FS + \gamma^{BE}} \qquad (4\text{-}136)$$

$$T^{coll} = \frac{\left(T^{proc}\left(FS + \gamma^{BE}\right)\right) + \left(T^{turb} F^{turb}\right)}{\left(\left(FS + \gamma^{BE}\right) + F^{turb}\right)} \qquad (4\text{-}137)$$

$$T^{boil} = T^{coll} + \frac{Q_{preheat}}{c_p\left(\left(FS + \gamma^{BE}\right) + F^{turb}\right)} \qquad (4\text{-}138)$$

$$\eta_b = \frac{q\left(\left(\left(FS + \gamma^{BE}\right) + F^{turb}\right)/F^U\right)}{\left(c_p\left(T^{sat} - T^{boil}\right) + q\right)\left[(1+b)\left(\left(\left(FS + \gamma^{BE}\right) + F^{turb}\right)/F^U\right) + a\right]} \qquad (4\text{-}139)$$

$$MinZ = \gamma^{BE} \qquad (4\text{-}140)$$

Therefore this formulation includes the HEN steam flowrate minimisation constraints found in Section 4.1, namely Constraints (4-1) to (4-29), with the objective function replaced by Constraint (4-140). Then the boiler efficiency constraints discussed

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above, Constraints (4-136) to (4-139) as well as the considerations for the limiting temperatures and the duty of the $i*$ heat exchanger, Constraints (4-132) to (4-134) make up the formulation to reduce steam flowrate to a HEN while maintaining the boiler efficiency with a dedicated boiler feed water pre heater.

This formulation contains a number of non linear terms making the problem an MINLP. The variable product terms are bilinear, making the problem nonconvex. Price and Majozi (2010a) catered for the bilinear terms in the sensible energy constraint by setting the outlet temperatures to their limits using the principle applied by Savelski and Bagajewicz (2000). The bilinear boiler efficiency terms were handled using the technique of Quesada and Grossmann (1994), described in Section 4.5. In this work the limiting temperature constraint of Savelski and Bagajewicz (2000) will be relaxed. All of the bilinear terms will be handled using the relaxation and linearisation technique discussed in Section 4.5 as well as the transformation and convexification technique discussed in Section 4.6.

4.8.4. Solution Strategy

The same bilinear terms exist in Constraint (4-15) as were found in the pressure drop minimisation problem. These terms will be dealt with in the same way as discussed in Section 4.5 and Section 4.6. Additional bilinear terms are found in the boiler efficiency constraints. These are listed below:

- T_i^{out} and FRL_i;
- T^{proc} and FS;
- T^{proc} and γ^{BE};
- T^{coll} and FS;
- T^{coll} and γ^{BE};
- T^{boil} and FS; and
- T^{boil} and γ^{BE}.

A number of bilinear terms are brought about by the variable nature of the duty for the $i*$ heat exchanger. Constraints (4-22) and (4-23) are typically linear, however with a variable duty two bilinear terms are formed. These are listed below:

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- Q_{i*} and y_{i*}; and
- Q_{i*} and x_{i*}.

As y_{i*} and x_{i*} are binary variables these bilinear terms can be dealt with by the Glover Transformation (Glover, 1975). This is discussed further in Appendix B.

Relaxation and Linearisation

The relaxation and linearisation technique was applied to the variables in the boiler efficiency constraints by Price and Majozi (2010a). The formulations will be used as such. The allowance for degenerate solutions will be catered for in the same way as was discussed in Section 4.5. Key focus elements of the solution strategy from Sections 4.5.2, 4.5.3 and 4.5.4 such as variable limits will also be applied, as well as those additional solver techniques as discussed in Section 4.7.

Transformation and Convexification

The various bilinear terms will have the ET or PT applied to them depending on their sign in the constraint they appear in. As they do not all occur in the same constraints, the signs of the various terms with respect to each other will be utilised to determine whether the ET or PT is applied to the various bilinear terms.

The transformations are designated and shown in **Table 4-1**.

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Table 4-1: Designation of Transformations for Boiler Efficiency Problem

Variables	Sign in Constraints	Transform	Transform Designation
T_i^{out} and FRL_i	+	ET	$T^{out,ET}$, FRL^{ET}
T^{proc} and FS	-	PT	$T^{proc,PT}$, FS^{PT}
T^{proc} and γ^{BE}	-	PT	$T^{proc,PT}$, $\gamma^{BE,PT}$
T^{coll} and FS	+	ET	$T^{coll,ET}$, FS^{ET}
T^{coll} and γ^{BE}	+	ET	$T^{coll,ET}$, $\gamma^{BE,ET}$
T^{boil} and FS	-	PT	$T^{boil,PT}$, FS^{PT}
T^{boil} and γ^{BE}	-	PT	$T^{boil,PT}$, $\gamma^{BE,PT}$

Constraints (4-136) to (4-139) contain the various bilinear terms and these terms will be replaced by the transforms shown in **Table 4-1**. As all of the boiler efficiency flow and temperature variables cannot take on zero values, these will not require translations. The first transform, FRL^{ET} , will require a translation as discussed in Section 4.3.3 as the variable FRL_i can take values of zero.

Additional solver techniques as discussed in Section 4.7 will also be applied to this formulation.

4.9. Summary

This section will summarise the formulations presented in this chapter for ease of reference.

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Formulation	Description	Solution Order
General		
Problem A	Basic HEN pressure drop formulation containing both nonlinear and convex as well as nonlinear and nonconvex terms	
Problem B	Basic HEN pressure drop formulation containing with pressure drop correlation constraints linearised	
Relaxation and Linearisation		
Problem C	Bilinear terms are replaced according to the relaxation and linearisation technique. With linearisations from problem B this can be solved as a MILP and form a starting point for problem D	
Problem D	A slack variable is added to sensible energy constraint and included in objective function with penalty factor. This is intended to provide feasible solutions.	Solved according to progression shown in **Figure 4-6**
Problem E	Solutions to problem D where the slack energy variable can be minimised to zero are used to fix outlet temperatures in order to solve problem E with nonlinear pressure drop correlations	
Transformation and Convexification		
Problem F	Bilinear terms are replaced according to the transformation and convexification technique. These changes are initially proposed to problem B, however due to the additional transformation constraints problem F remains a MINLP	Solved according to progression shown in **Figure 4-14**
Problem G	Test problem for comparison with problem F. If the slack variable is not reduced to zero this residual energy is added to problem G and the result compared to that of problem F	

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5. Case Studies

This chapter is intended to apply the degenerate HEN optimisation problem in order to minimise pressure drop and maintain boiler efficiency.

Firstly an analysis of the pressure drop problem portrayed by Price and Majozi (2010c) where the original base case study information from Coetzee and Majozi (2008) is described, then the minimum pressure drop solution first described by Price and Majozi (2010c) is analysed and compared to the solution found by applying the techniques described in Chapter 4. The degenerate solution formulations are then used to solve the pressure drop minimisation problem and the solutions are presented. The most effective solution procedure will then be tested on an additional case study.

The degenerate solution methodology will then be applied to a system where an attempt is made to maintain boiler efficiency with less steam, as discussed in Chapter 4.

5.1. Case Study HEN

The limiting temperature data and duties for the utility streams are shown in **Table 5-1**. The process streams originate from a petrochemical company where steam at a single pressure level is supplied and is required to satisfy the duties and adhere to the limiting temperature constraints. **Table 5-1** also shows the minimum steam flowrate required to satisfy the duty with latent heat. **Table 5-2** shows information relevant to the steam available to the system.

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Table 5-1: Hot utility stream data

Stream	T^L Target (°C)	T^L Supply (°C)	Duty (kW)	Flowrate (kg/s)
1	35	55	135	0.07
2	35	55	320	0.17
3	219	225	3 620	1.97
4	89	195	12 980	7.08
5	217	217	1 980	1.08
6	54	80	635	0.34
7	54	80	330	0.18
Total			**20 000**	**10.98**

Table 5-2: Steam system data Coetzee and Majozi (2008)

Description	T^{sat} (°C)	P (kPa)	λ (kJ/kg)
Process Pressure steam	225	2 550	1834.3

This information is used by Coetzee and Majozi (2008) to minimise the overall steam flowrate to the HEN. The steam flowrate for the system is reduced from 10.98 kg/s to 7.68 kg/s. In all formulations the minimum steam flowrate will be maintained and often used as a constraint as discussed in Chapter 4.

The pressure drop through a HEN is a combination of the series arrangement of piping and heat exchanger pressure drops. To calculate the individual piping and heat exchanger pressure drop coefficients Price and Majozi (2010c) used realistic piping dimensions and designed feasible heat exchangers according to guidelines from Sinnot (2005) to approximate actual heat exchangers to be used in the pressure drop minimisation formulation. The basis for the designs can be seen in Appendix A.

The resulting coefficients were used to approximate pressure drop as a function of mass flowrate. Price and Majozi (2010c) used a third order polynomial to approximate the pressure drop correlations for process piping and a second order polynomial approximation for the heat exchanger and condenser pressure drop. For simplicity in this work, all pressure drop approximations were made from second order polynomials. The coefficients of the various polynomials are shown in **Table 5-3**.

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The information contained in **Table 5-1**, **Table 5-2** and **Table 5-3** is sufficient to formulate and solve the minimum pressure drop problem as described in Chapter 4.

Table 5-3: Second order polynomial pressure drop coefficients

Description	K2(Pa.s2/kg2)	K1 (Pa.s/kg)	K0 (Pa)
Utility Stream 1 - Condenser	9.00E+06	3.73E+04	-1.07E+02
Utility Stream 2 - Condenser	1.00E+06	1.02E+04	-6.94E+01
Utility Stream 3 - Condenser	3.20E+04	9.34E+03	-7.20E+02
Utility Stream 4 - Condenser	4.35E+03	1.92E+03	-5.30E+02
Utility Stream 5 - Condenser	9.71E+04	1.60E+04	-6.74E+02
Utility Stream 6 - Condenser	3.81E+05	1.05E+04	-1.43E+02
Utility Stream 7 - Condenser	1.00E+06	2.03E+04	-1.43E+02
Utility Stream 1 – Heat Exchanger	8.19E+03	1.71E+03	-1.05E+02
Utility Stream 2 – Heat Exchanger	1.84E+03	8.27E+02	-1.20E+02
Utility Stream 3 – Heat Exchanger	6.19E+02	1.05E+03	-4.47E+02
Utility Stream 4 – Heat Exchanger	1.74E+03	3.24E+03	-1.38E+03
Utility Stream 5 – Heat Exchanger	5.46E+02	8.34E+02	-3.55E+02
Utility Stream 6 – Heat Exchanger	6.85E+02	5.51E+02	-1.22E+02
Utility Stream 7 – Heat Exchanger	2.53E+03	1.06E+03	-1.22E+02
Saturated Condensate Recycle/Reuse Pipework (SL)	1.03E+02	1.92E+03	1.53E+04
Sub-Cooled Condensate Recycle/Reuse Pipework (L)	1.76E+02	-3.28E+03	2.61E+04
Saturate Condensate Boiler Return Pipework (FRL)	2.64E+02	-4.91E+03	3.91E+04
Sub-Cooled Condensate Boiler Return Pipework (FRS)	1.03E+02	-1.92E+03	1.53E+04

5.2. System Pressure Drop with Fixed Outlet Temperature

This section discusses the original minimum pressure drop solution presented by Price and Majozi (2010c). The techniques used by the authors to overcome singularities which originate from zero flowrate values are described. The solution is then reworked with second order polynomial pressure drop approximations and

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translations to overcome the singularities. The formulation is then linearised as discussed in Section 4.3.2 so as to approximate a globally optimal solution.

5.2.1. Solution from Price and Majozi (2010c)

Price and Majozi (2010c) used the flowrate minimisation model derived in Price and Majozi (2010a) along with the pressure drop correlations shown in Chapter 4. As in Price and Majozi (2010a) the boiler efficiency for the case study was also maintained. This is done in Price and Majozi (2010c) by first solving for the relevant minimum steam flowrate that is able to maintain the boiler efficiency and then utilising this flowrate in the pressure minimisation model.

The formulation contains mixed integer terms as well as non linear terms making the pressure drop minimisation formulation an MINLP. The MINLP solver DICOPT was utilised in the optimisation software package GAMS.

The problem formulation in GAMS required some minor adjustments to the basic constraints presented in Chapter 4. These are as a result of singularities that occur when the steam or condensate flowrate is zero in nonlinear terms. The nonlinear terms in question are cubic and square terms in the polynomial representations of pressure drop through heat exchangers and pipework. In GAMS, an exponentiation such as a square or cubic function is calculated as $\exp[n.\ln(x)]$ where n is the exponent and x is the variable. The natural logarithm of zero is undefined in GAMS and causes errors in NLP solvers. As a large number of the possible heat exchangers and pipework connections in the heat exchanger network will not necessarily exist in the final solution the flowrates through these elements can be zero. This has the potential to cause singularities in the model resulting in model failures.

The technique utilised by Price and Majozi (2010c) was to shift the flowrates to non-existent heat exchangers and pipework connections away from zero by a small amount, a value of 0.0001 kg/s. This results in several constraint changes as well as a relaxation of the minimum steam flowrate to accommodate the offset values. Representative constraints such as Constraints (4.42) and (4.43) are changed as shown in Constraints (5-1) and (5-2)

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$$SL - SL^U\left(y^{SL}\right) - (0.0001)\left(1 - y^{SL}\right) \leq -0.0001 \quad (5\text{-}1)$$

$$SL - SL^L\left(y^{SL}\right) + (0.0001)\left(1 - y^{SL}\right) \geq 0.0001 \quad (5\text{-}2)$$

Using the changes above the minimum steam flowrate was then relaxed until a feasible solution was found in using the DICOPT MINLP algorithm in GAMS. A feasible pressure drop was found using a flowrate relaxation of 0.0405 kg/s, a relaxation of less than 1% of the minimum steam flowrate of 7.6806 kg/s. The pressure drop calculated using this relaxation is reported in Price and Majozi (2010c) as 344.40 kPa.

Optimality of solutions

The DICOPT solver can guarantee global optimality of solutions providing the nonlinear constraints are convex or quasi-convex within the feasible region (Kocis and Grossmann, 1989). The exponential functions used to represent pressure drop are nonconvex in the range of the mass flowrate. Therefore the global optimality of the solution found by Price and Majozi (2010c) cannot be guaranteed.

5.2.2. Solution with Exact Minimum Steam Flowrate

Several improvements to the formulation used by Price and Majozi (2010c) can be implemented in an attempt to attain a better solution. The first is to completely remove the possibility of singularities by creating a dummy variable to replace the nonlinear exponentials functions. This will allow a more effective shift of the operating area away from the singularities created by zero flows. The removal of binary variables from functions involving other variables can also improve the solution procedure of DICOPT Kocis and Grossmann (1989).

The first improvement is accomplished using translations as discussed in Section 4.3.1. This effectively removes the singularities from the formulation, removing errors when any of the variables involved in nonlinear functions approach zero. A further improvement is the removal of binary variables from constraints where other variables appear. This is discussed in more detail in Section 4.6.

5.2.3. Reworked Formulations

The replacement of third order polynomials as discussed in Section 4.2.2 will require the original optimum pressure drop calculated by Price and Majozi (2010c) to be recalculated using the square polynomial approximations. This was completed and the minimum pressure drop found when not restricting the number of split heat exchangers was 413.38 kPa using the technique of Price and Majozi (2010c). By individually varying the heat exchanger splits the minimum pressure drop was found to be 321.21 kPa with two heat exchanger splits.

Using the techniques demonstrated above the pressure drop can be slightly reduced to 321.18 kPa using the same mass flowrate relaxation. The formulations did however make it possible to find a minimum pressure drop without the need to relax the mass flowrate at all. Using the minimum flowrate found in Price and Majozi (2010c) the minimum pressure drop was calculated as 364,43 kPa. This result will be used for comparison going forward as this is the result obtained using the technique of Price and Majozi (2010c).

5.2.4. Solution

The flow network for the solution described above is shown in **Figure 5-1**. All flowrates are reported in kg/s.

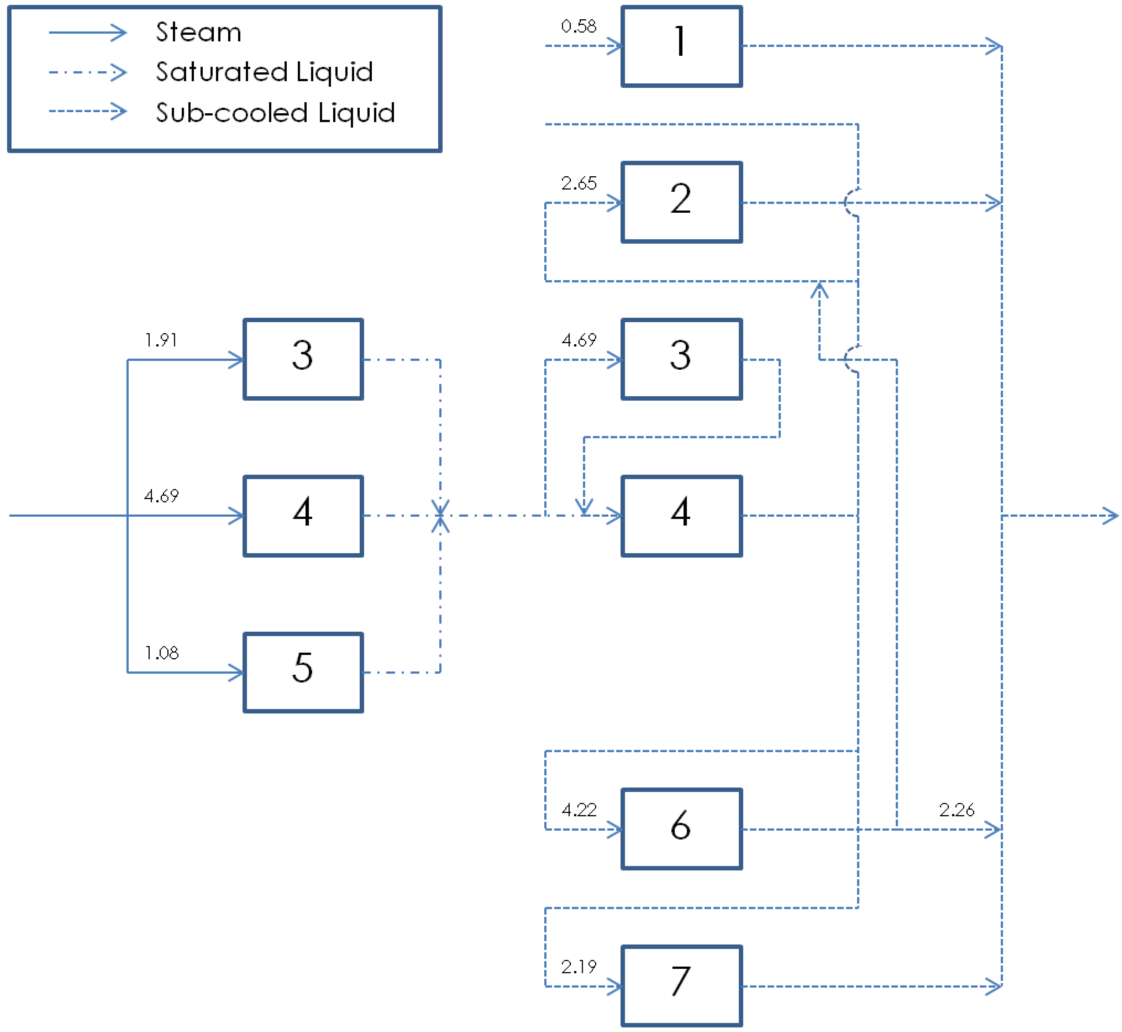

Figure 5-1: Heat exchanger network layout for minimal pressure drop

Including piecewise linear approximations of the nonlinear terms in the pressure drop constraints yielded a MILP model. The break points for the approximations were evenly distributed along the possible flow solution space. The solution strategy was to run the model in an iterative fashion, updating the break points continuously until a certain tolerance on the difference in break points and the actual flow variables is achieved. As the models are linear they can be solved to optimality.

Using the case study shown above, a minimum pressure drop of 365.41 was found with percentage errors between the break points and square flow variable approximations not exceeding 1.43%, with the majority of errors not exceeding 0.10%. As the pressure drop value is very close to the value of the solution found

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using the nonlinear representation of the pressure drop constraints it is likely that this is a globally optimal solution. It must be noted that this formulation is with fixed heat exchanger outlet temperatures.

The network for the solution of the piecewise linear problem is shown in **Figure 5-2** below. All flowrates are reported in kg/s.

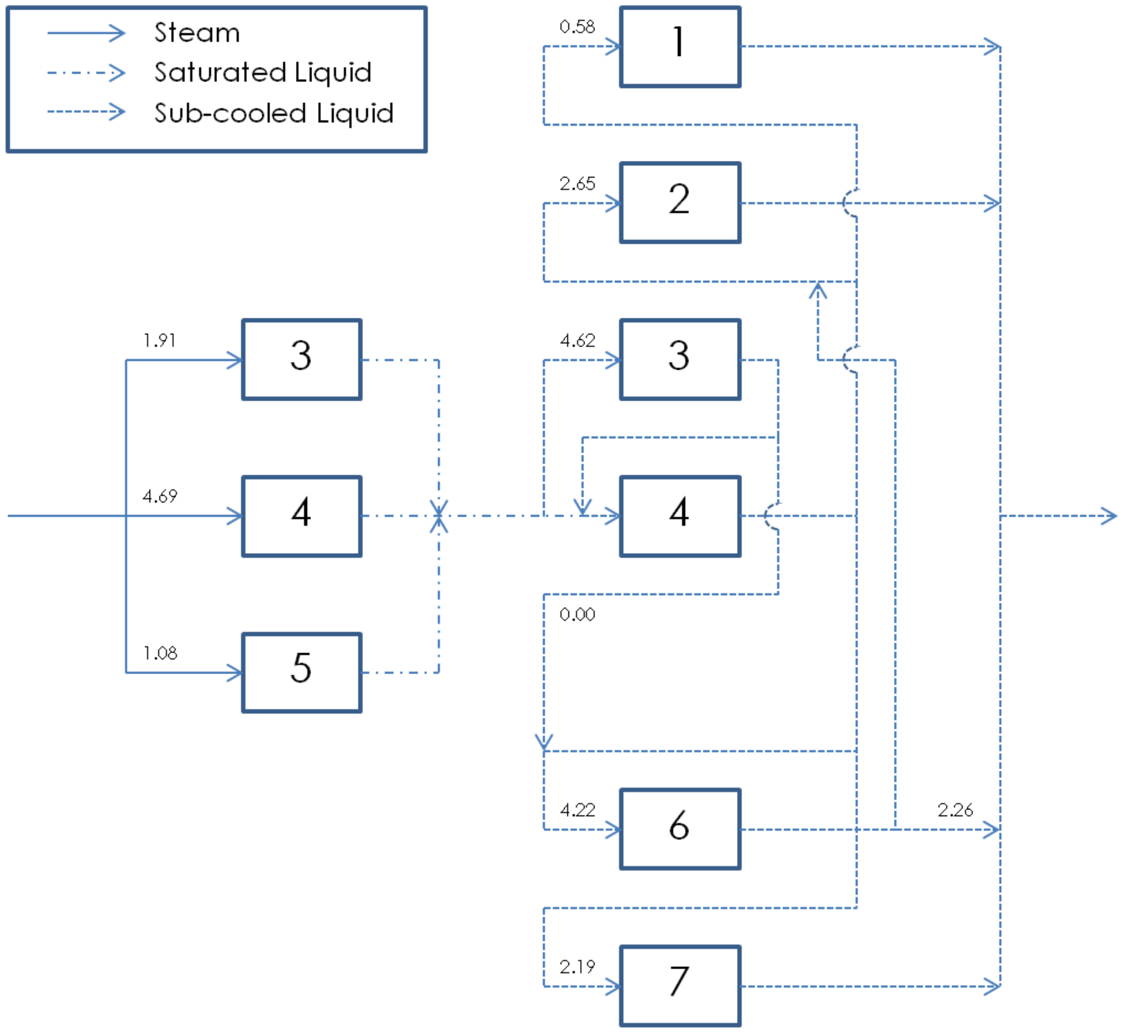

Figure 5-2: Heat exchanger network layout for minimal pressure drop using piecewise linear approximations

5.2.5. Discussion of Results

By implementing the same mass flowrate relaxation as Price and Majozi (2010c) a minimum HEN pressure drop of 321.18 kPa. The implementation of translations to allowed the minimum pressure drop to be found with the exact minimum steam

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flowrate. This was found to be 364.43 kPa. By comparing these results it can be seen that utilising a slightly relaxed minimum steam flowrate can lead to a substantial reduction in the minimum system pressure drop. The inclusion of translations allows the exact minimum steam flowrate to be utilised and the subsequent minimum pressure drop to be determined.

The inclusion of piecewise linear approximations to the pressure drop correlations allows the resulting MILP problem to be solved to optimality and therefore can give an indication of the minimum system pressure drop. As the piecewise linear approximations overestimate the pressure drop, the resulting solutions are likely to be slightly higher than the exact pressure drop. By comparing the solutions, one can make a judgement on the optimality of the precise formulation which is solved as an MINLP.

5.3. Degenerate Solution Pressure Drop with Relaxation and Linearisation Formulation

This section describes the solutions to the steam system minimum pressure drop problem found by the relaxation and linearisation formulation.

The solution techniques described in Section 4.5.4 were applied to the pressure minimisation model. The minimum steam flowrate for the system was expectedly identical to that of Coetzee and Majozi (2010) as 7.68 kg/s. The initial linearised model C showed a minimum pressure drop of 328.27 kPa.

A solution which effectively minimised the penalty function in problem D was not found. It is understood that this is as a result of system constraints pertaining to the nature of the heat exchangers requiring heating. Process stream 4 has a large duty as compared to the other process streams and it was found that this caused complications during the modelling process. Therefore an alternate penalty function which attempted to find a feasible solution as close to the initial linearised model C solution was attempted. This model utilised a single linear approximation for the pressure drop due to the potential reduced solution spaces found in MINLP solvers as described in Section 4.3.5.

The model solved to an objective function value of 514.89 kPa. The total value of the penalty function values was calculated to be 50.03 kPa. Therefore the return node pressure was calculated as 464.87 kPa.

As linear approximations for pressure drop were used, the actual system pressure drop for this solution is likely to be lower. It was found that the minimum pressure drop was indeed less than the reported solver values after they were process with the exact pressure drop coefficients. The minimum pressure drop path was found from the solution and the pressure drop of the individual elements recalculated exactly using the same coefficients as were found in the model. The exact minimum pressure drop was calculated to be 360.46 kPa. This shows a saving of 1.1%. The solution network has been created and shown in **Figure 5-3** while the minimum pressure drop path has been shown in **Figure 5-4**.

The problem formulation was unsuccessful at minimizing the objective function in problem D. In addition this result is not a large reduction in pressure drop and it was found that most network structures did not vary largely due to a single process stream requiring a large duty.

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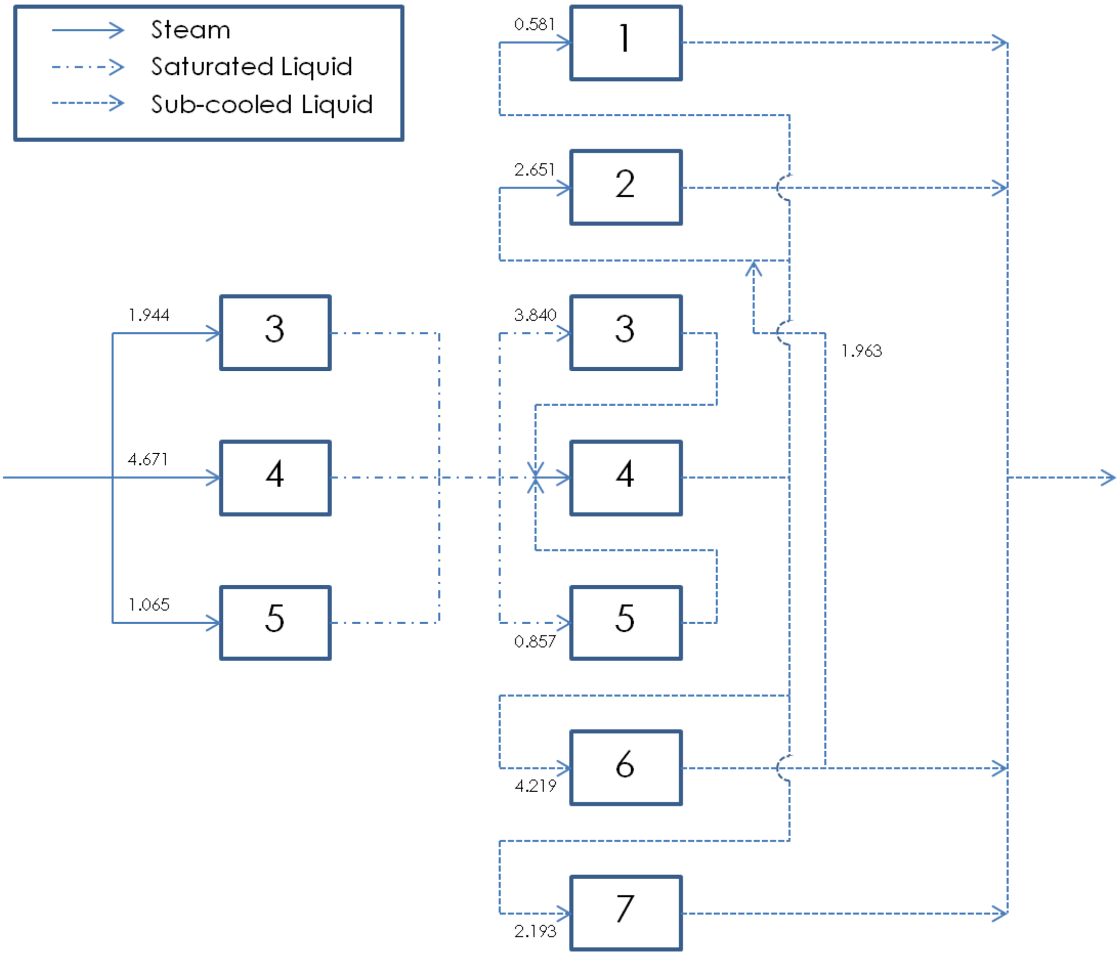

Figure 5-3: HEN layout for minimum pressure drop found using the Relaxation and Linearisation technique

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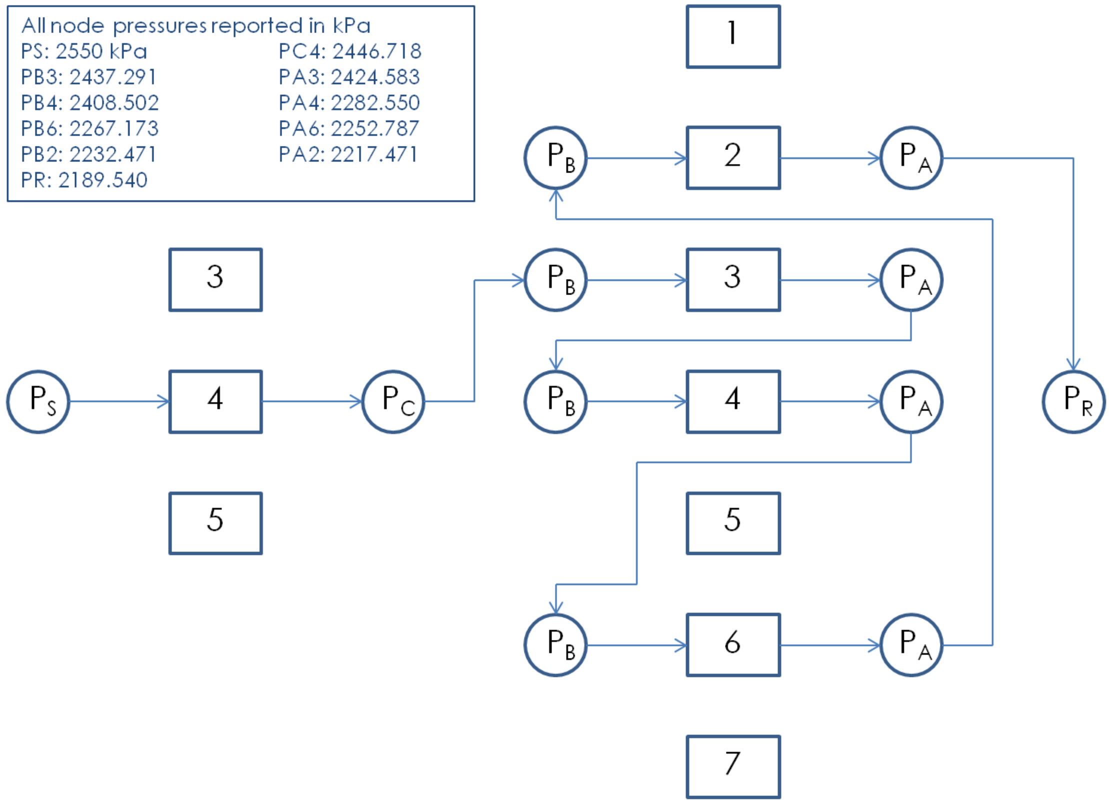

Figure 5-4: Maximum pressure drop path found through the Relaxation and Linearisation technique

The outlet temperatures of the various streams are shown in **Table 5-4** as compared to the minimum outlet temperatures used in the initial work by Price and Majozi (2010c).

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Table 5-4: Heat exchanger outlet temperatures for minimum pressure drop network found with Relaxation and Linearisation technique

Process Stream	Minimum Utility Outlet Temperature (°C)	Outlet T From Degenerate Solution (°C)
1	35.000	35.000
2	35.000	35.000
3	219.000	221.744
4	89.000	89.000
5	217.000	217.893
6	54.000	54.000
7	54.000	54.000

5.4. Degenerate Solution Pressure Drop with Transformation and Convexification Formulation

This section describes the solutions to the steam system minimum pressure drop problem found by the transformation and convexification formulation. A description of modelling experience with the transformation and convexification formulation is given initially, followed by the solution to the problem as described in Section 4.6.9.

5.4.1. Modelling Experience

The transformation and convexification technique of Pörn et al. (2008) was applied to the HEN pressure drop minimisation problem. This was attempted in order to transform the bilinear terms encountered when handling problems which are allowed to exhibit degenerate solutions into convex terms.

A number of variables alluded to in Chapter 4 were varied in an attempt to find the most optimal solution. It was however not the objective of this work to find a combination of variables that lead to the most optimal solution. Instead it was the intention to investigate feasible techniques to be used to overcome the difficulties encountered when solving the HEN pressure drop minimisation problem while allowing degenerate solutions.

This section describes some of the key modelling variables and attempts to describe the influence of these variables on the model outcomes.

Number of Tangents

The number of tangents used to approximate the nonlinear terms in the ET and PT can be varied. A larger number of tangents will lead to a closer approximation of the natural logarithm and square functions found in the ET and PT respectively. However the drawback of a large number of tangents is the large number of associated binary variables which need to be assigned to activate a particular tangent. These binary variables can be built into the formulation manually or if an MILP solver is capable of using SOS2 variables these can be used instead. This is discussed further in Section 4.3.5.

By utilising a branch and bound type MINLP solver, binary variables are fixed between the master MILP and nonlinear sub problems. By fixing binary variables only a certain portion of the solution space is available for the nonlinear sub problem to find a solution. This could negatively impact the final solution.

To ensure a larger solution space, initially low numbers of tangents were chosen ranging between 1 and 4. These solutions were then compared to larger numbers of tangents and it was found that solution spaces divided by between 5 and 10 tangents exhibited the best mix of solution time for the MILP master problem and feasible solutions in the NLP problems.

More powerful processors will likely be able to cater for larger numbers of tangents and the optimal number of tangents could be made a further field of investigation.

Slack Variable Penalty Constants

Slack variables are used to make the solution values tend closer to tangential points as shown in Section 4.6.6. These slack variables are intended to allow individual solutions to vary from the tangential points, however the iterative updating of tangential points is intended to find a solution.

The penalty constants assigned to the slack variables were attempted in a number of different ways. Initially a linear penalty constant where each heating stream i was penalised by a constant in the range of 0.1 to 10 was implemented. It was then found that varying the penalty constant based on the duty of the heating stream (where higher duty streams were penalised less) was implemented. This was

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achieved by setting the lowest duty stream penalty constant to 1 and varying all other streams accordingly, with stream 4 having a penalty constant of approximately 0.01. Other variations of these penalty constant approaches were also attempted.

A problem arises when making slack variables part of the objective function and that is the focus of the model can become directed at minimising these variables completely and not focussing on the network pressure drop. Therefore the penalty constants were also varied in orders of magnitude.

5.4.2. Problem solution

Additional Slack Variable

During the solution of the transformation and convexification problem it was found that feasible solutions were often only found when an additional slack energy variable was added to the sensible energy constraint. This additional slack variable adds energy to the system to allow the model to find starting solutions where it could not originally. This additional slack variable $\gamma_i^{SE,pos}$ is added to Constraint (4.122) and is shown in Constraint (5-3).

$$
\begin{aligned}
QL_i = SL_{j,i} Tsat &+ \left(\exp\left(L_{j,i}^{ET,PLT}\right) - \phi_L^{ET}\right)\exp\left(Tout_j^{ET,PLT}\right) \\
&- \left(\left(SL_{j,i}^{PT,PLT}\right)^{1/2} - \phi_{SL}^{PT}\right)\left(\left(Tout_i^{PT,PLT}\right)^{1/2} - \phi_{Tout}^{PT}\right) \\
&- \left(\left(L_{j,i}^{PT,PLT}\right)^{1/2} - \phi_L^{PT}\right)\left(\left(Tout_i^{PT,PLT}\right)^{1/2} - \phi_{Tout}^{PT}\right) \\
&- \gamma_i^{SE,neg} \\
&+ \gamma_i^{SE,pos} \qquad \forall i, j \in I
\end{aligned}
\tag{5-3}
$$

By including the additional slack variable the objective function has to find the minimum system pressure drop as well as minimise the two slack variables. The selection of appropriate penalty constants also applies to the positive slack variable.

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This variable essentially represents free energy and should therefore be heavily penalised for any use.

Both Constraint (4.122) and Constraint (4.122) were utilised to solve problem F. Many attempts to solve problem F were made with varying numbers of tangents. Many solutions of the pseudo exact problem revealed problem F having a better solution than problem G, but processing of the exact solution revealed the problem G solution to be better.

Solution Variants

Different numbers of tangents were utilised in an attempt to find solutions to problem F that showed an improved pressure drop to problem G. Solutions were tested with between 3 and 20 tangents. Those with few tangents typically showed large excess sensible heat values. Those with high numbers of tangents typically had poorer solutions which is likely due to restrictions on solution time. The most successful numbers of tangents ranged between 5 and 10 and solutions to these will be discussed.

The most successful solution using 5 tangents utilised Constraint (4.122) and exhibited penalty functions that varied according to the required duty of the various heat exchangers. . Problem F was solved to a pressure drop of 277.883 kPa. After processing, this solution was found to be 209.202 kPa. The initial solution to problem G was found to be 279.245 kPa and after processing was found to be 208.152 kPa. This solution shows the pressure drop for problem F to be higher than for problem G by 1.050 kPa.

The smallest difference between problem F and problem G was found from a model with 10 tangents utilising Constraint (4.122) and having the penalty functions vary according to the required duty of the various heat exchangers. Problem F was solved to a pressure drop of 282.788 kPa. After processing, this solution was found to be 211.525 kPa. The initial solution to problem G was found to be 287.187 kPa and after processing was found to be 210.994 kPa. This solution shows the pressure drop for problem F to be higher than for problem G by 0.531 kPa.

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The network arrangement for the solution to problem F and problem G are shown in **Figure 5-5** and **Figure 5-6** respectively. The largest pressure drop paths for both problems were found to be equal and are shown in **Figure 5-7** and **Figure 5-8** for problem F and problem G respectively.

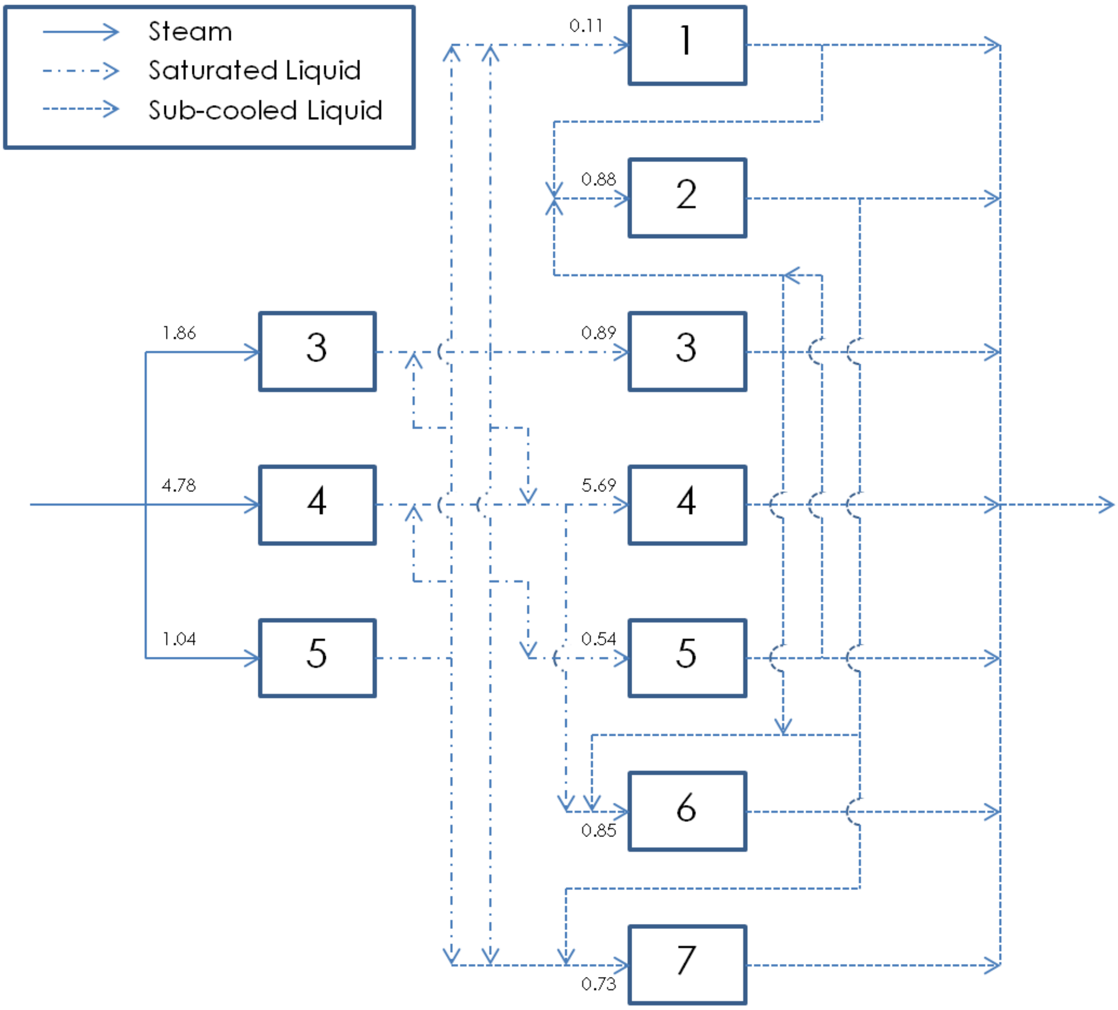

Figure 5-5: HEN layout for minimum pressure drop found using transformation and convexification technique

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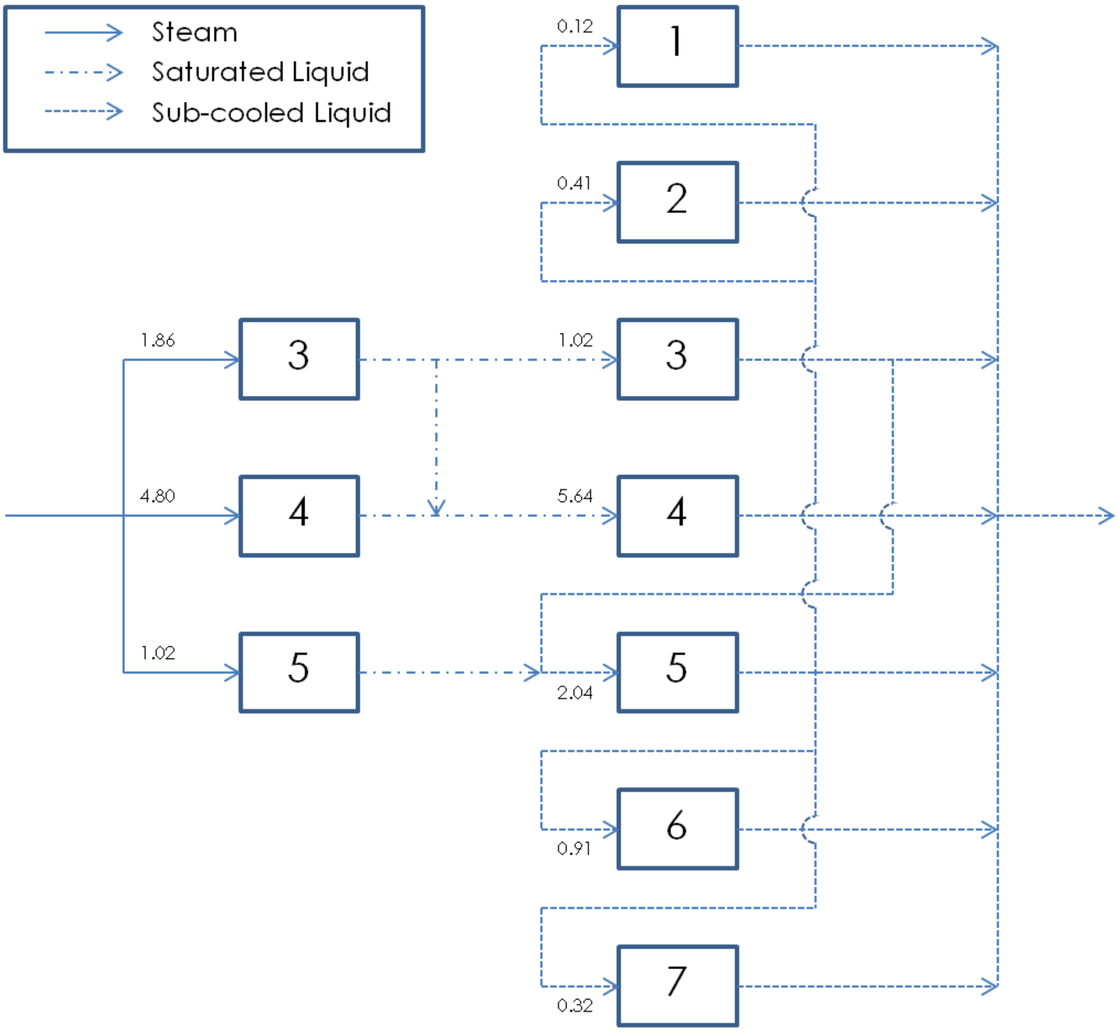

Figure 5-6: HEN layout for minimum pressure drop found using the test formulation for the transformation and convexification technique

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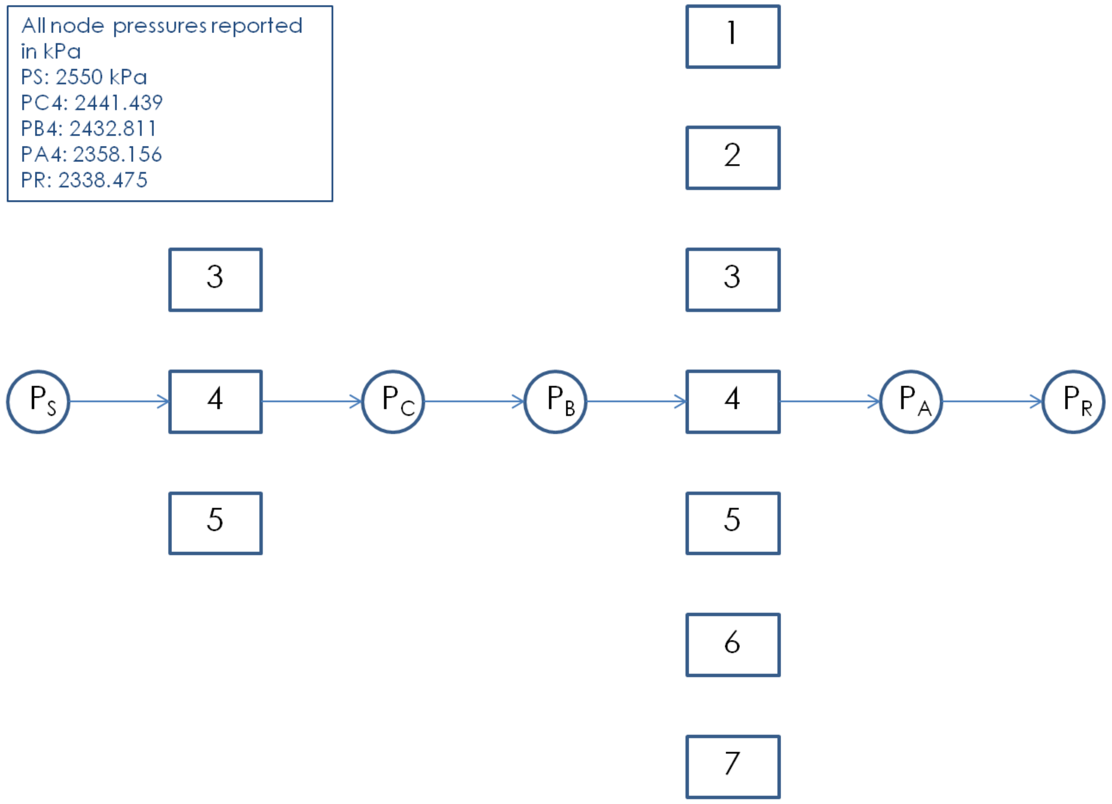

Figure 5-7: Maximum pressure drop path found through the transformation and convexification technique

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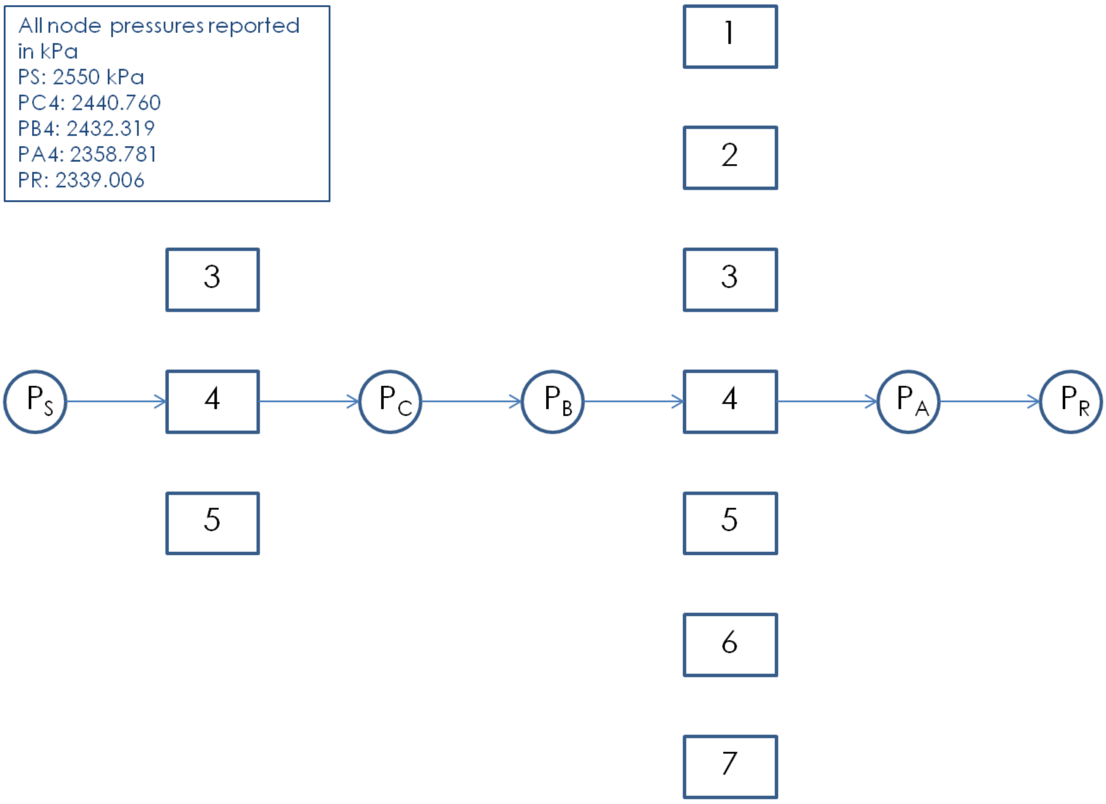

Figure 5-8: Maximum pressure drop path found through the test formulation for the transformation and convexification technique

From the results it can be proposed that solutions which focus on multiple objectives can occasionally lead to inferior solutions for the key objective, in this case network pressure drop.

5.5. Comparison of Results

By comparing the results from the relaxation and linearisation formulation and the transformation and convexification techniques it can be seen that the relaxation and linearisation technique is more effective as it yields a better network pressure drop by utilising a degenerate solution.

5.5.1. Relaxation and Linearisation Result

The relaxation and linearisation technique successfully improved the network pressure drop using a degenerate solution. The exact solution was found to differ from the relaxed solution, therefore the global optimality of the solution presented cannot be guaranteed.

5.5.2. Transformation and Convexification Result

The transformation and convexification technique fails to yield a better pressure drop than a solution found utilising the fixed outlet temperature approach of Savelski and Bagajewicz (2000). Furthermore this technique requires overestimation of the sensible energy terms. This will require additional design work to create a feasible HEN. The transformation and convexification technique of Pörn et al. (2008) is effective at solving MINLP problems, however it was found that this technique had difficulty being used alongside the critical path algorithm. This caused the objective function of problem F to minimise pressure drop along with slack variables. This trade off proved to be less effective than the pure pressure drop objective function utilised when the outlet temperatures were fixed.

It is likely that the manipulations employed in the transformation and convexification methodology presented in this work can be improved upon and this could be the basis of further research.

5.5.3. Conclusion

The outlet temperature of heat exchangers can be allowed to vary in an attempt to further reduce the pressure drop through a HEN. It was found that these degenerate solutions can successfully be used to reduce the pressure drop through a HEN as compared to a network where the outlet temperatures of the individual heat exchangers are fixed to their minimum values.

The relaxation and linearisation technique was found to successfully improve the HEN network pressure drop using a degenerate solution. This was done by overcoming the complications of a nonconvex MINLP problem utilising a technique successfully employed in literature. As the transformation and convexification technique was unable to find an improved solution, the relaxation and linearisation technique was found to be the most effective.

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5.6. Second Case Study HEN

A second case study was created in order to further test the relaxation and linearisation methodology to minimise steam system HEN pressure drop.

As for the first case study, the process stream parameters used for the second case study have been adjusted by the heat exchanger limiting temperature data to form the limiting hot utility stream data shown in. The steam utility information is identical to that used by Price and Majozi[14], as are the heat exchanger design principles.

Table 5-5: Hot utility stream data for second case study

Stream	TL Target (°C)	TL Supply (°C)	Duty (kW)	Minimum Flowrate (kg/s)
1	50	175	752.5	0.59
2	50	175	752.5	0.14
3	180	45	193.5	0.62
4	90	135	580.5	0.05
5	70	155	666.5	0.2
6	40	185	795.5	1.99
7	130	95	408.5	0.03
8	80	145	623.5	0.26
Total			**7 353**	**3.88**

The same hot utility stream data as shown in **Table 5-2** will be used. The second order pressure drop correlation polynomial constants are shown in . As before these heat exchangers have been designed with basic design principles of Sinnot (2005) which are shown in Appendix A.

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Table 5-6: Hot utility stream data for second case study

Description	K2(Pa.s2/kg2)	K1 (Pa.s/kg)	K0 (Pa)
Utility Stream 1 - Condenser	3.56E+04	2.69E+03	-6.10E+01
Utility Stream 2 - Condenser	1.44E+05	5.97E+03	-8.20E+01
Utility Stream 3 - Condenser	2.76E+04	3.77E+03	-1.38E+02
Utility Stream 4 - Condenser	1.59E+06	4.57E+04	-3.34E+02
Utility Stream 5 - Condenser	2.71E+05	4.73E+03	-3.00E+01
Utility Stream 6 - Condenser	3.23E+03	4.82E+02	-2.60E+01
Utility Stream 7 - Condenser	7.85E+05	1.61E+04	-1.11E+02
Utility Stream 8 - Condenser	2.05E+05	4.84E+03	-3.80E+01
Utility Stream 1 – Heat Exchanger	3.26E+03	1.67E+03	-2.62E+02
Utility Stream 2 – Heat Exchanger	1.96E+03	8.28E+02	-1.30E+02
Utility Stream 3 – Heat Exchanger	1.16E+04	7.95E+03	-1.25E+03
Utility Stream 4 – Heat Exchanger	8.00E+02	3.41E+02	-5.30E+01
Utility Stream 5 – Heat Exchanger	4.81E+03	2.60E+03	-4.07E+02
Utility Stream 6 – Heat Exchanger	6.87E+03	4.56E+03	-7.14E+02
Utility Stream 7 – Heat Exchanger	2.74E+03	1.28E+03	-2.00E+02
Utility Stream 7 – Heat Exchanger	2.09E+03	1.08E+03	-1.68E+02
Saturated Condensate Recycle/Reuse Pipework (SL)	1.09E+03	7.49E+03	2.19E+04
Sub-Cooled Condensate Recycle/Reuse Pipework (L)	1.86E+03	1.28E+04	3.74E+04
Saturate Condensate Boiler Return Pipework (FRL)	2.80E+03	1.92E+04	5.61E+04
Sub-Cooled Condensate Boiler Return Pipework (FRS)	1.09E+03	7.49E+03	2.19E+04

5.6.1. Minimum Steam Flowrate

The minimum steam flowrate for the system described in **Table 5-5** was found using the technique of Coetzee and Majozi (2010) and calculated as 2.80 kg/s. This steam flowrate can now be fixed to solve for the minimum pressure drop of the system.

This steam flowrate was also found by allowing the heat exchanger outlet temperatures to vary. Therefore the potential for degenerate solutions for this case study exists.

5.6.2. System Pressure Drop

Here the system pressure drop was solved for using the fixed heat exchanger outlet temperatures as well as with allowing the temperatures to vary.

Fixed Heat Exchanger Outlet Temperatures

By fixing the heat exchanger outlet temperatures to minimum described in **Table 5-5** the minimum pressure drop for the system was solved to 164.16 kPa.

This value can now be used as a basis for comparison for the degenerate solution.

Variable Heat Exchanger Outlet Temperatures

By allowing the hot utility stream heat exchanger outlet temperatures to vary, a minimum pressure drop of 151.95 kPa was found. This represents a 7.1% improvement on the previous solution.

The network flow diagram for this solution is shown in **Figure 5-9**.

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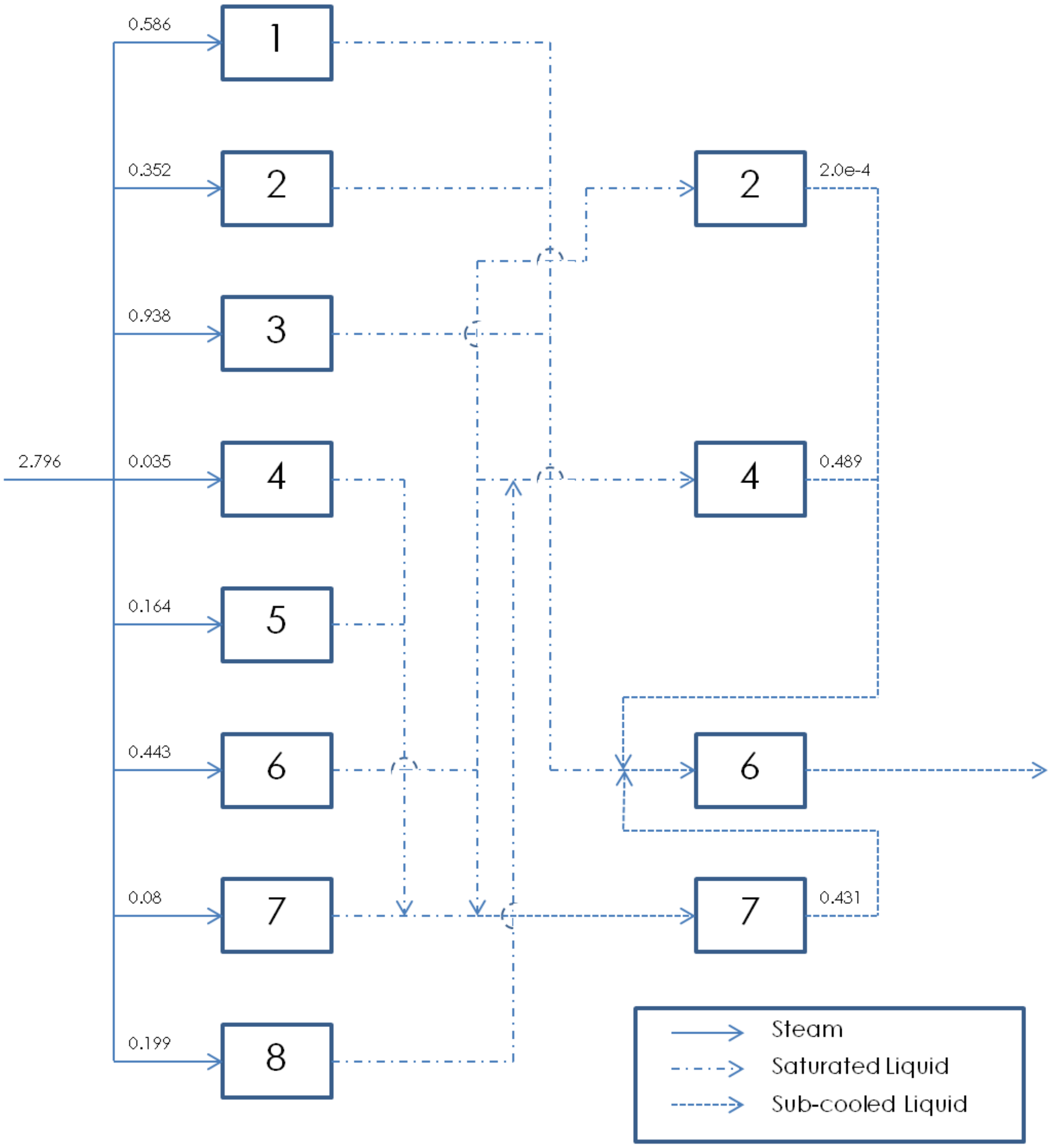

Figure 5-9: Network for the Degenerate Solution to the Second Case Study

The largest pressure drop path for the solution shown in **Figure 5-9** is shown in

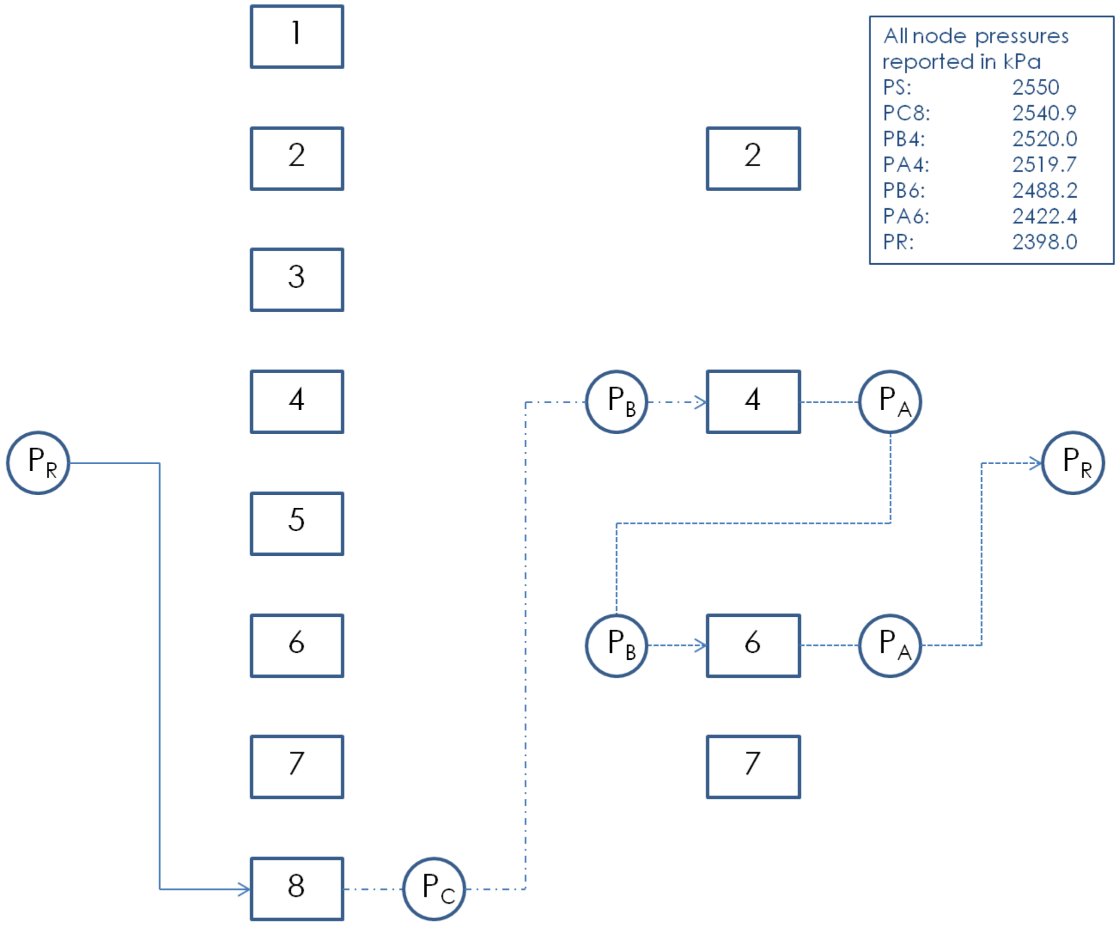

Figure 5-10: Largest Pressure Drop Path for the Solution in the Second Case Study

The outlet temperatures from the result are shown in **Table 5-7**. From this table it can be seen that two heat exchanger outlet temperatures vary to achieve the new minimum HEN pressure drop.

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Table 5-7: Utility Heat Exchanger Outlet Temperatures from Second Case Study

Process Stream	Minimum Utility Outlet Temperature (°C)	Outlet T From Degenerate Solution (°C)
1	50.00	50.00
2	50.00	154.01
3	180.00	180.00
4	90.00	91.87
5	70.00	70.00
6	40.00	40.00
7	130.00	130.00
8	80.00	80.00

5.6.3. Discussion of Results

From the results of the second case study it can be seen that by allowing the hot utility stream outlet temperature to vary, a better system minimum pressure drop can be achieved while still achieving the minimum steam flowrate for the system. Therefore degenerate solutions can be considered a viable option for HENs in order to minimise further design variables in addition to steam flowrate.

5.7. Maintaining Boiler Efficiency

This section is intended to compare the results of the case study used to maintain the boiler efficiency with the use of a dedicated pre heater as shown by Price and Majozi (2010a) to that of a problem which utilises degenerate solutions.

A number of parameters are used to create a base boiler efficiency in the work of Price and Majozi (2010a). **Figure 3.1** is reproduced along with typical steam system temperatures which were used to create a comparative boiler efficiency to compare results in Price and Majozi (2010a) and Price and Majozi (2010b). The steam system is shown in **Figure 5-11** and the typical temperature parameters are shown in **Table 5-8** which were taken from a survey of Harrel (1996).

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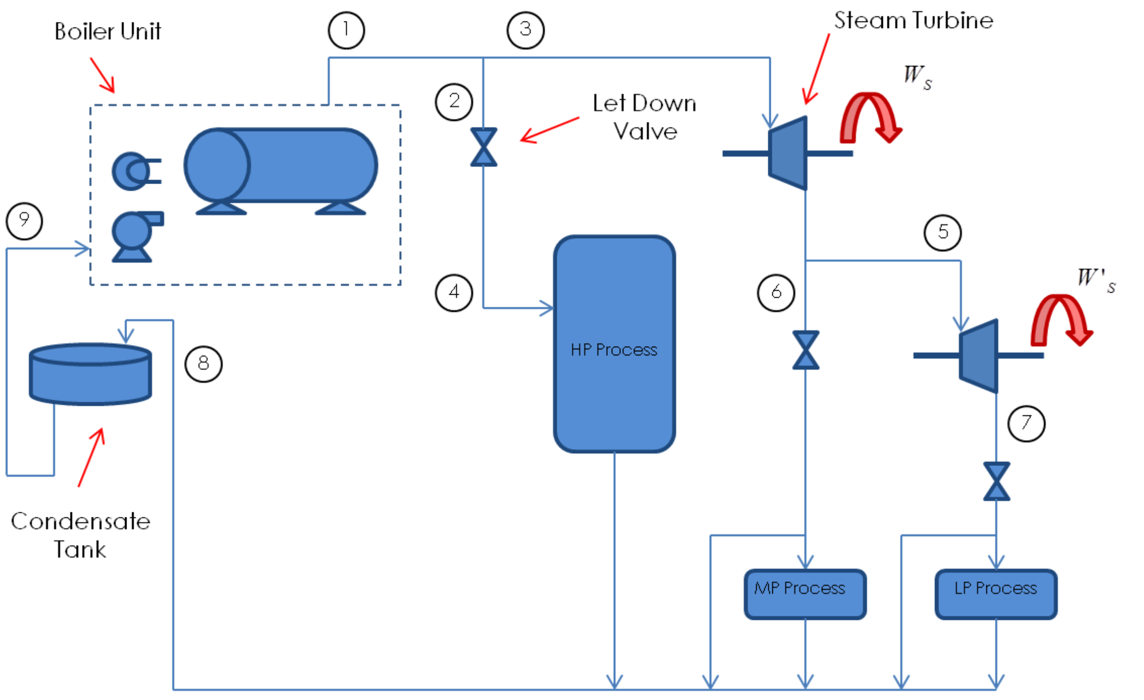

Figure 5-11: Steam System used to Show Boiler Efficiency Temperature Parameters

Table 5-8: Steam System Parameters (Harrel, 1996)

Description	T (°C)	P (kPa)	T^{sat} (°C)
High Pressure (HP) from boiler	399	4 238	254
Medium Pressure (MP)	327	1 480	197
Process Pressure (an example)	225	2 550	225
Intermediate Pressure (IP)	209	377	141
Low Pressure (LP)	221	164	113
Deaerator Outlet	113	164	113
Feed Pump outlet to the boiler	116	6 310	277

The HP steam from the boiler is shown as stream 1 in **Figure 5-11**. Stream 2 is at the same conditions and is let down to stream 4 at the process pressure. The stream entering the MP Process and LP Process are at medium pressure and low pressure respectively. The stream leading to the boiler feed water pump is indicated as deaerator outlet, while stream 10 is shown as the feed pump outlet to the boiler.

As discussed in Section 3.4, the boiler efficiency represented by Constraint (3.22) is not a strict definition of boiler efficiency but can however be used as a comparative

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tool to investigate the effects of changing parameters in the steam system. The boiler efficiency constraint is expanded in the context of the steam system of interest and is shown in Constraint (4.131). This constraint has been reproduced as Constraint (5.4) for clarity. To calculate the initial steam system boiler efficiency a number of other parameters are required. These constraints are derived from a number of sources and shown in **Table 3.1** which is reproduced in **Table 5-9** for clarity. The entire mass flowrate shown in **Table 5-9** as F comprises both the HP Process return flowrate as well as that of the two turbine processes MP Process and LP Process. This flowrate and temperature is shown in **Table 5-10**.

$$\eta_b = \frac{q\left(\left(FS + F_{turb}\right)/F^U\right)}{\left(c_p\left(T_{sat} - T_{boil}\right) + q\right)\left[\left(1 + b\right)\left(\left(FS + F_{turb}\right)/F^U\right) + a\right]} \tag{5-4}$$

Table 5-9: Steam System Data

Parameter	
q (sum of the latent and superheated energy)	2110 (kJ/kg)
F^U (maximum steam load of boiler)	20.19 (kg/s)
c_P (specific heat capacity of boiler feed water)	4.3 (kJ/kg.K)
a (regression parameter)	0.0126
b (regression parameter)	0.2156
T_{sat} (saturated steam temperature at boiler pressure)	253.20 (°C)
T_{boil} (initial return temperature to the boiler for 100% η_b calculation)	116.10 (°C)
F (initial return flowrate for 100% η_b calculation)	18.17 (kg/s)

Table 5-10: Turbine Outlet Data

Turbine condensate mass flowrate	7.27 kg/s
Turbine condensate return temperature	113 °C

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Thus using the initial steam system flowrate of 10.98 kg/s as well as the relevant temperatures from **Table 5-8** and parameters from **Table 5-9** and **Table 5-10** the initial steam system boiler efficiency is calculated as 63.4%.

5.7.1. Solution from Price and Majozi (2010a)

As described in Section 3.4 and Section 4.8, by reducing the steam flowrate to a HEN the boiler efficiency is negatively affected by both the reduction in the circulating steam through the system as well as the associated decrease in the condensate return temperature to the boiler. It was however found that increasing the condensate return temperature would be able to maintain the boiler efficiency. Price and Majozi (1010a) showed how after reducing the steam flowrate to a HEN an additional pre heater can be added to the HEN in order to elevate the condensate return temperature to such an extent that the boiler efficiency is maintained.

The same steam system described in Section 5.1 was used as a case study for this technique. The steam flowrate for the system was reduced from 10.98 kg/s to 7.68 kg/s. The original outlet temperature of the steam system was at the saturated temperature of 225°C. By reducing the steam flowrate and utilising condensate to heat a portion of the process streams the subsequent outlet temperature was calculated as 46°C. Using the other parameters of the steam system which remained unchanged, the boiler efficiency for the system was calculated as 59.8%, a decrease of 3.6%.

By incorporating a dedicated pre heater into the HEN it was found that the boiler efficiency could be effectively maintained at 63.4%. The steam flowrate required to maintain the boiler efficiency at this level was found to be 8.76 kg/s. this is 13.9% higher than the minimum steam flowrate of 7.68 kg/s but still a saving of 19.6% of the original 10.98 kg/s. The process outlet temperature was found to be 60.4°C. This resulted in a temperature of 84.2°C when combined with the turbine stream. The duty of the additional heat exchanger was calculated as 2 256.4 kW. The return stream to the boiler thus had a temperature of 117.0°C which was sufficient to maintain the boiler efficiency for the reduced steam flowrate. The HEN arrangement

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is shown in **Figure 5-12**. The additional heat exchanger is used to heat stream 8 and is identified with an asterisk (*).

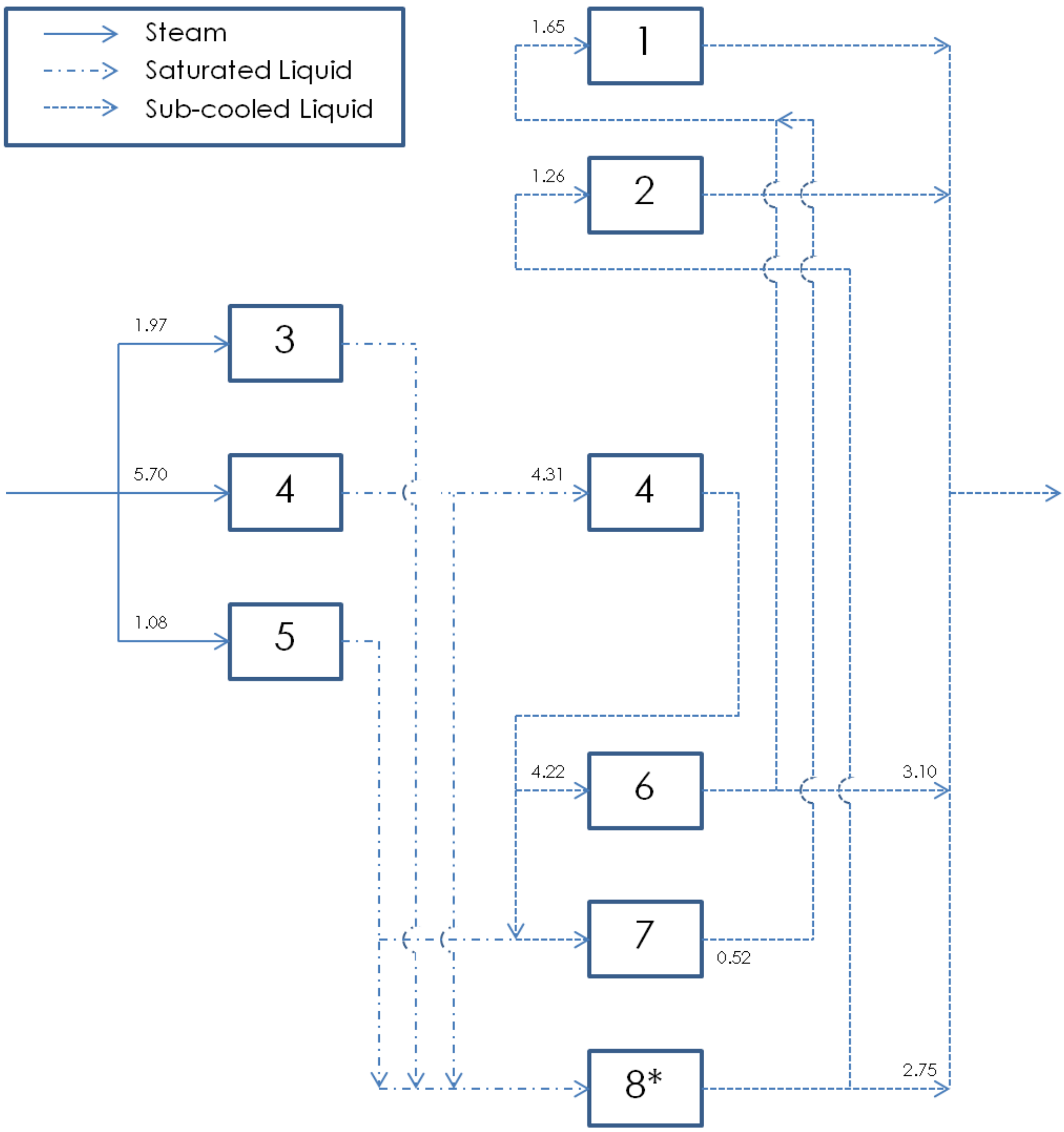

Figure 5-12: HEN with Additional Heat Exchanger

The solution technique utilised to account for the bilinear boiler efficiency terms, as discussed in Section 4.8.3, was that of Quesada and Grossmann (1995). Price and

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Majozi (2010a) found the solution to the MILP starting model to be 7.68 kg/s, insinuating that the boiler efficiency could be maintained without the need for any additional steam in the HEN. The solution of the exact MINLP revealed a steam flowrate of 8.76 kg/s.

The pressure drop minimisation solution of Price and Majozi (2010c) was reworked to remove singularities in the pressure drop constraints. This is not the case for the boiler efficiency constraints and as such the solution of Price and Majozi (2010c) will be maintained.

5.7.2. Degenerate Solution with Relaxation and Linearisation Formulation

This section describes the solution to the problem of maintaining boiler efficiency with a dedicated pre heater while allowing for degenerate solutions within the problem formulation.

The relaxation and linearisation formulation requires a large number of replacement variables for those in the sensible energy constraint as was found for the pressure drop minimisation case along with those found in calculating the boiler efficiency.

The relaxation and linearisation technique requires the solution of a linearised model which becomes the starting point of the exact model. Unlike the solution of Price and Majozi (2010a), the solution allowing for degenerate solutions will require the terms in the sensible energy constraint to be treated in the same way as those of the boiler efficiency constraints.

By incorporating the degenerate solutions to minimise the steam flowrate required to maintain the boiler efficiency with an additional dedicated heat exchanger, the solution to the MILP starting point problem was found to be 7.68 kg/s. This is identical to that found by Price and Majozi (2010a). This suggests the boiler efficiency could be maintained without the need to preheat the boiler return stream. Based on observations and the boiler efficiency calculated after heat integration was applied to the steam system this solution appears to be a large underestimate.

The solution to the exact MINLP was found to be 8.76 kg/s. This is identical to the value found by Price and Majozi (2010a). The HEN arrangement however is quite different and is shown in **Figure 5-13**.

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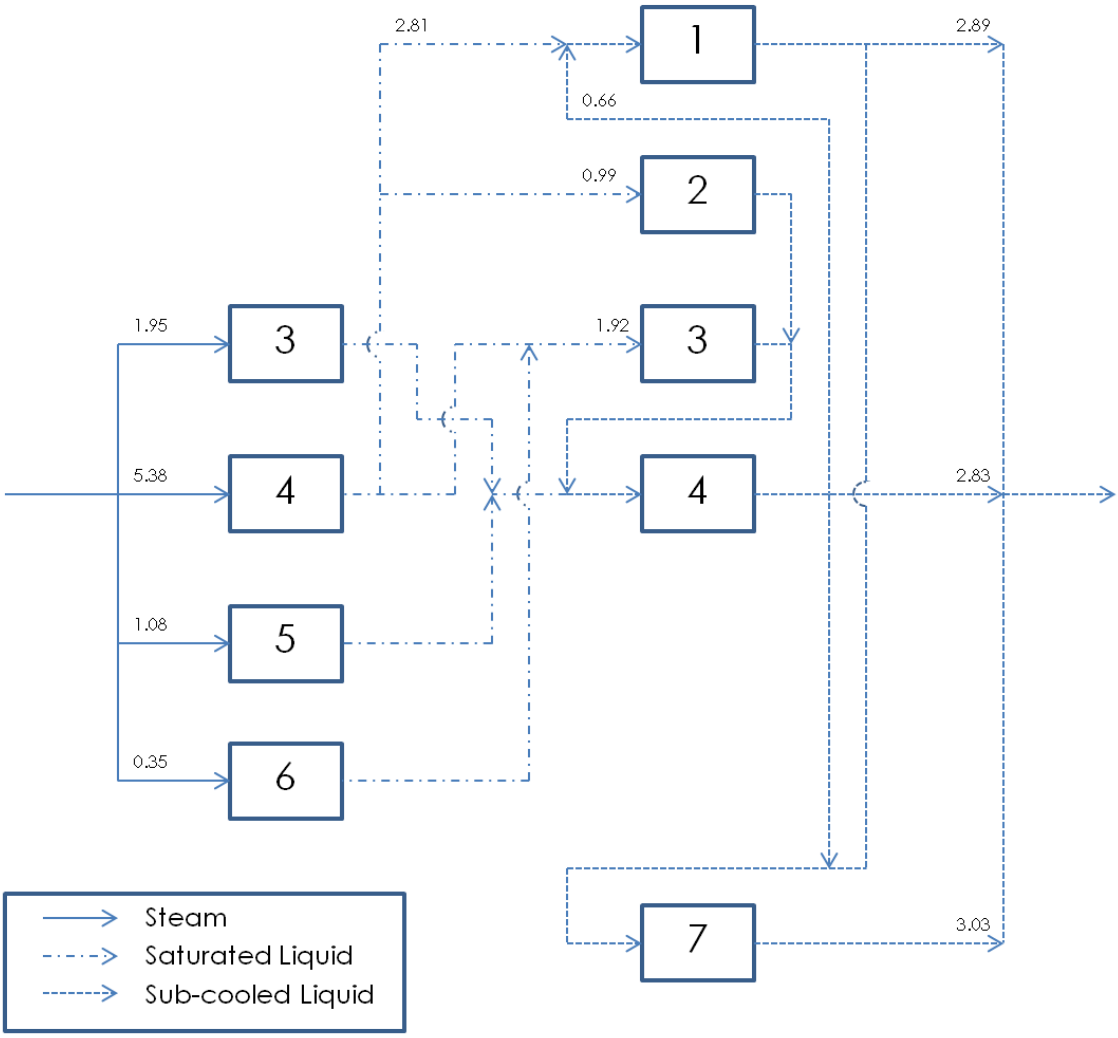

Figure 5-13: HEN with Additional Heat Exchanger Allowing for Degenerate Solutions

From **Figure 5-13** it can be seen that an additional heat exchanger is not required to preheat the boiler feed water. This is as a result of the higher outlet temperatures from the various heat exchangers. The outlet temperatures of the three streams returning condensate to the steam boiler as well as the resultant HEN outlet conditions F and T^{proc} are shown in **Table 5-11**. In the table it can be seen that the high return temperature of stream 1 is sufficient to lift the return temperature of the entire HEN to such a level that the boiler efficiency can be maintained without the need for an additional heat exchanger.

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Table 5-11: Outlet Conditions of Streams in Degenerate HEN in **Figure 5-13**

Stream	T (°C)	Flow (kg/s)
Stream 1	190.0	2.89
Stream 4	89.0	2.83
Stream 7	83.0	3.03
Heat Exchanger Network	120.3	8.76

The HEN arrangement shown in **Figure 5-13** does not require an additional pre heater to maintain the boiler efficiency. This could be seen as a large advantage over the HEN arrangement shown in **Figure 5-12** as the dedicated pre heater is needed to heat the entire return stream to the boiler which has a high flowrate as compared to the internal streams and hence likely a more costly heat exchanger. Another factor however is the resulting inlet temperature to the boiler feed water pump. From the results this temperature is calculated as 117.0°C. Unless certain precautions are taken, there is a large risk of cavitation for the boiler feed water pump.

A number of process steam systems maintain pressurised condensate return lines and condensate collection tanks. For such systems where the condensate can be pressurised to such an extent as to prevent the risk of cavitation this problem can be avoided. For other systems condensate is collected in an open condensate return tank. Elevating the condensate return temperature to 117.0°C, above the boiling temperature at atmospheric conditions, would result in flashing in the condensate return tank. This would result in large water losses from the steam system as well as wasted energy. The condensate in the condensate tank would still be close to saturated conditions. For these systems the only pressurisation to occur before condensate enters the feed water pump is as a result of the head of pressure from the condensate tank to the pump. Many plants keep condensate return tanks elevated for this reason. In these situations it is likely that the pressure head from the elevated condensate return tank would not be sufficient to prevent cavitation in the feed water pump as the conditions in the condensate tank would be close to saturation. Such systems could require a condenser/cooler to prevent flashing losses as well as protect the boiler feed water pump.

An alternative solution would be to restrict the feed water pump inlet temperature in the HEN design. This can be achieved by restricting T^{coll} in the formulation to a safe pumping temperature sufficiently below the flashing temperature of condensate at atmospheric conditions. An additional constraint was therefore added to the formulation to restrict the inlet temperature to the boiler feed water pump. This is shown in Constraint (5-5).

$$T^{coll} \leq T^{coll,U} \qquad (5\text{-}5)$$

In Constraint (5-5) the limiting collection temperature is denoted as $T^{coll,U}$ and can be set at a level deemed safe for the boiler feed water pump. The lower the temperature is set to, the larger the duty required for the additional pre heater is likely to be. As an exercise the limit was set to 80°C.

The boiler efficiency was able to be maintained with a limiting collection temperature. The steam flowrate was also able to be maintained at the level found in Price and Majozi (2010a) of 8.76 kg/s. The HEN arrangement is shown in **Figure 5-14**.

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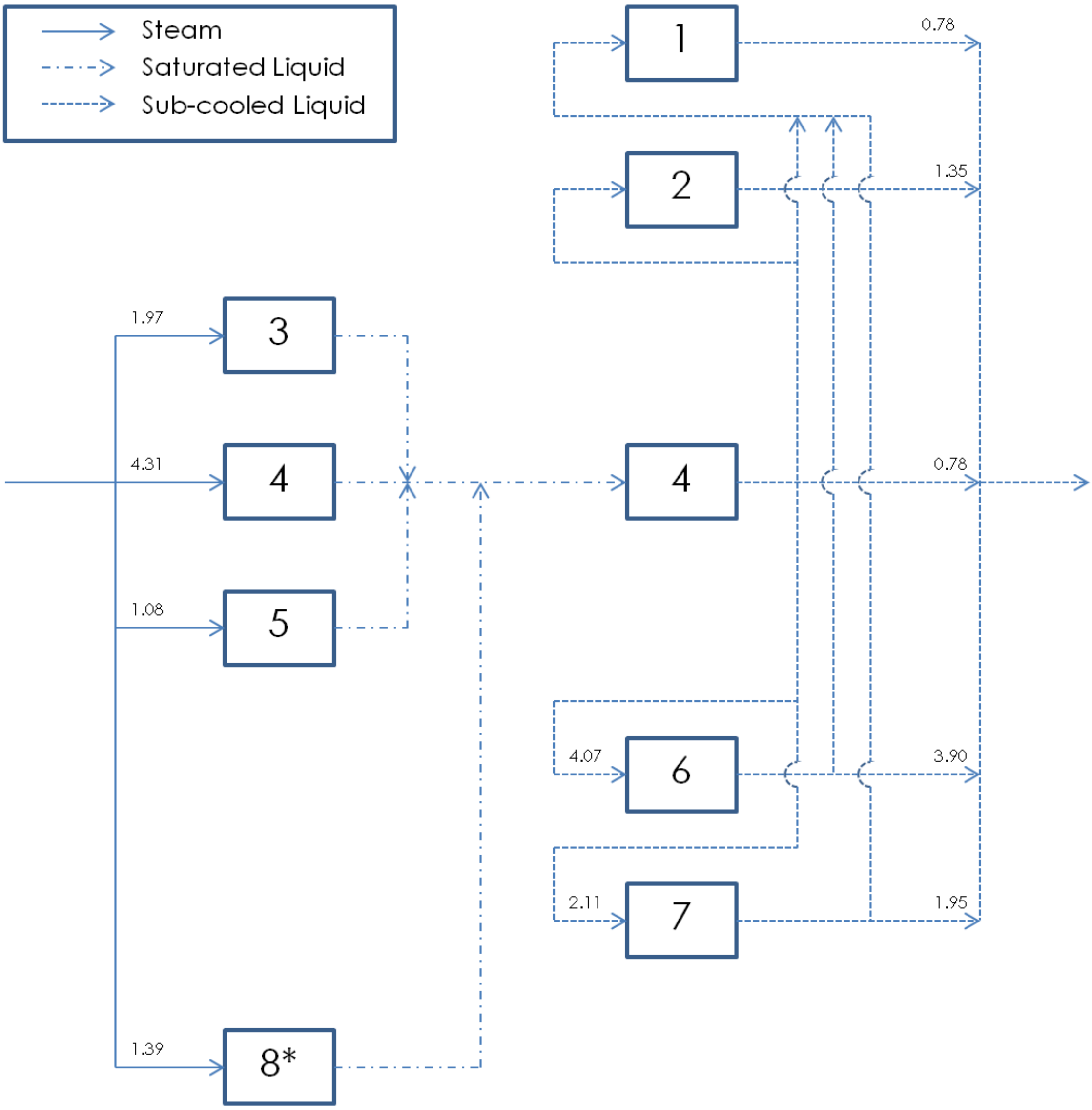

Figure 5-14: HEN with Additional Heat Exchanger with Limited Collection Temperature

In the HEN arrangement in **Figure 5-14** the process return temperature is significantly reduced from that of the HEN arrangement in **Figure 5-13**. The outlet temperature is now 52.6°C, thus, along with the turbine streams a collection temperature of 80°C is achieved. The additional heat exchanger then elevates the return temperature to the boiler by 37°C. The duty of the additional pre heater is calculated as 2 548.4 kW.

The duty of the pre heater is higher than that found by Price and Majozi (2010a) of 2256.4kW. The variable outlet temperature for the HEN can therefore be used to vary the required size of the pre heater. As seen for the arrangement in **Figure 5-13**, the

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additional pre heater can be eliminated entirely with high return temperatures. Restrictions on the condensate collection and pumping temperature should however be taken into account for these formulations, which can now be achieved with variable heat exchanger outlet temperatures. The design freedom provided by incorporating degenerate solutions into the boiler efficiency framework can result in savings in capital cost for new equipment as well as potentially allowing the system to be further optimised for other network variables.

5.7.3. Degenerate Solution with Transformation and Convexification Formulation

Initial Solution

This section describes the results attained for the problem of maintaining the boiler efficiency of a steam system using a dedicated pre heater after the steam flowrate to the system was minimised using methods of process integration.

As the steam flowrate to the system is unknown, no additional energy can be allowed for by over estimations from the various transforms found in the formulation. As such the same penalty functions as utilised in Constraint (4.122) were used in this formulation. The positive slack variable described in Constraint (5-3) was included to provide a feasible starting point where necessary.

The discretised solution process described in Section 4.6.5 is also problematic in the boiler efficiency formulation due to the equality constraints relating the various pre heater temperatures. This is due to the over estimation of the discretisations not necessarily being equal to one another, unless the solution values appear at the tangential point. This phenomena was observed with the pressure drop minimisation formulation and was catered for with slack variables as shown in Constraint (5-3). Slack variables were therefore also added to each of the temperature definition constraints described by Constraints (4.136) to (4.138). The variables were then added to the objective function which can be seen in Constraint (5-6).

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$$MinZ = FS + \begin{pmatrix} \sum_i QL_i^{slackpos} + \sum_i QL_i^{slackneg} + T_{proc}^{slackpos} + T_{proc}^{slackneg} + \\ T_{coll}^{slackpos} + T_{coll}^{slackneg} + T_{boil}^{slackpos} + T_{boil}^{slackneg} \end{pmatrix} \Omega \qquad (5\text{-}6)$$

Where Ω is some penalty function constant. This constant is likely to take on a high value as additional energy will distort the solution greatly.

As discussed in Section 5.4.1, a number of modelling variables play a part in the solution process. Using the modelling experience from Section 5.4.1 a number of these modelling variables were attempted but no feasible solution was found.

Equality constraints were also simplified to two inequality constraints as is advised in Pörn et al. (2008). This formulation did not result in any feasible solutions.

Further Modelling

The transformation and convexification formulation presented with linearised functions for the convexification variables is complex to solve when ET and PT transforms appear in many constraints. As the linearisations are not necessarily equivalent, the constraints cannot always be represented as equality constraints but rather as inequality constraints to allow for variations in the degree of linearisation. This is particularly prevalent in the boiler efficiency problem as many of the bilinear terms appear in equality constraints. These constraints can be represented with a combination of inequality constraints which was completed for the formulation. Slack variables were provided to the formulation in an attempt to counter this phenomenon with limited success.

Linearisations allow the entire problem to be convexified, however, as described in Pörn et al. (2008), by transforming the complex bilinear terms into convex terms and effectively transferring the nonconvexity to a single term in a constraint this can simplify the problem. This approach was attempted for the boiler efficiency problem. All transformation variables were formulated without discretisations. The resultant MINLP is nonconvex due to the natural logarithm and square functions in the formulation for the ET and PT respectively.

As was noted on the solution to the boiler efficiency problem utilising the relaxation and lineariasation technique of Section 5.7.2, the boiler feed water pumping temperature can be limited to prevent cavitation. Therefore Constraint (5-5) was incorporated into this formulation. The limiting temperature was once again set to 80°C. The minimum flowrate found in the formulation was 8.76 kg/s. This solution value is identical to that found by Price and Majozi (2010a) as well as using the relaxation and linearisation technique. The network layout is shown in **Figure 5-15**.

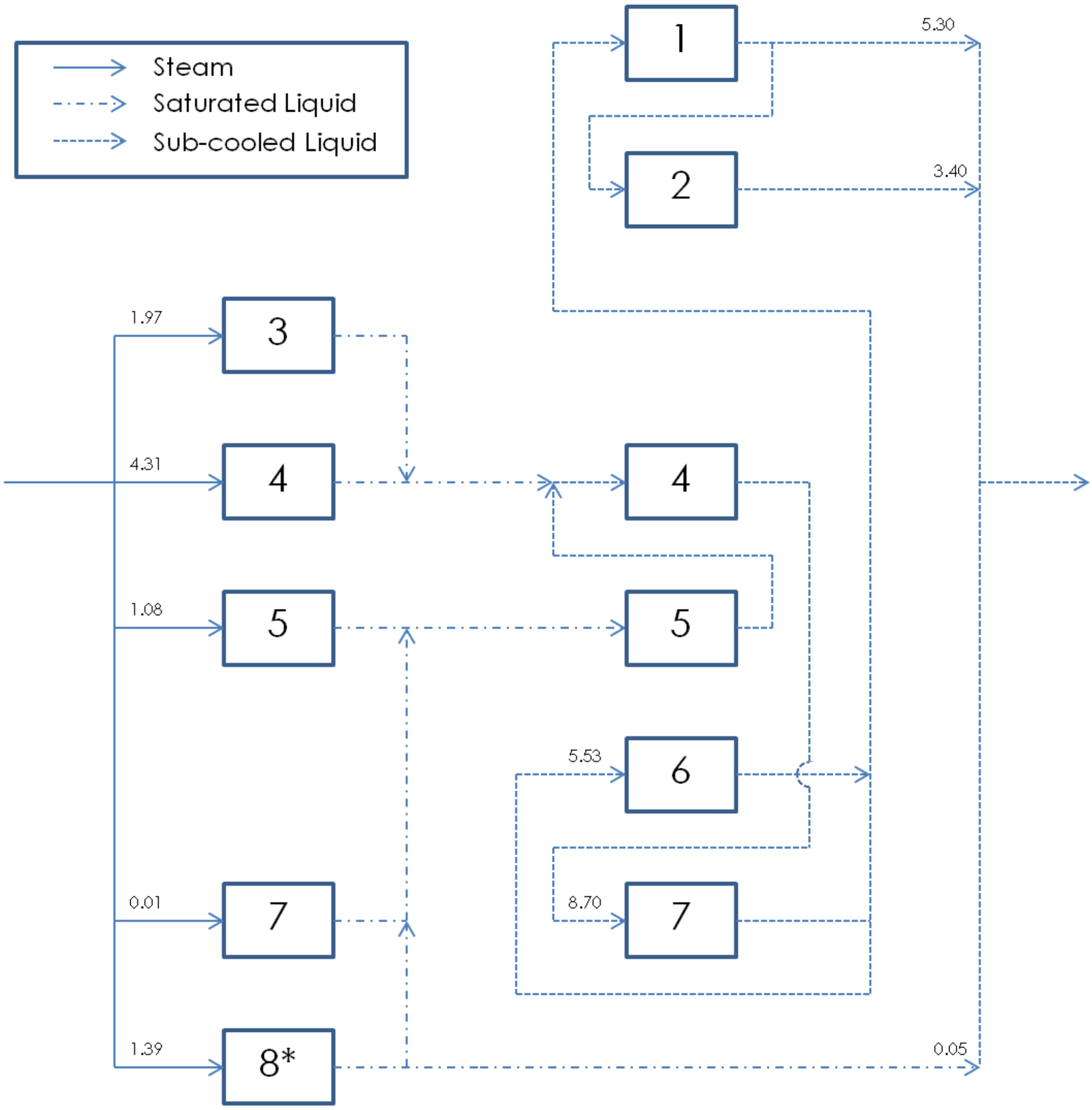

Figure 5-15: HEN found Using Transformation and Convexification Technique

The various stream temperatures for the boiler return are shown in **Table 5-12**. This result shows how the transformation and convexification can be utilised to provide alternate means to solve the boiler efficiency problem. By comparing the outlet temperatures in **Table 5-12** to the limiting temperatures in **Table 5-1** it can be seen that significant changes in the outlet temperatures are realised, adding a large range of solutions.

Table 5-12: Outlet Conditions of Streams in Degenerate HEN in **Figure 5-15**

Stream	T (°C)	Flow (kg/s)
Stream 1	60.13	5.30
Stream 2	38.25	3.40
Stream 4	89.00	8.70
Stream 5	223.88	2.42
Stream 6	54.0	5.53
Stream 7	80.71	8.70
Heat Exchanger Network	52.6	8.76

5.7.4. Comparison of Results

By comparing the results of the boiler efficiency problem solved with the relaxation and linearisation as well as the transformation and convexification formulations, it can be seen that the both formulations resulted in the same solution. The transformation and convexification technique makes use of discretisation to completely transform the formulation to one exhibiting only convex terms. This did not yield a feasible result and as such these discretisations were removed. The resulting formulation, while nonconvex, did still simplify the problem and the resulting solution was found to be the same as that found by the relaxation and linearisation technique.

For the boiler efficiency optimisation problem, utilisation of degenerate solutions was shown to give larger flexibility to the network design by varying the process outlet temperature, T^{proc}, and limiting the size of the additional pre heater required to provide sufficient energy to the boiler feed water stream to maintain the boiler efficiency. The minimum steam flowrate found by both the relaxation and

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linearisation technique as well as the transformation and convexification technique was found to be the same as those found by Price and Majozi (2010a). The network structures for these solutions all differ significantly, suggesting further optimisation potential for another network variable such as heat exchange area or pressure drop.

No feasible solution was found using the discretised transformation and convexification formulation. It is believed that complexities arise when utilising the discretised form of the formulation when working with branch and bound type MINLP solvers due to limited solution space. This result mimics the experience from the pressure drop minimisation problem.

5.8. References

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6. Conclusions and Discussion

This chapter summarises the findings of this work and discusses areas of further application and potential research.

6.1. Conclusions

Minimum heating and cooling utilities can be determined for process HENs. A technique used to find the heating or cooling utility flowrate is a condition of network optimality where the limiting temperatures of the heat exchangers are set to their bounds. This approach typically results in a linear problem which can be solved to global optimality. The minimum flowrate can be achieved with an infinite number of network arrangements therefore additional system variables can be optimised while still maintaining the minimum steam flowrate.

Once a minimum utility flowrate is found the conditions of network optimality can be relaxed in order to further optimise additional system variables. This is due to the solution space for the system being enlarged by allowing the limiting temperatures of utility streams leaving heat exchangers to vary.

By allowing the outlet temperatures to vary bilinear terms are created in the energy constraints in the formulation. Bilinear terms are nonlinear and nonconvex and therefore present difficulties to conventional optimisation solvers.

This work presents the optimisation of two system variables, namely heat exchanger network pressure drop for heating systems as well as boiler efficiency. Two methods are proposed to cater for the bilinear terms created by relaxing the conditions of network optimality. The results from case studies were compared with previous work in order to determine the effectiveness of the methods.

6.1.1. Pressure Drop Comparison

The minimum HEN pressure drop presented by Price and Majozi (2010c) was achieved by relaxing the minimum steam flowrate. This is due to singularities formed when flow variables take zero values. The model was resolved using translations to shift the flow variables away from zero. This allowed the minimum pressure drop to be found while still retaining the exact minimum steam flowrate. The model was solved successfully as an MINLP problem.

The minimum HEN pressure drop for this system was found to be 364.430 kPa. This result shows how translations can be used effectively to overcome singularities. An effective means to find a network that exhibits the minimum pressure drop while still achieving the minimum steam flowrate has been created successfully. A second case study was used to determine the rigorousness of this technique and a minimum system pressure drop of 164.16 kPa was achieved.

By allowing degenerate solutions to the HEN pressure drop minimisation problem the size of the solution space is enlarged. This comes at the expense of nonlinear, nonconvex bilinear terms being added to the formulation. These bilinear terms can be reformulated using the relaxation and linearisation formulation. Using this technique a better pressure drop for the system was found using two case studies. The first case study resulted in a minimum pressure drop of 360.46 kPa, an improvement of 1.1%. This result shows how degenerate solutions can be used to improve the solutions to nonlinear network optimisation problems. A solution of the second case study was found to be 151.95 kPa. This is an improvement of 7.1% from the fixed heat exchanger outlet temperature solution.

The same problem was attempted using the transformation and convexification technique to create a convex problem which is much more easily solvable with conventional MINLP solvers. This technique was not found to be as successful in finding a minimum pressure drop. This is understood to be due to the nature of the discretisation process which accompanies the transformation step of the formulation. The discretisation is accomplished using binary variables which limit the NLP sub problem solution space when using branch and bound type MINLP solvers. The solution was found not to converge to a point where the discretisation did not unduly benefit the formulation, skewing the minimum pressure drop results. The use of this technique to address degenerate solutions and their benefits over formulations utilising only the conditions of network optimality was tested by comparing the solution of the two problems with the same degree of relaxation provided by the

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discretisation of the transformation and convexification technique. The pressure drop found by effectively adding the same degree of sensible energy to the fixed outlet temperature formulation was 208.15 kPa. The solution utilising degenerate solutions was found to be 209.20 kPa.

By a comparison of the results the relaxation and linearisation technique allowed a feasible solution to be found and a better minimum HEN pressure drop was achieved in two case studies. The discretised transformation and convexification technique was unable to find a feasible solution to the network pressure drop minimisation problem. Therefore it is concluded that the relaxation and linearization technique was the favoured of the two investigated in this work.

6.1.2. Boiler Efficiency Comparison

The steam flowrate to a HEN can be minimised by utilising saturated and sub cooled condensate as a source of energy. The resulting reduction in steam flowrate and condensate return temperature negatively affects the efficiency of the steam boiler. The boiler efficiency can however be maintained by incorporating an additional dedicated heat exchanger into the HEN to pre heat the boiler feed water return. This was accomplished by Price and Majozi (2010a).

The minimum steam flowrate from the system was slightly compromised by this alteration as additional energy was required to pre heat the boiler feed water. This minimum flowrate was found to be 8.76 kg/s with an additional pre heater duty of 2256.4kW.

As described in Section 6.1.1, incorporating degenerate solutions enlarges the size of the solution space for the HEN arrangement. The variables required to calculate the boiler efficiency can therefore vary more, allowing for more flexible solutions. The minimum steam flowrate found using the relaxation and linearisation technique was 8.76 kg/s which is identical to that found by Price and Majozi (2010a). The required duty of the pre heater for the two cases was however different, with the degenerate solution case being able to vary depending on the outlet temperatures of the individual heat exchangers. With no limitation to the HEN outlet temperature the need for an additional pre heater was removed due to high return temperatures. This could potentially cause cavitation in the boiler feed water pump and therefore

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the pumping temperature was limited. The resulting duty was found to be 2548.4 kW. In general, the duty of the pre heater can be varied by changing the outlet temperature of the HEN which was not previously feasible with limited heat exchanger outlet temperatures.

The transformation and convexification technique was utilised with discretised transformation variables as described by Pörn et al. (2008). This formulation did not result in a feasible solution. The undiscretised transformation and convexification formulation did however result in a minimum flowrate of 8.76 kg/s, once again identical to that of Price and Majozi (2010a). Once again the HEN arrangement was found to be more flexible and the pre heater duty could be varied by limiting the HEN outlet temperature. By not discretising the transformation variables in the transformation and convexification formulation the resulting MINLP is nonconvex and therefore the global optimality of the solution cannot be guaranteed.

The relaxation and linearisation as well as the transformation and convexification techniques were found to be successful at dealing with the bilinear terms arising from incorporating degenerate solutions in the formulation. The results using the two techniques were identical in terms of minimum steam flowrate, however the transformation and convexification technique could not guarantee global optimality due to the undiscretised and hence nonconvex formulation providing the only feasible solution.

6.2. Discussion

This work shows that degenerate solutions should be investigated to optimise network variables once a minimum utility flowrate has been found. For network pressure drop it is suggested that the minimum network flowrate is found, then the minimum pressure drop is found using conditions of network optimality and then degenerate solutions are investigated in an attempt to further minimise the network pressure drop. Similarly, for boiler efficiency optimisation, a minimum steam flowrate for the HEN should be found using established techniques. The boiler efficiency for the system can then be maintained for retrofit steam systems using sources of heat within the steam systems or a dedicated additional heat exchanger. By

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incorporating degenerate solutions, the steam system is allowed additional degrees of freedom to accommodate more design constraints, such as boiler feed water pumping temperature. The size and duty of additional equipment can be optimised due to the variable HEN outlet temperature brought about by the allowance for degenerate solutions.

It must be noted that improvements in HEN pressure drop and the series heat exchanger connections discussed in this work will result in higher HEN interconnectivity which could make general operability as well as abnormal operations such as startup or shutdown more difficult. When incorporating any aspects of process integration into design, aspects such as operability and process control should also be considered. By formalising better techniques for process integration, a more effective iterative approach which gives consideration to aspects such as control are more feasible and less time consuming.

The techniques utilised in this work are not necessarily the only techniques that are effective at dealing with bilinear terms. Further, other solvers may also be more effective at finding a more optimal solution.

From the outset of this research and that of preceding work stochastic type optimisation algorithms such as Genetic Algorithms (GA) were not as effective at solving nonconvex MINLP problems. Therefore the focus of this and preceding work was on the operation of deterministic algorithms and how these behave when applied to the formulations presented. Subsequently large advances in the robustness and effectiveness of stochastic algorithms have resulted in them becoming competitive as compared to deterministic algorithms. Future work could include the use of stochastic algorithms to explore the potential benefits of including degenerate solutions in exchange network optimisation.

Future work in this field could also include the update of the transformation and convexification technique which may be found to yield a more optimal HEN pressure drop. Boiler efficiency optimisation using the discretised transformation and convexification technique should be further explored as this technique was found to not result in a feasible solution. The undiscretised formulation was successful at

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finding a solution however due to the nonconvex nature of the constraints the global optimality of the solution cannot be guaranteed.

The relaxation and linearisation technique was found to be effective at achieving an improved network pressure drop with degenerate solutions.

The transformation and convexification technique has been shown to be effective at aiding the solutions of complex nonconvex problems however the application with branch and bound type MINLP solvers was not as effective as the relaxation and linearisation technique. The use of tangential piecewise linear approximations for the purposes of discretising certain variables is effective at ensuring a variable can take the value above or below a particular limit if necessary. These techniques have the potential to yield better solutions to network optimisation problems where nonlinear constraints are present.

6.3. References

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Appendix A.

This section of the Appendix is intended to show how the unknown terms relating to the heat exchanger and piping pressure drop correlations have been derived for the pressure drop mathematical model.

A.1. Heat Exchanger Guidelines

Constraints (3-2) and (3-3) contain the following heat exchanger design based variables; heat transfer area A, the number of tube passes n_{tp}, the number of tubes N_t, the inside tube diameter d_i and the outside tube diameter d_o.

For the various heat exchangers in the relevant case study the heat transfer area is determined using the general equation for heat transfer defined in Sinnot (2005), shown in Constraint (A.1)

$$Q = UA\Delta T_m \qquad (6\text{-}1)$$

In Constraint (6-1) Q is the relevant duty for the stream to be heated, U is the overall heat transfer coefficient, A is the heat transfer area and ΔT_m is the log mean temperature difference. The stream duty is known for the case studies. An approximate overall heat transfer coefficient is taken from Sinnot (2005). This value is 1000 W/m^2.K for the condensers and 800 W/m^2.K for the condensate heat exchangers. The ΔT_m for condensers is determined using Constraint (6-2) as defined by Sinnot (2005).

$$\Delta T_m = \frac{t_2 - t_1}{\ln\left(\frac{T^{sat} - t_1}{T^{sat} - t_2}\right)} \qquad (6\text{-}2)$$

In Constraint (6-2), T^{sat} is the saturated steam temperature, t_2 is the cold stream inlet temperature and t_1 is the cold stream outlet temperature. The ΔT_m for the condensate heat exchangers is assumed to be the minimum global approach temperature, $\Delta T_{\min}$ for the case study so as to give a conservative approximation for the area. With the Q, U and ΔT_m known the heat transfer area can be calculated using Constraint (6-1).

This area must then be made up by the outside area of the tubes in the heat exchanger. The area is a function of the area of one tube multiplied by the number of tubes, as stated by Nie (1998) and shown in Constraint (6-3).

$$A = N_t \pi d_o L \qquad (6\text{-}3)$$

In Constraint (6-3), L is the length of a tube. With A known, the variables N_t, L and d_o must be selected. There are several design guidelines given in Sinnot (2005) that aid in the selection of these variables. One of the major considerations for heat exchangers is the fluid velocity. Low fluid velocities often lead to fouling while high fluid velocities increase the pressure drop. Velocity is calculated by Constraint (6-4), shown in Nie (1998).

$$u = V \frac{4}{\pi d_i^2} \frac{n_{tp}}{N_t} \qquad (6\text{-}4)$$

The number of tube passes are assumed to start at 2 for the smaller duties and increasing up to 16 for the larger duties. Sinnot (2005) indicates generally accepted velocity ranges for fluids and gases in pipes, which can be assumed equivalent to heat exchanger tubes. These ranges are shown in **Table 3-1**.

Table 6-1: Steam System Data

Fluid	Velocity (m/s)
Liquids	1 – 3
Gasses and Vapours	15 - 30

The lower limit is in place to prevent fouling. Since steam and steam condensate contains very little impurities this lower limit is assumed to be flexible for the approximate heat exchanger design. Since the pressure drop through the steam pipes is assumed to be negligible the only steam flowrate to be considered is inside the condensers. Thus the gas and vapour flowrate range is used simply as a guideline.

The relation between the inside and outside pipe diameter is assumed to be a ratio of 0.8, since this is the ration indicated by the most commonly chosen pipe diameters in Sinnot (2005).

A relationship between the tube length and the number of tubes exists in the form of the bundle diameter to tube length relationship defined in Sinnot (2005). The bundle diameter is calculated using the number of tubes and the tube pitch. A square pitch is assumed for all heat exchangers.

By alternating the inside diameter, number of tubes, tube length and number of tube passes while maintaining the heat transfer area and bearing the design guidelines in mind the various heat exchangers are designed for the grassroot case. In the retrofit case the actual heat exchanger dimensions can be used. It must be emphasised that the objective is not to design an optimal heat exchanger but simply to simulate the pressure drop for a realistic heat exchanger such that the pressure drop can be included in the flowrate minimisation framework.

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A.2. Piping Guidelines

Constraint (3.5) is a fairly simple piping pressure drop estimation. Since an economic design guideline of Peters and Timmerhaus (1991) has already been used to derive the constraint the only choice left is the pipe length. In the model the various types of pipe length are varied. The recycle and reuse pipes are assumed to be longer than the pipes joining the heat exchangers to the central condensate return hub.

A.3. References

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Appendix B.

This section of the Appendix includes a description of the linearisation techniques used in this dissertation. Two linearisations are described. The first is applicable for the bilinear product of two continuous variables and the technique is illustrated by Quesada and Grossmann (1995). The second is applicable for the bilinear product of a continuous variable and a binary variable and this method is explained by Glover (1975).

B.1. Relaxation Linearisation Technique Described by Quesada and Grossmann (1995)

Let

$xy = \Gamma$, where x and y are both continuous variables in the formulation. In the case of this dissertation x is a temperature and *y* is a flowrate.

with each variable displaying the following bounds

$$X^L \leq x \leq X^U \qquad (6\text{-}5)$$

$$Y^L \leq y \leq Y^U \qquad (6\text{-}6)$$

each of the bounds expressed as individual equations

$$x - X^L \geq 0 \qquad (6\text{-}7)$$

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$$X^U - x \geq 0 \quad (6\text{-}8)$$

$$y - Y^L \geq 0 \quad (6\text{-}9)$$

$$Y^U - y \geq 0 \quad (6\text{-}10)$$

performing the following multiplications

$$C-3 \times C-6 \Rightarrow \Gamma = xy \leq xY^U + X^L y - X^L Y^U \quad (6\text{-}11)$$

$$C-4 \times C-5 \Rightarrow \Gamma = xy \leq xY^L + X^U y - X^U Y^L \quad (6\text{-}12)$$

$$C-3 \times C-5 \Rightarrow \Gamma = xy \geq xY^L + X^L y - X^L Y^L \quad (6\text{-}13)$$

$$C-4 \times C-6 \Rightarrow \Gamma = xy \geq xY^U + X^U y - X^U Y^U \quad (6\text{-}14)$$

This linearisation technique is not exact. It does however create a convex solution space where the linearised model is solved. This solution is then used as a starting point for the exact, nonlinear model. To implement this technique Constraints (6-11) to (6-14) are included in the formulation for the linear model and all the bilinear terms are replaced with *Γ*. If the solution to the nonlinear model equals that of the linear model it can be concluded that a globally optimal solution exists. If the solutions differ then it can be concluded that the solution for the exact, nonlinear model is feasible but not globally optimal.

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B.2. Glover (1975) Transformation

Let

$xy = \Omega$, where $x \in \Re$ and $y \in [0,1]$

the following restrictions also hold

$$0 \leq \Omega \leq 0 \text{ when } y = 0 \qquad (6\text{-}15)$$

$$x \leq \Omega \leq x \text{ when } y = 1 \qquad (6\text{-}16)$$

the following bounds are applicable

$$M^L \leq \Omega \leq M^U \qquad (6\text{-}17)$$

then the following constraints on Ω hold

$$M^L y \leq \Omega \leq M^U y \qquad (6\text{-}18)$$

$$x - M^U(1-y) \leq \Omega \leq x - M^L(1-y) \qquad (6\text{-}19)$$

Constraints (6-18) and (6-1) are then added to the formulation and the bilinear term xy is replaced with the new linearisation variable Ω. This linearisation technique is exact and will therefore result in a globally optimal solution if all of the other constraints in the formulation are linear.

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