Design of Crude Oil Distillation Systems with Preflash Units

A thesis submitted to the University of Manchester for the degree of Doctor of Philosophy in the Faculty of Science and Engineering

2019

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Design of Crude Oil Distillation Systems with Preflash Units

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The University of Manchester
2019
Abstract – PhD Thesis

Refining technology has evolved considerably over the last century in response to the need for more energy-efficient processes. Crude oil distillation is a complex and energy-intensive process with a large number of degrees of freedom that interact. A crude oil distillation system comprises one or more complex distillation units with side strippers and pump-arounds, a preheat train (heat recovery system) and a furnace providing fired heating. In addition, pre-separation units may be introduced, where a preliminary separation of some low-boiling components is carried out at a relatively low temperature, reducing the high-temperature heating requirements of the process. Design of these complex, integrated systems is challenging due to a large number of degrees of freedom and process constraints involved. The high operating costs dominated by the need for fired heating in the furnace and the complexity of the crude oil distillation system motivates the development of systematic approaches for optimal system design.

In this work, the design methodology is developed using simulation models in Aspen HYSYS v8.8; these models are linked to MATLAB R2016a through an interface that allows communication between the two software packages. A simulation file is created for two different configurations with and without a preflash unit upstream of the atmospheric column. Two optimisation-based design approaches are proposed, the first one extracts streams and column information needed to perform the optimisation directly from the simulation model in Aspen HYSYS while in the second approach, artificial neural networks (ANN) are developed to represent the distillation process. The

scope of the methodology consists of finding optimal operating and structural conditions for the crude oil distillation system that minimises hot utility demand in the furnace accounting for product quality and yield. Current design systematic methods have not focused on the role of preflash units.

The strong interactions between the crude oil distillation unit, the preflash unit, and the heat recovery system make this a challenging optimisation case, especially because both operational and structural variables are to be optimised simultaneously. Therefore, a stochastic optimisation method (a genetic algorithm) is applied. As the simulation-optimisation approach is computationally intensive, it motivates the use of surrogate models that have the advantage of performing the optimisation of the system in less time (i.e. 4-6 hours vs 1.6 hours).

In industrial practice, heat integration is of prime importance for the energy-efficient operation of crude oil distillation systems. This work applies pinch technology using the grand composite curve to evaluate the minimum heating and cooling requirements for each converged simulation rather than addressing detailed aspects of design and costing of the heat recovery system so that no details about investment costs and the complexity of the heat recovery system are taken into account. The novel optimisation-based design approach developed is extended to minimise fired heating demand. To date, no previous research studies focused on minimising the total fuel consumption of the system and the design or operation of crude oil distillation columns have been reported.

Results obtained from industrially-relevant case studies indicate that introducing a preflash unit within a crude oil distillation system can reduce its energy demand by 14% to 16%. Using surrogate models, instead of rigorous models, considerably reduce the computational time (from 6.1 hours to 103 seconds per each optimisation run for the case with a preflash). Excellent agreement between the surrogate and rigorous models is also reported; rigorous optimised results vs ANN-optimised results for the case without a preflash unit are 44.5 MW and 44.6 MW respectively, demonstrating the effectiveness of the new approaches. On the other hand, it is demonstrated that minimising only the hot utility demand of the system does not give complete information about the demand for fired heating and it does not necessarily minimise the total fuel consumption of the system.

Declaration

No portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

Minerva Ledezma Martínez

Copyright Statement

Acknowledgement

A PhD journey is enclosed in this Thesis, a journey that I did not walk alone. I want to express my deepest gratitude to those who have been walking with me; without their support, encouragement, company and friendship this journey would have not been the same.

First of all, a special acknowledgement to my Supervisors:

Professor Megan Jobson: with my great and deepest appreciation for your patience, professionalism and for always encouraging me to go further. Your unconditional support, constructive feedback and invaluable guidance in all the stages of this work were outstanding. Thank you for your time to have weekly meetings and to provide feedback for posters and oral presentations. I deeply appreciate your willingness to be in touch at any time during the writing period of this Thesis. No words to describe all the lessons learned from you through my PhD journey. I really enjoyed your Distillation classes; being part of your demonstrator's team was truly rewarding, helping the new generations of Chemical Engineers to grow up and to enhance their abilities with process simulators.

Professor Robin Smith, thank you for sharing your industrial experience and for your valuable comments and contributions to enhance this work. In particular, during our meetings for the Process Integration Research Consortium, where I had the opportunity to present the work to industry representatives. It was great pleasure to me have the opportunity to learn from you and to be part of your demonstrator's team in the Oil and Gas processing course. My deepest gratitude for your empathy and willingness to help me with everything related to this work and for your unconditional personal support.

Working under the supervision of both, *Megan and Robin*, was an extraordinary and more than inspirational experience because I had the balance between academia and industrial experience. On top of that, you were always there supporting me with personal situations, which is something that I sincerely appreciate. Thank you both!

Now, I would like to thank all of those special people whose company and friendship helped me to keep going, all of you made a huge difference during my PhD studies:

Family Carmona-Dourdou: no words to thank you all for your everyday company, unconditional support and for all the special and unique moments shared. I am going to keep all our memories together in my heart forever. Jesús, I believe that life joined our paths for a reason. You are a wise man who always makes me see the world from a different perspective. Thanks! for all your personal and academic support, even before I started the PhD, for all our 'clubbing nights-out' which I really enjoyed. Delphine, thank you! for being always pending on me, for your day-to-day company and absolute support. Lily, you will always be my favourite princess in the world.

Mrs Benton and Family: *Alex, Matthew and Phil*, thank you for the time shared, for all your support and empathy. I will always remember our irreplaceable and extraordinary moments together. *Mrs Benton*, my "Angel" in England, I am going to keep all our days shared in my heart, you made me felt always protected in all senses. Thank you! for all your smiles and hugs and for always made time to celebrate my birthday. You were always there for me, listening, encouraging, supporting even from distant places. We share the passion for classical music, and I found a "sweet" way to let you know how special you are to me. All of you are part of those rare people who are willing to go that extra mile for others. Thank you for everything!

My friends in Spain, *Salvador*, we have been sharing paths in almost 20 years! Thank you for your company and for being part of this adventure, for

all your support and daily encouragement; your messages every morning made me always smile. *Nadia,* you are a really special friend, thank you for always being there and for cheering me up since the beginning of my PhD. You made my work trip to Barcelona unforgettable. Thank you both for your amazing friendship.

Thanks to all CPI students who enriched my day-to-day path at office. Especially to my “Musketeers”, *Gonzalo and Fernando* for being always close to me since day one of our PhD journeys, for all your support and for all the moments shared. I will always remember our trips together, all our adventures discovering England and our Nero coffee afternoons!

In Mexico:

Mrs Mary Baz, I thank you for all the special things you have done for me, for helping me to overcome many difficult situations to be able to be here making my biggest dream come true. I know you have walked with me even in the distance during these years in England.

(Señora Mary Baz, ¡gracias! por todas las cosas especiales que ha hecho por mí, por ayudarme a superar muchas situaciones difíciles para poder estar aquí y hacer realidad mi mayor sueño. Sé que ha caminado conmigo incluso en la distancia durante estos años en Inglaterra).

Finally, I thank the financial support of the National Council of Science and Technology México (CONACyT), scholarship number: 381926.

This is just the start of a new Chapter in my life as a professional. Some years ago, I had a dream, a dream that came true after long waiting, but at the right time and surrounded by the right people. I thank all of those who contributed academically and personally to the completion of this exciting and challenging journey through the world of Process Integration at the birthplace of Chemical Engineering, The University of Manchester.

Dedication

To my Mother, for all her support and unconditional love, for always encouraging me to go further and taught me to be brave, for all your days and nights taking care of me; working always hard, building a better life to me.

Thank you for giving me the wings and courage to pursue my dreams!

A mi Madre, por todo tu apoyo y amor incondicional, por siempre alentarme a llegar más lejos y por enseñarme a ser valiente, por todos tus días y noches cuidando de mí; trabajando siempre muy duro, construyendo una vida mejor para mí.

¡Gracias por darme las alas y el coraje de perseguir mis sueños!

To the memory of my grandparents, you both taught me to be a hard-working person. Thank you! grandfather, you gave me the best advice for life: do always your best at school. Always remember where you come from, be proud of your origin, but never be afraid to dream big.

A la memoria de mis abuelos, ambos me enseñaron a ser una persona trabajadora. ¡Gracias abuelo! me diste el mejor consejo de vida: da siempre lo mejor de tí en la escuela. Siempre recuerda de dónde vienes, siéntete orgullosa de tu origen, pero nunca tengas miedo de soñar en grande.

About the Author

Minerva Ledezma Martínez received her Bachelor's degree in Chemical Engineering in 2005 and a Master's degree in Chemical Engineering (Process Integration) in 2007 from the University of Guanajuato, Mexico. In 2014, she started her PhD studies in the Centre for Process Integration at The University of Manchester sponsored by the National Council of Science and Technology (CONACyT) Mexico, working on crude oil distillation systems design. A complete list of publications and conference presentations delivered during her PhD studies are presented in Appendix E. Minerva is an Associate Member of the Institution of Chemical Engineers (IChemE).

Since 2015, Minerva has been part of the staff at The University of Manchester as a Graduate Teaching Assistant for several course units including Distillation Systems Design, Process Design and Simulation, Oil & Gas Processing among others. She was involved in several extra-curricular activities during her PhD studies: President, Manchester Mexican Society, 2015-2016. Student Representative, Centre for Process Integration, 2016-2017. Student Ambassador and volunteer during the undergraduate open days at the School of Chemical Engineering and Analytical Science 2016-2019.

Chapter 1

Introduction

Petroleum refining industry has existed for around a century, it supplies a wide range of essential products to a variety of end-user markets. These products are manufactured from natural deposits of oil and gas located around the world. Both crude oil and gas are the major sources to meet world energy demand (Clews, 2016).

An overall objective in a refinery is to add value to a crude oil feed through the production of fuels and materials at the lowest possible cost meeting product specifications. Separation processes constitute the initial processing stage in a refinery. Crude oil distillation is the core separation process in any refinery; it fractionates the crude oil into several distillation products according to their boiling points (Clews, 2016).

This Chapter aims to give a brief introduction to the research topic addressed in this work; it is divided into four sections: first, the main features on crude oil distillation are presented, explaining some concepts and terminology that are used in this work. Second, the design of heat-integrated crude oil distillation systems is introduced. Third, research aim and objectives are outlined to conclude with a general Thesis overview.

1.1. Features on crude oil distillation

Crude oil is a mixture of hydrocarbon compounds ranging in size from the methane, with one carbon atom to large compounds containing more than 300 carbon atoms (Jones, 1995). Crude oil extracted from natural reservoirs is a basic raw material for the petroleum industry; however, it has limited value in its natural state. There are many types of crude oils, each of them is categorised according to their density, the presence of impurities (sulphur content - the measure of total sulphur in the oil) and its location. High sulphur contents in oil make it ‘sour’ while low sulphur content in a crude oil makes it ‘sweet’ (Kayode, 2010).

Crude oil characterisation and cut points

Crude oil characterisation is usually the first step taken to facilitate other calculations and the minimum requirements are: (a) whole crude True Boiling Point (TBP) curve, (b) whole crude American Petroleum Institute (API) gravity and (c) whole crude light-ends analysis (Watkins, 1979). Crude oil is characterised to provide a good representation of it during modelling. When modelling complex hydrocarbon mixtures within commercial simulation packages, the original mixture is substituted by a mixture comprising two different groups of components: the light-ends components and a group of pseudo-components (Eckert and Vaněk, 2005).

Because of the complex composition, crude oil and petroleum fractions are usually characterised as a mixture of discrete pseudo-components (Nelson, 1958). Each pseudo-component corresponds to several or more unknown actual hydrocarbons, and is assigned an average boiling point on the TBP distillation curve (Fahim et al., 2010). This allows crude oil to be treated as a defined multicomponent mixture. To simulate refining processes, the first step is to define a pseudo-component scheme to characterise the crude oil feed.

Data requirement and definition of the pseudo-components depend on the type of the refining process to be modelled. The composition of the crude oil is indicated in terms of bulk and distillation based-properties. Bulk properties refer to those taking the whole crude into account such as density and viscosity. Distillation-based properties refer to the bulk properties measured for small amounts of crude based on its boiling point i.e. density distributions and boiling points distributions (TBP, D86). The collection of bulk and distillation-based properties form a *crude oil assay* that indicates how much of a cut (or product) can be produced for a given crude (Chang et al., 2012).

The pseudo-components for crude oil distillation units have to accurately characterise volatilities of the hydrocarbons in the crude oil feed in order to calculate vapour-liquid equilibrium in distillation columns (Chang et al., 2012).

In order to define the number of pseudo-components, it is necessary to cut the entire boiling range of the crude oil into a number of ‘cut-point ranges’ which are used to define the pseudo-components. The determination of number of cuts is arbitrary. The number of pseudo-components for each cut point range can vary depending on the product range desired (Chang et al., 2012). To maintain agreement with previous works (Chen, 2008; Ochoa-Estopier, 2014; Enríquez-Gutiérrez, 2016; Ibrahim, 2018), 25 pseudo-components are chosen to represent the crude oil boiling range in this work.

Most commercial process simulators have the capability to generate pseudo-components based on boiling-point ranges representing the oil fractions (Chang et al., 2012). Aspen HYSYS v8.8 is used in this work to carry out the characterisation of the crude oil. See Appendix F for a detailed explanation about how does Aspen HYSYS carries out the crude oil characterisation.

An indicator of the composition of crude oil and the facility in which it can be processed is the density. The density of crude oil is measured using the American Petroleum Institute, API gravity, a method of measuring the density of petroleum compared to water; it is related to specific gravity as follows:

$$Degress\ API = (141.5/Specific\ gravity) - 131.5 \quad (1.1)$$

Both specific gravity and API gravity are expressed relative to the density of water at 60°F (15.9°C). Lighter crudes are generally more valuable than heavier ones due to a greater volume of light components can be produced with less processing costs (Clews, 2016).

To facilitate crude oil compounds identification, petroleum refining community adopted crude oil characterisation through crude oil assays. An assay is the product of laboratory tests that provide detailed physical and chemical analysis of crude oil (Clews, 2016). A crude oil assay describes a specific crude oil type in terms of increasing boiling point temperatures at which specific parts of the crude oil evaporate. The first step in building a crude distillation model is the transformation of the crude oil assay data into petroleum pseudo-components or cuts. Figure 1.1 shows the boiling point curves for five distillation products light naphtha (LN), heavy naphtha (HN), light distillate (LD), heavy distillate (HD) and residue (RES).

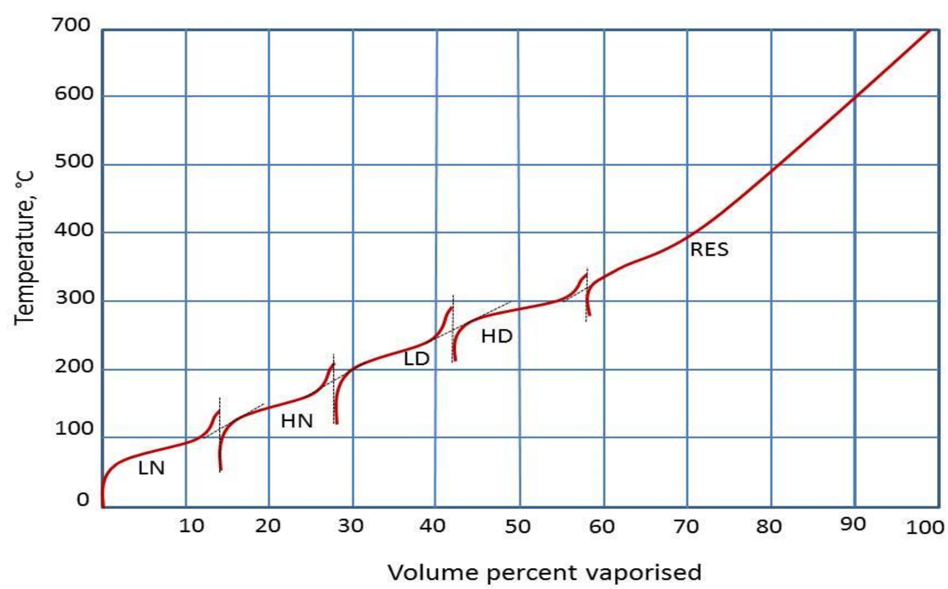

Figure 1.1 Product boiling point curves (adapted from Liebmann, 1996).

Figure 1.2 illustrates the region around the end point of a light product and the initial boiling point of a heavy product showing an overlap in temperatures, the width of this overlap is a measure for the quality of separation. The smaller the width of the overlap, the sharper the separation is. The overlap is defined as the difference between the 5% point of the heavier product (T5H) and the 95% point of the lighter product (T95L), this is called the '5-95 gap'. The larger the value of this difference, the sharper the separation is between two adjacent products (Liebmann, 1996).

A 'cut point' is defined by the volumetric yield point between two adjacent fractions and the corresponding temperature on the boiling point curve. This temperature is equal to the arithmetic mean of the end (T100) and initial (T0) boiling points of two products (Liebmann, 1996).

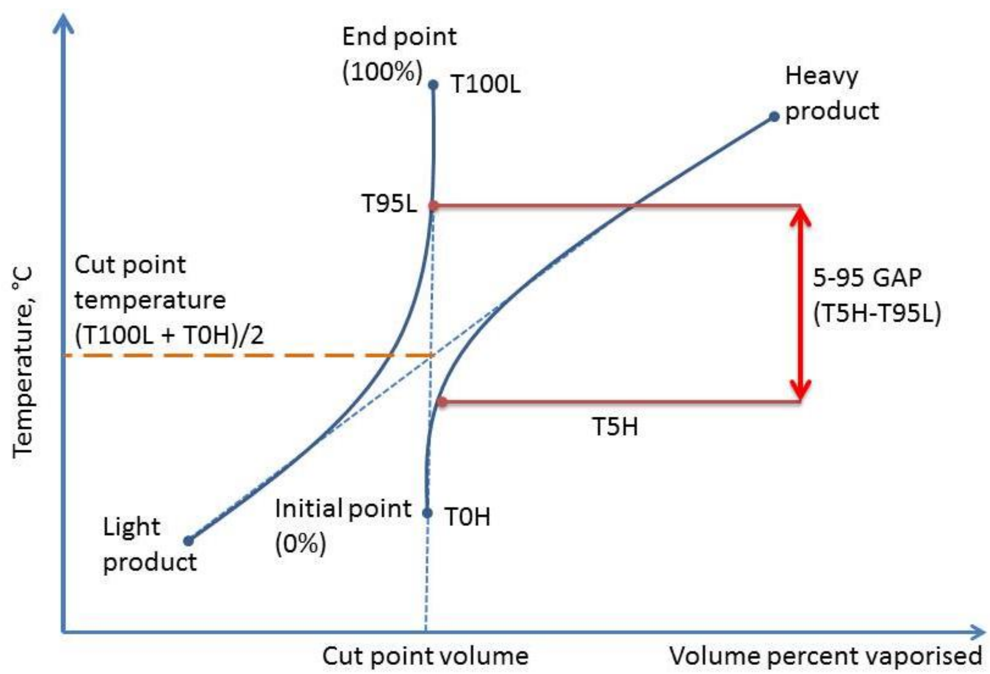

Figure 1.2 Gap and cut point between crude distillation products (adapted from Liebmann, 1996).

As single components of crude oil are not identified, properties defining the quality of a crude oil distillation product are found by a standardised test suchas the American Society for Testing and Materials, ASTM D86.

Crude oil distillation carries out the transformation of crude oil into useful products; it is a complex and energy-intensive process. The processing steps required for a particular refinery are mainly driven by the quality of the crude oil being processed and the product specifications of the products. Every refinery is different so that many possible refinery configurations can be found around the world.

The next section presents a brief introduction about the design of heat-integrated crude oil distillation systems.

1.2. Design of heat-integrated crude oil distillation systems

A typical crude oil distillation system, as illustrated in Figure 1.3 comprises a heat recovery network (two preheat trains where the crude oil is preheated and partially vaporised), an atmospheric furnace, a crude distillation unit equipped with a condenser (required to cool the naphtha product into a usable liquid form), one steam-injected side stripper, two reboiled side strippers which remove light components from side draws, and three pump-arounds that pull a certain amount of liquid on a tray, cool it down by heat recovery and then return it to the column two or four stages above the withdrawal. Pump-arounds provide local reflux to the crude distillation unit, which does have a huge impact on the separation quality. They also create heat recovery opportunities between the distillation column and the heat recovery system.

Side withdrawals are fed to side-strippers, which strip the lighter components and return them to the main tower (Liu, 2012). The main function of a side stripper is to improve the fractionation between a side distillate and the distillate drawn from above (Fraser, 2014).

Steam is injected into the column at the bottom in order to enhance vaporisation and separation of the heavier components. The presence of the steam decreases the partial pressure of hydrocarbons so that they can be vaporised at lower temperatures.

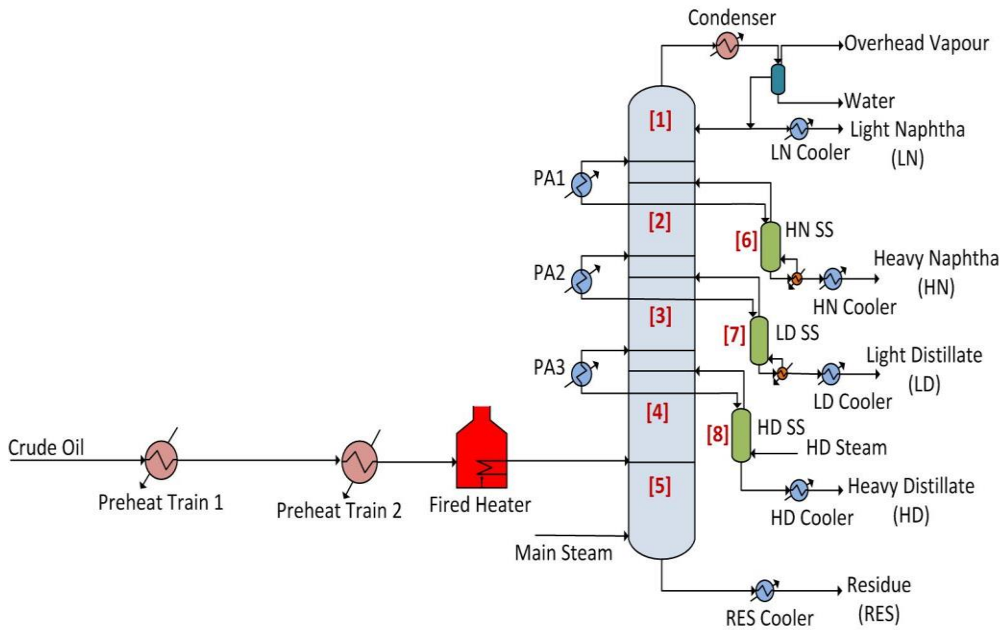

Figure 1.3 Crude oil distillation system.

Crude oil is first pumped into a series of heat exchangers (preheat trains 1 and 2) where heat is transferred from hot process streams to the cold crude oil. Next, it is sent to a furnace where the crude oil is heated up by exhaust of fuel combustion. Finally, crude is fed to the crude distillation unit (Liu, 2012).

Table 1.1 illustrates column sections, stages and temperatures of the crude oil distillation column showed in Figure 1.3.

The crude oil distillation unit has strong connections with its associated heat recovery system i.e. the hot streams (pump-arounds, condenser and distillation products streams, are heat-integrated with the cold streams, in particular with the crude oil feed.

Table 1.1 Column sections, stages and temperatures of a crude oil distillation column

Column section	Stage	Temperature, °C
1	1	93.7
	9	146.5
2	10	147.4
	17	227.5
3	18	238.6
	27	304.9
4	28	310.9
	36	341.3
5	37	341.3
	41	335.1

Duty of pump-arounds can be used as heating utility in other sections of the process. The rest of the energy requirements of the system are provided by fuel oil in the atmospheric furnace and cooling water.

Even though the system is heat-integrated, it consumes fuel at the equivalent of 2% of the crude processed (Bagajewicz and Soto, 2001). Typically, energy usage is on the order of 10 to 200 MW per crude oil distillation unit. In order to maximise the recovery of atmospheric products, the crude oil distillation unit operates at high temperatures around 360ºC to 370ºC. Consequently, these units need large fired heaters (furnaces) to heat the raw crude (Fraser, 2014). It should be noted that most of the energy necessary to carry out the distillation process is added in the fired heater.

Heat integration is implemented within a crude oil distillation system to enhance its energy efficiency interchanging heat between hot streams that require cooling and cold streams that require heating.

The interactions between the crude oil distillation process and the heat recovery system have a critical effect on the performance of the overall process. These interactions are represented by the operating conditions of the crude oil distillation unit such as pump-around duties and temperature drops, steam flow rates, reflux ratio and column inlet temperature. There are many degrees of freedom (variables that have a significant impact on process operation and also that can be manipulated and measured in the plant) available for the design and operation of a crude oil distillation system. From a design perspective, it is important to take into account both structural and operational degrees of freedom (Ochoa-Estopier, 2014).

Changing the operating conditions of a crude oil distillation system may benefit heat recovery opportunities in the heat exchanger network, HEN. Furthermore, modifying the column structure by adding a preflash unit does not only allow more capacity to be processed but also help the overall system to reduce its energy consumption increasing heat recovery opportunities (Gadalla, 2003).

Preflash units are commonly placed upstream of the crude oil distillation unit as shown in Figure 1.4, aiming to debottleneck either the distillation column or the furnace. A preflash unit allows bypassing the preflashed vapour from the furnace and sending it to an appropriate location in the main column (Golden, 1997). In this way, it is possible to reduce the heat duty of the distillation unit and it also improves the hydraulic performance of the heat exchanger network (Feintuch, 1985).

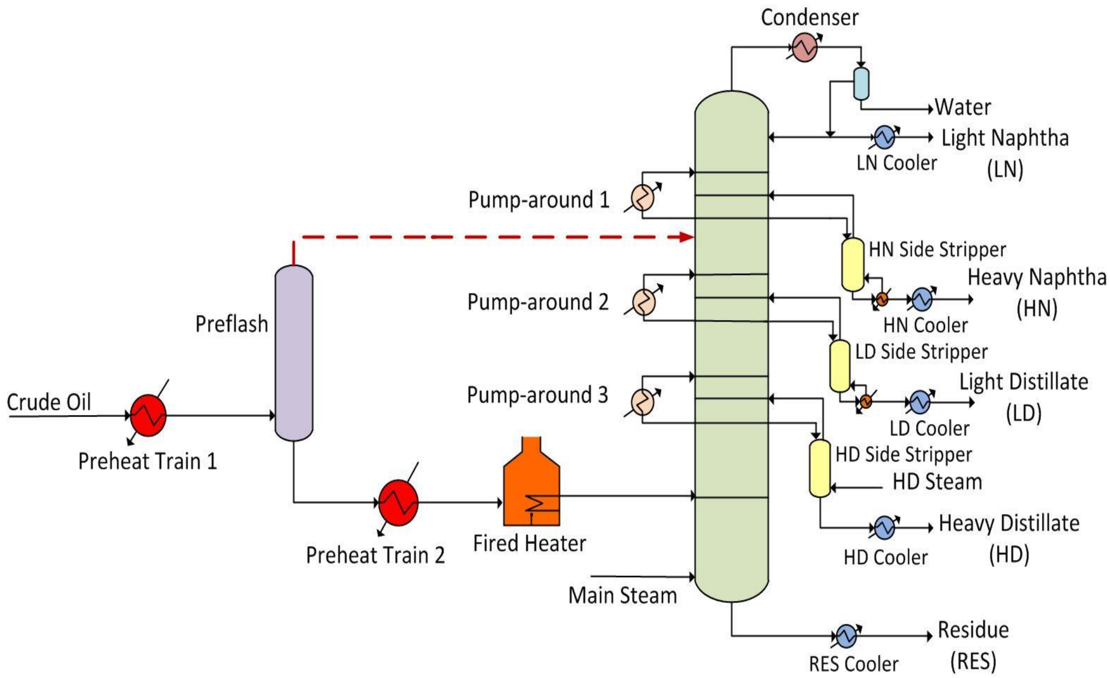

Figure 1.4 Crude oil distillation system with a preflash unit.

Implementing a preflash unit helps to remove light components of the crude oil mixture before entering in the fired heater. The main advantages of a preflash implementation will be discussed in Chapter 2.

Design of heat-integrated crude oil distillation systems has attracted research interest due to the possibility to reduce their energy consumption by implementing new design methodologies.

Main focus of early design methodologies (Nelson, 1958; Watkins, 1979; Jones, 1995) was to implement heuristics, engineering experience and empirical correlations that require trial and error and do not account for interactions within the system, i.e. design of the distillation column was performed first, followed by the design of the heat recovery network.

Later research works (Suphanit, 1999; Gadalla, 2003; Rastogi, 2006; Chen, 2008) followed the work of Liebmann (1996) proposing methodologies to address the design of heat-integrated crude oil distillation systems.

Design methodologies based on rigorous models (Ji and Bagajewicz, 2002) and recent developments on surrogate models (Ochoa-Estopier and Jobson, 2015; Ibrahim et al., 2018) have not included a pre-separation unit within the crude oil distillation system. Both rigorous and surrogate models have their own advantages and disadvantages, for instance, rigorous models tend to be accurate but they require large computational time. In addition, the implementation of rigorous models into optimisation frameworks is not as simple as it is when implementing surrogate models. In particular, artificial neural network models are able to represent the distillation process with accuracy and they are faster in convergence than rigorous models. On the other hand, there is a trade-off between model accuracy and computational effort which needs to be taken into account when implementing models into an optimisation framework (Ochoa-Estopier, 2014).

Nowadays, new computational tools are leading to the development of sophisticated design methodologies that employ optimisation algorithms and models to facilitate the design of complex crude oil distillation systems. Reliable simulation modelling is of prime importance for a successful process evaluation. Within the modern petroleum industry, process simulation is widely used to design and to analyse the crude distillation unit performance. However, accurate simulation modelling requires a deep understanding and knowledge of the entire crude oil distillation process (Lee, et al., 2009).

Hence, the development of new design methodologies for crude oil distillation systems with and without a pre-separation unit that enable a reduction in energy consumption and CO_2 emissions can bring substantial benefits to the refining industry. Nevertheless, due to the high complexity of the system, it is challenging to develop optimisation-based design approaches that exploit interactions between the separation units and their associated heat recovery system simultaneously, while meeting product quality and quantity specifications.

1.3. Motivation

Crude distillation is the oldest and most important part of any refinery, the distillation of crude provides refined products such as gasoline and diesel for direct sale and feed stocks to further processing. Recent emphasis has been highlighted in reducing energy consumption and CO_2 emissions (Chang et al., 2012). Figure 1.5 illustrates the energy use by type of industry; petroleum refining is the highest energy consumer.

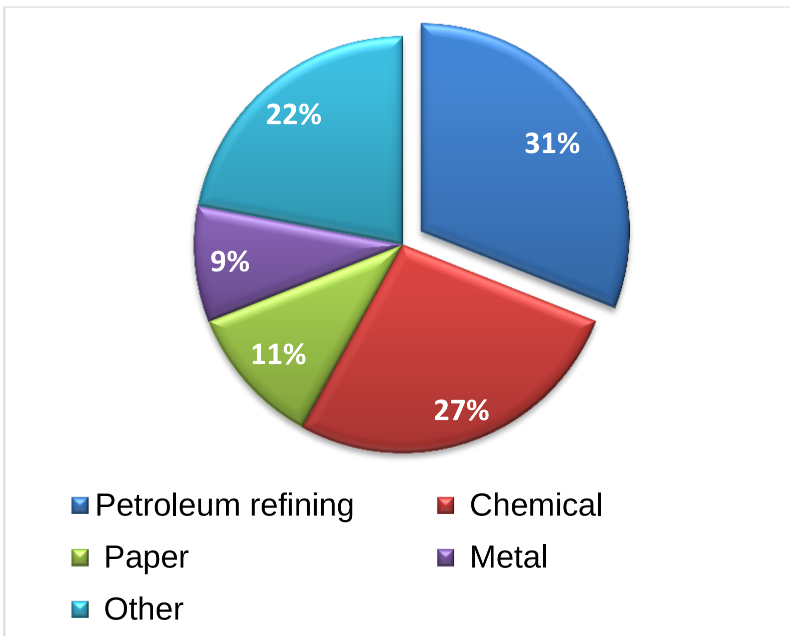

Figure 1.5 Energy use by type of industry (Source: US Energy information administration, manufacturing energy consumption survey, 2010).

Currently, research on how to reduce the energy consumption of atmospheric distillation units in a refinery has become a top priority. It is estimated that a crude oil distillation unit consumes 20-30% of the total energy required to separate a given crude into products. Therefore, it is critical to recover as much heat as possible from hot streams throughout the refinery to optimally heat and vaporise the crude oil (Chang et al., 2012).

On the other hand, the atmospheric furnace is the main energy conversion equipment, it is estimated that about 1/3 of the comprehensive energy consumption of refinery conversion and consumption is achieved through the furnace; thereby, increasing refinery furnace efficiency has become a main priority within the refining industry (Ping et al., 2012).

Energy savings can be achieved by exploiting interactions between separation units and the heat recovery system. Heat recovery is essential in design due to its impact on energy costs of process. In a crude oil distillation system, heat recovery is carried out via a heat exchanger network (HEN). In this work, the design of a heat exchanger network is out of scope; however, previous studies have addressed this part (Smith et al., 2010).

In order to simplify the problem and to reduce computational time, in this work pinch analysis (using the grand composite curve) is selected to evaluate minimum hot utility requirements for the crude oil distillation system, taking into account that pinch technology has provided industry with a systematic tool for design and optimisation of processes.

To date, there is no study that focuses on hot utility demand and fired heating demand of a crude oil distillation system with emphasis on adding a preflash unit. Therefore, the present work represents a starting point for further analysis to capture the trade-offs between yield and energy demand or by maximising net profit. The following section presents the research aim and objectives of this work.

1.4. Research aim and objectives

This research work aims to develop a systematic methodology to design energy-efficient crude oil distillation systems that exploit interactions between the separation units and the associated heat recovery system while meeting product quality and quantity specifications. Heat recovery is systematically evaluated using pinch analysis to account for the impact of operational variables on minimum energy demand.

The optimisation-based design framework enables the selection of operational and structural variables within the crude oil distillation system. Product quality and quantity constraints are taken into account. This research has the following objectives:

1. Develop an optimisation-based design methodology using rigorous models and pinch analysis simultaneously to simplify the design of heat-integrated crude oil distillation systems with and without a preflash unit taken into account operational and structural variables.

2. Incorporate surrogate models (in particular, Artificial Neural Networks, ANN) into the optimisation-based design methodology aiming to reduce optimisation time without compromising model accuracy, column performance, product qualities or product yields.

3. Enable minimisation of fired heating demand using rigorous and surrogate models.

4. Apply the modelling and optimisation approaches to both objectives, minimum hot utility demand and minimum fired heating demand to demonstrate the capabilities of the methodology, and to gain understanding about opportunities to reduce energy demand

through appropriate selection of structural and operational design degrees of freedom.

1.5. Thesis Overview

This PhD Thesis is organised in seven Chapters. In Chapter 1, a brief introduction to the design of crude oil distillation and heat-integrated crude oil systems is presented.

Chapter 2 outlines an overview of previous research related to the design and optimisation of heat-integrated crude oil distillation systems emphasising the cases including pre-separation units. Stochastic optimisation methods applied for crude oil distillation design are addressed, and standard methods for analysing heat integration potential are explained.

An optimisation-based design methodology for crude oil distillation systems with preflash units is proposed in Chapter 3. In this Chapter, 'direct optimisation' is applied to design crude oil distillation systems with and without a preflash unit. Two scenarios are explored and presented as case studies. In the first case study, the structure of the main column is fixed in terms of the numbers of trays. In the second case study, the structure of the main column and the operating conditions of the crude oil distillation system are optimised simultaneously.

Chapter 4 introduces an optimisation-based design framework developed applying surrogate models for crude oil distillation systems with and without a preflash unit. The models are developed using data from rigorous simulations and Artificial Neural Networks, ANN. Case studies demonstrate the capabilities of the optimisation framework and allow comparison to the 'direct optimisation' approach of Chapter 3.

A novel optimisation-based design methodology to minimise fired heating demand of crude oil distillation systems is presented in Chapter 5. No previous research is known to have taken into account the optimisation of fired heating demand and the associated fuel consumption of the atmospheric furnace. In this research work results of optimisations using both ‘direct optimisation’ and ANN-based optimisation regarding minimum hot utility demand and fired heating demand are compared for two different case studies: with and without a preflash unit.

An overall Thesis summary is included in Chapter 6, linking results from case studies presented in Chapters 3, 4 and 5. The base case in each case study (with and without a preflash unit) is outlined, comparing best optimised designs.

Finally, Chapter 7, summarises this research work discusses its limitations and recommends future work.

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Chapter 2

Literature Review

This Chapter includes information published in:

> Ledezma Martínez, M., Jobson, M., and Smith, R. (2018a). Simulation-optimization-based Design of Crude Oil Distillation Systems with Preflash Units. *Industrial and Engineering Chemistry Research*, *57*(30), doi.org/10.1021/acs.iecr.7b05252.

2.1 Introduction

Crude oil distillation is the core part of a refining process and also the major energy consumer. Design and operation of crude oil distillation columns involve strong trade-offs between energy use and product recovery. Optimising these trade-offs by applying optimisation-based design methodologies can lead to increase energy savings in crude oil distillation systems.

This Chapter presents a brief review about relevant previous research on design and optimisation of crude oil distillation systems; benefits of a preflash implementation in a crude oil distillation system are also discussed.

Stochastic optimisation methods are described in summary. Then, an introduction to surrogate models is presented. Finally, heat integration in crude oil distillation systems is addressed.

2.2 Design and optimisation of crude oil distillation systems

The design of chemical processes can be classified into grassroots design and retrofit design; the former refers to the design the process equipment to meet required product specifications and certain economic criteria. In crude oil distillation processes, grassroots design aims to find the most energy-efficient option to separate the crude oil into the desired products.

Designing crude oil distillation systems comprises the definition of operating and structure conditions; over the years, researches have been applying different design methodologies following traditional methods, integrated methods or optimisation-based design methods.

Challenges in the crude oil distillation columns have been influenced by the rise in the cost of energy. Consequently, new design approaches need to be developed in order to meet energy demand, e.g. heat integrated designs in crude oil distillation, which involves the design of columns and heat exchangers simultaneously taking into account the interactions between them.

Packie (1941) was the pioneer in designing crude oil distillation columns, he reported empirical charts based on experience to show the relation among 5-95 gaps used as separation criteria. In his design, no heat-integration was taken into account because his designs followed a sequential method.

Nelson (1958) proposed a methodology for the design of atmospheric crude distillation units. Years later, Watkins (1979) included a design procedure for atmospheric and vacuum crude oil distillation units, based mainly on mass and energy balances, using empirical models and by trial and error. Because of the low cost of energy and lack of computational tools in those years, they do not include improvements regarding energy efficiency in their designs. Later, alternative configurations were developed including a pre-separation unit.

Later works reported by Bagajewicz and Ji. (2001a); Bagajewicz and Soto (2001b); Ji and Bagajewicz (2002a) present the design of distillation systems to be used with different types of crude oils. However, their approach does not include the interactions between the crude oil distillation unit and its HEN.

2.3 Preflash implementation in a crude oil distillation system

Energy savings in a crude oil distillation system can be achieved by exploiting interactions between separation units and the heat recovery system. Preflash units are useful for reducing the fired heat demand for crude oil preheating prior to distillation. A preflash unit removes some light components and some of the light naphtha; the vapour stream bypasses the fired heater, helping to reduce its fuel consumption. The vapour stream can then be mixed with the stream leaving the furnace or be fed to the main column at a suitable location; this helps to reduce the heat duty of the column and can bring enhancements of the hydraulic performance of the HEN (Errico et al., 2009).

Preflash units are added to existing crude units mainly for three reasons: a) to increase capacity, b) to improve heat integration and c) to improve the quality of the separation. Generally, preflash units are added to crude oil distillation units already built; however, few crude distillation units are designed with preflash units since the beginning (Sloley, 2001).

2.3.1 Previous works with focus on prefractionation units

Several published studies consider the design and optimisation of crude oil distillation systems and how to maximise the benefits of including preflash units.

Brugma (1942) is considered as a pioneer on prefractionation investigations. He suggested a configuration of three columns to separate a mixture of four components (ABCD) to symbolise petroleum products. He used a prefractionator to separate the two lightest components. Then a further separation is carried out in a column. He did not report energy consumption of his proposed configuration.

Petlyuk et al., 1965 investigate the performance of a prefracionator in the separation of a ternary mixture, known as fully thermal coupled configuration. Results indicate that there was a reduction regarding mixing effects in the column due to a better match between the feed composition and the column feed stage.

Golden (1997) provides useful insights into how key parameters, such as flash temperature and flashed vapour feed location, affect the performance of the main distillation column.

Bagajewickz and Ji (2001); Li and Bagajewickz (2002a; 2002b) present a rigorous approach for setting the inlet and outlet stream conditions when designing a crude oil distillation unit with a preflash. The preflash temperature and feed location of preflash vapour in the main column are addressed, while pinch analysis is applied to assess minimum utility requirements.

Sloley (2001) developed a complete review of the types of prefractionator and gas oil towers used in industrial practice. His work explains the advantages and disadvantages to the equipment, and evaluates the influence of prefractionation units on crude oil distillation design, considering product yields. But the analysis did not include HEN interactions; on the other hand, he concluded that only if product yields were kept constant, prefractionation units can bring energy savings on the overall system.

Errico et al., 2009 explore an industrial crude oil distillation unit analysing the feed conditions when installing a preflash drum or a preflash plate column. They compare the performance of a distillation system with and without a preflash unit, considering product flow rates, product quality and potential for energy savings. A limitation of this study is that column operating conditions and the preflash temperature are constant. Their results showed better performance for the preflash column than those obtained for a preflash drum.

Wang et al., 2011 apply thermodynamic metrics to select the best pre-separation scheme for heavy crude oils. Nine predistillation arrangements are explored, and the option with two preflash units is found to perform best. Heat recovery is not explicitly considered, so the results do not relate directly to demand for fired heating; in addition, product quality specifications appear to be only partially addressed, via stream or 'cut' temperatures.

Benali et al., 2012 demonstrate that preflash units can bring benefits in terms of exergy destruction, although their methodology for adjusting the column operating conditions and for analysing the impact of the process changes on heat recovery opportunities is not discussed.

Gadalla et al., 2013 present a methodology for the design of the crude oil distillation column and heat exchanger network simultaneously, considering process changes and structural modifications together with the interactions between them. Their work also reports the addition of a preflash drum, concluding that large energy savings of around 32% are obtained with this which also impact the utility costs.

Kuboski (2014) investigates prefractionation upstream and downstream of the atmospheric distillation column in crude oil distillation. His results reveal variations on process streams due to the allocation of prefractionation equipment, showing the importance of heat-integration to improve energy efficiency on grassroots design.

Other researchers explore using optimisation to improve the performance of the crude oil distillation system when a preflash unit is added:

Al-Mayyahi et al., 2014 utilise multi-objective optimisation techniques to study the effects of single and multiple preflash units on both energy consumption and yield. Their study investigates the vapour feed location and considers heat integration with and without preflash units. The optimisation variables varied include the steam flow to the main column and the furnace outlet temperature, as well as the vapour fraction from each flash unit; significantly, pump-around duties and temperature drops are not considered.

Enriquez-Gutiérrez (2016) applies a simulation-optimisation strategy to explore the option of installing a preflash unit as a retrofit option in a crude oil distillation system when increasing capacity. This study confirms that installing a preflash unit can help to alleviate hydraulic constraints in the column (Fraser, 2014), thus avoiding the need to replace column internals.

Table 2.1 summarises selected previous works about the design of crude oil distillation systems including a preflash unit. Table 2.2 presents an overview of previous works related to the optimisation of crude oil distillation systems with preflash units.

Table 2.1. Selected works on design of crude oil distillation systems with preflash units

Authors	Remarks
Golden, 1997	Flash temperature and vapour feed location insights.
Ji and Bagajewicz, 2002b	Pinch analysis is applied.
Errico et al., 2009	Compare the performance of columns with preflash units.
Benali et al., 2012	Demonstrate the benefits of preflash units in terms of exergy destruction.

Table 2.2. Optimisation of crude oil distillation systems with preflash units

Authors	Remarks
Al-Mayyahi et al., 2014	Use of multi-objective techniques to study effect of single and multiple preflash units.
Wang et al., 2016	Simulation-optimisation study for two different feedstocks.
Enríquez-Gutiérrez, 2016	Optimisation-based retrofit approach for heat integrated crude oil distillation systems with a preflash unit.

None of the methodologies discussed above provides a systematic design methodology for optimisation of crude oil distillation systems with preflash units that account for an extensive set of operating variables, as well as heat integration, product quality and yield constraints as it is addressed in this work.

2.4 Optimisation methods

2.4.1 Introduction

The need for efficient and systematic approaches drives the development of optimisation strategies. In Chemical Engineering, optimisation has been playing a key role in the design and operation of separation processes. It refers to finding the best solution to a problem within a certain range; where an objective function is needed to provide a measure to the performance of the system, this can be system costs, profit, etc.

Optimisation can be applied for minimisation or maximisation of the objective function with respect to (decision) variables subject to (process) constraints and bounds on the variables (Rangaiah, 2010). The constraints comprise a feasible region that defines limits of performance for the system. Process variables must be adjusted to satisfy the constraints.

In practice, engineers need to consider optimisation tasks on a regular basis so that a systematic approach with a fundamental knowledge of optimisation algorithms is essential.

Optimisation approaches can be classified as:

a) Gradient-based and
b) Metaheuristics

Gradient-based (deterministic) approaches aim to find the gradients of the response variables due to they rely on derivatives of the objective function. Although they require continuity of functions in the optimisation problem, less iterations are needed to find the final solution which is usually a local optimum. The quality of the solution depends on the initial values. Detailed descriptions of deterministic optimisation methods are provided in Edgar et al, 2001; Trespalacios and Grossman (2014) and Biegler (2014).

In the context of crude oil distillation, various researchers have used gradient-based approaches to meet diverse objectives, Gadalla (2003), applied a successive quadratic programming algorithm, SQP to improve the energy efficiency of a crude oil distillation unit and to find the optimal process conditions of a heat-integrated crude oil distillation system respectively. López et al., 2013, applied a gradient-based method to find the operating conditions that maximise the profit of an existing crude oil distillation system.

On the other hand, metaheuristic approaches are derivative-free algorithms which are designed to solve complex optimisation problems (Bianchi et al., 2009). Two main methods have been widely used to solve complex chemical processes such as crude oil distillation system design namely, genetic algorithms and simulated annealing. Motlagli et al., 2008 use a genetic algorithm to optimise product yields according to their market values. Chen (2008) proposes an optimisation-based retrofit approach for maximising the net profit of crude oil distillation systems using a simulated annealing algorithm. Ochoa-Estopier (2015) also uses a simulated annealing algorithm to optimise column operating conditions and the heat exchanger network structure of a heat-integrated crude oil distillation system.

To date, there are no optimisation-based design approaches that include a wide range of operational and structural variables for the design of crude oil distillation systems with a preflash unit. Chapter 5, will present a novel optimisation based-design methodology for the optimisation of fired heating demand in crude oil distillation systems with and without a preflash unit.

The following Sections present an overview of two optimisation algorithms widely applied in the context of crude oil distillation that are used in this work, a genetic algorithm and simulated annealing.

2.4.2 Genetic Algorithm

Genetic algorithms as an optimisation technique were proposed by Holland (1975). They mimic the process of natural selection starting from an initial encoded solution, a population is generated. The population is evaluated according to its fitness function, which is similar to the survival capacity of the species. Based on the fitness function, individuals are sorted and selected to be parents of the next generation. Then, they are combined to generate a new generation of children. Children are mutated and the elitism operator allows keeping the best solution during the optimisation process. The entire population evolves, with the fitness improving over generations (Bhaskar et al., 2000).

The application of the genetic algorithm for optimisation used in Chapters 3, 4 and 5 of this work, is described as follows and illustrated in Figure 2.1 (Ledezma-Martínez et al., 2018).

1. The search space is defined. In particular, upper and lower bounds are defined for the optimisation variables;
2. The optimisation parameters are selected, namely the size of the initial population size and the number of generations;
3. The initial generation is created randomly by the *gaoptimiset* algorithm;
4. The algorithm evaluates the objective function for all individuals in the population, applying penalties as required;
5. After evaluating the 'fitness' of individuals, the algorithm selects a sub-set of best-performing individuals;
6. The algorithm populates the next generation using genetic operators (crossover and mutation), applying the default parameters; the objective function is evaluated again for all individuals;

7. If a termination condition is met (e.g. maximum number of generations, or a very small change in the average value of the objective function over a certain number of generations), the solution corresponding to the 'best' solution is retrieved. This solution, including the corresponding set of optimised variables, represents the best-performing design, i.e. with lowest hot utility demand.

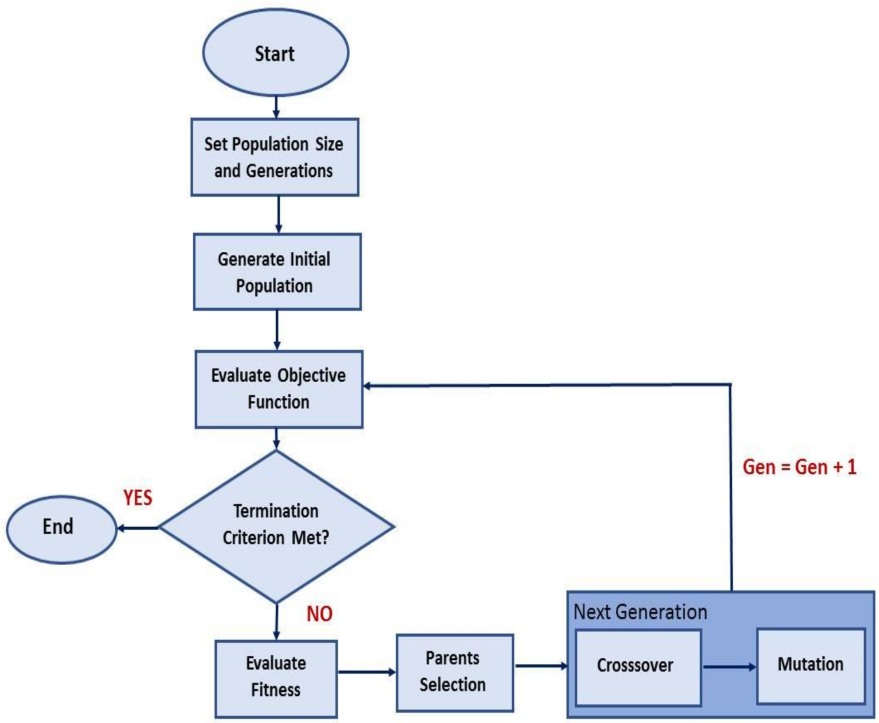


Figure 2.1 Overview genetic algorithm.

2.4.3 Simulated Annealing

Simulated Annealing is an optimisation method inspired by the process of annealing of metals. First, the metal is heated by raising the energy of the molecules allowing freely movement between them. Second, a cooling process is performed to minimise the energy of the particles by their accommodation in a crystalline structure. If the cooling process is done very quickly, then an amorphous structure is obtained, leading to a higher energy state. This simulation of the annealing of metals was proposed by Metropolis et al., 1953; however, Kirkpatrick et al., 1983 and Cerny, 1985 pointed out the analogy between this process and an optimisation strategy where the objective function is represented by the energy of the particles; the temperature and the cooling path are the operators which will need to be tuned. Simulated annealing algorithm uses only one solution from the entire search space; therefore, the acceptance of a new individual is based on a probability value.

The application of the simulated annealing method for optimisation used in this work in Chapter 4, as shown in Figure 2.2 is described as follows:

1. Initial operating conditions for the optimisation variables are used as a starting point within the search space.
2. Optimisation tuning parameters are selected; in particular, an initial value for the annealing temperature is needed.
3. A random nearby solution, called move, is generated around the current solution.
4. The objective function of the new proposed solution is calculated and compared with the current solution.
5. If the new value of the objective function is lower than the initial calculated value, the new solution is accepted. Otherwise, it is accepted by applying a suitable acceptance criterion.

6. If the acceptance criterion is met, the annealing temperature is updated applying a cooling schedule.
7. At each annealing temperature, the process is repeated, before the annealing temperature is reduced, and the whole cycle is repeated.
   The algorithm stops when a defined termination criterion is met.

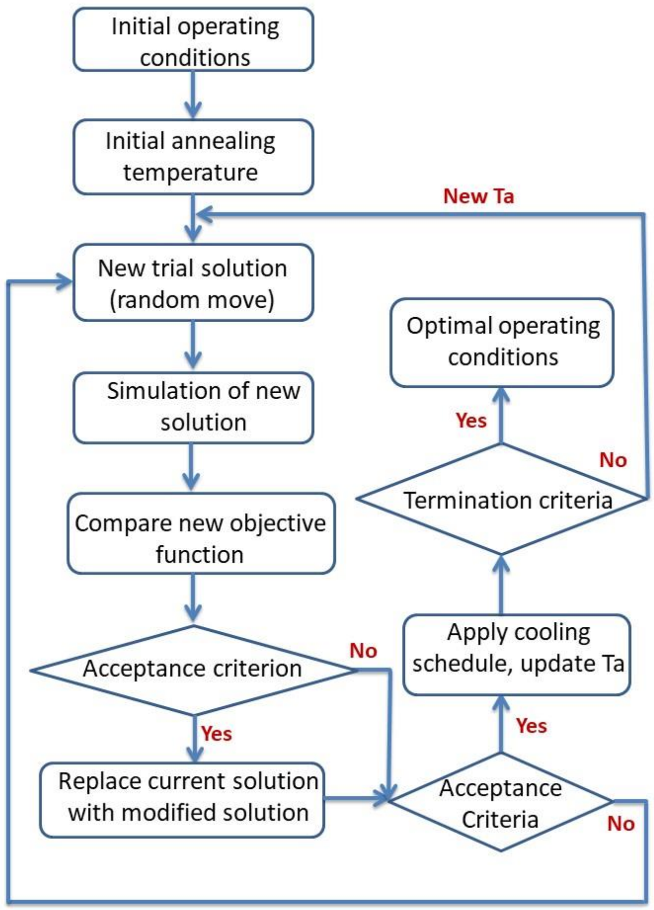


Figure 2.2 Simulated annealing algorithm (adapted from Chen, 2008).

In this work, solvers (*gaoptimset, and simulannealbnd)* embedded within the Global Optimisation Toolbox in MATLAB R2016a are used to perform the optimisations of the crude oil distillation system with and without a preflash unit. See Appendix B, Tables B2 and B9 for details about the number of function evaluations that are needed for the optimisation using simulated annealing that will be presented in Chapter 4. In general, genetic algorithm performed better than simulated annealing based on the objective function values obtained after carrying out optimisation of the system.

2.5 Crude oil distillation systems design by optimisation

In the case of complex Chemical Engineering problems such as the design of crude oil distillation systems, a process simulator is generally integrated as a black box model into the evaluation step of an optimisation framework, which mainly uses the degrees of freedom of the process (i.e. pump-around duties and temperature drops, steam flow rates). Process models are usually implemented within simulation software such as Aspen HYSYS, while additional software (i.e. MATLAB) can be linked to the process simulator via an interface to facilitate data transfer.

In addition to the solution of the simulation model, the software may also facilitate the integration of additional constraints, e.g. product quality specifications. However, not all constraints can be handled by the process simulator so that constraint violations need to be implemented in an optimisation framework (Skiborowsky et al., 2015). Therefore, genetic algorithms make use of ‘penalty functions’ as will be presented in Chapter 3. This is especially important because failure in the simulation convergence can result in a failure of the optimisation (Caballero, 2015).

From the perspective of the optimiser, a lack of convergence of the simulation and infeasible design specifications are indistinguishable (Silva and Salcedo, 2009) so that the determination of an infeasible design can become the bottleneck of stochastic optimisation.

Some authors assume that nonconvergent simulations correspond to an infeasible solution (Linke and Kokossis, 2003; Moddla, 2013) but this may limit the optimiser to suboptimal solutions due to a lack of convergence.

Therefore, having a high convergence ratio (ratio of converged solutions for the evaluation of a set of feasible degrees of freedom) is of prime importance for a successful optimisation (Silva and Salcedo, 2009).

To summarise, the optimisation of complex engineering design problems such as the design of crude oil distillation systems is not straightforward due to the high computational effort (several hours to days) that is needed to perform an optimisation. Consequently, there is a need for alternative approaches that allow a reduction in computational time without compromising the performance of the system and also guarantee that constraints in product qualities are met.

Recent developments (Ochoa-Estopier, 2014; Ibrahim, 2018) regarding the implementation of surrogate models, such as artificial neural networks, within an optimisation framework, have demonstrated to be a good alternative to overcome high computational effort in the optimisation of crude oil distillation systems. Figure 2.3 summarises the design of crude oil distillation systems by optimisation followed in this work. A brief review on artificial neural networks is presented in the next Section.

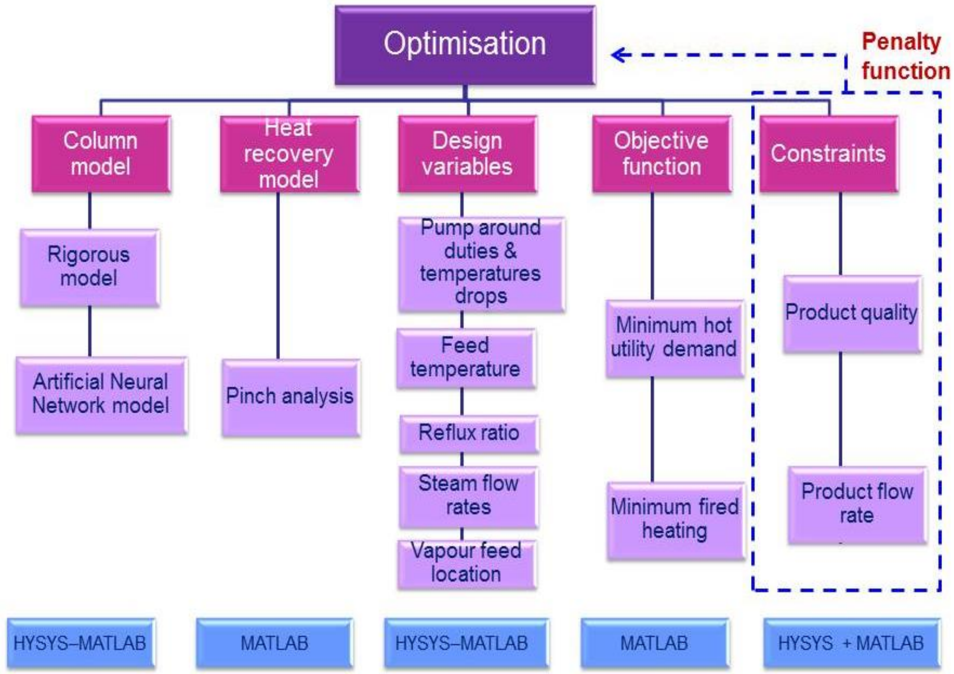


Figure 2.3 Crude oil distillation system design by optimisation (adapted from PRES 17 workshop presentation, Jobson M., 2017).

2.6 Artificial Neural Networks, ANN

An artificial neural network is a structure built by many interconnected basic elements called neurons. It is similar to the natural tissues in the human brain so that early work on the field of the neural networks was focused on modelling the behaviour of neurons found in the human brain (Himmelblau, 2000).

Artificial neural networks consist of a number of neurons (simple processors) which are arranged into layers as can be seen in Figure 2.4. A group of neurons called the input layer receive a signal form an external source; the output layer, return signals to the environment and the layers between the input and output layer are called hidden layers (Himmelblau, 2000).

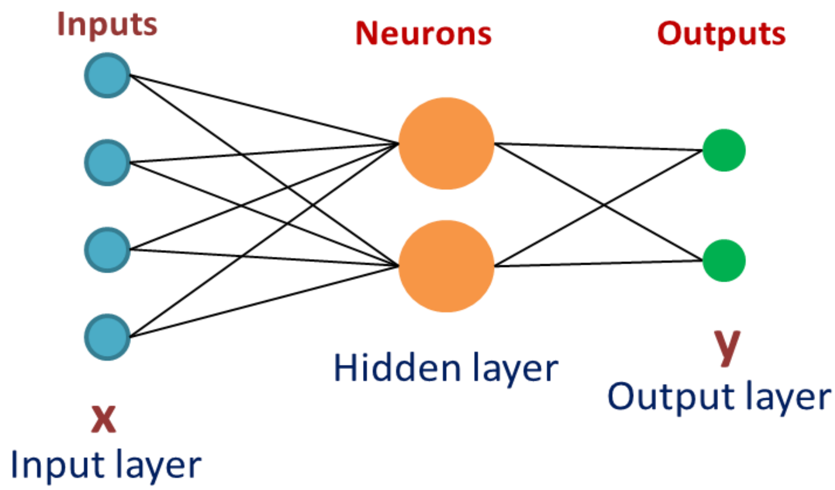


Figure 2.4 Artificial neural network, ANN.

Neurons in adjacent layers of the artificial neural network are connected by weighted links passing signals from one layer to the next adjacent layer. Those links have numerical weights that are applied to the inputs of a neuron. An artificial neural network learns through the repeated adjustment of the weights to obtain the desired output signal.

Artificial neural networks can be divided based on the type of connections between neurons. In this work, multilayers, feedforward networks are used. It means that the signal that they receive is directed from the input to the output layer, without cycles.

The feedforward structure of ANN consists of a multilayer structure whereby there are hidden nodes in between the input and output layers. However, there is no specific method to obtain the number of the hidden nodes and it is commonly based on trial and error basis to find the appropriate number of nodes that will provide the best results (Aliet et al., 2015). Table 2.3 shows the principal elements of an artificial neural network and Figure 2.5 illustrates the architecture of a network neuron.

Table 2.3. Elements and description for an ANN

Element in an ANN	Description	Symbol
Inputs	Independent variables	x
Outputs	Dependent variables	y
Neurons	Number of relations	S
Layer	Stages of connections	
Transfer function	Form of equations	f
Weights	Regression coefficient	W
Bias	Regression coefficient	b

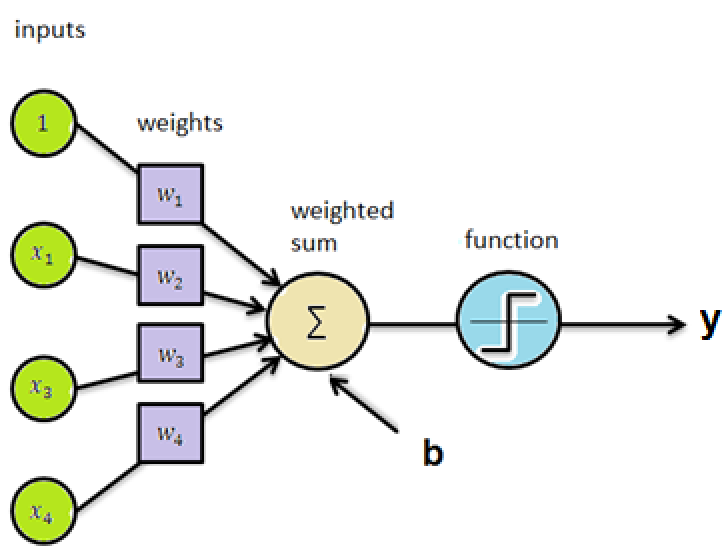


Figure 2.5 Architecture of a network neuron.

Feedforward network is the most common architecture due to it is easy to implement within an optimisation algorithm. In this type of architecture, information is processed in the forward direction only (Beale et al., 2015).

The summation point (weighted sum) adds the product of all inputs along with their corresponding weights and bias. The transfer function takes an input (x) to produce an output (y). In this work, both sigmoidal and linear functions are used in the hidden and output layers respectively.

A neural network needs to be "trained" to be able to replicate the behaviour of the input-output data. This training is performed using an optimisation method such as the Levenberg-Marquardt; this method provides a faster training to the neural network, so it is selected to perform the training process of the network in this work. In order to facilitate the training and enhance their performance of a neural network, all the input-output data sets need to be scaled between -1 and +1 (Beale, et al, 2015).

The mean squared error is used in this work to evaluate the performance of a neural network, it is defined as follows:

$$mse = \frac{1}{N}\sum_{i=1}^{N}(t_i - a_i)^2 \qquad (2.1)$$

where, t and a are the target and predicted output: N is the total number of samples.

Surrogate models have gained popularity over the past three decades due to their simplicity to represent complex models. One of the advantages of using ANN models is that once the network is trained, it provides a response with a few simple calculations.

The use of surrogate models within an optimisation framework, resulting in significant savings in terms of computational time. In particular, artificial neural networks (ANN) are used for process modelling, process control and optimisation.

2.7 Modelling crude oil distillation systems using artificial neural networks

In response to the demand for increasing oil production levels and strict product quality specifications, the intensity and complexity of the operation of oil refineries have been increasing during the last three decades. To improve the operating requirements associated with new market demands, design engineers are increasingly looking into the implementation of new design methodologies (Bawazeer and Zilouchian, 1997).

Mathematical models are important for the design of chemical and petrochemical plants. However, the high computational time required in solving models is a major problem for on-line applications so that there is a need to look for alternative approaches to solve high non-linear models such as a crude oil distillation column model (Yusof et al., 2003). Traditional approaches of solving chemical engineering problems have their limitations in the modelling of these highly complex and non-linear systems (Himmelblau, 2000). Because of the non-linear interactions between the operating input and output variables in a crude oil distillation column, maintaining optimal operating conditions of the column is a challenging task.

Artificial neural networks had generated interest in Chemical Engineering since late eighties as an alternative approach to model a process. ANN modelling approach is efficient and accurate for a system with non-linear interactions among several variables. An ANN model can represent the knowledge of the process operation. The model is constructed to describe the relationship between input and output variables of a crude oil distillation unit (Motlaghi, 2008).

Research on crude oil distillation system design and optimisation using artificial neural networks has been increasing in the last ten years. Liau et al., 2004 and Motlaghi et al., 2008 develop an artificial neural network (ANN) model of a crude oil distillation column using data from existing plants. Liau et al., 2004 solved an optimisation problem to determine the operating conditions to achieve better product yields maintaining the required product specifications; however, no details about energy efficiency were included into their optimisation approach. In the work of Motlaghi et al., 2008, product flowrates were optimised according to their market value. They use a genetic algorithm to perform the optimisation but again, no heat integration was taken into account in their optimisation framework.

Yao and Chu, 2012 used a non-linear regression method known as support vector regression to optimise the operating conditions of a crude oil distillation unit. A wide range of optimisation variables was included into their optimisation framework such as product flow rates, pump-around temperature drops, stripping steam, column inlet temperature, reflux ratio. They used rigorous simulations in Aspen Plus to generate the samples used to regress the model. Energy requirements were calculated without including heat exchanger network details.

López et al., 2013 developed an optimisation framework to improve net profit of a crude oil distillation system with three atmospheric distillation columns and two vacuum columns. Rigorous simulations in PRO/II were performed to generate the data to regress the model based on second order polynomial functions. Optimisation variables pump-around temperatures and flow rates, stripping steam flow rates and temperatures for the furnace and condenser.

Ochoa-Estopier and Jobson, 2015 used artificial neural networks to carry out operational optimisation of crude oil distillation systems. Their optimisation framework is developed using the simulated annealing method to optimise net profit. Data generated via rigorous simulations in Aspen HYSYS is used to regress the column model. They took into account the dependence of thermal properties on temperature in process streams using linear and third order polynomial correlations. Optimisation variables include pump-around temperatures drops and duties, product and steam flow rates and the feed inlet temperature.

Osuolale and Zhang, 2017 included a prefractionator within the crude oil distillation system. They used a bootstrap aggregate artificial neural network where the predictions for all the artificial neural network build are aggregated and used as the network output with the aim to improve the accuracy on the ANN. They used a successive quadratic programming algorithm to optimise a profit objective.

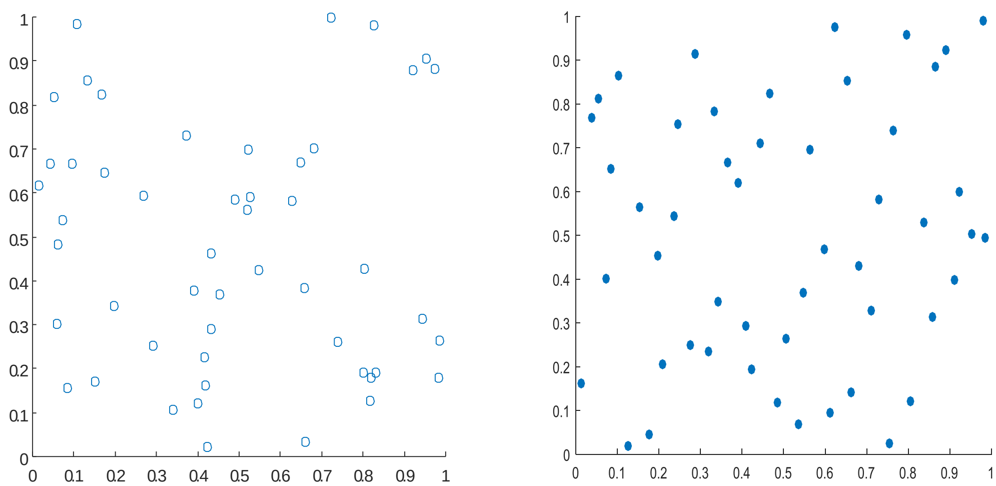
Ibrahim et al., 2018 propose a novel optimisation framework for the optimal design of flexible crude oil distillation systems. The crude oil distillation unit is modelled using a rigorous tray-by-tray model where the number of trays active in each section is also a design degree of freedom. They used a support vector machine as a feasibility constraint. The support vector machine is a classifier which filters infeasible design alternatives form the search space reducing computational time and improving the quality of the final solution. Pinch analysis is considered to maximise heat recovery.

To date, the modelling of a crude oil distillation system with a preflash unit using artificial neural networks accounting for a wide range of optimisation variables (i.e. pump-around duties and temperature drops, stripping steam flow rates, reflux ratio, column inlet temperature), including the vapour feed location in the main column has not been reported.

Training the artificial neural network takes only a few seconds, from the total samples generated, they are randomly divided into three sets: training (70%), validation (15%), and testing (15%). Number of hidden neurons can be adjusted until the desired performance of the network is achieved. Maximum number of iterations is defined by the neural fitting tool in MATLAB, usually set as 1000.

2.8 Latin Hypercube Sampling (LHS)

As it has been presented in the previous Section, initial data needed to create a model using artificial neural networks is the generation of samples. McKay, Beckman and Conover (1979) proposed Latin Hypercube Sampling, LHS as an attractive alternative to simple random sampling in computer experiments. The main feature of LHS is that it simultaneously distributes the samples in all input dimensions as can be seen in Figure 2.6.



a) Random sampling

b) LHS sampling

Figure 2.6 Random and LHS samples generated in MATLAB.

This sampling method, allows the samples to be randomly generated, but no two points share input parameters of the same value (Loh, 1996). The samples are divided into homogeneous subgroups with the aim to improve the precision of the sample by reducing sampling error.

In this work, the samples used to build the distillation column model are generated using the Latin Hypercube Sampling function (*lhsdesign*) embedded in MATLAB R2016a.

2.9 Heat integration in distillation systems design

In general, crude oil distillation systems are energy-intensive: it is estimated that 7 to 15% of the crude oil input is consumed in refinery processes, of which 35 to 45% is used for crude oil distillation (Szklo and Schaeffer, 2007).

In practice, heat integration is crucial for energy-efficient operation of crude oil distillation systems. Heat integration, the recovery of heat between streams requiring cooling and streams requiring heating, reduces the need for hot and cold utilities. In these systems, the crude oil feed needs to be heated, usually from ambient conditions, to the temperature of the desalter and then to the temperature of the column feed; this 'cold stream' is heated by other 'hot' streams in the system that require cooling – these include pump-arounds and product streams (Ochoa-Estopier et al., 2015).

Early design procedures do not include the interactions between the distillation column and the heat exchanger network. Therefore, design methodologies which consider both the distillation column, and its heat recovery network provide an opportunity to explore energy efficiency in the systems.

Liebmann (1996) reported an integrated approach for the design of heat-integrated crude oil distillation systems; he used the grand composite curve to find the appropriate design of an integrated crude oil distillation column. This work has the advantage that he considered the distillation column and its heat recovery system simultaneously.

Suphanit (1999) used shortcut distillation models in order to simulate a crude oil distillation system in a grassroots design, taking into account pinch analysis and an optimisation framework to produce energy-efficient column designs. As a result, it was found that optimising the operating conditions of the distillation column reduce energy consumption for a given minimum temperature approach.

Rastogi (2006) analysed a distillation column and HEN simultaneously for grassroots and retrofit designs; his work is an extension of the shortcut models of Suphanit (1999) and Gadalla (2003) considering the effect of pressure drop in the atmospheric distillation column. Then, he developed a methodology to be applied to the vacuum distillation column.

Chen (2008) extended the work published by Rastogi (2006), she proposed a methodology that can be applied either to grassroots designs and retrofit designs including refining specifications in short-cut models, eluding the need of identifying key components and its recoveries.

It is important to point out that the methodology proposed by Rastogi (2006) and continued by Chen (2008) has the consideration to join the distillation unit and the HEN into an optimisation framework, expanding the number of design options.

Ochoa-Estopier and Jobson (2015) evaluated a new methodology for optimising heat-integrated crude oil distillation systems applying artificial neuronal networks models to avoid convergence issues. They reported a case study that is validated with the grand composite curve (GCC) in terms of heat recovery comparing minimum energy requirements when assuming temperature–dependent and constant properties.

Enríquez-Gutiérrez et al. (2015) proposed a systematic retrofit methodology of distillation systems and heat exchanger networks to revise and evaluate hardware adjustments to increase capacity. Their work highlights the necessity of considering both the distillation column and HEN when modelling crude oil distillation systems.

2.9.1 The Grand Composite Curve

The grand composite curve (GCC) as shown in Figure 2.7 is a plot of interval temperatures against enthalpy. It can be described as a profile of the net heat surpluses and heat demands of process streams at different ranges of shifted temperature intervals. The grand composite curve is a tool for understanding the interface between the process and the utility system (Smith, 2016).

Hot streams are represented $\Delta T_{min}/2$ colder and cold streams $\Delta T_{min}/2$ hotter than they are in practice. The heat recovery pinch is the point of zero heat flow in the grand composite curve. The open “jaws” at the top and bottom are the hot utility (Q_{Hmin}) and cold utility (Q_{Cmin}), respectively. Shaded areas, known as *pockets* represent areas of additional process-to-process heat transfer (Smith, 2016).

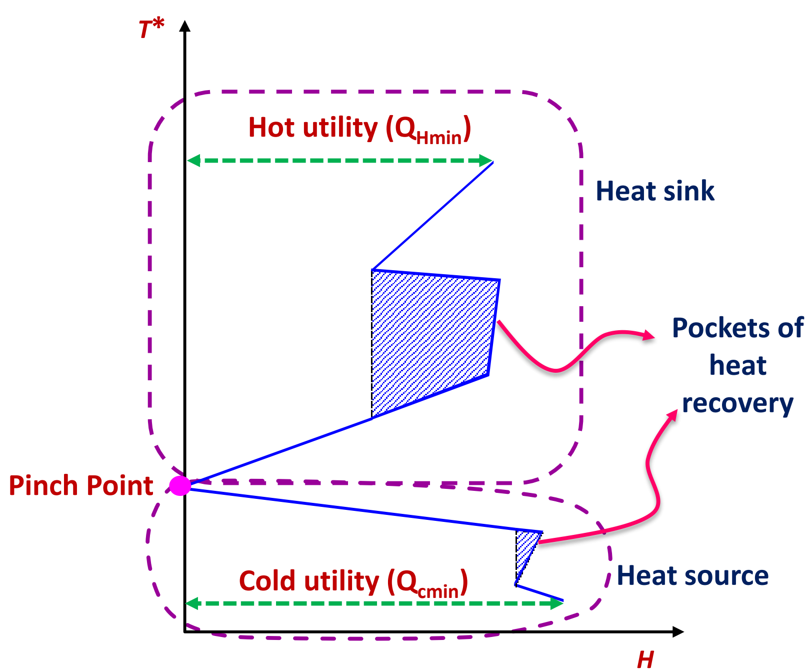


Figure 2.7 Grand Composite Curve, GCC (Source: Smith, 2016: Figure 17.24).

In this work, it is important to capture the impact of process design choices on opportunities for heat recovery and utility demand, but there is no need for detailed information about the heat exchanger network design.

Therefore, the grand composite curve will be used to represent the net heating and cooling demands of the process and the corresponding temperatures.

2.9.2 Fired heaters (Furnaces)

Fired heaters are essential in refineries; they are used to heat all types of hydrocarbons, hot coils, steam or air. The largest energy consumption in any refinery is associated with its fired heater.

In a fired heater, gaseous, liquid or solid fuels are burnt to provide high-temperature heat to process streams by heat transfer from the flame and combustion gases. In a refinery, waste gases blended with natural gas, heavy or light fuel oils, etc. may be used as fuels for heaters. Fuel is combusted with air or oxygen to produce hot flue gas. Inefficient furnaces contribute to fossil fuels problems due to higher fuel demand and higher carbon emissions (Izyan and Shuhaimi, 2014). The minimum fuel consumption targets in the furnace represent minimum fuel cost. Nevertheless, there are unavoidable stack losses (energy taken from the fuel being burnt along with the flue gases that is unutilised).

Figure 2.8 illustrates a furnace model. The flue gas represented by the slopping line, starts at its theoretical flame temperature (T_{FT}), shifted for a given $\Delta T_{min,}$ ending at the ambient temperature (T_{amb}).

The theoretical flame temperature of 1800°C is used as a reference. Stack temperature (T_{stack}) should not be lower than the corrosion limit which is usually 160°C (Delaby, 1993).

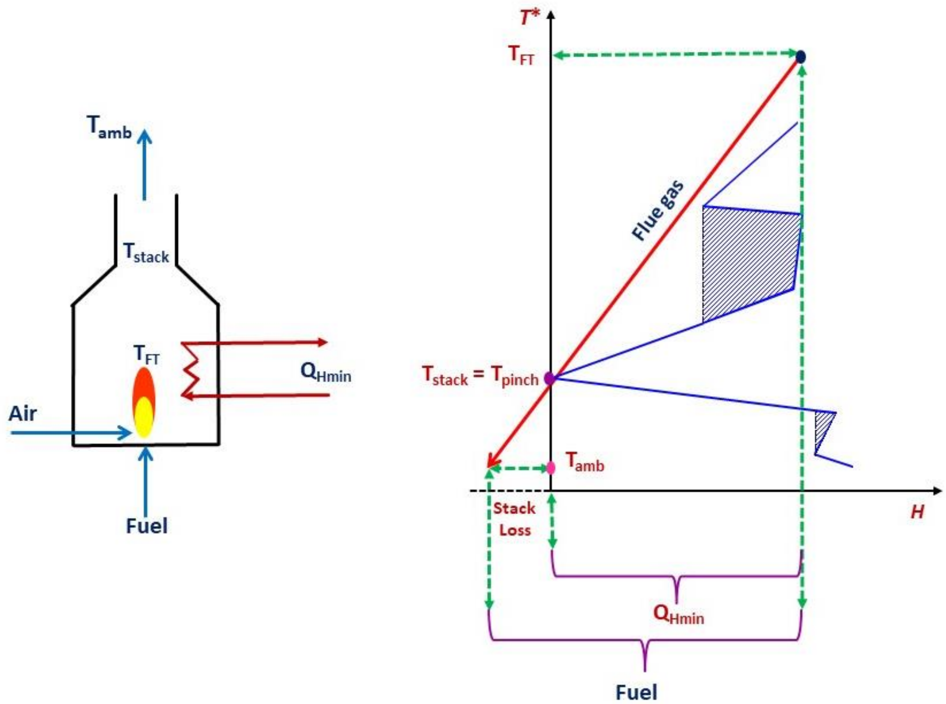


Figure 2.8 Simple furnace model (Source: Smith, 2016: Figure 17.27).

Three different cases (see Figure 2.9) are considered to evaluate the total fuel consumption in a crude oil distillation system:

- Case 1: Process pinch limitation
- Case 2: Utility pinch limitation
- Case 3: Dew point temperature limitation

The role of heat integration within an optimisation framework will be addressed in the next section as an introduction to the optimisation-based design methodology that will be presented in Chapter 5.

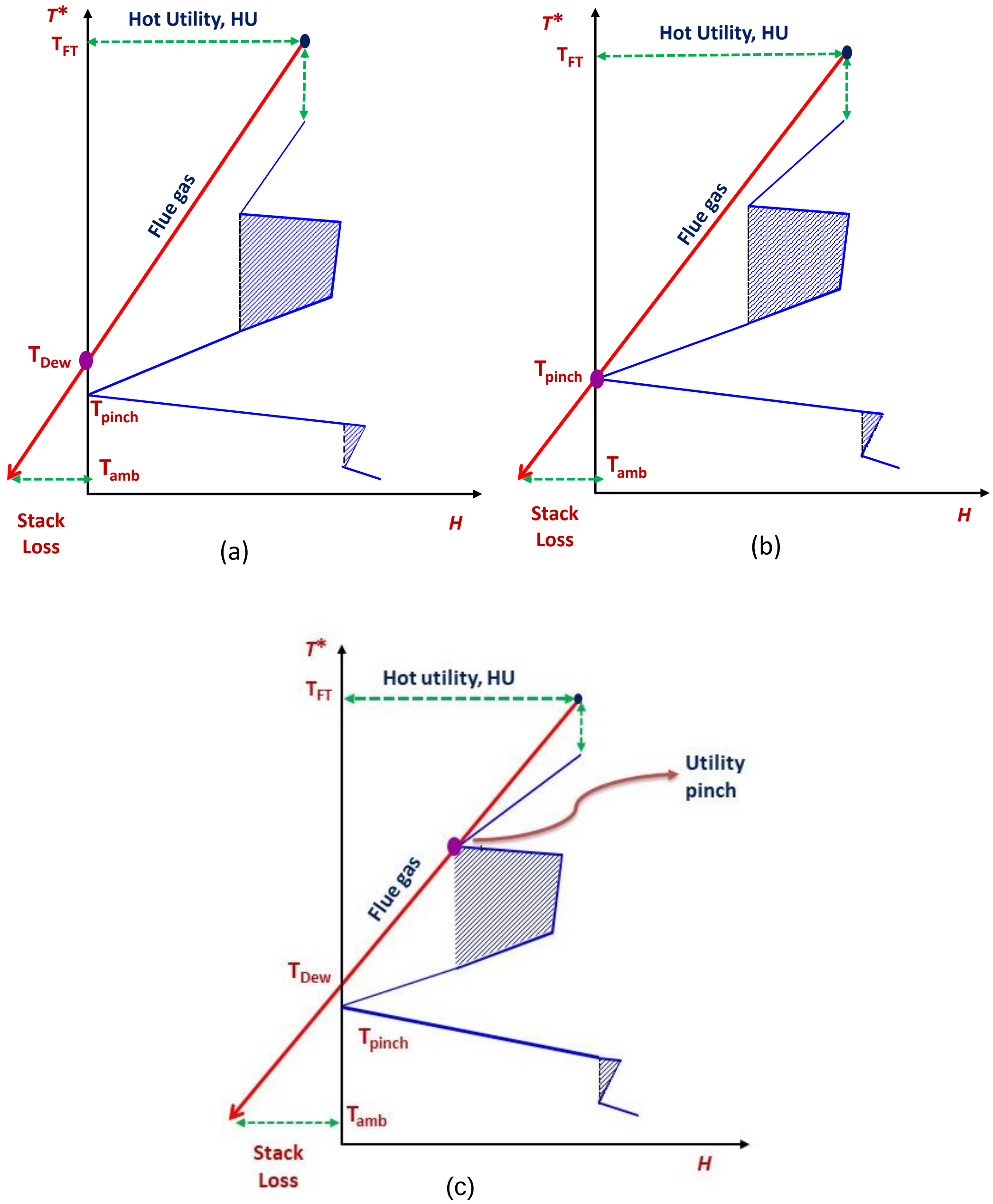


Figure 2.9 Flue gas line: (a) Limited by dew point temperature, (b) Limited by process pinch; (c) Limited by match between process and utility. (Source: Smith, 2016: Figures 17.28 & 17.29).

2.9.3 Role of heat integration within an optimisation framework

Oil refining is a major traditional area for pinch studies. Pinch analysis method has some disadvantages mainly due to the fact that the method is based on heuristic rules and it is best suitable for the design of small-scale problems (Shenoy, 1995). In particular, the Grand Composite Curve (GCC) has the limitation that details about the individual streams are not shown.

To overcome the limitation of the use of pinch analysis in big-scale problems such as a crude oil distillation system, mathematical programming provides a framework for an 'automatic design' reducing optimisation time which is a limiting factor in any refinery.

This work applies 'pinch technology' to evaluate the minimum heating and cooling requirements, after all opportunities for heat recovery have been exploited (Smith, 2016). In particular, the grand composite curve is used to assess the minimum hot utility demand; in these systems, the temperature at which heat is needed requires fired heating. This approach allows minimum utility requirements to be calculated for each converged simulation, without requiring more detailed analysis and design of the heat recovery system. The disadvantage of this approach is that the investment costs and complexity of the heat recovery system that could achieve these utility targets are not considered (Ledezma-Martínez et al., 2018).

In the context of the optimisation of this complex distillation system, designing a HEN for each possible column design would require very significant computational effort. Therefore, the design of the heat exchanger network is not addressed in this work. Previous research (Smith et al., 2010) proposes a relevant approach.

Pinch analysis is carried out within MATLAB R2016a using an open source algorithm (Morandin, 2014), where relevant stream data (supply and target temperatures and duties) are extracted from Aspen HYSYS for each proposed design. This algorithm is extended in this work to allow the evaluation of the fired heating demand in a crude oil distillation system as explained in the following section.

2.9.4 Algorithm to evaluate fired heating demand

The subroutine used in Chapters 3 and 4 to calculate the minimum hot utility demand of the crude oil distillation system is extended to account for the calculation of fired heating as follows:

1. From the cascade information, a new matrix (matrix A) is created including supply and target temperatures, heat capacity flow rate and change in enthalpy for each stream.

2. The heat capacity flow rate is identified using the function *sign* in MATLAB.

3. The value for the theoretical flame temperature (T_{FT}) is set to be equal to 1800ºC (Smith, 2016).

4. The slope of the flue gas line, m (flue gas profile for a fired heater) is calculated using the line equation:

$$m = \frac{T_{FT} - T_T}{HU - \Delta H} \tag{2.2}$$

where T_T is the target temperature, HU is the minimum hot utility demand, T_{FT} is the theoretical flame temperature and ΔH is the change in enthalpy.

5. A temperature dew point limitation is set to be equal or greater than 160ºC.

6. A new matrix (C = [T, DH, M]) is created to include only values of target temperatures (T) greater than the dew point limitation, change in enthalpy values (DH) and the flue gas line slope (M).

7. The *min* function in MATLAB is used to find the minimum slope value (M) and the minimum change in enthalpy value (DH), from matrix C.

8. As the length of matrix C will be changing on each iteration, the function *position* in MATLAB is used to find the position of the target temperature, (T) that corresponds to the minimum slope, (M) of the flue gas line.

9. The position of the new value for the change in enthalpy (DH_{new}) of matrix C, which will be changing on each iteration, is also found applying the *position* function in MATLAB.

10. Three different cases (See Figure 2.8) according to the temperature values of matrix C are defined within the MATLAB subroutine using an *if clause* as follows:

- Case 1: T = Pinch point, a process pinch limitation.
- Case 2: T ≠ Pinch point, a heat recovery pocket limitation.
- Case 3: $T<T_{dew}$, a dew point temperature limitation.

11. To calculate the stack losses of the crude oil distillation system, three important points are identified numerically which represent the flue gas line: point 1: minimum hot utility demand and theoretical flame temperature, $P_1 = (Q_{Hmin}, T_{FT})$; point 2: intersection of the flue gas line on "y" axis, $P_2 = (0, T_T)$ and point P_3: stack loss value, P_3: = (stack loss, 0) as illustrated in Figure 2.10.

12. Values for the stack losses are calculated based on the specific case according to the value of the target temperature (T) as follows:

- Case 1: Stack loss 1 (SL_1) = T/M
- Case 2: Stack loss 2 (SL_2) = f/M; f = (T-DH/M)
- Case 3: Stack loss 3 (SL_3) = g/M; g= (T-DH_{new}) * M

13. The total fuel consumption of the system (FH) is evaluated as the sum of the minimum hot utility demand (Q_{Hmin}) plus the corresponding stack loss.

$$FH = Q_{Hmin} + SL \tag{2.3}$$

14. The objective function (min fired heating, min FH) is expressed as:

$$\min FH = FH + Penalty * (g_{x1} + g_{x2} + g_{x3}) \tag{2.4}$$

where g_{x1}, g_{x2} are the inequality constraints for product qualities and g_{x3} is the inequality constraint for the residue flow rate.

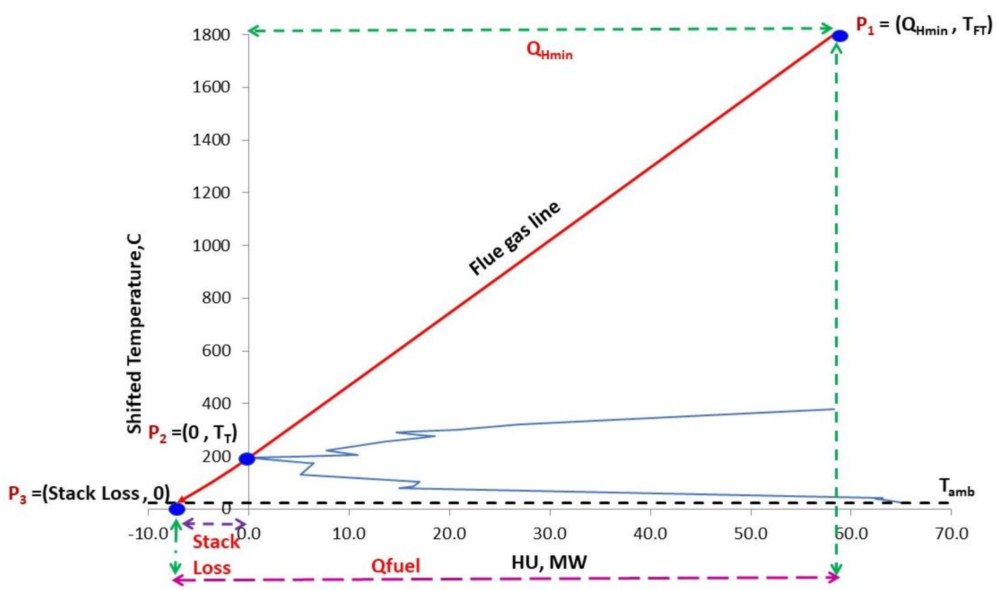


Figure 2.10 Flue gas line representation.

2.10 Hydraulic considerations in distillation

Distillation is based on the concept of vapour-liquid separation stage in which vapour and liquid loads are in contact in the column internals. Internals can be divided into two categories: trays and packings (Kister, 1992, Ch. 6).

To meet fixed product specifications, there will be a maximum feed flow rate that can be separated for an existing distillation process with a fixed feed composition. Flooding will occur on those stages with the highest traffic due to it is associated with the combination of the liquid and vapour flows (Liu and Jobson, 2004). Typically, the distillation column is designed with 80-85% tray flooding. In operation, the column can operate harder to reach 90-95% of the flood limit (Zhu, 2014).

This Section introduces hydraulics of trayed columns and presents the results obtained after optimisation by using correlations embedded in Aspen HYSYS v8.8 for conventional trays.

2.10.1 Hydraulics of trayed columns

Sieve tray is a flat perforated plate where the vapour velocity keeps the liquid from flowing down through the holes (weeping effect). With a low vapour velocity, liquid weeps through the holes reducing its efficiency (Kister, 1992). Figure 2.11 shows a tray hydraulic model and a sieve tray.

Figure 2.12 illustrates the flow limits at which trays can operate efficiently. Flooding is an excessive accumulation of liquid inside the column; it sets the upper limit and can be caused by spray entrainment flooding or froth entrainment flooding. Downcomer backup flooding occurs when aerated liquid is backed up into the downcomer due to a pressure drop in the tray, if it exceeds the tray spacing, liquid accumulates on the above tray, causing downcomer backup flooding (Kister, 1992). Weeping sets the lower limit of operation when liquid descends through the tray perforations, caused by a low vapour flow.

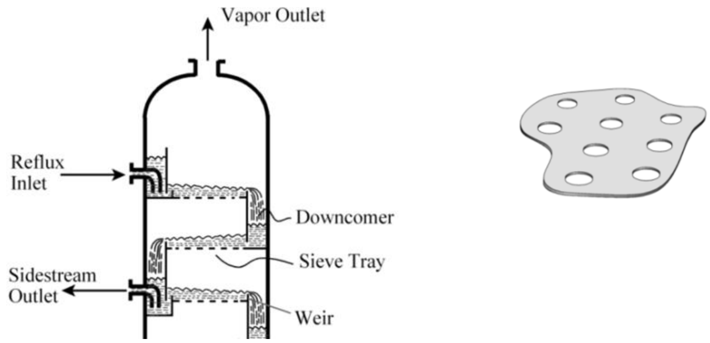


Figure 2.11 Tray hydraulic model and sieve tray (adapted from Figure 8.6, Smith 2016).

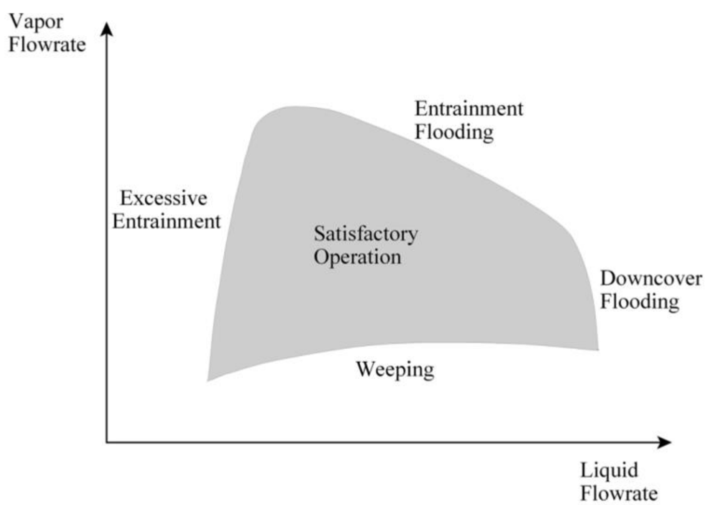


Figure 2.12 Tray operation region (Source: Figure 8.24, Smith 2016).

The most popular criteria for the maximum velocity of clear liquid at the downcomer entrance are the Glitsch, Kosch and Nutter correlations. Glitsch correlation is set by default in Aspen HYSYS equipment design package, this correlation is used in this work as a jet flooding method.

To account for the hydraulic constraints related to the liquid loads, this work assesses two hydraulic parameters: the downcomer exit velocity and the approach to downcomer flooding. To prevent tower malfunction, it is recommended that the approach to downcomer flooding does not exceed 80-85% of the design limit (Koch-Glitsch, 2013).

Weir loading is another important parameter for tray ratings. It is calculated as the clear liquid volume divided by the length of the tray outlet weir. This value has a direct influence on the froth height on the tray as higher weir loadings increase the fluid crest over the weir. If the weir loading is too high, leading to an excessively high weir crest, the number of downcomers can be increased by introducing multiple passes as shown in Figure 2.13.

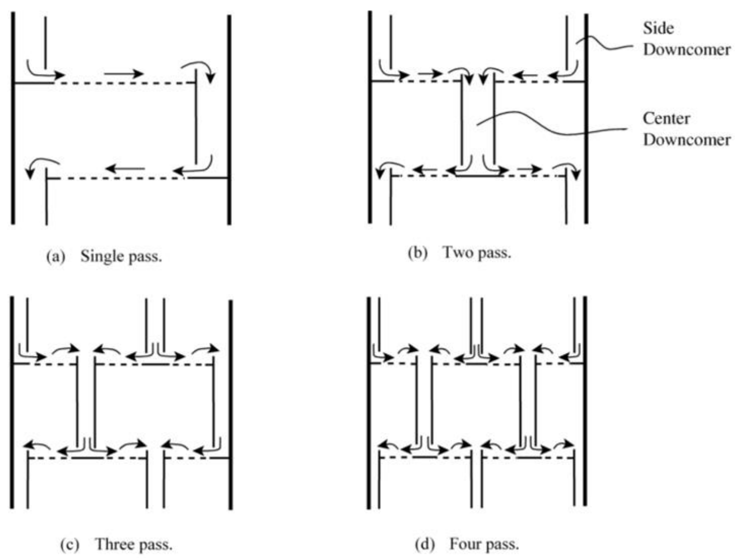


Figure 2.13 Multipass tray layouts (Source: Figure 8.9, Smith 2016).

2.10.2 Hydraulic performance for a CDU with and without a preflash unit

Figure 2.14 shows the diagram for a crude oil distillation unit without a preflash unit. Figure 2.15 illustrates the configuration for the preflash case. In both cases, the crude oil distillation column has eight sections starting from top to bottom; stage numbering is presented in Table 2.4 where it can be noted that the stages in the side-strippers are numbered sequentially for easy understanding. Note that column sections and stage numbering are the same for the crude oil distillation system with a preflash unit.

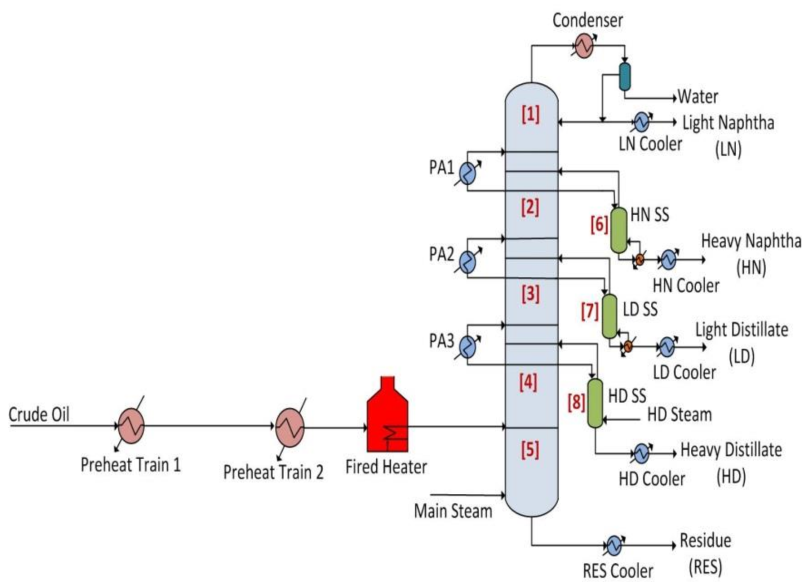


Figure 2.14 Crude oil distillation column configuration without a preflash unit.

For flooding calculations within Aspen HYSYS, the main distillation column is divided into five sections as shown in Table 2.4, while only one section is considered per stripper. The maximum flooding condition considered for all sections and strippers is 85%.

Table 2.4. Crude oil distillation column stage numbering

Column section	**Stage numbering**
Section 1*	1-9
Section 2*	10-17
Section 3*	18-27
Section 4*	28-36
Section 5*	37-41
Section 6 (HN SS)	42-47
Section 7 (LD SS)	48-54
Section 8 (HD SS)	55-59

*Main column

After optimisation of both systems (with and without a preflash unit), the hydraulic performance of them is analysed, noticing that key parameters such as downcomer flooding and downcomer backup are under design limits for all sections of the column due to the design constraints specified in Aspen HYSYS. For each optimisation run the algorithm takes into account these design constraints avoiding possible flooding problems related to column hydraulics.

Detailed data for each crude oil distillation system including hydraulic results, internals and geometry are presented in Tables 2.5 and 2.6. Figures 2.16 and 2.17 show performance comparisons of the crude oil distillation systems with and without a preflash unit studied in this work.

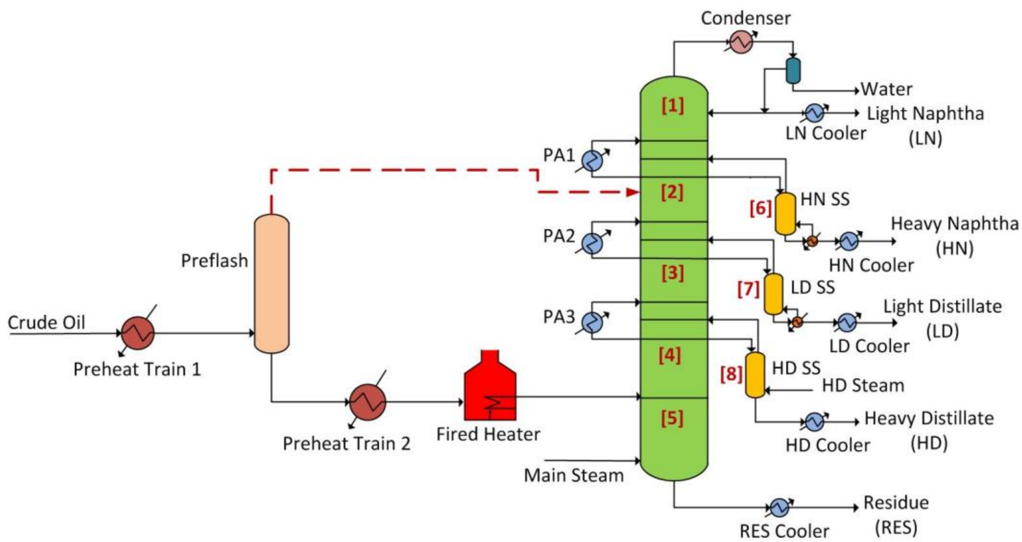


Figure 2.15 Crude oil distillation configuration with a preflash unit.

Table 2.5. Detailed hydraulic and column geometry for a crude distillation unit

Column Section	**[1]**	**[2]**	**[3]**	**[4]**	**[5]**	**[6]**	**[7]**	**[8]**
Hydraulic Results								
Max Flooding [%]	85.8	82.8	78.7	82.1	83.4	60.3	55.6	31.2
Max DC Backup [%]	43.7	46.1	41.1	37.4	44.6	28.0	30.1	23.10
Max Weir Load [m^3/h-m]	52.0	63.2	53.1	37.2	60.9			
Internals	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve
Number of Flow Paths	4	4	4	2	2	2	3	3
Jet Flooding Method	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch
Column Geometry								
Section Diameter [m]	5.2	5.5	5.6	5.3	5.0	1.7	2.6	2.4
Tray Spacing [m]	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
Section Height [m]	6.1	5.5	6.7	5.5	3.7	3.0	4.3	3.7

Table 2.6. Detailed hydraulic and geometry: preflash case

Column Section	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]
Hydraulic Results								
Max Flooding [%]	82.0	80.3	82.4	77.6	74.9	75.7	67.9	67.9
Max DC Backup [%]	46.1	46.4	40.0	31.3	35.2	40.9	33.4	36.3
Max Weir Load [m^3/h-m]	64.6	66.1	47.9	14.6	40.4			
Internals	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve
Number of Flow Paths	4	4	4	4	4	1	3	2
Jet Flooding Method	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch	Glitsch
Column Geometry								
Section Diameter [m]	5.2	5.3	4.6	4.1	4.0	1.5	2.6	1.8
Tray Spacing [m]	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
Section Height [m]	6.1	5.5	6.7	5.5	3.7	3.0	4.3	3.7

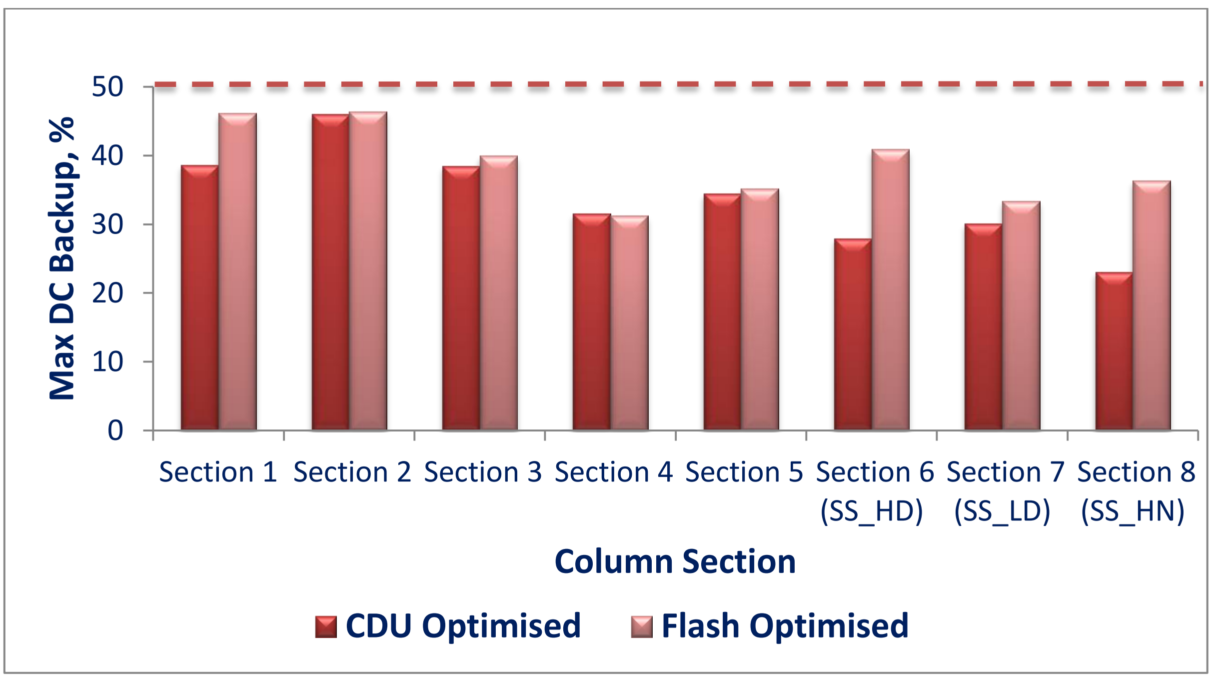


Figure 2.16 Downcomer flooding performances.

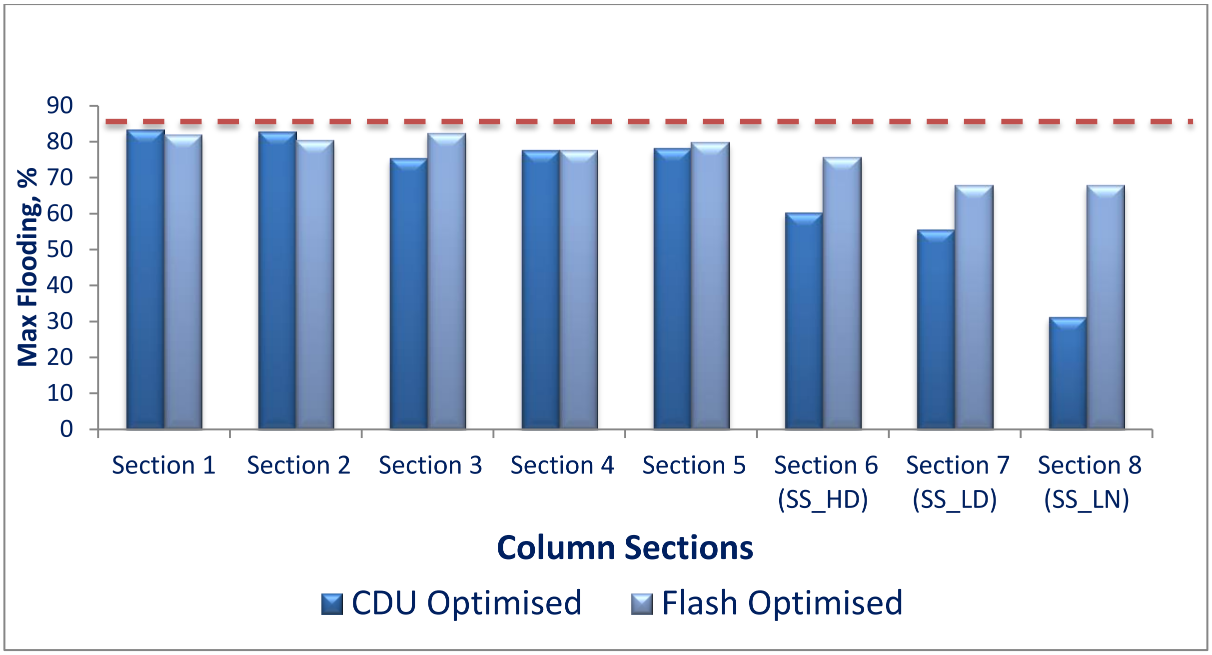


Figure 2.17 Jet flooding profiles.

2.10.3 Summary

In this Section, concepts about distillation column hydraulics are presented including sieve trays definition, tray operation region, flow limits, flooding methods and tray layouts. Then, the hydraulic performance of a crude oil distillation system with and without a preflash unit is evaluated in terms of their downcomer flooding and jet flooding profiles. Results obtained show that all the column sections are below flooding due to the constraints imposed within the equipment design option in Aspen HYSYS v8.8; in this way, for each optimisation run column hydraulics is taken into account. Finally, as all sections are below flooding, there is no need to add constraints in the optimisation framework developed in MATLAB; if necessary, they can be added as constraints within the optimisation algorithm as reported by Ochoa-Estopier and Jobson, 2015 and Enríquez-Gutiérrez, 2016.

2.11 Concluding remarks

This Chapter summarises developments on the design and optimisation of crude oil distillation systems over the years. Initially, traditional design methods were based on heuristic rules, involving trial an error. Later on, integrated design methods applied rigorous simulations in commercial software packages such as Aspen HYSYS, Aspen Plus and PRO/II. Pinch analysis is used to evaluate energy consumption within the heat exchanger network, HEN. Recently, optimisation-based design methods have been widely applied. In these methods, the design of the crude oil distillation system is supported by optimisation. Objective functions vary depending on the requirements of the refinery.

Exploiting the operating conditions of a crude oil distillation system can improve heat recovering opportunities, as it was discussed in this Chapter. Furthermore, adding a preflash unit to a crude oil distillation system helps to reduce the flow rate of the crude entering to the furnace, which in turn can reduce hot utility demand of the system.

However, there are some limitations of the current approaches available on the literature:

1. Design and optimisation methodologies developed over the years have been focussed mainly on the atmospheric distillation column only.

2. Modelling approaches using artificial neural networks have not been applied to the case when a preflash is added to a crude oil distillation system.

3. Process constraints are typically related to product specifications without paying attention to the residue flow rate.

4. Fired heating demand (including stack losses) of crude oil distillation systems with and without a preflash unit has never been explored and optimised simultaneously with its operating variables.

The above limitations of existing design methodologies and the importance of crude oil distillation processes in the refining industry motivate the present work. To date, no systematic optimisation-based design methodologies are available to design crude oil distillation systems with preflash units that account for heat integration and yield constraints. On the other hand, the importance of taking into account the role of fired heating demand within the evaluation of heat recovery opportunities has not been addressed in any published work. Today, new technologies/methodologies are increasingly sought; energy management and process integration of any refinery continues to be of prime importance.

Outcomes of this work can be of interest for industrial application in crude oil distillation processes with and without a preflash unit.

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Chapter 3

Optimisation-based Design of Crude Oil Distillation Systems with a Preflash Unit

This Thesis Chapter is based on two published papers:

1. Ledezma Martínez, M., Jobson, M., Smith, R. (2018a). Simulation-optimization-based Design of Crude Oil Distillation Systems with Preflash Units. *Industrial & Engineering Chemistry Research*, *57*(30). doi.org/10.1021/acs.iecr.7b05252.

2. Ledezma-Martínez, M., Jobson, M., Smith, R. (2018b). A new optimisation-based design methodology for energy-efficient crude oil distillation systems with preflash units. *Chemical Engineering Transactions*, 69, 385-390. doi.org/10.3303/CET1869065.

3.1 Introduction

Petroleum continues to be crucial in meeting global energy demand and crude oil distillation systems continue to play a central role in petroleum refining. World refining industry today is facing new challenges to meet strict requirements related to product quality, maximise the yield of valuable products in an energy-efficient way along with environmental regulations such as reducing CO_2 emissions. Particularly, crude oil distillation is a highly energy-intensive process; on average a crude oil distillation unit consumes around 20% of total energy consumption in a refinery (Fu and Mahalec, 2015).

Modelling crude oil distillation systems is not a trivial task due to the complexity of the crude oil mixture, column configuration and its interactions with the heat recovery system. Models need to describe the process accurately as they are used to perform the optimisation of the system. The effectiveness of the optimisation relies on the optimisation algorithm selected, the lower and upper bounds for the optimisation variables and on the complexity and accuracy of models (Jobson et al., 2017).

To date, systematic and accurate approaches for modelling and optimisation of crude oil distillation systems with a preflash unit are lacking. In practice a crude oil distillation system is likely to include a preflash unit. Hence, systematic and accurate approaches for modelling and optimisation of crude oil distillation systems with a preflash unit are needed.

A typical crude oil distillation system, as illustrated in Figure 3.1, comprises a preheat train, crude oil distillation units with side strippers and pump-arounds and sometimes pre-separation units, such as flash units and prefractionation columns. These systems are energy-intensive: it is estimated that 7 to 15% of the crude oil input is consumed in refinery processes, of which 35 to 45% is used for crude oil distillation (Szklo and Schaeffer, 2007). Preflash units can be useful for facilitating heat recovery within the system and thus reducing demand for fired heat for crude oil preheating prior to distillation. The preflash unit carries out a partial separation – the vapour recovers some low-boiling components and some material in the boiling range of light naphtha. This vapour stream bypasses the fired heater, helping to reduce its fuel consumption; the vapour may then be mixed with the stream leaving the furnace or be fed to the main column at a suitable location.

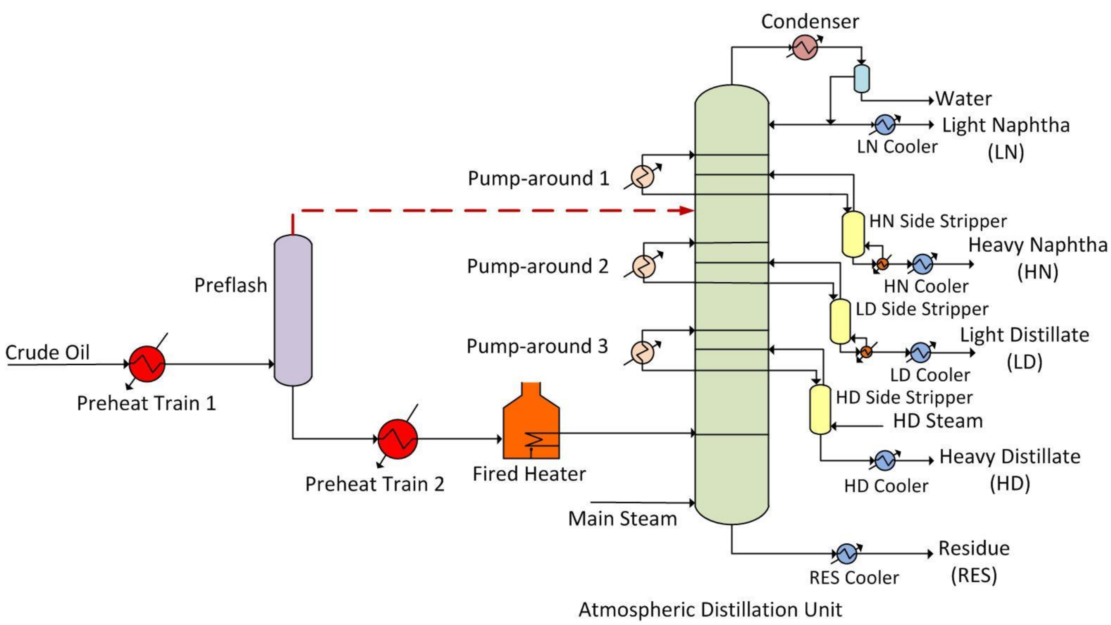


Figure 3.1 Crude oil distillation system with a preflash unit.

Global concerns about carbon emissions and pressure on refining process economics encourage design of crude oil distillation systems that maximise process yield and minimise energy consumption, and therefore also operating costs. Furthermore, the high capital and operating costs of these systems, together with their considerable complexity, motivate development of systematic approaches to develop optimised designs.

Crude oil distillation system design methods employ experience, trial-and-error and heuristics, as well as process simulations and heat recovery analyses, typically using pinch analysis, to identify cost-effective and energy-efficient design solutions. Design methods that are systematic and employ optimisation effectively continue to be developed, but these have not focused on the role of pre-separation units, such as preflash units and prefractionation towers.

The aim of this work is to develop a systematic approach to design cost-effective, energy-efficient crude oil distillation systems with preflash units, accounting for product quality constraints, yield and heat integration. The design methodology is developed using simulation models in Aspen HYSYS v8.8; these models are linked to MATLAB R2016a through an interface that allows communication between the two software packages.

3.2 Simulation-based design methodology

This section introduces the proposed simulation-optimisation-based design methodology for the design of a crude oil distillation system with a preflash unit. First, the Aspen HYSYS simulation model is presented, along with the use of an interface between Aspen HYSYS and MATLAB. Second, heat integration is addressed. Next, the optimisation approach is described. The strong interactions between the crude oil distillation unit, the preflash unit and the heat recovery system, make this a challenging optimisation problem, especially since both operational and structural variables are to be optimised.

Two different scenarios are explored and presented as case studies in section 3.3. In the first case study, the structure of the main column is maintained unaltered - no change in the number of trays (Ledezma-Martínez et al., 2018). In the second case study, the structure of the main column is simultaneously optimised with the operating conditions of the crude oil distillation system (Ledezma-Martínez et al., 2018b).

3.2.1. Simulation model and Aspen HYSYS-MATLAB interface

The crude oil distillation process is modelled using Aspen HYSYS v8.8; in such commercial simulation software, models for crude oil characterisation are well established in industrial practice and rigorous distillation models have demonstrated their potential to provide highly accurate representations of this complex process. The models require the crude oil feed, the process and the column configuration to be fully defined.

At the design stage, it is appropriate to use heaters and coolers, rather than heat exchangers, because this simplifies process simulation and also because it allows the details of the heat recovery system to be decoupled from process design. Nevertheless, the minimum heating and cooling requirements of a proposed design can be readily ‘targeted’ using pinch analysis; this simplifies process simulation while still allowing evaluation of utility demand.

A simulation file is created for two configurations – that without and that with a preflash unit. The column structure – number of stages in each section, number and location of pump-arounds, draw and return stages for all side-strippers – is identical in both cases, as are the feed, operating pressures and product specifications. This work follows the approach in related studies (Ochoa-Estopier and Jobson, 2015; Ibrahim et al., 2017) by expressing the product quality in terms of points on the boiling profile, namely the temperatures at which 5 vol% (T5) and 95 vol% (T95) of each product are vaporised, according to the ASTM standard D86.

For the configuration with a preflash unit, heating of the crude oil is modelled using two heaters; one represents the heating upstream of the preflash unit and the other represents the preheating of the flash liquid by heat recovery and fired heating. The vapour leaving the flash unit is divided, using a stream splitter, into five streams, each of which is connected to a different stage of the main column, where there is one feed stage per section. The split fractions are defined in MATLAB such that all but one of these five streams will have zero flow, i.e. that all the material is directed to a single feed location. The extract of the MATLAB file included in Appendix A provides further detail. The approach builds on the simulation–optimisation technique (Caballero et al., 2005) for the design of distillation columns, facilitated by an Aspen HYSYS–MATLAB interface. The simulation model in Aspen HYSYS is linked to MATLAB R2016a via an 'automation' interface that allows the user to send inputs to and collect outputs from the simulation software (Aspen HYSYS Customization Guide). Spreadsheets within Aspen HYSYS are found very useful for viewing and storing results and for facilitating data-transfer between Aspen HYSYS and MATLAB. For example, HYSYS spreadsheets are useful for storing the current value of the objective function and values of other variables that need to meet specified constraints (e.g. product quality specifications).

The column simulation is set up to allow its convergence. In addition, a set of variables is defined, corresponding to the design degrees of freedom. In this work, the variables are cooling duty and temperature drop of each pump-around; flow rate of stripping steam to all steam-stripped column sections; reflux ratio; column feed inlet temperature and preflash feed temperature. One structural variable, the feed location in the main column to which the flash vapour is sent, is included as a degree of freedom.

For the case with a preflash unit, the flash temperature is an important degree of freedom. Higher temperatures allow more vaporisation of the crude oil feed and thus more of the feed to bypass the fired heater; heating only the preflash liquid reduces the fired heating duty. On the other hand, if a large fraction of the crude oil feed bypasses the fired heater, there is a risk that the total enthalpy of the two feed streams is too low to allow the desired separation to be achieved. The vapour leaving the flash unit is sent to a stream splitter which facilitates the vapour stream to be sent to any one of several potential feed locations. Initially, it is assumed that the vapour is sent to the same stage as the main feed, i.e. is effectively mixed with the crude oil leaving the fired heater. Product quality specifications aim to ensure that the product streams meet the requirements of downstream processing and of the market. Some of these specifications can be defined (as 'specifications') within the rigorous distillation model, but the limited number of degrees of freedom of the column means that not all products can be fully specified. Therefore, the remaining product specifications are defined within MATLAB as inequality constraints, where compliance with specifications is checked and, in the optimisation, a penalty term is added to the objective function. In line with industrial practice, where specifications are defined in terms of characteristic boiling temperatures within a tolerance ε (typically $\pm 10°C$), the constraints are defined accordingly.

When using the 'automation' feature for direct simulation-based optimisation, there is a risk that the rigorous simulation will not converge, either because the simulation has been poorly initialised or because, for a particular set of inputs, the specifications cannot be met. If the simulation does not converge, the optimisation may not be able to proceed or taking steps to facilitate convergence, such as re-initialising the simulation or increasing the number of iterations, may be computationally intensive. Therefore, the automation code instructs the Aspen HYSYS simulation to stop if it does not converge within the specified maximum number of iterations. In the case that the Aspen HYSYS simulation does not converge, a penalty is applied to the objective function within MATLAB. This penalty helps to reject spurious results during the optimisation.

3.2.2. System Optimisation

Experience showed that deterministic non-linear optimisation techniques (such as *fmincon* in MATLAB) for optimising the operating variables frequently led to the optimisation reaching a local optimum. Furthermore, the vapour feed location introduces an integer variable into the problem, which cannot be handled effectively by such an algorithm. Therefore, randomised search methods, also known as stochastic optimisation or metaheuristics, are applied. These methods are known to help to overcome the limitations of non-randomised methods (Osman, 1996) by 'learning' about the problem during the optimisation and tailoring the search strategy accordingly. However, it is well known that such algorithms find 'near-optimal' solutions, rather than the globally optimal solution (Osman and Kelly, 1996).

Two options from MATLAB R2016a Global Optimisation Toolbox were tested both simulated annealing (*simulannealbnd*) and a genetic algorithm (*gaoptimset*). The latter was found to be far more robust in reaching good solutions and therefore is adopted, (See Chapter 2, Section 2.4 for details about the optimisation methods).

The objective function can be expressed mathematically as:

$$min\, F(x) = f(x) + \gamma_1 |h(x)| + \sum_{j=1}^{n} \gamma_j \left[max\left(0, g_j(x)\right)\right]^2 \qquad (3.1)$$

$$h(x) = 0 \quad g_j(x) \leq 0$$

where x is the vector of optimisation variables (i.e. cooling duty and temperature drop of each pump-around, the flow rate of steam to the main column and to any other steam-stripped sections, the column feed temperature and the preflash feed temperature, if applicable); *F(x)* is the overall objective function; *f(x)* is the objective function before applying any penalty terms; *h(x)* represents the set of equality constraints; $g_j(x)$ represents inequality constraints and γ_j is a set of scalar penalty factors that scale the penalty according to the significance of the constraint and the magnitude of the violation of the constraint (Ibrahim et al., 2017).

Product quality constraints are included as inequality constraints $g_j(x)$ in the objective function as follows:

$$T5_i^* - \varepsilon \leq T5_i \leq T5_i^* + \varepsilon \qquad i = 1,2, \ldots\ldots, N_{products} \tag{3.2}$$

$$T95_i^* - \varepsilon \leq T95_i \leq T95_i^* + \varepsilon \qquad i = 1,2, \ldots\ldots, N_{products} \tag{3.3}$$

where $T5_i$ and $T95_i$ correspond to the T5 and T95 ASTM D86 temperatures for product *i*, where the lower bound is ε less than the specified temperatures ($T5_i*$ and $T95_i*$, respectively) and the upper bound is ε greater than the specified temperature. These specifications are conveniently represented using the *max* function in MATLAB:

$$g_1(x) = \sum_{i=1}^{n}[max(0,(T5_i^* - \varepsilon) - T5_i)^2] + [max(0, T5_i - (T5_i^* + \varepsilon))^2] \tag{3.4}$$

$$g_2(x) = \sum_{i=1}^{n}[max(0,(T95_i^* - \varepsilon) - T95_i)^2] + [max(0, T95_i - (T95_i^* + \varepsilon))^2] \tag{3.5}$$

The squared term ensures that a positive penalty is applied only when the inequality constraint is violated (Biegler, 2003).

In Case 2 (case study 3.1), a third inequality constraint is added to ensure that the volumetric flow rate of the atmospheric residue, $m_{RES,}$ is no greater than that in the base case, m_{RES}^0:

$$g_3(x) = max(0, m_{RES} - m_{RES}^0) \tag{3.6}$$

Table 3.1. Variables and constraints for system optimisation

Optimisation variables	Constraints	Objective function
3 Pump-around duties	Product quality T5% and T95% ASTM D86 ± 10°C Residue flow rate, no greater than the value for the base case	Minimum hot utility demand Q_{Hmin}
3 Pump-around temperature drops		
Main steam flow rate		
HD steam flow rate		
Reflux ratio		
Column inlet temperature		
Preflash temperature		
Flash vapour feed location		

3.3 Case studies

Case studies presented in sections 3.3.1 and 3.3.2 aim to demonstrate the capabilities of the proposed design methodology for two different scenarios and to illustrate that a preflash unit can bring significant energy savings, even when product flow rates are constrained.

The first case study is limited to the case that the column design – the number of sections and number of stages in each section – is fixed, and to a given crude oil feed and a given set of products, with associated quality specifications. The constraints on product quality partially fix the distribution of the crude oil into the various products; the option of including constraints on product quantity, as well as quality, is also explored. The methodology focuses on reducing the fired heating demand of the system, without compromising the quality and quantity of products. Therefore, the objective function is the minimum hot utility demand (Q_{Hmin}), calculated using pinch analysis, where penalty terms ensure that the optimal solution meets product specifications and also successfully converged when simulated.

3.3.1. Case study 3.1: main column structure fixed

The case study is based on the data presented by Watkins, 1979. Appendix A provides details of the crude oil assay in Tables A1 and A2, design specifications (Table A3), column structure (Table A4), base case product properties and flow rates (Table A5) and base case stream data (Table A6). The oil characterisation tool in Aspen HYSYS v8.8 is used to 'cut' the oil into a set of 25 pseudo-components and to calculate the physical and thermodynamic properties of each pseudo-component (e.g. molecular weight, density and viscosity). These pseudo-components, together with the six-real low-boiling components, represent the crude oil mixture. The Peng-Robinson equation of state is used to simulate the mixture of pseudo-components.

The crude oil distillation system comprises an atmospheric distillation unit with a condenser, three pump-arounds, one steam-injected side stripper and two reboiled side strippers. The case study addresses the system with and without a preflash unit upstream of the column. The main column operates at a uniform pressure of 2.5 bar and has 41 theoretical stages, distributed in five sections, and numbered from top to bottom. Figure 3.2 illustrates the crude oil distillation system, showing details of the section numbers, distribution of stages in the main column, locations of pump-arounds and of draw and return streams, and stripping steam feed locations. Table A4 in the Appendix A, presents the distribution of trays in the main column and side-strippers; note that the numbering continues from 42 to 59 for stages in the side strippers. Figure 3.3 illustrates how the flowsheet is implemented in Aspen HYSYS – in particular, it shows how the flash vapour stream may be directed to five different feed locations in the main column, and how several spreadsheets are used to facilitate data transfer to and from MATLAB.

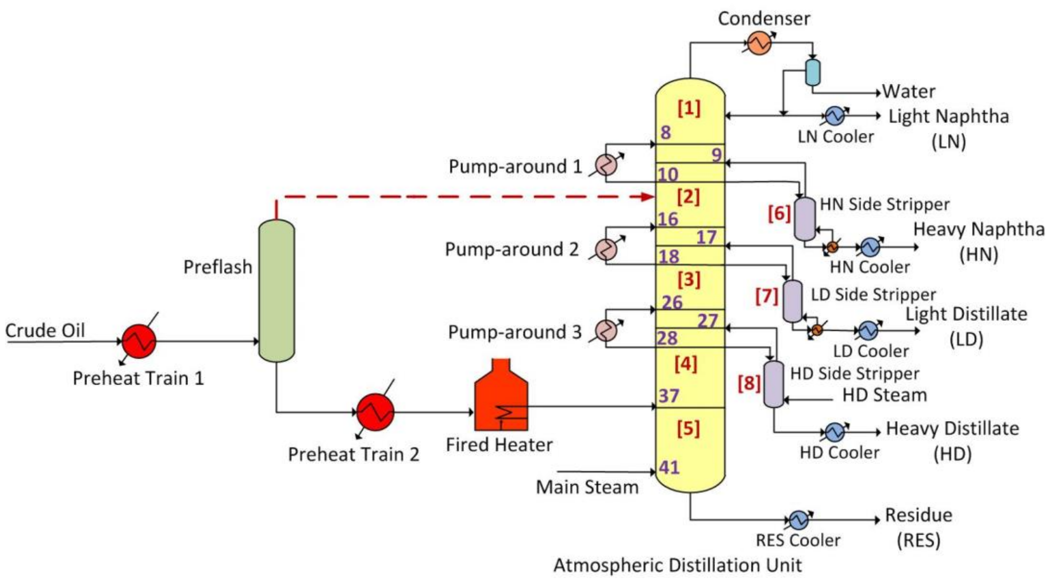


Figure 3.2 Crude oil distillation system with a preflash unit.

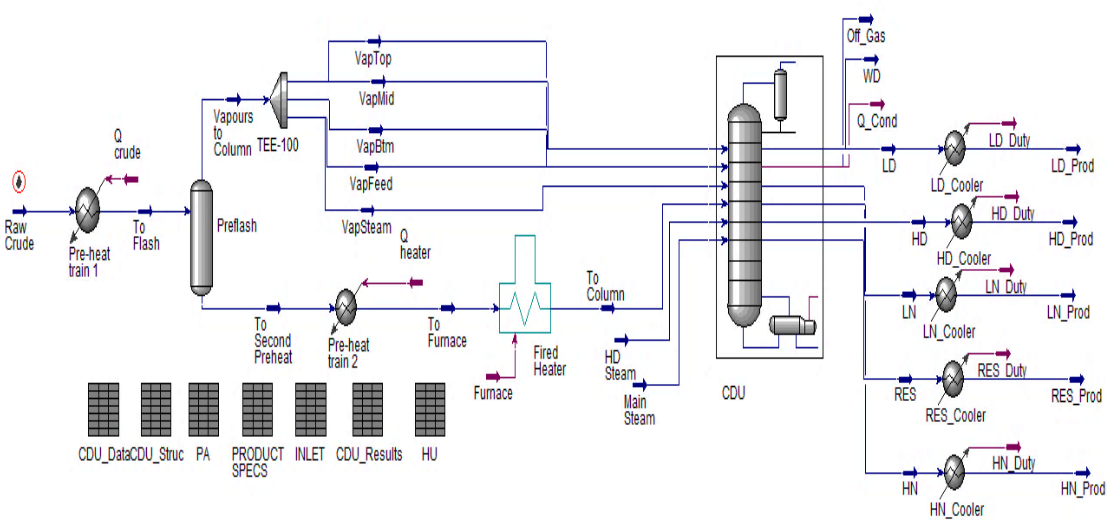


Figure 3.3 Screenshot of Aspen HYSYS simulation.

The system processes 100,000 bbl day^{-1} (662.4 m^3 h^{-1}) of Venezuelan Tia Juana light crude oil. The crude oil distillation column produces five products: Light Naphtha (LN), Heavy Naphtha (HN), Light Distillate (LD), Heavy Distillate (HD) and Residue (RES). The unoptimised base case design is derived from a study by Chen, 2008. Table A6 (Appendix A) provides details about the process stream data for the not optimised base case (without a preflash unit) and Figure A1 shows its grand composite curve and minimum utility requirements. Vapour leaving the preflash unit is initially mixed with the stream leaving the fired heater; the mixture is sent to the feed stage in the main column. Steam is utilised as a stripping agent in the main column and in the HD stripper. The HN and LD strippers use reboilers, rather than live steam. Product specifications are expressed in terms of ASTM T5 and T95 (in °C).

3.3.1.1 Operational variables

The crude oil distillation system has eleven operational variables and one structural variable (vapour feed location), as shown in Figure 3.4. The base case operating conditions and product specifications are listed in detail in Table A3 in Appendix A; the vapour feed location is selected to be the main feed stage, in Section 5 of the main column. The preflash temperature and vapour feed location are two important operating variables that significantly influence the performance of the crude oil distillation system. Product quality specifications and base case product flow rates (expressed in m^3 h^{-1} and kmol h^{-1}) are presented in Table A5 in the Appendix A. The study assumes a minimum temperature approach of 30°C in all heat exchangers for the heat recovery calculations.

Prior to process optimisation, the initial case forms the basis for sensitivity studies. These studies facilitate understanding of the system and performance trends, in terms of hot utility demand, as each design variable is changed. The results of the sensitivity studies help to define suitable bounds for the optimisation, considering the effect of design variables on performance and on ease of convergence of the flowsheet simulation.

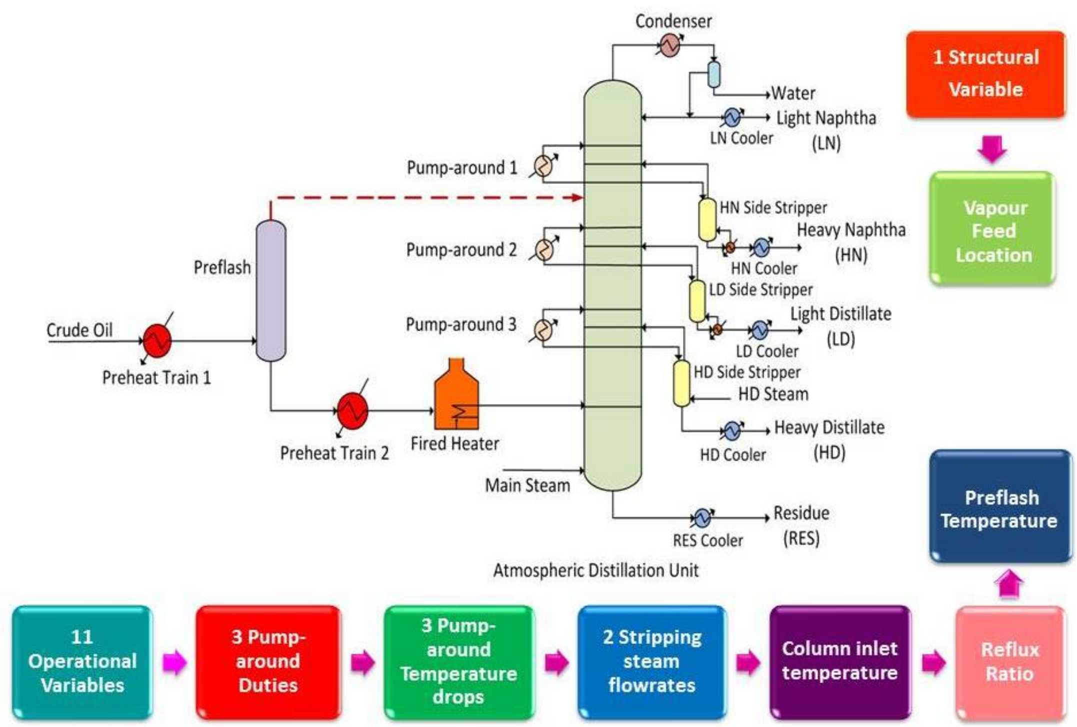


Figure 3.4 Operational and structural variables, crude oil distillation system with a preflash unit.

3.3.1.2 Optimisation framework: Case study 3.1

Figure 3.5 illustrates a general optimisation-based design methodology for case study 3.1 where the number of trays in the main column is fixed. Aspen HYSYS v8.8 is applied for flowsheet simulation while MATLAB R2016a is used to carry out pinch analysis on proposed solutions and to drive the optimisation. Relevant streams to calculate minimum hot utility demand of the system are the supply and target temperatures and duties of the preheat trains, fired heater, products coolers, condenser, pump-arounds and side-strippers.

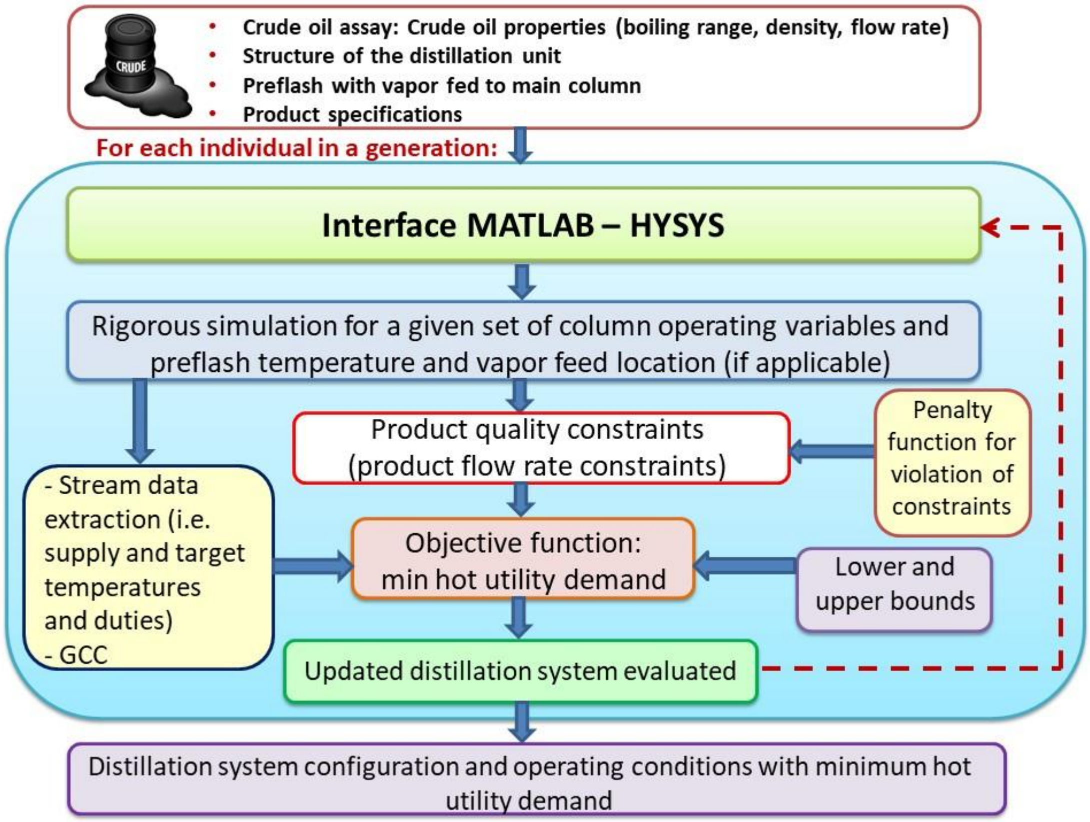


Figure 3.5 Optimisation-based design methodology, case study 3.1.

3.3.1.3 Optimisation parameters

The aim of the optimisation is to identify a flowsheet configuration and a corresponding set of operating conditions that minimise the hot utility demand. The optimisation is carried out as described in Section 3.2.3. The parameters selected for the genetic algorithm are 500 for the maximum number of generations and 100 for the initial population; the 'function tolerance', the average change in the value of the objective required before the optimisation is terminated, is set to 1×10^{-10}. These optimisation parameters were selected after running the optimisation several times with different values for population size and number of generations and considering the best value of the objective function and the effect on the computation time.

Three optimisation runs are performed for each case. Multiple runs help to give confidence that the optimisation is effective and robust; wide variations in the value of the objective function could suggest that the optimisation algorithm and/or parameters are unsuitable.

3.3.1.4 Optimisation results

Two cases are considered, Case 1, where constraints relate to product quality only, and Case 2, where both qualities of products and the flow rate of the atmospheric residue (RES) are constrained. Details of the optimisation results are provided in Tables A7 and A9 (for Case 1) and Tables A8 and A10 (for Case 2) in the Appendix A. Optimisation runs took between 4 and 6 hours of CPU time on an HP desktop PC with Intel Core i5 processor running at 3.20 GHz and 16 GB of RAM.

Case 1: Crude oil distillation system without and with a preflash unit, where constraints relate to product quality only. A summary of optimisation results and bounds (selected after performing sensitivity analyses) for operational and structural variables obtained for the crude oil distillation system with and without a preflash unit is presented in Table 3.2. (Note that pump-around duties are negative values in HYSYS; the MATLAB code takes this into account when defining upper and lower bounds on the duties).

Table 3.2 shows that the initial conditions of the base case were far from optimal. More importantly, Table 3.2 shows that the minimum hot utility demand could be reduced by 17% by introducing a preflash unit to the flowsheet. It is also noteworthy that the optimiser selected Section 3 for the feed location of the preflash vapour. (This result was obtained in all successful optimisations).

It was observed that the location for the vapour feed was always chosen to be in the section with the temperature closest to the preflash temperature. For the solution shown in Table 3.2, the optimised feed location corresponds to stage 18 in section 3 of the main column. It may be observed that the column inlet temperature is 4°C higher in the case that the flash vapour bypasses the furnace; this result indicates that, with a preflash, the crude oil feed needs to be hotter, to compensate for the lower enthalpy of the preflash vapour when it enters the column. Table 3.2 also shows that the optimiser maximises the temperature of the flash unit (to the upper bound of 230°C), indicating that the benefits of allowing some material to bypass the fired heater outweigh the drawbacks of feeding relatively cold vapour to the column.

Table 3.3 presents results for Case 1 related to product quality in terms of ASTM T5 and T95 (in °C). It may be seen that the product quality constraints are all met within the allowed range of temperatures (±10°C). Table 3.4 shows the results for the optimised product flow rates and vapour for Case 1. These results confirm that the product yields for most of the valuable products (LN, HN, HD) change relatively little, which is a consequence of the product quality being constrained, and therefore the distribution of the crude oil feed into products being constrained. However, the 2.4% and 3% increases in the flow rate of the atmospheric residue (RES), compared to the not optimised base case, represents a loss of more valuable products. Therefore, Case 2 addresses this problem by adding a constraint on the flow rate of the atmospheric residue, in line with previous studies (Ibrahim et al., 2017).

Table 3.2 Optimisation results and bounds for the crude oil distillation system Case 1

Variable	Units	Base Case	Lower Bound	Upper Bound	Optimisation Results	
					No Preflash	With Preflash
Main Steam Flow Rate	kmol h^{-1}	1200	900	1800	900	1190
HD Steam Flow Rate	kmol h^{-1}	250	200	375	200	211
PA1 Duty	MW	12.8	6	14	6.0	6.8
PA2 Duty	MW	17.8	6	18	9.8	8.3
PA3 Duty	MW	11.2	6	12	11.9	8.8
PA1 ΔT	°C	30	20	50	48.6	25.5
PA2 ΔT	°C	50	15	60	33.8	23.0
PA3 ΔT	°C	20	10	40	39.9	39.3
Column Inlet Temperature	°C	365	350	385	350	354
Flash Temperature	°C	115	110	230	–	230
Reflux Ratio		4.17	3.0	4.5	3.7	3.0
Vapour Feed Location[a]		5	1	5	–	3
Minimum Hot Utility	MW	58.3			43.4	35.9

[a] Number of section in main column

PA: pump-around

ΔT: pump-around temperature drop

Table 3.3. Product qualities, optimised crude oil distillation system: Case 1

Product	Base Case ASTM (°C)		Optimisation Results No Preflash ASTM (°C)		Optimisation Results With Preflash ASTM (°C)	
	T5 %	T95%	T5%	T95%	T5%	T95%
LN	27	110 [a]	25	110	25	110
HN	143	196 [a]	133	196	133	196
LD	218 [a]	300 [a]	218	300	218	300
HD	308	354 [a]	305	354	302	354
RES	363	755	354	753	353	753

[a] Specified in HYSYS

Table 3.4. Product flow rates, optimised crude oil distillation system: Case 1

Flow rate ($m^3\ h^{-1}$)	Base Case	Optimised No Preflash	Optimised With Preflash
LN	102	101	101
HN	87	88	89
LD	128	126	123
HD	54	48	49
RES	292	299	301

Case 2: Crude oil distillation system with constraints on both product quality and product flow rates. Again, the crude oil distillation system is optimised without and with a preflash unit. The optimisation results for Case 2 are summarised in Tables 3.5 to 3.7, providing details of operating conditions and flowsheet structure, product quality and product flow rates. Note that bounds for HD steam flow rare, pump-around 3 duty and flash temperature are different of those presented in Case 1, bounds were updated according to a

better performance of the optimisation for the case when a residue constraint is added to the objective function.

Table 3.5 Optimisation results and bounds for the crude oil distillation system Case 2

Variable	Units	Base Case	Lower Bound	Upper Bound	Optimisation Results	
					No Preflash	With Preflash
Main Steam Flow Rate	kmol h^{-1}	1200	900	1800	1247	1195
HD Steam Flow Rate	kmol h^{-1}	250	180	375	188	180
PA1 Duty	MW	12.8	6	14	7.4	8.5
PA2 Duty	MW	17.8	6	18	9.8	8.8
PA3 Duty	MW	11.2	6	14	14.0	13.0
PA1 ΔT	°C	30	20	50	31.9	38.8
PA2 ΔT	°C	50	15	60	34.9	31.6
PA3 ΔT	°C	20	10	40	39.9	21.0
Column Inlet Temperature	°C	365	350	385	362	383
Flash Temperature	°C	115	110	240	–	240
Reflux Ratio		4.17	3.0	4.5	4.1	3.1
Vapour Feed Location [a]		5	1	5	–	3
Minimum Hot Utility	MW	58.3			46.6	37.9

[a] Number of section in main column
PA: pump-around
ΔT: pump-around temperature drop

As shown in Table 3.5, in Case 2 the use of a preflash unit again leads to a significantly lower minimum hot utility demand (18%). However, for both configurations – without and with a preflash unit – when the residue flow rate is constrained, the minimum hot utility demand increases significantly, by 6% and 5%, compared to the optimised flowsheets without product flow rate constraints (i.e. Case 1). This increased demand for fired heating is consistent with the higher column inlet temperature of Case 2 (362°C and 383°C), compared to Case 1 (350°C and 354°C). The increased column feed temperatures achieve greater vaporisation of this stream, compensating for both an increased vapour fraction entering the column at a relatively low temperature (240°C) and the need to vaporise more of the feed in order to meet the flow rate constraint on the atmospheric residue. Consequently, and aligned with previous work (Ibrahim et al., 2017) demand for fired heating increases.

It is noted that, as in Case 1, the flash temperature selected by the optimiser is at the upper bound of the range (240°C), indicating that there are benefits for the heat recovery system (and few penalties for the separation performance) of using a preflash unit. It is also observed that the stream flow rate to the HD side-stripper is at the minimum value; a lower requirement for stripping steam is consistent with the removal of lighter material from the column feed.

Again, the flash vapour is directed to the section of the column with the temperature that is most similar to that of the vapour. This result implies that the optimisation search space could be narrowed appropriately, with corresponding reductions in computation time.

The greater duties of the pump-arounds in Case 2 indicate that the higher feed temperature also allows more heat to be recovered in the heat recovery system. It may be observed from Tables 3.2 and 3.5 that, in both Cases 1 and 2, introducing a preflash, i.e. allowing a fraction of the feed to bypass the fired heater, tends to reduce the amount of high-temperature heat recovered.

In particular, heat recovery from pump-arounds 3 and 2 is reduced in favour of rejecting lower-grade heat from pump-around 1. This trend would also reduce the temperature to which the heat recovery system could preheat the crude oil feed before it enters the fired heater.

In Table 3.6 it may be seen that the product quality constraints are all met within the allowed range of temperatures (±10°C), as are those in Case 1. Results also confirm that the residue flow rate is unchanged, indicating that there is no loss of valuable products.

Table 3.6. Product qualities, optimised system: Case 2

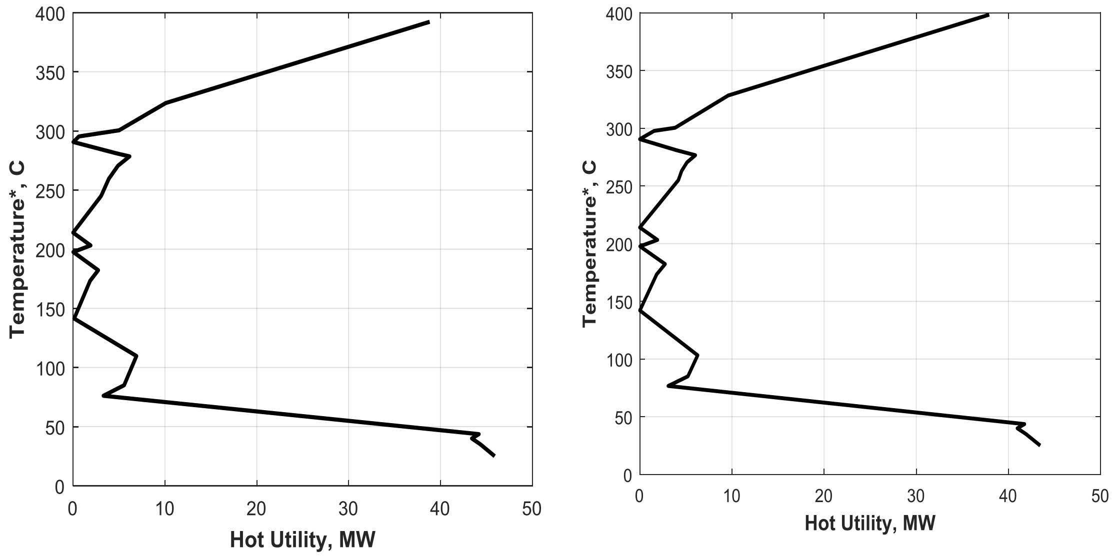
Product	**Base Case ASTM (°C)**		**Optimisation Results No Preflash ASTM (°C)**		**Optimisation Results With Preflash ASTM (°C)**	
	T5%	**T95%**	**T5%**	**T95%**	**T5%**	**T95%**
LN	27	110 [a]	25	110	25	110
HN	143	196 [a]	133	196	135	196
LD	218 [a]	300 [a]	218	300	218	300
HD	308	354 [a]	307	354	303	354
RES	363	755	361	754	362	754

[a] Specified in HYSYS

Figure 3.6 presents the grand composite curves for the two optimised cases with a preflash unit, where Case 1 considers product quality constraints and Case 2 considers both product quality and product flow rate. The grand composite curves show that the minimum hot utility demand increases when product flow rates are considered. In both cases, the existence of several pinches (or near-pinches) indicates that heat recovery is maximised at a wide range of temperature levels: that is, the column operating conditions have been optimised to maximise heat recovery. This is a strength of the methodology, where each proposed solution is assessed in terms of its net heating demand, after heat recovery, rather than by considering heat recovery only after the design of the system. The results in Figure 3.6 and Tables 3.2 and 3.5 highlight the trade-offs between the fired heating demand and the yield of valuable products. Table A8 of the Appendix A provides stream data for the optimised system applying the constraint on the atmospheric residue flow rate.

Table 3.7. Product flow rates, optimised system: Case 2

Flow rate (m^3 h^{-1})	Base Case	Optimised No Preflash	Optimised With Preflash
LN	102	101	101
HN	87	88	89
LD	128	126	123
HD	54	55	58
RES	292	292	292



(a) Case 1   (b) Case 2

Figure 3.6 Grand composite curves of optimised crude oil distillation system with preflash.

3.3.1.5 Case study summary

A systematic design optimisation approach is proposed for crude oil distillation systems with preflash unit, applying a rigorous simulation model and using pinch analysis to determine the minimum hot utility demand of the heat-integrated system. The methodology accounts for industrially relevant constraints related to product quality and yield and the main operating cost of the distillation system, that of fired heating. Especially because of the rigorous simulations involved, the optimisation is relatively computationally intensive, requiring 4 to 6 hours of CPU time per optimisation run.

The case study confirms that introducing a preflash unit, while also optimising the column operating conditions, can bring significant improvements in the hot utility demand. However, the preflash clearly impacts on the separation performance of the column, and thus potentially could reduce the value added by the distillation system to the crude oil, for example, if more of the crude oil leaves the column in the residue stream. These results highlight the trade-off between yield and energy demand, and suggest that the objective function should capture both aspects, for example, as net profit, as in previous studies (Ochoa-Estopier and Jobson, 2015).

The problem formulation described in this case study keeps the design of the distillation column (number of stages in each section) fixed in all cases. Case study 3.2 will address this limitation taking into account column design, together with the use of a preflash unit, taking advantage of recent developments in this area (Ibrahim et al., 2017). The change in flow rate and composition of the feeds after introducing a preflash unit, would logically require a different distribution and/or number of stages in the distillation unit, and would also significantly affect the cost of the column because of changes in required column diameter.

3.3.2. Case study 3.2: design of main column structure optimised

This second case study is also based on data reported by Watkins, 1979 and the base case is an unoptimised design presented by Chen, 2008. The crude oil distillation system analysed is exactly the same as that presented in Section 3.3.1. The crude oil distillation unit is modelled in Aspen HYSYS v8.8, applying the '3ss crude' column template for this purpose; this software has been employed in industrial practice because of its ability to generate accurate simulation results. The Aspen HYSYS simulation model represents the flowsheet structure and the column design (number of stages in each section and location of feed and draw stages and locations of pump-arounds, stripping steam feeds and side-stripper reboilers).

The flowsheet shown in Figure 3.7 includes a preflash unit, where the destination of the preflash vapour is a design degree of freedom. Therefore, the flash vapour is fed to a stream splitter with n outlets, each of which is connected to a different location in the main column. The stream splitter is specified to send 100% of the inlet stream to only one outlet stream; in this way, the flowsheet configuration can be varied using the stream splitter specifications.

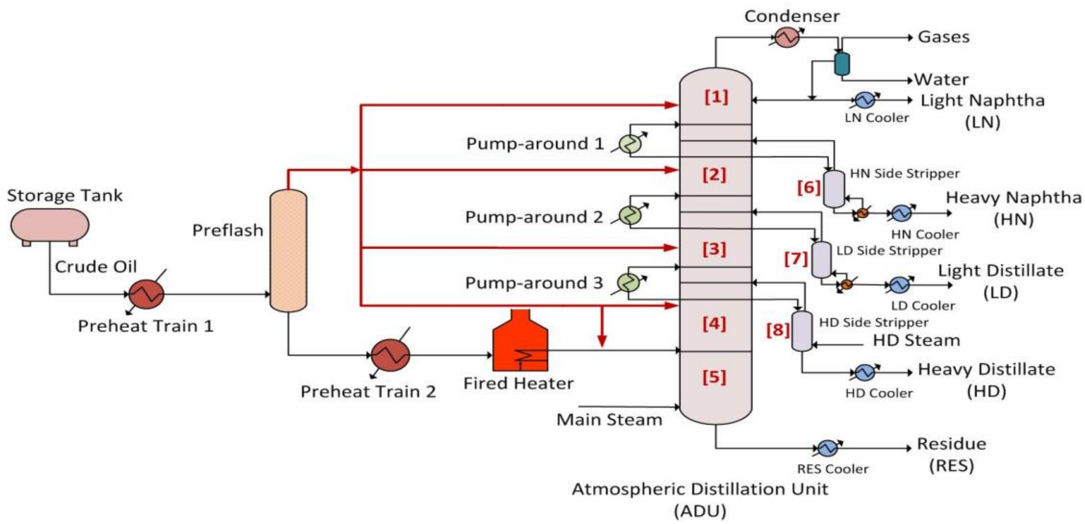


Figure 3.7 Crude oil distillation system showing vapour feed locations.

3.3.2.1 System modelling and operating conditions

The model also represents process operating conditions. Within the flowsheet, the heating of the crude oil from ambient conditions to the furnace inlet temperature is modelled using one heater upstream of the flash unit and one heater representing a second preheat train upstream of the furnace. The outlet temperature of the upstream heater, i.e. the preflash temperature, is an important degree of freedom in the flowsheet design. Other design variables to be selected include column operating conditions, namely pump-around duties and temperature drops, stripping steam flow rates, column feed temperature, preflash temperature and reflux ratio.

In the simulation model in Aspen HYSYS, product quality may be specified in terms of product boiling ranges (e.g. T5% and T95%, the boiling temperature when 5% and 95% of the material, respectively, has vaporised using a standard test, such as ASTM D86). Independent variables are then manipulated by the simulation algorithm to attempt to meet these specifications and converge the simulation.

The optimisation problem shown on Figure 3.8 has 11 operating variables (3 pump-around duties, 3 temperature drops, 2 stripping steam flow rates, column feed temperature, preflash temperature and reflux ratio). The feed location in the main column of the flash vapour and the column structure (number of trays in each of 8 sections, including the side strippers) are the 9 structural optimisation variables. The objective function is to minimise hot utility demand, calculated using pinch analysis. The optimisation algorithm provides a systematic search for the set of operating and structural variables that maximise the performance of the system in terms of demand for fired heating. A minimum approach temperature of 30°C is assumed for all heat exchangers when generating the grand composite curve.

The design of the column sections is addressed by including redundant stages in each section and defining the Murphree stage efficiency for each stage in each section of the column to be zero or one. In this way, existing trays can be activated (by setting the stage efficiency to 1), to allow mass transfer, or deactivated (by setting the stage efficiency to 0), to disallow mass transfer (Ibrahim et al., 2017). As a result, the number of active stages in each section and therefore the total number of stages in the column can be altered easily, by changing a process variable, without needing to explicitly change the column structure.

The model can be used repeatedly, with trial and error or systematic searches, to search for designs that perform well in terms of the performance indicator. Instead, following Caballero et al. (2005) and Ibrahim et al. (2017), the search is automated: an interface is created between MATLAB R2016a and Aspen HYSYS v8.8 which permits MATLAB to read from and write to Aspen HYSYS (AspenTech, 2010). A MATLAB subroutine (Morandin, 2014) uses the results of each converged simulation to apply pinch analysis and to generate a grand composite curve for the process, from which the minimum hot and cold utility demand is calculated.

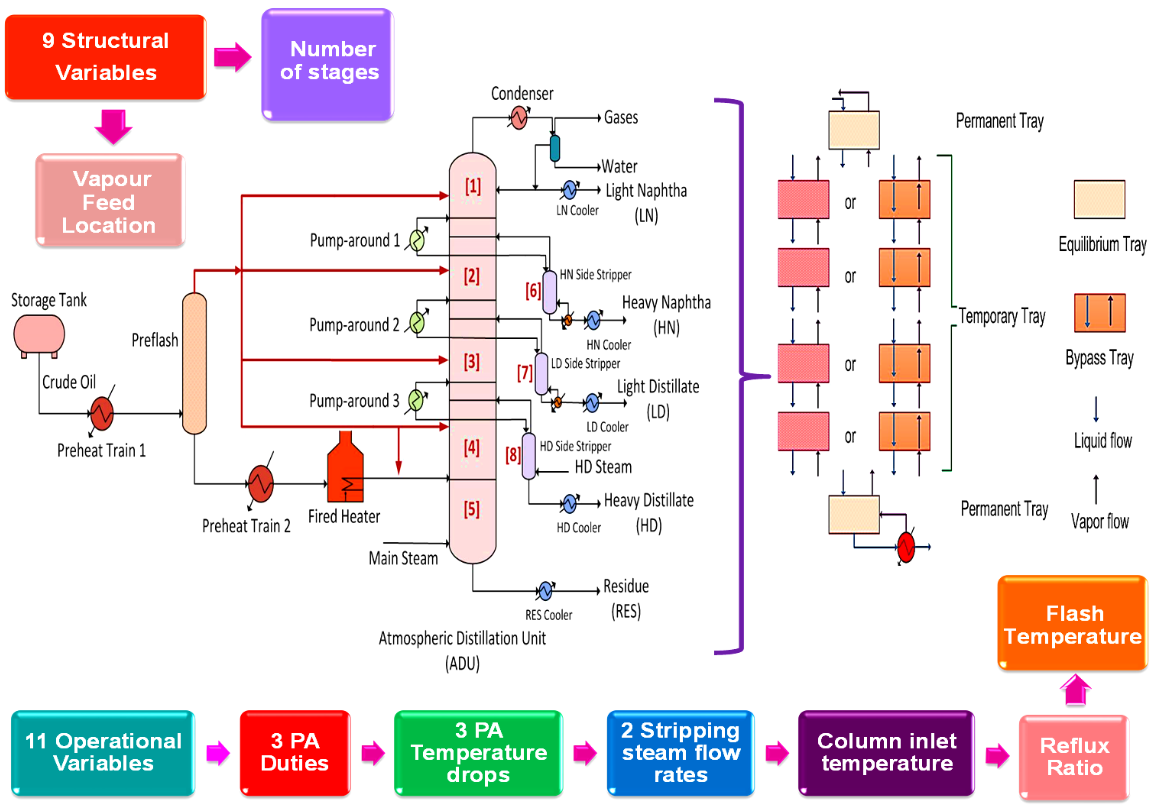


Figure 3.8 Operational variables and superstructure representation, crude oil distillation system with a preflash unit.

3.3.2.2 Optimisation framework: Case study 3.2

The optimisation framework for the case study 3.2 as shown in Figure 3.9, selects values of process variables, including those determining the flowsheet or column structure, simulates the corresponding flowsheet, evaluates it and then selects a new set of inputs.

A genetic algorithm is selected as the optimisation technique because it is known to be effective in finding good solutions to complex process design problems involving both continuous and discrete design choices (Kotecha et al., 2010). It is also simple to implement a genetic algorithm, using MATLAB R2016a Global Optimisation Toolbox. The optimisation parameters for the genetic algorithm are: population size, number of generations, and termination criteria. In this work, the optimisation terminates after a given number of generations or if the objective function does not improve by more than a certain tolerance over a given number of generations. Optimisation parameters for the genetic algorithm are: population size (100), maximum number of generations (500) and the objective function tolerance ($1\cdot10^{-10}$). Optimisation runs took 8 to 8.5 hours of CPU time on an HP desktop PC with Intel Core i5 processor running at 3.20 GHz and 16 GB of RAM.

Relevant optimisation constraints include the upper and lower limits of optimisation variables and constraints on integer variables (e.g. only one stream from the flash vapour has a non-zero flow rate; the maximum and minimum number of stages is specified for each column section). If an Aspen HYSYS simulation does not converge within a given number of iterations, a penalty term (a scalar of the same magnitude as the objective function) is applied to the objective function.

Pinch analysis is applied to evaluate the minimum utility demand of the system, assuming heat recovery within the crude oil distillation system is maximised. The grand composite curve (GCC) is generated for each simulated design – using results of the simulation relating to stream inlet and outlet temperatures and heating and cooling duties; the minimum approach temperature is specified by the user. The grand composite curve is then used to evaluate the minimum demand for fired heating, which is an important performance indicator. Detailed heat exchanger design is not directly addressed (Ledezma-Martínez et al., 2018a).

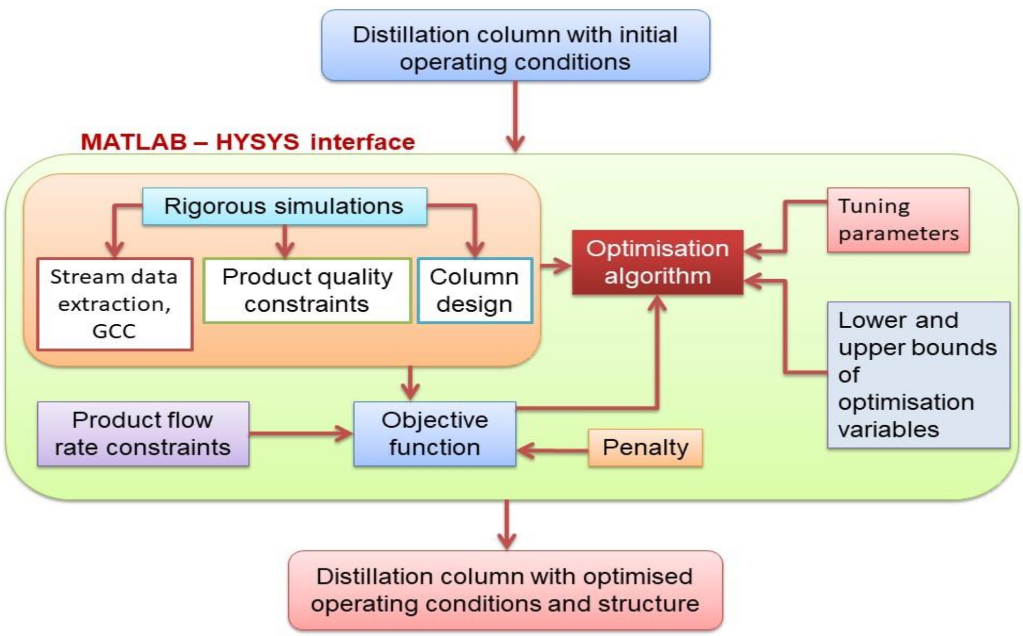


Figure 3.9 Optimisation-based design methodology, case 3.2.

Typically, in the process simulation model, there are fewer degrees of freedom than there are specifications, so some important specifications are expressed as constraints in the optimisation problem. In line with industrial practice and the flexibility of downstream units, product quality constraints related to boiling range (ASTM D86 T5% and T95%) may be set with a wide tolerance (±10°C). In addition, even though product quality specifications are imposed, it is possible for these to be met but the yield of products to decrease (i.e. more of the column feed is relegated to the residue stream, for further processing in a vacuum tower, and flow rates of more valuable product streams may decrease). Therefore, the flow rate of the Residue stream is constrained to be no more than that in the base case design (Ledezma-Martínez, et al., 2018a). If the product quality or residue flow rate constraints are violated, a penalty term – a scalar multiplied by amount by which the constraint is exceeded – is added to the objective function.

3.3.2.3 Optimisation results

To provide a reasonable basis for comparison, the base case is first optimised without a preflash unit, then the base case design is optimised with a preflash unit (but without making any changes to column design); finally, the column design is optimised.

A summary of the optimised operating variables is provided in Table 3.8 for: 1) the base case, where the column design is fixed (without a preflash unit); 2) the column design is fixed (no change in number of trays per section) and a preflash unit is added; 3) the column design is optimised for both operational and structural variables. Table 3.9 confirms that product specifications are satisfied within the tolerance (±10°C) in all three cases. Product flow rates for all cases are presented in Table 3.10. Residue flow rate is constant and other product flow rates change relatively little, as a consequence of product quality constraints. Table 3.11 provides detail of the base case (fixed) column structure and the optimised column structure. As shown in Table 3.8, introducing a preflash unit to the crude oil distillation system reduces the minimum hot utility demand by 20%, compared to the base case (without a flash). The significant increase in the column feed temperature compensates for the large flow rate of vaporised crude oil that bypasses the fired heater and enters the column at a relatively low temperature (230°C). Nevertheless, more high-temperature heat is recovered within the system: pump-around duties are reduced in pump-around 1, PA1 and pump-around 2, PA2, at lower temperatures, but increased in pump-around 3, PA3, where higher-temperature heat is more useful. When a preflash is used and the column design is also optimised, there is a marginal decrease in demand for fired heating. This result suggests that the additional stages and new distribution of stages do not effectively improve the separation performance and heat recovery opportunities simultaneously.

Table 3.8. Optimisation results Case 3.2

Variable	**Units**	**Base Case (no flash)**	**Base Case (with flash)**	**Optimised Design**
Main steam flow rate	kmol h^{-1}	1298	1287	1262
HD steam flow rate	kmol h^{-1}	275	200	209
PA1 duty	MW	9.3	8.5	7.2
PA2 duty	MW	10.1	8.7	8.8
PA3 duty	MW	10.5	12.0	11.9
PA1 ΔT	°C	23.7	31.7	33.4
PA2 ΔT	°C	36.2	31.8	31.1
PA3 ΔT	°C	39.8	16.9	21.3
Column feed temperature	°C	363	377	377
Flash temperature	°C	–	230	230
Reflux ratio		4.0	3.2	3.3
Vapour feed location[a]		–	3	3
Minimum hot utility	MW	48.4	38.8	38.6

[a] Number of section in main column
PA: pump-around
ΔT: pump-around temperature drop

Table 3.9. Product quality specifications Case 3.2

Product	Base Case (no flash) ASTM (°C)		Base Case (with flash) ASTM (°C)		Optimised Design ASTM (° C)	
	T5 %	T95 %	T5 %	T95 %	T5 %	T 95 %
LN	27	110 [a]	25	110	25	110
HN	134	196 [a]	133	196	133	196
LD	218[a]	300 [a]	218	300	218	300
HD	309	354 [a]	304	354	298	354
RES	362	754	361	754	361	754

[a] specified in HYSYS.

Table 3.10. Product flow rates in m3 h^{-1}, Case 3.2

Product	Base Case (no flash)	Base Case (with flash)	Optimised Design
LN	105	101	101
HN	84	89	89
LD	128	124	122
HD	53	57	58
RES	292	292	292

Table 3.11. Crude oil distillation column design (number of stages in each section)

Column Section	Number of trays		
	Base Case (no flash)	Base Case (with flash)	Optimised Design
1	9	9	6
2	8	8	10
3	10	10	11
4	9	9	9
5	5	5	10
6	6	6	3
7	7	7	8
8	5	5	7
Total	59	59	64

For both cases with a preflash unit, the optimum flash temperature was 230°C, the upper bound of the range; this suggests that the constraints on the search space should be revised. The insensitivity of the performance to the design of main column was unexpected. Note that the cost of the column is not considered in this work so that the extra stages obtained by the optimised design do not have an impact on the objective function as it only takes into account the minimum hot utility demand of the system.

3.3.2.4 Case study summary

This second case study proposes a new optimisation-based design methodology for a crude oil distillation system with a preflash unit including a wide set of operational and structural variables. The approach allows the vapour leaving the flash unit to be fed to a suitable location to the main column (according to the temperature of the tray) while column structure is modified simultaneously on each optimisation run. Pinch technology is applied using the Grand Composite Curve (GCC) to evaluate minimum hot utility demand of the system but it does not account for the fuel demand of the fired heater nor take into account the detailed design and costing of the heat recovery system.

The optimisation results show that adding a preflash unit – while applying product quality constraints and a flowrate constraint to the residue and taking into account both operational and structural variables – can reduce the energy consumption of the system. It is evident that the simulation–optimisation approach is computationally intensive; this motivates the use of surrogate models, building on recent developments, e.g. Ibrahim et al., 2017.

3.4 Conclusions

This Chapter addressed the first objective stated in the introduction (See Section 1.3) regarding the development of an optimisation-based design methodology using rigorous models and pinch analysis simultaneously. Direct optimisation was performed to select the optimal operational and structural variables of a crude oil distillation system with and without a preflash unit.

Two scenarios are explored aiming to reduce minimum hot utility demand of the crude oil distillation system when a preflash is added. Case study 3.1 demonstrates that a decrease in energy demand for fired heating of 17% is achieved for case 1; for case 2, a decrease of 19% is obtained. On the other hand, in Case study 3.2 energy savings are about 20% between the optimised base case with no flash and the optimised base case with flash (no change in number of stages); however, a marginal saving (0.5%) is obtained when optimising both operational variables and the structure of the main column. Further examination of capital–separation–energy trade-offs can be beneficial to this case study, where the column capital cost and operating costs are considered in the objective function.

Limitations of the proposed design methodology are the use of pinch analysis, rather than addressing detailed aspects of design and costing of the heat recovery system. Also, the relatively high computational demand of this study cases – which could certainly be reduced by using software that is more time-efficient than MATLAB – points to the possibility of adapting recent developments in the use of surrogate models for distillation system optimisation (Ochoa-Estopier and Jobson, 2015; Ibrahim et al., 2017) as will be presented in the next Chapter.

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Chapter 4

Modelling and Optimisation of Crude Oil Distillation Systems with a Preflash Unit using Artificial Neural Networks

4.1 Introduction

The use of artificial neural network models rather than rigorous models to solve complex optimisation problems, as crude oil distillation systems are, has been preferred in practice because they are suitable for on-line applications taking advantages of shortest computational times required compared with rigorous models (Yusolf, et al., 2013). Specifically, artificial neural network models have been successfully used to model chemical processes including crude oil distillation systems (Motlaghi et al., 2008, Liau et al., 2004; Shalini et al., 2012; Popoola et al., 2013).

Optimising a crude oil distillation system is a highly complex task due to the interactions between the distillation column and its heat recovery system. Moreover, there is a trade-off between model accuracy and computational effort (Ochoa-Estopier and Jobson, 2015b).

Process optimisation based on process simulation as presented in Chapter 3, is usually time-consuming due to the flowsheet created in Aspen HYSYS v8.8 needs to be evaluated several times; however, it is strongly desirable that the distillation model can be simulated in a short period of time.

To overcome large optimisation times using simulation based-design optimisation approaches, artificial neural network models (ANN) can be implemented within an optimisation framework. The replacement of a rigorous model by an equivalent artificial neural network model takes advantage of a high-speed processing as a result of non-iterative algebraic calculations (Gao et al, 2005).

Previous research works (Ochoa et al., 2013; Ochoa et al., 2015a, 2015b; Ibrahim et al., 2018) have shown that surrogate models are useful and nearly as accurate as rigorous models; however, previous works have not addressed the design and optimisation of crude oil distillation systems that include a preflash unit using surrogate models.

Surrogate models of the distillation column have demonstrated their ability to reduce computational times compared with conventional simulation-optimisation approaches (Ibrahim et al., 2018a) as presented in the previous Chapter.

This Chapter extends the use of artificial neural network models for the optimisation-based design of crude oil distillation systems with a preflash unit. The proposed approach takes into account both discrete and continuous variables within the heat-integrated crude oil distillation system and it is applied to cases with and without a preflash unit.

As presented in Chapter 2, Section 2.4, there are two popular stochastic search methods that are used to solve optimisation problems: a genetic algorithm and simulated annealing. These methods are inherently more robust than gradient-based optimisation techniques as discussed previously in Chapter 3, section 3.2.3. In this Chapter, both optimisation methods are implemented within the optimisation framework of the system to explore and compare their capabilities for a better performance of the system in terms of optimisation time and to search for the ‘best’ structural and operating conditions of the system which minimise fired heating demand.

Similarly, to what was discussed in Chapter 3, Section 3.2.2, pinch analysis is used due to it allows calculations for minimum utility requirements for each converged simulation without detailed analysis and design of the heat recovery system represented by the heat exchanger network.

4.2 Modelling crude oil distillation systems using artificial neural networks

Increased attention regarding the use of surrogate models in crude oil distillation has emerged because they are easy to implement within an optimisation framework. Following the work of Ochoa-Estopier (2014) and Ibrahim (2018), the surrogate modelling framework developed in this research work starts with data generation (known as sampling); column modelling is performed using artificial neural networks, including a feasibility model extending previous work (Ochoa-Estopier, 2014) to the case when a preflash unit is added to the crude oil distillation system in order to predict whether a set of inputs can lead to feasible operating scenarios (i.e. the simulation converges so that material and energy balances, phase equilibrium relationships, as well as product constraints, are satisfied).

To date, systematic and accurate approaches to identify optimal operating conditions for crude oil distillation systems with preflash units are needed, as discussed in Chapter 2, Section 2.3.1. The purpose of generating an ANN column model is to correlate inputs and outputs of the heat-integrated crude oil distillation system which can easily be implemented within an optimisation framework, hence representing a good alternative for practical application in industry.

The following Sections describe in some detail the procedure to create the distillation model for a crude oil distillation system with and without a preflash unit followed in this work.

4.2.1. Data generation

The first step to create an artificial neural network model is data generation, as the performance of the entire model will depend on the quality of the data used to train the network (Ibrahim et at., 2018). In the context of simulating a crude oil distillation column, the neural network represents complex nonlinear relationships between process inputs and outputs. In this work, selected inputs or independent variables are those that can be manipulated or adjusted during column operation and also have an impact on heat recovery of the system as reported in previous research works (Ochoa-Estopier and Jobson, 2015a; Ibrahim et al., 2018). Inputs for the crude oil distillation system without a preflash unit analysed in this work are operational variables (namely pump-around duties and temperature drops, stripping steam flow rates, the column inlet temperature, and reflux ratio. On the other hand, inputs for the crude oil distillation system with a peflash are the same as for the case without a preflash unit plus the preflash temperature. The preflash vapour feed location is the structural variable due to it will change during the optimisation process.

The outputs of the ANN model are dependent variables needed to evaluate the desired objective function and to verify if process constraints are met. A penalty function added to the objective function will ensure that other product quality and flow rates specifications are met. Both sets of constraints relate to feasible outputs but only those defined in Aspen HYSYS v8.8 relate to converged solutions. Therefore, output variables selected in this work, as presented in Chapter 3, section 3.2.1, comprise those related to product quality for each product (namely ASTM D86 T5% and T95%), product flow rates and all the stream information required to calculate minimum heating and cooling requirements of the heat-integrated crude oil distillation system, namely the supply and target temperatures and enthalpy changes of relevant streams (See Chapter 3, Section 3.3.1.2).

Once the inputs and outputs of the system are defined, the next step is to apply a sampling technique to generate random samples for each input variable. In this work, Latin Hypercube Sampling (LHS) is selected. LHS is a method of sampling from a given population (data) where all members are divided into homogeneous subgroups, aiming to guarantee a uniform distribution as presented in Section 2.8. Generation of data is carried out using in MATLAB R2016a.

After sampling generation, rigorous simulations in Aspen HYSYS v8.8 of the crude oil distillation system with and without a preflash unit are performed separately in order to create ANN models for each case. Results of these rigorous simulations are recorded for each sample. To facilitate data collection from Aspen HYSYS v8.8, an automation code in MATLAB R2016a is used; the code works as an interface between the two software packages; first, it calls the set of input variables generated using the LHS method and sends each vector of inputs to Aspen HYSYS which automatically runs a simulation; then, the outputs of the system are generated.

Each set of input variables is classified depending on the convergence of a rigorous simulation in Aspen HYSYS as reported in previous works, Ochoa-Estopier et al., 2013, 2015a, 2015b; where the use of a feasibility model is discussed in detail. A binary value is assigned to each set of inputs, 1 if a set of input variables leads to a converged simulation; otherwise, a 0 value is assigned. This classification facilitates the ‘training’ of each neural network so that only the sets of input variables which produce a converged simulation in Aspen HYSYS are used to fit the network. Figure 4.1 summarises the steps followed in this work to generate the data (sets of input vectors) needed to build the ANN model.

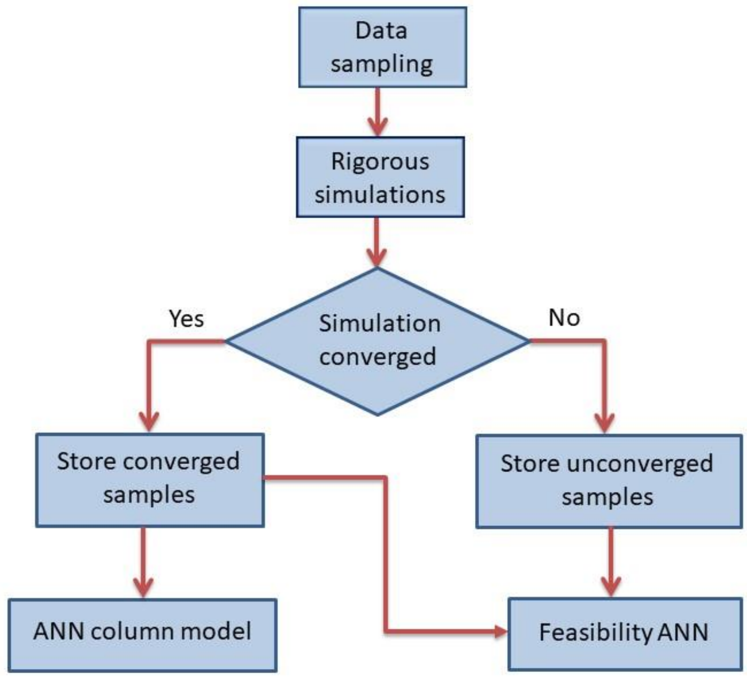

Figure 4.1 Data generation.

After data generation is completed, a regressed model for the atmospheric distillation column is created using artificial neural networks. The following section presents details about column modelling using surrogate models.

4.2.2. Creating the ANN model

To create the ANN model, it is necessary to define the structure, transfer functions and number of neurons (Beale et al., 2011). Different approaches have been followed by the research community: (Sarle, 1995; Heaton, 2005) suggest the use of heuristic rules to determine the number of layers and neurons for a neural network; Nolfi and Parisi, (2002) used an approach based on a genetic algorithm. However, for simplicity, the number of layers and neurons used in this work are chosen by trial and error as was reported in previous work (Ochoa-Estopier, 2013). The ANN structure used to model the distillation column for the cases with and without a preflash unit is a feedforward backpropagation network with one hidden layer, one output layer a hyperbolic tangent function and a linear transfer function for the hidden and output layers respectively (Beale et al., 2011).

4.2.3. ANN column modelling: crude oil distillation system with and without a preflash unit

In this work, two different flowsheets are modelled using artificial neural networks, 1) a crude oil distillation system without a preflash unit and 2) a crude oil distillation system with a preflash unit. For the first case, there are 10 inputs (i.e. independent variables) and 38 outputs (i.e. dependent variables); while for the second case, the system comprises 12 input variables and 41 outputs. To build the distillation model, several neural networks are required. In order to facilitate training of the neural networks, the outputs of both scenarios are grouped into six categories: product qualities (ASTM D86 T5% and T95%), product flow rates (See Chapter 3, Section 3.3.1.4), and stream data (i.e. supply and target temperatures and enthalpy changes) needed to evaluate the objective function. Thus, six ANN models are built to represent the distillation column. The difference between the modelling for the case with a preflash unit with respect to the case without a preflash unit are the number of streams that are taking into account for each group (i.e. 11 supply temperatures and 9 enthalpy change streams, for the case without a preflash vs 12 supply temperatures and 11 enthalpy change streams, for the case with a preflash).

The ANN models are developed using the Artificial Neural Network Toolbox embedded in MATLAB R2016a to build, validate and test the column model. These artificial neural networks models are structured as reported in previous works (Ochoa-Estopier and Jobson, 2015b; Ibrahim et al., 2018a) as multilayer feedforward networks, with one input layer, one hidden layer and one output layer.

The hidden layer comprises 10 hidden neurons as it was seen to provide a better performance in line with previous work (Ibrahim et al., 2018). The number of neurons of the output layer depends on the number of output variables in the network (Beale et al., 2011. For example, the neural network built for product qualities (ASTM 5%) in the preflash case has 12 inputs and 5 outputs as shown in Figure 4.2 corresponding to the five products namely, light naphtha, heavy naphtha, light distillate, heavy distillate and residue as will be presented and discussed in Section 4.4.2.

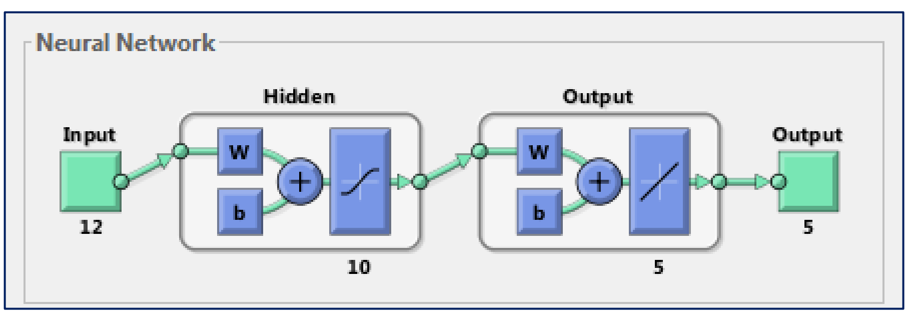

Figure 4.2 MATLAB screenshot of a neural network for product qualities.

The transfer function (also known as the system function or network function is a mathematical representation of the relation between inputs and outputs) selected in this work for the hidden layers is a sigmoidal function, while an identity function is used for the output layers (Beale et al., 2011).

All the converged samples for the column model generated using rigorous simulations are randomly divided into three sets: training (70%), validation (15%) and testing (15%); each set has a specific function within the ANN model, the training set is used to build the ANN model while the validation and testing sets are used to avoid model overfitting and to check the performance of the model respectively (Ibrahim et al., 2018b).

The accuracy of the fitting is measured by the mean squared error (MSE) and the coefficient of determination, R. The error is defined as the difference between the values predicted by the ANN model and those generated during the sampling process. MSE is an interpretation of how close are the values generated by the ANN model to those against they will be compared. Both indicators are used to evaluate whether a group of variables is well-trained or not, more details are given in Sections 4.4.1 and 4.4.2.

4.2.3.1 Feasibility ANN model

Apart from the six ANN models required to develop the crude oil distillation model, another ANN model is created using a new sampled data set from rigorous simulations in Aspen HYSYS v8.8 to predict whether a set of inputs lead to a feasible operating scenario. A feasibility ANN model helps to predict whether a set of inputs (i.e. operating conditions) are feasible (Ochoa-Estopier and Jobson, 2015a), the ANN distillation model provides stream data information (outputs) needed to evaluate the objective function value and to verify that process constraints on product quality are met. A feasibility ANN model guides the optimiser (clalsifying a set of outputs) towards operating points which satisfy all the specifications in the simulation model only; hence, facilitating the convergence of an Aspen HYSYS simulation. Using a feasibility ANN increases the likelihood that if the inputs associated with the ‘optimal’ solution are given as inputs to the rigorous simulation, it will converge. Process constraints in HYSYS aim to ensure that a limited number of product quality and flow rate specifications are met.

The feasibility ANN is built using the Neural Net Pattern Recognition application embedded in MATLAB R2016a, following the approach developed by (Ochoa-Estopier et al., 2013) as a feedforward network containing one hidden layer with 10 neurons (which were determined by trial an error) and one output layer. Hyperbolic transfer functions are used in both layers (default options in MATLAB Neural Pattern Recognition application).

The output of this pattern recognition network (a feedforward network that can be trained to classify inputs according to target classes, MATLAB, 2016) is an integer, either 0 for infeasible scenarios or 1 for the feasible ones.

Parity plots created for each ANN model represent a specific group of inputs correlated with the outputs of the system (i.e. product qualities, product flow rates and stream data). The goodness of fit of the feasibility ANN is validated using a so-called confusion matrix; a table that indicates the performance of a pattern recognition model on a set of inputs, more details will be given in Sections 4.4.1.2 and 4.4.2.2.

The feasibility ANN model reported by Ochoa-Estopier, 2014 for the case of a heat-integrated crude oil distillation system is adapted in this work, and extended to the case when a preflash unit is added. It was observed that without a feasibility ANN model within the optimisation framework for both case studies – with and wihout a preflash unit, the likelihood of converged simulation in Aspen HYSYS v8.8 was low (i.e. after 10 optimisation runs only 1 or 2 converged). The feasibility ANN helps the optimiser to search only in the regions where the samples for the optimisation variables that are sent to

Aspen HYSYS lead to a converged simulation, meeting all product quality and quantity specifications.

4.3 Optimisation framework using surrogate models

The main feature of the optimisation methodology presented in this Chapter is the implementation of surrogate models into the optimisation framework presented in Chapter 3, Section 3.3.1.2, which has been adapted to apply surrogate models rather than rigorous simulation models to represent the distillation process, aiming to reduce optimisation times while accounting for product quality, yields and heat integration. This Section describes the approach proposed for optimisation of the crude oil distillation systems with and without a preflash unit using surrogate models.

4.3.1. Objective function and process constraints

The role of optimisation-based design methodologies is to select the best design alternative from a set of available options in a systematic way. In this work, the performance indicator used to identify an optimal solution is the minimum hot utility demand of the heat-integrated crude oil distillation system as presented in Chapter 3, Section 3.3.1.2.

The optimisation methodology is formulated as a mixed integer nonlinear programming (MINLP) problem involving the distillation column model based on artificial neural networks, the feasibility ANN and additional inequality constraints related to product quality and quantity specifications. These additional constraints are incorporated into the objective function via penalty terms (i.e. product constraints in Aspen HYSYS v8.8 and in MATLAB R2016a which are within a tolerance of ±10°C). Therefore, the objective function used in this work can be expressed mathematically as given in Chapter 3 by the equation (3.1) where product quality constraints are included as inequality constraints $g_j(x)$ in the objective function as given by equations (3.4) and (3.5) in Chapter 3. A third inequality constraint is added to ensure that the volumetric flow rate of the atmospheric residue, m_{RES}, is no greater than that in the base case, m^0_{RES} (Ibrahim et al., 2017; Ledezma-Martínez et al., 2018) as stated by equation (3.6), Chapter 3.

The surrogate model includes six artificial neural networks; each group of ANN's predicts a set of dependent variables of the system. Hence, the equality constraints $h(x)$ in equation (3.1) presented in Chapter 3 can be expressed as follows:

$$
\begin{aligned}
h_1 &= ANN1\ [T5_i] \qquad (4.1)\\
h_2 &= ANN2\ [T95_i]\\
h_3 &= ANN3\ [FR_i]\\
h_4 &= ANN4\ [TS_i]\\
h_5 &= ANN5\ [TT_i]\\
h_6 &= ANN6\ [EC_i]\\
h_7 &= \ [FC]
\end{aligned}
$$

where $T5_i$ and $T95_i$ represent product qualities in terms of ASTM D86, FR_i is the flow rate of each product, TS and TT are supply and target temperatures respectively, EC_i is the enthalpy change of each stream and; FC represents the *feasibility constraint* according to a convergence criterion (0 or 1) as explained in Section 4.2.2.

Inequality constraints $g_j(x)$ represent the upper and lower bounds of the optimisation variables (pump-around duties and temperature drops, steam flow rates, column inlet temperature, preflash temperature, reflux ratio and vapour feed location for the preflash case).

Process optimisation is performed in MATLAB R2016a. Two optimisation search methods are applied: a) genetic algorithm and b) simulated annealing to explore their performance. For the genetic algorithm, two tuning parameters need to be selected; the initial population size and the maximum number of generations, both make a difference to the optimisation results. For the simulated annealing algorithm, tuning parameters are the initial temperature and a function tolerance. General MINLP convergence refers to the stopping criteria for each method (i.e. maximum number of generations for the genetic algorithm and function tolerance for simulated annealing method). Figure 4.3 summarises the proposed optimisation framework.

In order to gain confidence in results obtained by the optimiser, several runs should be performed. The solution with the lowest objective function is selected as the 'optimal' solution.

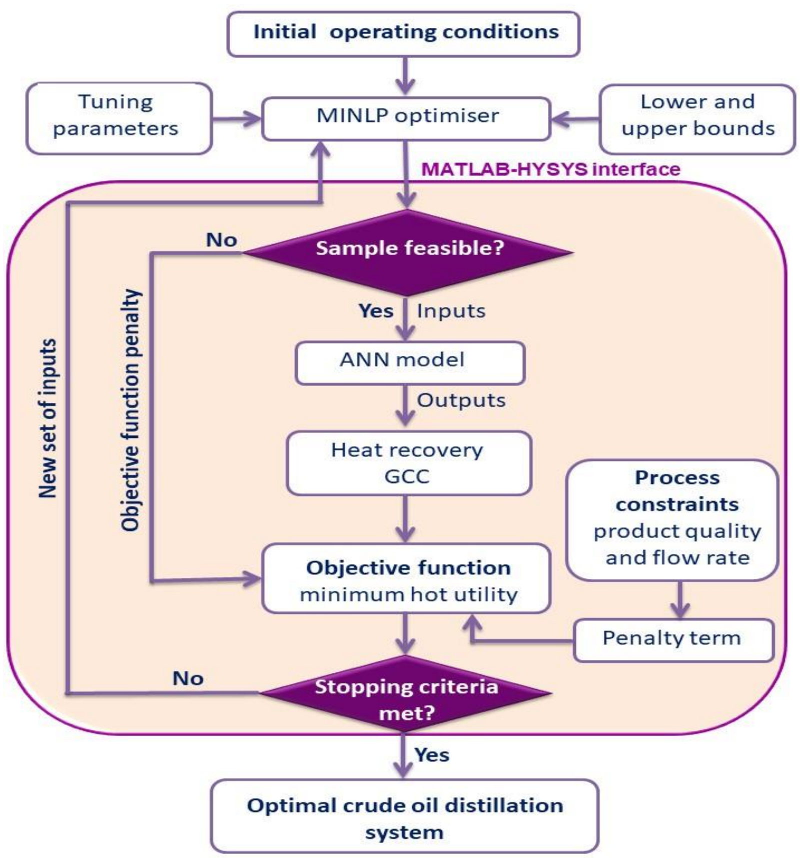

Figure 4.3 Optimisation framework using surrogate models.

4.3.2. Validation of ANN model results on rigorous models in Aspen HYSYS

To gain more confidence in results obtained using surrogate models into an optimisation framework as shown in Figure 4.3 a final validation is performed as reported in previous work (Ibrahim, 2018), and extended to the case of a crude oil distillation system with a preflash unit.

The validation of optimisation results on rigorous models is performed as follows: the set of optimal operating and structural conditions obtained after performing the optimisation of the system using surrogate models, (10 for the case without a preflash and 12 for the case with a preflash) is automatically send from MATLAB R2016a (via an interface) to the corresponding flowsheet, either with or without a preflash unit, in Aspen HYSYS v8.8 as inputs to verify:

1. Convergence of the corresponding flowsheet in Aspen HYSYS v8.8.
2. Agreement between objective function values (minimum hot utility demand) obtained using surrogate models and rigorous models.
3. Accuracy and effectiveness of the proposed approach (Ibrahim, 2018).

In practice, it is common to judge the effectiveness of surrogate models results comparing them with actual plant measurements (Arce-Medina and Paz-Paredes, 2009). Validating optimisation results from surrogate models on rigorous simulation models is useful in industrial practice and for process controls (Mittal, 2013).

4.4 Case studies

The design approach presented in this Chapter is illustrated with two case studies to demonstrate the capabilities of the proposed optimisation methodology. The objective function is the minimum hot utility demand.

The first case study refers to a crude oil distillation system without a preflash unit. The second case study includes a preflash unit within the crude oil distillation system. Here, the flash temperature and vapour feed location are added as optimisation variables. Heat recovery is evaluated as discussed in Chapter 3, Section 3.2.2. The next Sections describe each case study and present their optimisation results.

4.4.1. Case study 4.1: crude oil distillation unit

The atmospheric distillation unit processes 100,000 bbl/day (0.184 m^3h^{-1}) of Venezuela Tia Juana light crude oil (Watkins, 1979) into five products, namely, light naphtha (LN), heavy naphtha (HN), light distillate (LD), heavy distillate (HD) and residue (RES). The structure of the column as shown in Figure 4.4 includes a condenser, three pump-arounds numbered from top to bottom (PA1, PA2, PA3) one steam-injected side stripper (HD SS) and two reboiled side strippers (HN SS, LD SS). The column has 41 theoretical stages over five sections numbered from top to bottom; it operates at a uniform pressure of 2.5 bar. Initial column configuration and initial operating conditions are taken from Chen (2008) based on a study case presented by Watkins (1979). The Peng-Robinson equation of state is used to simulate the mixture of pseudo-components as previously discussed in Chapter 3, Section 3.3.1.

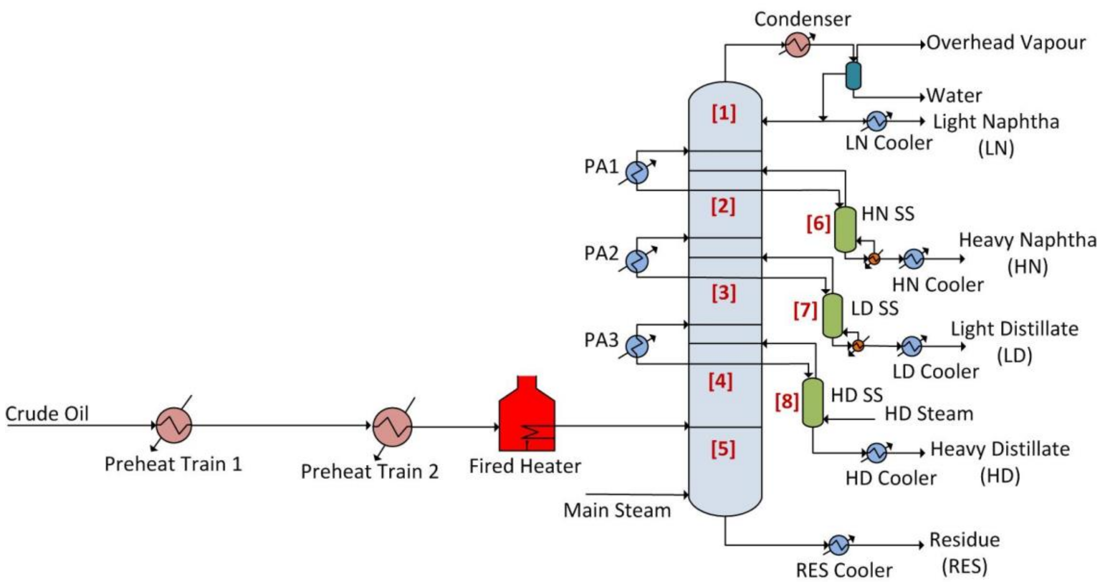

Figure 4.4 Crude oil distillation system.

4.4.1.1 ANN model for a crude oil distillation system without a preflash unit

The procedure to set up the crude oil distillation model starts with a rigorous simulation (base case) ensuring that product quality specifications are met. Then, a Latin Hypercube Sampling method (see Chapter 2, Section 2.8) is applied to generate 7000 samples in line with previous research work (Ibrahim et al., 2018a). Note that each sample has a set of independent variables that can be manipulated within the system. Lower and upper bounds for each independent variable are presented in Table 4.3. All bounds are the same as those used in Chapter 3, for Case 2 (Case study 3.1).

From the 7000 simulated set of samples, 1713 converged (rigorous simulations took 1.6 hours). Results from the converged simulations only are used to train the artificial neural network model, while all samples are used to train the feasibility ANN. Details about the 10 input variables selected to correlate the 38 outputs present in this case study as well as the number of streams grouped on each ANN are shown in Table 4.1.

Table 4.1. ANN inputs-outputs model for Case 4.1 (without a preflash)

Inputs **10**	**Outputs** **38**	**Streams**	**ANN group**
PA1 Duty			
PA2 Duty	Product quality ASTM 5%	5	1
PA3 Duty	Product quality ASTM 95%	5	2
PA1 ΔT	Product flow rates	5	3
PA2 ΔT	Supply temperatures	11	4
PA3 ΔT	Target temperatures	3	5
Main Steam	Stream enthalpy change	9	6
HD Steam			
Column inlet temperature			
Reflux Ratio			

PA: pump-around
ΔT: pump-around temperature drop

Inputs of the surrogate model are all optimisation variables while the outputs of the model represent the information needed to calculate minimum hot utility demand and to allow inequality constraints related to product quality to be checked.

Figure 4.5 shows the parity plots for the six artificial networks developed to describe the distillation model according to Table 4.1. These plots compare the ANN distillation model predictions against rigorous simulations for the 6 groups of regressed variables. As can be seen, there is an excellent agreement between the rigorous simulations and ANN models.

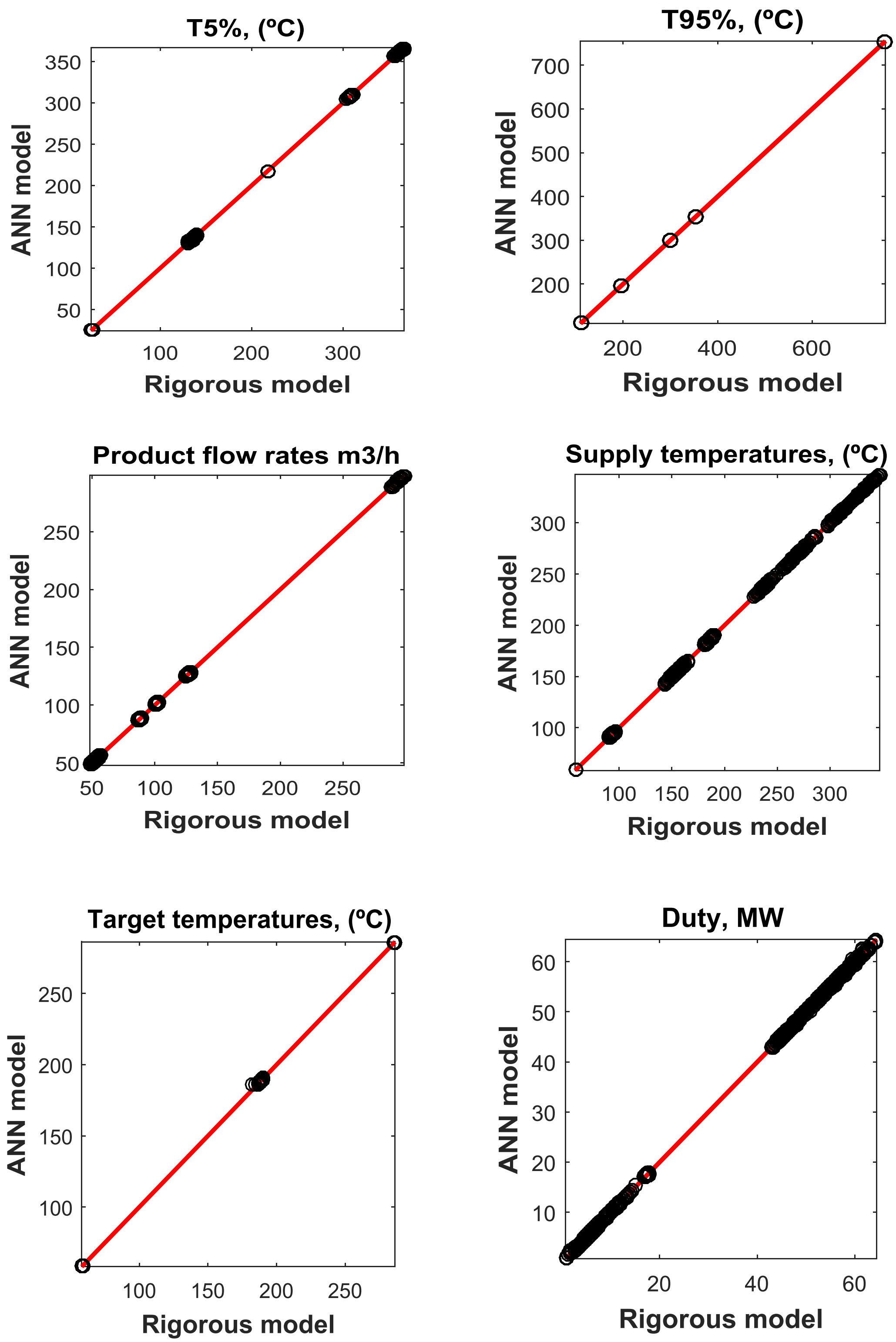

Figure 4.5 Parity plots generated using 70% data, Case 4.1 (without a preflash).

Table 4.2 shows the group of variables for each ANN created in this case study; the goodness of fit for each network is also shown in terms of MSE and coefficient of determination R.

Table 4.2. ANN models and goodness of fit for Case 4.1 (without a preflash)

ANN group	Variables	Units	Mean Squared Error, MSE	Coefficient of determination, R
1	Product quality, T5%	ºC	$3.5 \cdot 10^{-2}$	1
2	Product quality, T95%	ºC	$9.6 \cdot 10^{-3}$	1
3	Product flow rates	kmol h^{-1}	$1.4 \cdot 10^{-2}$	1
4	Supply temperatures	ºC	$1.6 \cdot 10^{-2}$	1
5	Target temperatures	ºC	$3.2 \cdot 10^{-2}$	1
6	Enthalpy change (duty)	MW	$7.7 \cdot 10^{-2}$	1

A well-trained ANN should have low values (close to zero) for the mean squared error. The coefficient of determination, R is an indication of the relationship between sampled and model outputs.

4.4.1.2 Prediction of feasibility, Case 4.1

The feasibility ANN is validated using a confusion matrix; it shows how well the feasibility ANN predicts convergence for this particular case study as shown in Figure 4.6. During the training stage for this ANN model, 4900 samples are used for training, 1050 samples for validation and 1050 samples for testing.

In a confusion matrix, four categories can be identified (Thing, 2011): true positives (TP), for correct true predictions, true negatives (TN), for correct false predictions, false positives (FP), for those predictions that are expected to be true but they are not (i.e. when a set of inputs is expected to lead to a feasible solution in Aspen HYSYS but it is not); false negatives (FN), for predictions expected to be unfeasible but they are (i.e. a set of inputs is likely to be unfeasible when simulated in Aspen HYSYS but actually, they might lead to a feasible solution).

From the square with double shading (bottom left) in the confusion matrix, it can be seen that there is a high accuracy of 97.7% (overall, how often is the classifier correct for the predicted values) while the classifier is wrong for 2.3% of cases. True positive and true negative predictions are 25% and 72.7% respectively. Between the two false predictions classes, the false positive ones are the least desired because they will allow unfeasible inputs to be used by the optimiser, thus leading to unrealistic results (Ochoa-Estopier and Jobson, 2015a). Feasible (convergeable) solutions that are correctly identified represent 25% while 72.7% represent unconvergeable solutions.

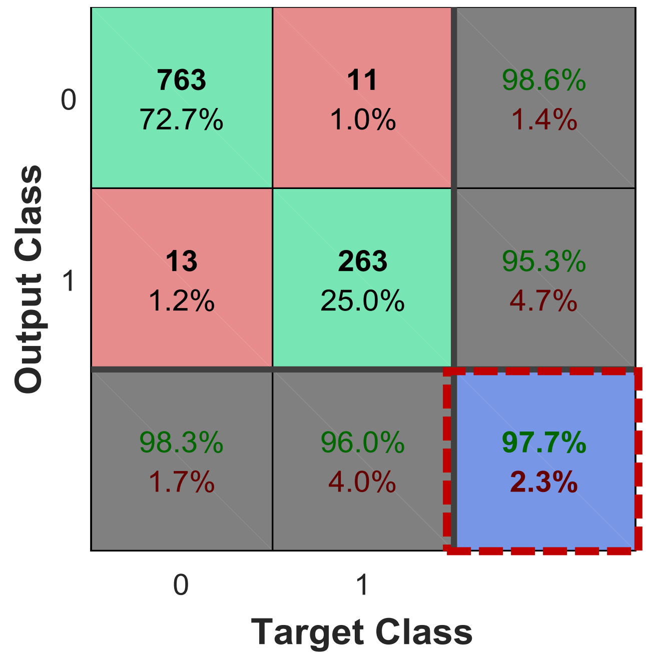

Figure 4.6. Confusion matrix for Case 4.1 (without a preflash).

4.4.1.3 Optimisation results, crude oil distillation system without a preflash unit

This Section presents optimisation results for a crude oil distillation system without a preflash unit; constraints on both product quality and residue flow rate (as discussed in Chapter 3, Section 3.3.1.4) are included within the optimisation framework in Figure 4.3. Two options from MATLAB R2016a Global Optimisation Toolbox were selected and tested as MINLP optimisers – both simulated annealing (*simulannealbnd*) and a genetic algorithm (*gaoptimset*) to solve the problem stated earlier in this Chapter, Section 4.1.

The application of the genetic algorithm for optimisation is described in Chapter 2, Section 2.4.1 and illustrated in Figure 2.1. Simulated annealing algorithm is presented in Section 2.4.2 and illustrated in Figure 2.2. Tuning parameters selected for the genetic algorithm are 500 for the maximum number of generations and 100 for the initial population size. For the simulated annealing algorithm, tuning parameters are the initial temperature of 100ºC and a function tolerance of 1e-30.

The independent variables (inputs) are randomly varied by the optimiser between their lower and upper bounds. Optimisation runs using a HP desktop PC with Intel Core i5 processor running at 3.20 GHz and 16 GB of RAM for the genetic algorithm took 95 to 98s of CPU time while for the simulated annealing algorithm optimisation runs took 41 to 122s of CPU time as can be seen in Appendix B, Tables B1-B3. Optimisation results are summarised in Tables 4.3 to 4.5.

After generating results using artificial neural networks, the independent variables for the optimal solutions are simulated provided as inputs to Aspen HYSYS v.8.8 to perform a final validation (See Section 4.3.2 and Appendix B, Tables B.6 and B.7.

Table 4.3. Optimisation results, Case 4.1 (no preflash)

Variable	Units	Base Case	Lower Bound	Upper Bound	Optimisation Results ANN model GA	SA
Main Steam Flow Rate	kmol h^{-1}	1200	900	1800	1607	1353
HD Steam Flow Rate	kmol h^{-1}	250	180	375	209	234
PA1 Duty	MW	12.8	14	6	6.0	9.5
PA2 Duty	MW	17.8	18	6	9.4	11.8
PA3 Duty	MW	11.2	14	6	14.0	14.0
PA1 ΔT	°C	30	20	50	20.0	31.5
PA2 ΔT	°C	50	15	60	29.6	37.8
PA3 ΔT	°C	20	10	40	40.0	33.9
Reflux Ratio		4.17	3.0	4.5	4.1	3.7
Optimisation CPU time	s				96	41

PA: pump-around
ΔT: pump-around temperature drops
GA: genetic algorithm
SA: simulated annealing

It can be seen from Table 4.3 that increasing column inlet temperature requires less stripping steam in the case using simulated annealing, where the column inlet temperature of 360ºC requires less steam flow rate (1353 kmol h^{-1}) compared with the genetic algorithm results (1607 kmol h^{-1}). Large stripping steam flow rates increase the vapour and liquid traffic in the bottom of the atmospheric column.

High pump-around duty values mean there is more heat to be recovered by the heat recovery system which will be pre-heating the crude oil before entering to the furnace. Optimisation results using a simulated annealing algorithm show the highest values for the 3 pump-around duties, in line with a high column inlet temperature of 360ºC. This high temperature also increases the minimum hot utility demand of the system by 2.4 MW compared with a lower temperature of 350ºC when using a genetic algorithm.

The lowest value for the minimum hot utility demand (44.5 MW) is obtained for the case using a genetic algorithm, which also corresponds to a lower column inlet temperature of 350ºC. A reduction in the column inlet temperature reduces the fired heating duty.

Appendix B, Tables B1 to B3 show details (objective function value, CPU optimisation time) for 10 optimisation runs performed for this case study.

Product quality specifications (for the best solutions found by the two optimisation methods) in terms of ASTM D86 T5% and T95% (in °C) are listed in Table 4.4. It can be seen that all the product quality constraints are met within the allowed range of temperatures selected in this work (± 10°C). Both sets of constraints are met (i.e. the specifications within Aspen HYSYS v8.8 and the constraints within the optimisation).

Table 4.5 shows results for the best solutions regarding the distribution of product flow rates. Residue flow rate value is kept almost unchanged as a result of the constraint added in MATLAB.

Table 4.4. Product specifications results for best solutions (Case 4.1)

Product	Base Case ASTM D86 (°C)		Optimisation Results ANN model			
			GA ASTM D86 (°C)		SA ASTM D86 (°C)	
	T5%	T95%	T5%	T95%	T5%	T95%
LN	25.6 [b]	109.7 [a]	25.0	109.7	25.2	109.7
HN	140.2 [b]	196.0 [a]	132.5	196.0	134.3	196.0
LD	217.5 [a]	300.1 [a]	217.5	300.1	217.6	300.1
HD	308.5 [b]	353.5 [a]	306.4	353.5	307.8	353.6
RES	361.6 [b]	754.4 [b]	361.4	754.3	361.9	754.5

[a] Specified in HYSYS GA: genetic algorithm SA: simulated annealing
[b] Specified in MATLAB

Table 4.5. Product flow rates for best solutions (Case 4.1)

Product flow rate ($m^3\ h^{-1}$)	Base Case	ANN model	
		GA	SA
LN	102.4	100.7	101.4
HN	86.8	88.8	88.0
LD	127.6	125.9	126.8
HD	53.7	55.1	54.7
RES	292.1	292.1	291.8

GA: genetic algorithm
SA: simulated annealing

Table 4.6 summarises and compares optimisation results and CPU times for each optimisation run obtained using rigorous models via the direct simulation-optimisation approach presented in Chapter 3 against those generated by the ANN model.

Table 4.6. Optimisation results summary and validation on rigorous model (Case 4.1)

Case 4.1	**HU, MW**	**CPU Time**	**Rigorous model, MW**	**Difference MW**
Direct simulation-optimisation using GA	44.8	4.1 h		
GA - ANN optimisation	44.5	96 s	44.6	-0.1
SA - ANN optimisation	46.9	41 s	46.9	0.0

GA: genetic algorithm
SA: simulated annealing

4.4.1.4 Case study summary

This case study illustrates how the implementation of artificial neural networks within an optimisation framework helps to reduce computational time to perform the optimisation of the crude oil distillation system without a preflash unit. An excellent accuracy between direct-simulation optimisation and GA-ANN optimisation routes is achieved as shown in Table 4.6. Product qualities and flow rates are maintained within the specified ranges as it is required in industrial practice.

See Appendix B, Tables B6 and B7 for detailed information regarding the validation of results of the artificial neural network model on the rigorous model in Aspen HYSYS V8.8.

In general, the artificial neural network model was easy to implement into the optimisation framework; the generation of samples via rigorous simulations took 1.6h, generation of samples took 0.5s, model training between 5 – 10min and each optimisation run took around 122s for the case using a simulated annealing algorithm and less than 98s for the case of using a genetic algorithm as an optimisation method. Note that all times reported are CPU times.

The next case study will extend the approach followed in this case study when a preflash unit is added to a crude oil distillation system.

4.4.2. Case study 4.2: Crude oil distillation system with a preflash unit

This case study aims to demonstrate the capabilities of the modelling approach using artificial neural networks when a preflash unit is added to a heat-integrated crude oil distillation system as shown in Figure 4.7. The main column structure is the same as that presented for the case without a preflash unit (Section 4.4.1). The crude oil distillation system has 11 operational variables and one structural variable (vapour feed location). In the base case, the vapour leaving the preflash unit is sent to the same stage in the main column as the main feed; the best vapour feed location is selected by the optimiser during the optimisation process.

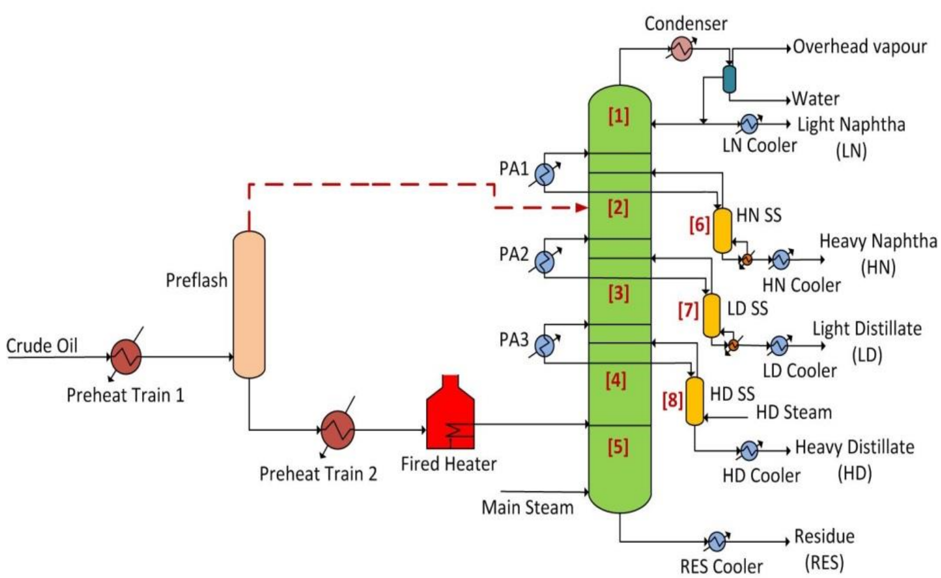

Figure 4.7 Crude oil distillation system with a preflash unit (Case 4.2).

4.4.2.1 Artificial neural network model for a crude oil distillation system with a preflash unit

The modelling of the crude oil distillation system with a preflash unit starts by setting up a base case in Aspen HYSYS v8.8 ensuring that product quality specifications are all met within a tolerance of ±10ºC. Next, the Latin Hypercube Sampling method is used to generate 7000 samples. To construct the ANN model, 7000 rigorous simulations in Aspen HYSYS v8.8 are performed, of which 3340 converged.

Simulation results from the converged simulations are used to train the artificial neural network models which describe the flowsheet comprising the preflash unit and atmospheric distillation column; while full set of samples is used to train the feasibility ANN. Details about the 12 input variables selected to correlate the 41 outputs present in this case of study as well as the number of streams grouped on each ANN are shown in Table 4.7.

Table 4.7. ANN model, case study 4.2 (with preflash)

Inputs 12	**Outputs 41**	**Streams**	**ANN group**
PA1 Duty			
PA2 Duty	Product quality, ASTM D86 5%	5	1
PA3 Duty	Product quality, ASTM D86 95%	5	2
PA1 ΔT	Product flow rates	5	3
PA2 ΔT	Supply temperatures	12	4
PA3 ΔT	Target temperatures	3	5
Main Steam	Stream enthalpy change	11	6
HD Steam			
Column inlet temperature			
Reflux Ratio			
Preflash temperature			
Vapour feed location			

PA: pump-around
ΔT: pump-around temperature drop

Table 4.8 shows the group of variables for each ANN created in this case study; the goodness of fit for each network is also shown in terms of MSE and coefficient of determination R.

Table 4.8. ANN models and goodness of fit for Case 4.2

ANN group	Variables	Units	Mean Squared Error, MSE	Coefficient of determination, R
1	Product qualities, T5%	ºC	$6.8 \cdot 10^{-1}$	0.9999
2	Product qualities, T95%	ºC	$1.7 \cdot 10^{-2}$	1
3	Product flow rates	kmol h^{-1}	$4.7 \cdot 10^{-1}$	0.9999
4	Supply temperatures	ºC	$1.6 \cdot 10^{-0}$	0.9999
5	Target temperatures	ºC	$1.3 \cdot 10^{-1}$	1
6	Enthalpy change	MW	$2.9 \cdot 10^{-1}$	0.9997

Figure 4.8 shows the parity plots generated after training each artificial neural network. Each parity plot compares the predictions of the ANN model and the original samples. It can be seen from Figure 4.8 that there are some issues with accuracy in parity plots for the supply temperatures and duties.

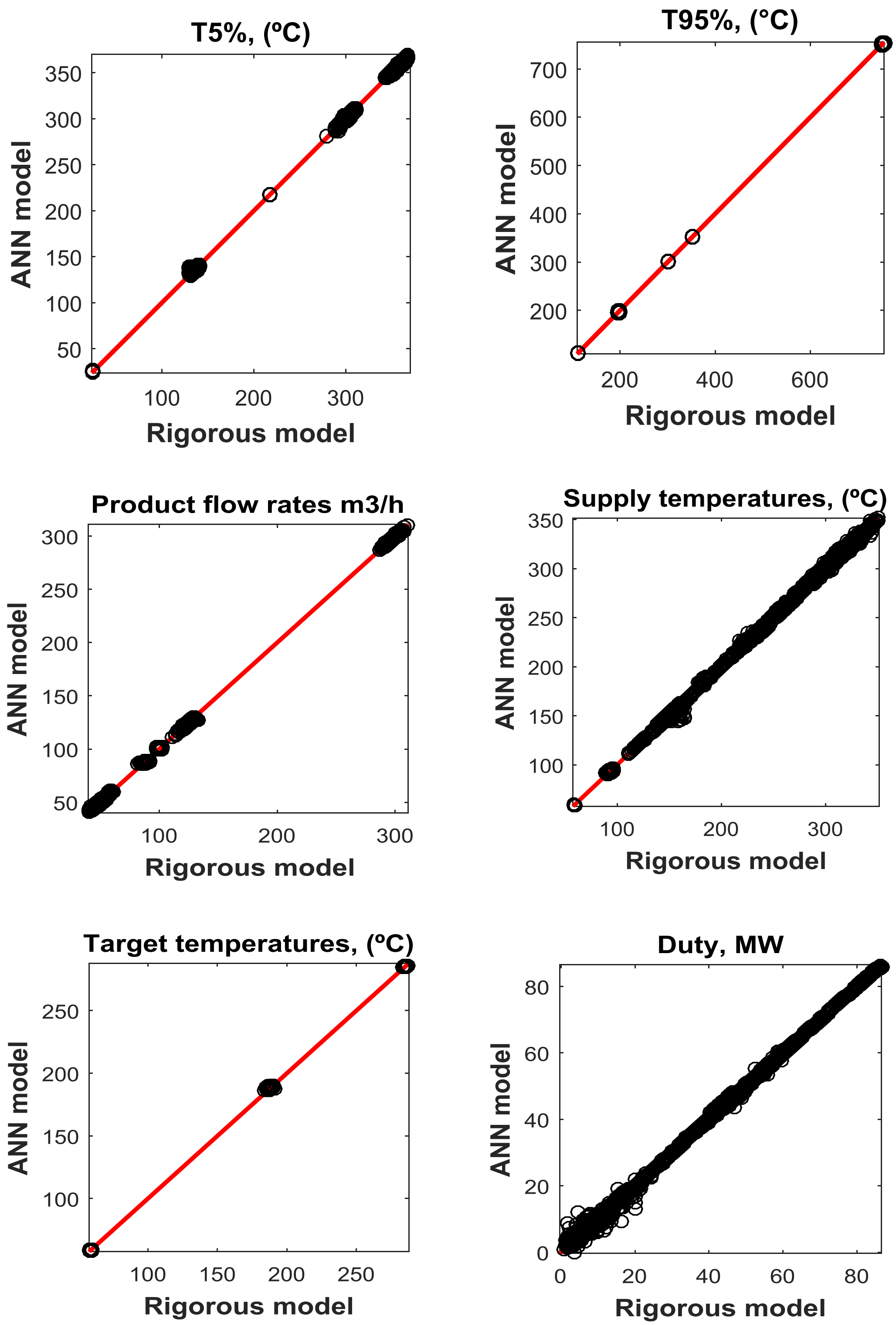

Figure 4.8 Parity plots generated using 70% data for Case 4.2 (with preflash).

4.4.2.2 Model validation (Case 4.2)

The feasibility ANN model is validated using a confusion matrix as explained in Case study 4.1. For Case 4.2, the overall accuracy of the feasibility ANN model, as shown in the bottom right of the matrix (dashed square) is 93.6%, while the misclassification rate is 6.4%. Feasible (convergeable) solutions that are correctly identified represent 46.9% while 46.8% represent unconvergeable solutions. To create the matrix, 7000 samples are used, from them 4900 are used to train the feasibility ANN, 1050 for validation and 1050 for testing.

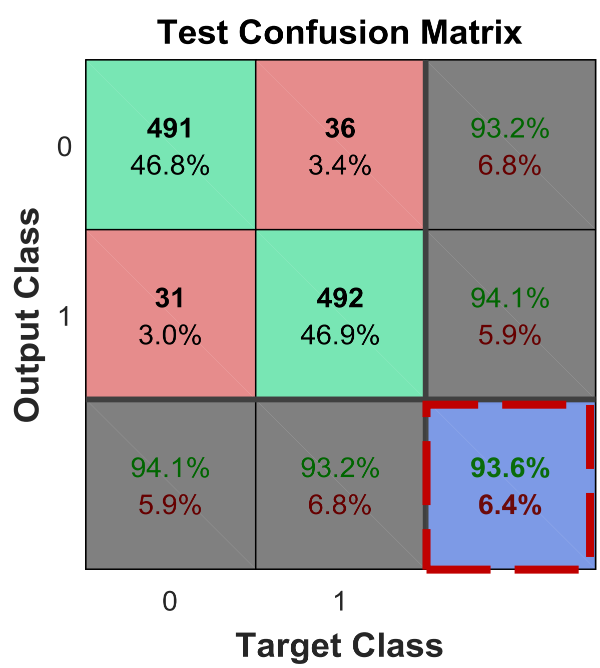

Figure 4.9 Confusion matrix, Case 4.2 (with preflash).

4.4.2.3 Optimisation results, Case 4.2: Crude oil distillation system with a preflash unit

In this Section, optimisation results for the crude oil distillation system with a preflash unit are presented. Again, two options from MATLAB R2016a Global Optimisation Toolbox are selected and tested as MINLP optimisers – simulated annealing (*simulannealbnd*) and a genetic algorithm (*gaoptimset*) to solve the problem stated in Equation 4.1. Optimisation results are summarised in Table 4.9. Appendix B, Tables B8 to B10 show detailed information about objective function values (minimum hot utility) and CPU time for optimisation.

For the genetic algorithm optimisation runs took 102 to 110s of CPU time while for the simulated annealing algorithm optimisation runs took 38 to 118s of CPU time

Product quality specifications are listed in Table 4.10. It can be seen that all the product quality constraints are met within the allowed range of temperatures selected in this work (± 10°C, in Aspen HYSYS v8.8 and MATLAB R2016a).

Table 4.9. Optimisation results case 4.2 (with preflash)

Variable	Units	Base Case	Lower Bound	Upper Bound	Optimisation Results	
					ANN model	
					GA	SA
Main Steam Flow Rate	kmol h^{-1}	1200	900	1800	1684	1374
HD Steam Flow Rate	kmol h^{-1}	250	180	375	193	345
PA1 Duty	MW	12.8	14	6	6.8	6.4
PA2 Duty	MW	17.8	18	6	8.1	7.9
PA3 Duty	MW	11.2	14	6	10.5	13.1
PA1 ΔT	°C	30	20	50	29.8	46.5
PA2 ΔT	°C	50	15	60	30.2	40.1
PA3 ΔT	°C	20	10	40	39.3	29.4
Column Inlet Temperature	°C	365	350	385	367	384
Reflux Ratio		4.17	3.0	4.5	3.8	3.8
Preflash temperature	°C	115	110	240	235	239
Vapour feed location (column section)[a]		5	1	5	3	3
Minimum Hot Utility	MW	57.7			38.2	39.4
Optimisation time	s				103	118

[a] Number of section in main column

PA: pump-around

ΔT: pump-around temperature drop

GA: genetic algorithm

SA: simulated annealing

It may be seen from Table 4.9 that the minimum hot utility demand of the crude oil distillation system deceased compared with optimisation results from case study 4.1 as follows: 15% for direct optimisation, 14% when a genetic algorithm is used as optimisation method and 16% using simulated annealing. Therefore, demonstrating that adding a preflash unit within the crude oil distillation system reduce its energy consumption. A preflash unit also allows more capacity to be processed in the distillation column as it reduces the vapour and liquid flow rates inside the column.

Energy savings are dependent on the value of preflash temperature, which is an important degree of freedom in this case study. High preflash temperatures (235ºC and 239ºC) allow more material to be vaporised from the crude, decreasing the flow rate entering to the furnace which will also decrease the furnace duty.

The vapour feed location in the main column is the same (column section 3) for the two optimisation methods used in this work. The optimiser selects a feed stage with a similar temperature as the flashed vapour (i.e. stage 18 in the main column).

Column inlet temperatures increased with respect to the base case in 2ºC (GA) and 19ºC (SA); therefore, different values for the minimum hot utility demand were obtained. Pump-around duties 1 and 2 for the two optimisation methods are lower than those in the base case, which in turn will reduce the temperature of the crude oil stream before entering to the furnace.

Table 4.10. Product specifications for best solutions, Case 4.2

Product	**Base Case ASTM D86 (°C)**		**Optimisation Results ANN model**			
			GA ASTM D86 (°C)		**SA ASTM D86 (°C)**	
	T5%	**T95%**	**T5%**	**T95%**	**T5%**	**T95%**
LN	25.6 [b]	109.7 [a]	25.4	109.7	25.1	109.7
HN	140.2 [b]	196.0 [a]	138.0	195.8	134.8	195.8
LD	217.7 [a]	300.1 [a]	217.5	300.1	217.5	300.1
HD	308.5 [b]	353.5 [a]	304.7	353.5	307.8	353.5
RES	361.4 [b]	754.3 [b]	362.2	754.4	363.0	754.6

[a] Specified in HYSYS GA: genetic algorithm SA: simulated annealing
[b] Specified in MATLAB

Table 4.11. Product flow rates for the best solutions, Case 4.2

Product flow rate (m^3 h^{-1})	**Base Case**	**ANN model**	
		GA	**SA**
LN	102.4	101.9	101.3
HN	86.8	87.1	87.8
LD	127.6	124.9	126.2
HD	53.5	56.5	56.2
RES	292.3	292.2	291.1

GA: genetic algorithm
SA: simulated annealing

Results obtained by the distillation column model using artificial neural networks are simulated in Aspen HYSYS v.8.8 to perform a final validation, showing good agreement. See Appendix B, Tables B.13 and B.14.

Table 4.12 summarises optimisation results and show the accuracy of the artificial neural network model with respect to the direct simulation-optimisation route. The validation of results on the rigorous model using a genetic algorithm has a difference of 2.2 MW with respect to predicted value from the ANN model; while for the simulated annealing algorithm has a better agreement. Validation of results is performed sending automatically from MATLAB to Aspen HYSYS a set of optimised operational variables.

These results confirm the importance of exploring two optimisation algorithms within the same optimisation framework; depending on the case study they might have different performance.

Table 4.12. Optimisation results summary and validation on rigorous model Case 4.2

Case 4.2	**HU, MW**	**CPU Time**	**Rigorous model, MW**	**Difference MW**
Direct simulation-optimisation using GA	38.1	6.2 h		
GA - ANN optimisation	38.2	103 s	40.4	2.2
SA - ANN optimisation	39.4	118 s	39.5	0.1

GA: genetic algorithm
SA: simulated annealing

4.4.2.4 Case study summary

This case study demonstrates the capabilities of the approach reducing optimisation times to the case of adding a preflash unit into a crude oil distillation system. Modelling the distillation process involves a deep understanding of the interactions between the operating conditions and how do they affect the performance of the whole system.

Artificial neural network models are easy to implement, as discussed in the previous case study. Main differences between the models developed in case studies 4.1 and 4.2 are the number of streams that are grouped to construct them. A detailed error analysis is presented in Appendix B, Tables B11 and B12.

Adding a preflash unit into a crude oil distillation system helps to avoid unnecessary heating of light components in the furnace and to reduce energy consumption as the flow rate entering the furnace is reduced.

4.5 Conclusions

The second objective of this work is addressed in this Chapter; surrogate models are incorporated into the optimisation-based design methodology presented in Chapter 3, aiming to reduce optimisation time without compromising model accuracy, column performance, product qualities or product yields.

An artificial neural network model can represent and describe the distillation process for its input and output relations.

Two case studies, with and without a preflash unit, demonstrate the capabilities of introducing artificial neural networks models into an optimisation framework. It has been demonstrated that an artificial neural network model, can represent and describe the distillation process for its input and output relations (Motlaghi et al., 2008).

Adding a preflash unit to a crude oil distillation system enable a considerable reduction on minimum hot utility demand of the system, i.e. 14% for the case using a genetic algorithm, and 16% for the case using simulated annealing.

The flowsheet structure for Case study 4.2 changed after optimisation was performed (i.e. vapour feed location) with respect to the base case where the vapour is fed to the same stage in the atmospheric column as the crude oil stream. Optimisation results shown in Table 4.5, confirm that both optimisation search methods (genetic algorithm and simulated annealing) selected column section 3 as the optimum location to introduce the flashed vapour, rather than in column section 5 as in the base case. It is worthy to mention that the feed stage selected by the optimiser as optimum to introduce the vapour leaving the preflash unit corresponds to that with a similar temperature of the vapour so that the separation performance (liquid-vapour equilibrium) on that stage is barely altered.

It is important to note that optimisation results obtained in this Chapter regarding the direct simulation-optimisation differ to those presented in Chapter 3 (Section 3.3.1.4) even though the bounds for the operational variables and tuning parameters for the optimisation algorithms are the same. Three new optimisation runs for each case study are carried out as reported in Appendix B, Table B3 for Case 4.1 and Table B10 for Case 4.2.

As can be seen from Figures 4.10 and 4.11, the lowest value for the hot utility demand corresponds to the case when an artificial neural network model is introduced to an optimisation framework where a genetic algorithm is employed; confirming its effectiveness in handling a variety of operational and structural variables.

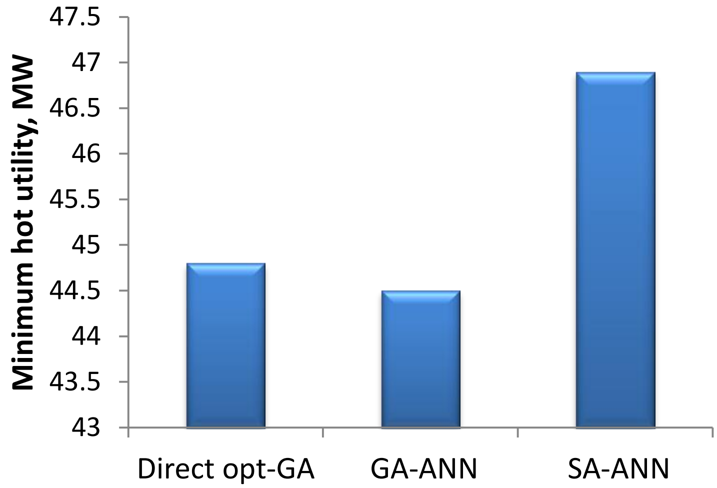

Figure 4.10 Optimisation results summary, Case 4.1 (no preflash).

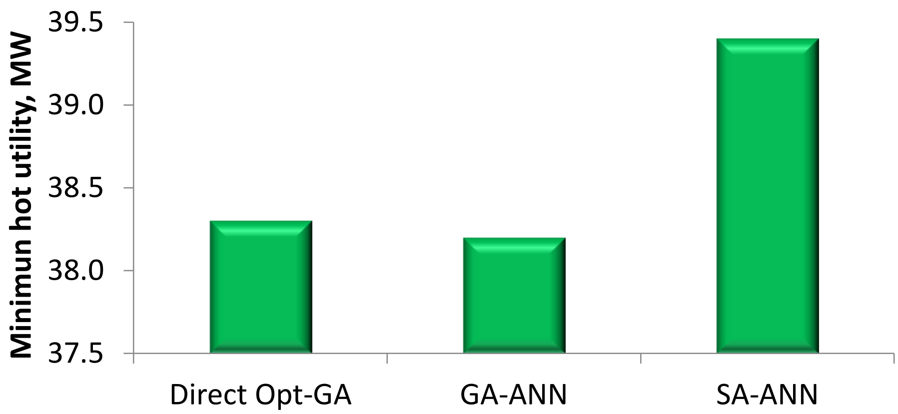

Figure 4.11 Optimisation results summary, Case 4.2 (with preflash).

The overall CPU time required for the complete simulation-optimisation process was around 1.6h for both case studies. Specifically, for case study 4.1 generation of samples took 0.5s, sampling (via rigorous simulations) 1.6h, model construction and validation 5min, and system optimisation 77s for the case using a genetic algorithm, and 41s when a simulating annealing algorithm is selected. For case study 4.2, generation of samples took 0.6s, sampling 1.6h, optimisation time using a genetic algorithm 103s and 118s using simulated annealing. Therefore, a considerable reduction of CPU time (74% for case study 4.2 and 62% for case study 4.1) compared with the direct simulation-optimisation approach presented in Chapter 3, is obtained following the proposed approach in this Chapter.

The next Chapter will introduce a novel optimisation-based design methodology for optimising fired heating demand which could lead to further energy savings within the crude oil distillation system.

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Chapter 5

Optimisation-based Design of Fired Heating Demand in Crude Oil Distillation Systems

5.1 Introduction

Petroleum refineries are increasingly required to address stringent environmental regulations. This incentivises the reduction of the use of primary energy, and hence reduced the generation of greenhouse gas emissions (mainly CO_2) and other combustion gases, such as NO_x and SO_x, which are harmful to the environment. Furthermore, given the energy-intensive nature of crude oil refining, even small improvements in the use of primary energy can yield considerable savings and environmental benefits.

Research on crude oil distillation systems has generally focused on minimum hot utility demand, without considering details of the type and quality of the hot utility. Focusing on the minimum hot utility demand is rather simplistic, as it does not recognise that the source of heat of interest is fired heating so that the figures related to the minimum hot utility demand (Q_{Hmin}) does not give completely useful information about the demand for fired heating, because the amount of fuel combusted depends on the demand for fired heating and also the amount of heat that can be recovered from the combustion gases. In particular, the temperature at which the gases leave the stack (T_{stack}), affect the amount of fuel that is consumed. Therefore, a deeper analysis is required; yet for optimisation purposes, the simplicity of pinch analysis is appealing, because it quickly and simply allows the impact of process changes on utility demand to be determined. To date, the literature search has not revealed any studies that consider both the efficiency of the fired heater (ratio of heat to process and heat released by fuel) and design or operation of the crude oil distillation column. This Chapter extends the methodology presented in Chapters 3 and 4 to account for the efficiency of the fired heater.

5.2 Role of fired heating in crude oil distillation

Petroleum refineries typically use a furnace to pre-heat crude oil before it enters the atmospheric distillation unit. The heat input is provided by burning fuel, usually oil or gas. The pre-heat train (heat recovery system) aims to minimise the demand for hot utility – i.e. fired heating, bringing benefits in terms of the demand for fuel, and the associated fuel cost and emissions (Mahmoud and Sunarso, 2018).

Approximately 75% of energy consumption in refineries is used by furnaces and heaters. Furnace efficiency can be affected by ambient air conditions (i.e. pressure and temperature) and operating conditions such as combustion air preheating and the use of excess air for combustion (Masoumi and Izakmenri, 2011).

Operating furnaces efficiently is a major operating concern in any refinery due to two-thirds of a plant fuel budget is needed for furnace fuel cost. Furthermore, furnace efficiency is directly linked to environmental regulations that stipulate a clean operation of the whole plant (Salih, 2018).

Taking into account the following considerations:

1) Fired heaters are inherently inefficient.
2) Crude oil distillation processes have many degrees of freedom for design (and for operation and retrofit).
3) Results presented in Chapters 3 and 4, have shown that optimisation can be effective for achieving the required separations in the atmospheric distillation units, while also maximising the opportunities for heat recovery.
4) No studies are known to have accounted for the effect of the process design variables on the performance (efficiency) of the fired heater.

The aim of this Chapter is to develop a new optimisation-based design methodology to reduce the fuel consumption in the furnace, while simultaneously optimising operational and structural variables of a crude oil distillation system with a preflash unit, accounting for product quality, product yield and heat integration.

5.3 Optimisation based-design of fired heating demand

The simulation-optimisation framework developed in this work is extended to minimise fuel consumption by the fired heater. Continuing with the case studies that have been presented in Chapters 3 and 4, two configurations of the atmospheric distillation unit are studied, with and without a preflash unit.

The design of the atmospheric distillation column is fixed and the initial operating conditions are exactly the same as those used in case studies presented in Chapters 3 and 4, (pump-around duties and temperature drops, flow rates of stripping steam to the main column and side-strippers, column inlet temperature, reflux ratio and preflash temperature). Product quality specifications are expressed in terms of product boiling ranges (T5% and

T95%, which are related to boiling point temperatures when 5% and 95% of the mixture has vaporised using a standard test e.g. ASTM D86). Additionally, a product quantity constraint (residue flow rate) is added within the optimisation framework to ensure that the sum of the flow rates of all other products is maintained. The flow rates of the individual products may change, as long as the product specifications are met.

The crude oil distillation system is modelled in Aspen HYSYS v8.8. Initially, the flowsheet is modelled for the case without a preflash unit. In the case of including a preflash unit, the destination of the flashed vapour is an important degree of freedom. The model also represents process operating conditions such as pump-around duties and temperature drops, stripping steam flow rates, column feed temperature, and reflux ratio (Ledezma-Martínez et al., 2018).

Pinch analysis is applied to evaluate the minimum fuel consumption of the fired heater, using the grand composite curve. However, it is important to point out that: 1) the heat exchanger network design is not considered in any detail, 2) the minimum approach temperature is assumed to be the same in all heat exchangers, 30ºC.

Main considerations for system optimisation are:

1) After extracting the stream data needed to generate the grand composite curve, it is systematically evaluated to identify the flue gas line that satisfies all the constraints (i.e. when the stack temperature is higher than the dew point temperature).

2) The slope of the flue gas line is minimised and it must not “cut” the grand composite curve.

3) Total fuel demand is calculated in terms of energy content to allow this to be calculated in the objective function.

Following the approach presented in Chapter 4, and based on the results obtained for the lowest minimum hot utility demand, two optimisation techniques are evaluated to compare their performance in terms of optimisation time and objective function value: (a) direct optimisation using genetic algorithms (GA), and (b) surrogate models using artificial neural networks (ANN).

The optimisation-based design methodology accounting for the demand for fired heating is illustrated through its application to cases studies: a crude oil distillation system with and without a preflash unit; results are compared to those of optimisation studies considering only the minimum hot utility demand.

5.3.1. Optimisation framework using direct optimisation

The crude oil distillation system (with and without a preflash unit) that is considered for optimisation in this Section is the same as that presented in Chapter 4 (See Figures 4.4 and 4.7). The operating conditions of the unoptimised base case are also the same as those used to perform the direct optimisation in the previous Chapter (See Tables 4.3 and 4.9).

The purpose of the optimisation is to minimise the demand for fuel consumption in the furnace. It is calculated by the sum of the minimum hot utility (Q_{Hmin}) plus the amount of heat loss to the ambient by the system, called stack loss (Smith, 2016, Ch. 17).

There are 10 optimisation variables for the case without a preflash unit and 12 optimisation variables for the case with a preflash unit as previously discussed in Chapters 3 and 4.

Starting with a set of operating conditions for the crude oil distillation system, rigorous simulations are carried out in HYSYS v8.8 via a MATLAB interface. The interface is embedded within the optimisation framework. The optimisation algorithm selects process variables values, simulates the corresponding flowsheet (with and without preflash unit), evaluates its fuel consumption and then selects a new set of inputs until the stopping criterion is met.

A genetic algorithm (GA) is selected to perform the direct optimisation due to it showed a better performance compared with the simulated annealing as discussed in Chapter 4. Tuning parameters required by the genetic algorithm are population size, number of generations, and termination criteria. Product and flow rate constraints are defined as in Chapters 3 and 4.

The simulation-optimisation framework developed in this work in Chapter 3 is extended to minimise fuel consumption by the fired heater using direct optimisation, as summarised in Figure 5.1. The algorithm coded in MATLAB for calculating the fuel consumption in the fired heater is explained in detail in Chapter 2, Section 2.9.4.

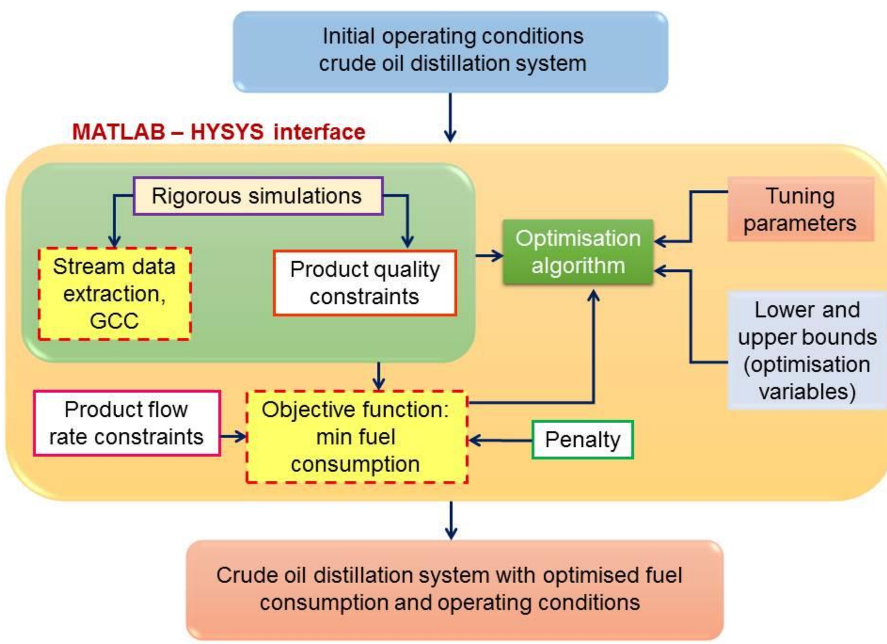

Figure 5.1 Direct optimisation framework, minimising fuel consumption.

It is important to remark that during the optimisation process, the shape of the grand composite curve will be changing on each iteration, one of the strengths of the proposed approach is that the algorithm developed in MATLAB is capable to identify the minimum slope for the flue gas line which represents the minimum amount of heat released to the ambient (stack loss). The algorithm also identifies the sign of the heat capacity flow rate which is related to the surplus-demand of energy within the system; as a result, the algorithm systematically evaluates both the minimum hot utility demand (Q_{Hmin}) and the minimum fuel consumption (Q_{fuel}) of the crude oil distillation system without the need to look at the shape of the grand composite curve.

The capabilities of the proposed simulation-optimisation-based design methodology are illustrated in the following Section as a case study.

5.4 Case study

The case study presented in this Chapter includes two different flowsheets for a crude oil distillation system with and without a preflash unit as has been presented in Chapters 3 and 4. A preliminary analysis is carried out for each flowsheet without performing optimisation of the system to evaluate the base case for each alternative, calculating their minimum hot utility, fired heating demand and heat released to the ambient which will be referred as stack loss.

Then, direct simulation-optimisation is carried out for each flowsheet, with and without a preflash unit. Optimisation results are compared with those obtained for the case of optimising minimum hot utility only, reported in Chapter 4 in order to gain some insight about the performance of the system and the importance to take into account stack losses for the evaluation of the complete fuel consumption.

5.4.1. Crude oil distillation system without a preflash unit

The standard configuration found in most refineries around the world is the atmospheric crude oil distillation column with side-strippers and pump-arounds as shown in Figure 5.2. Reboilers and steam are used for vapour generation (Gadalla, 2003).

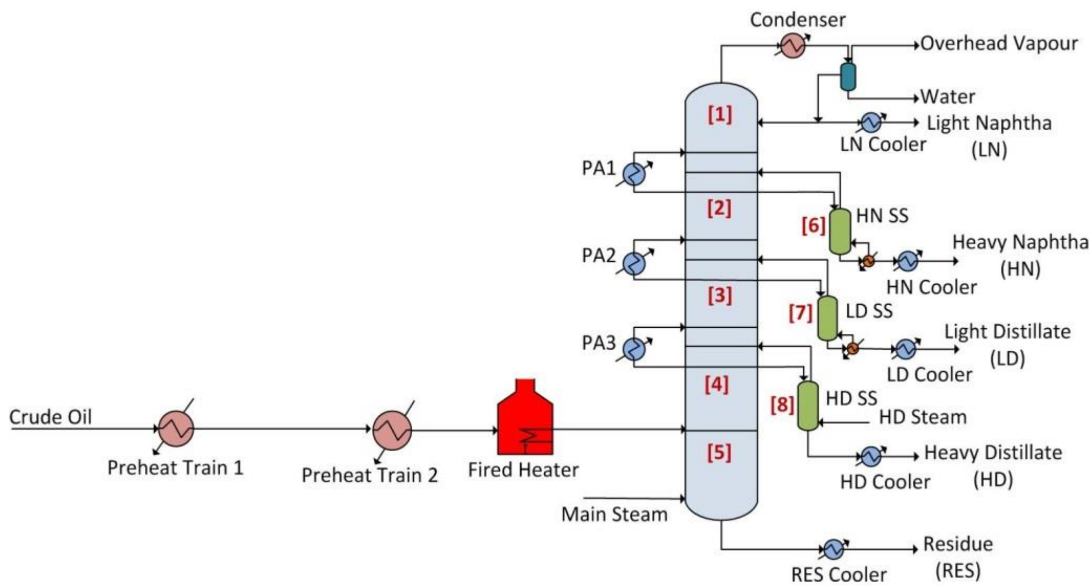

Figure 5.2 Crude oil distillation system.

The grand composite curve shown in Figure 5.3 corresponds to the base case for a crude oil distillation system without a preflash unit (See Figure 5.2). It can be seen that the flue gas line touches the grand composite curve (GCC) at the process pinch point so that there is a process pinch limitation within the system. Dew point temperature limitation is at 160°C.

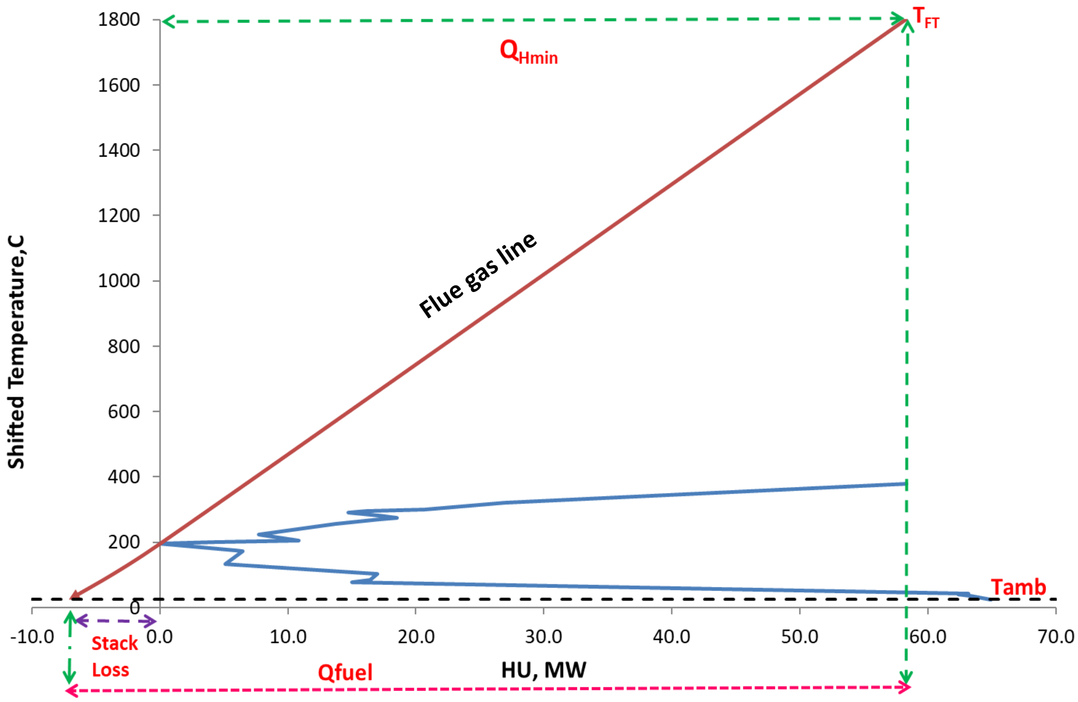

Figure 5.3 Grand composite curve base case: no preflash.

Initial calculations obtained from the MATLAB subroutine for the minimum hot utility demand (Q_{Hmin}), amount of heat loss (stack loss) and total fuel consumption (Q_{fuel}) respectively are 58.3 MW, 7.1 MW and 65.4 MW. These results are summarised in Table 5.1 together with the optimisation results for the cases of optimising minimum hot utility demand only, and optimising fired heating demand. Table 5.2 summarises values obtained after optimisation for the degrees of freedom of the system.

Optimisation results no preflash case

Table 5.1. Summary optimisation results: no preflash

	Base Case	Optimising Hot Utility	Optimising Fired Heating
Hot Utility, MW	58.3	44.8	45.7
Cold Utility, MW	64.9	57.6	58.3
Stack Loss, MW	7.1	8.1	6.0
Fired Heating, MW	65.4	53.0	51.7
CPU Time, h		4.1	4.2

As can be seen from Table 5.1, fired heating demand of the crude oil distillation system decreases from 53.0 to 51.7 MW when the objective function is to minimise it. This trend confirms that when the objective function focuses only on minimising hot utility demand, the information about energy consumption of the system is not complete; fired heating in the furnace is not reduced as a result of the high value for the stack loss. Even though the hot utility has an increase of 1.9%, the stack loss is 2.1 MW less than for the case when only the hot utility is optimised. Consequently, there is a reduction in the flue gas emissions to the ambient.

From Table 5.2, it can be seen that compared with the base case, pump-around duties 1 and 2 decreased, while pump-around duty 3 increases for both cases, optimising hot utility and fired heating. As a result, pump-around temperature drop 3 also increases, reducing the vapour traffic around the pump-around 3 due to more condensation.

Higher values for the column inlet temperature are desired as it creates more opportunities for heat recovery within the system, it also requires less stripping steam as it is shown for the case when the objective is to minimise fired heating, even one degree of temperature difference may lead to energy savings.

The high value of 4.2 for the reflux ratio when the minimum hot utility is to be optimised implies that the column condenser duty will also increase.

Table 5.2. Optimisation variables and results, direct optimisation no preflash case

		Direct simulation-optimisation	
	Base Case	**Minimising HU**	**Minimising Fired Heating**
PA1 Duty, MW	12.84	6.4	10.0
PA2 Duty, MW	17.89	9.2	8.5
PA3 Duty, MW	11.20	14.0	13.7
ΔT PA1, ºC	30	20.2	22.3
ΔT PA2, ºC	50	28.1	29.4
ΔT PA3, ºC	20	33.3	39.9
Main Steam, kmol h^{-1}	1200	1700	1620
HD Steam, kmol h^{-1}	250	200	264
Reflux Ratio	4.17	4.2	3.9
Column inlet temperature, ºC	365	350	351

PA: pump-around
ΔT: pump-around temperature drop

Figure 5.4, shows the grand composite curve obtained with data after optimisation of fired heating is performed. Its corresponding flue gas line profile starts from the theoretical flame temperature (1800ºC) to the ambient temperature (T_{amb}), 25ºC.

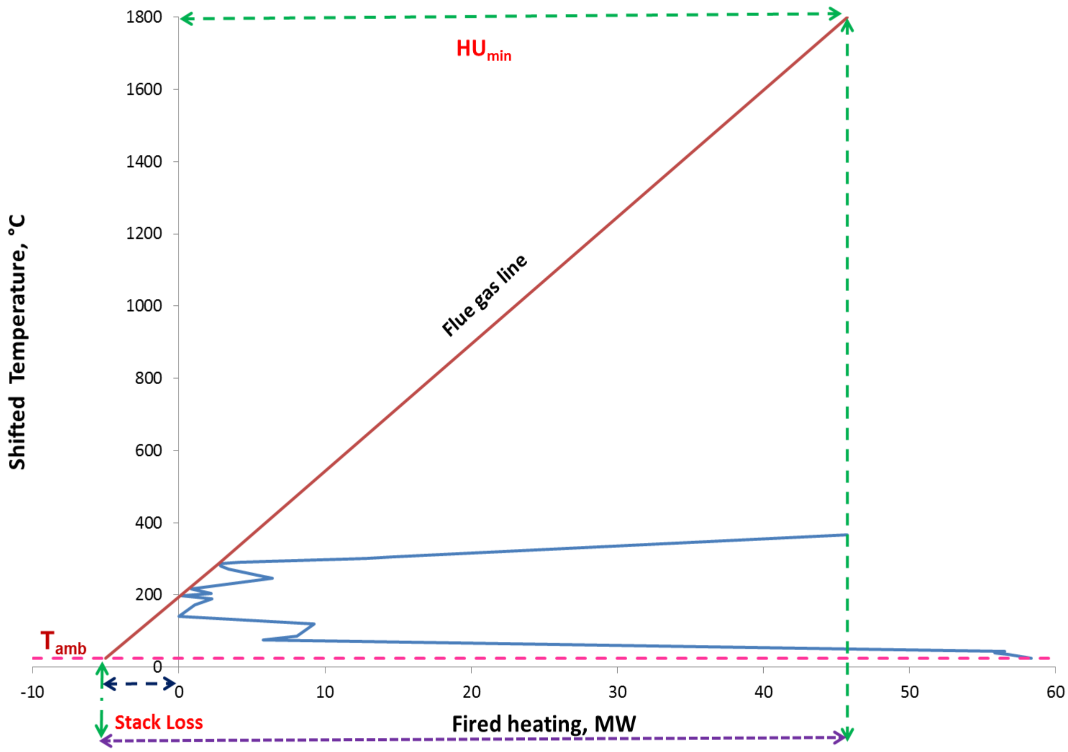

Figure 5.4 Grand composite curve, best result with direct optimisation: no preflash case.

From Figure 5.4, it may be seen that the flue gas line touches the grand composite curve three times (heat recovery pockets), the first point is of interest due to matching the flue gas line with the grand composite curve at this point ensures that it will not be crossing the curve; it also limits the slope of the flue gas line and hence the stack loss.

5.4.2. Crude oil distillation system with a preflash unit

Energy consumption of a crude oil distillation system can be reduced by installing a preflash unit as shown in Figure 5.5. As discussed in Chapter 3, there are five locations (one per column section) in which the vapour leaving the flash can be introduced in the main column; in the base case, the flashed vapour is introduced at the column feed stage at the bottom of the column so that it is mixed with the hot crude oil leaving the furnace. Column structure is the same as that presented in Chapters 3 and 4.

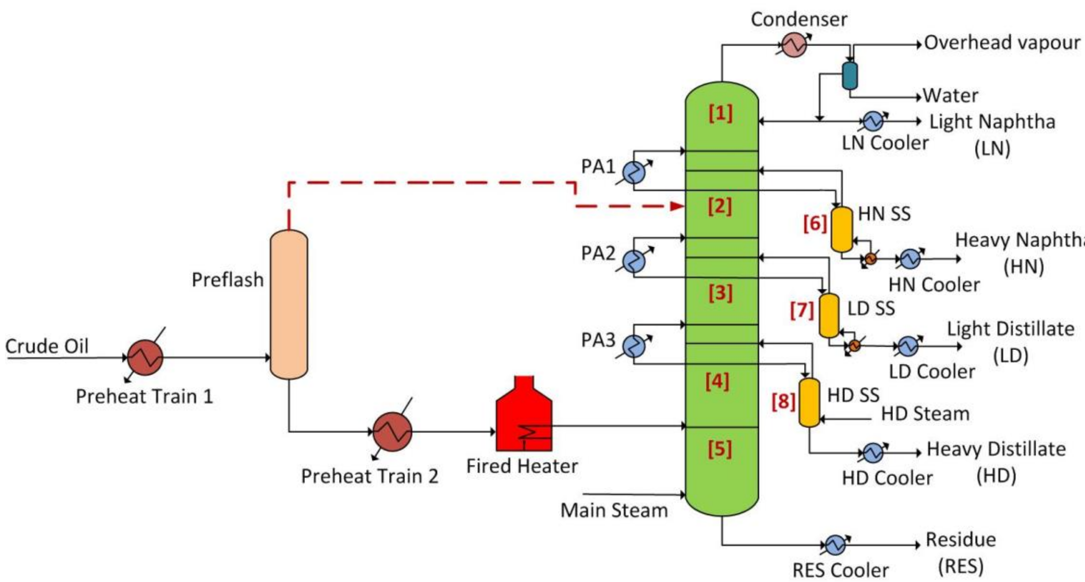

Figure 5.5 Crude oil distillation system with a preflash unit.

Figure 5.6 shows the grand composite curve obtained for the base case (without performing optimisation). In this case, the stack temperature (the temperature at which the flue gas leaves the furnace) is limited by a process utility pinch.

Total fuel consumption for the base case of a crude oil distillation system with a preflash unit is 64.1 MW, minimum hot utility demand is 57.7 MW with a stack loss of 6.4 MW. All values are lower than those for the base case without a preflash unit, confirming that adding a preflash unit to the crude oil distillation system can help to reduce energy consumption within the system.

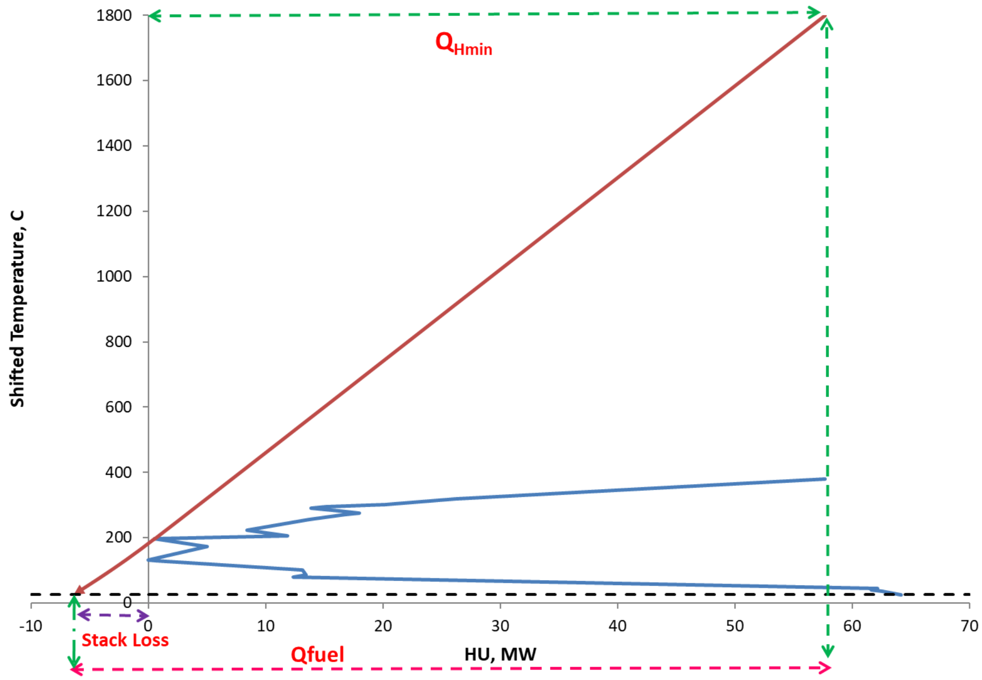

Figure 5.6 Crude oil distillation system with a preflash unit (base case).

Optimisation results

Tables 5.3 and 5.4 show results and degrees of freedom for the optimisation of the fired heating of the system with a preflash unit using a direct simulation-optimisation approach; they are compared with optimisation results when the objective is to minimise hot utility demand as presented in Chapter 4.

Table 5.3. Summary direct optimisation results: preflash case

	Base Case	Optimising Hot Utility	Optimising Fired Heating
Hot Utility, MW	57.7	38.1	41.4
Cold Utility, MW	64.1	44.6	53.6
Stack Loss, MW	6.4	7.3	3.5
Fired Heating, MW	64.1	45.4	44.9
CPU time, h		6.2	6.7

From Table 5.3, it may be seen that energy savings on hot utility demand of 15% are obtained after adding a preflash unit to the crude oil distillation system based on optimisation results for the case without a preflash unit (44.8 MW). On the other hand, stack loss decreased in 3.8 MW when optimising fired heating, reducing the amount of heat escaping to the ambient unutilised.

Fired heating demand decreased 0.5 MW compared with its value when the objective is minimising hot utility demand only; however, taking into account that fired heaters are major consumers of energy in a refinery, even smallest efficiency improvements on it can bring economic benefits.

Table 5.4. Optimisation results crude oil distillation system with a preflash

		Direct simulation-optimisation	
	Base Case	**Minimising HU**	**Minimising Fired Heating**
PA1 Duty, MW	12.84	8.2	6.6
PA2 Duty, MW	17.89	9.8	6.9
PA3 Duty, MW	11.20	12.6	8.3
ΔT PA1, ºC	30	41.1	39.4
ΔT PA2, ºC	50	34.1	26.5
ΔT PA3, ºC	20	21.4	20.1
Main Steam, kmol h^{-1}	1200	1269	1672
HD Steam, kmol h^{-1}	250	180	182
Reflux Ratio	4.17	3.1	4.1
Column inlet temperature, ºC	365	381	370
Flash temperature, ºC	115	240	240
Vapour feed location (column section)	5	3	3

PA: pump-around

ΔT: pump-around temperature drop

As shown in Table 5.4, column inlet temperatures increased compared with those presented in Table 5.2 for the case without a preflash unit. When a preflash is added to the crude oil distillation system, the crude oil needs to be heated to a higher temperature to allow more vaporisation within the column. Column inlet temperature is decreased 11 °C when fired heating is optimised which is related to an increase of the steam flow rate compared with the case when hot utility is optimised. Reflux ratio also increases, from 3.1 to 4.1 improving the separation within the column as there is more liquid returning to the column that cools and condensate the vapour up flowing.

Figure 5.7 shows the grand composite curve obtained after fired heating optimisation for this case.

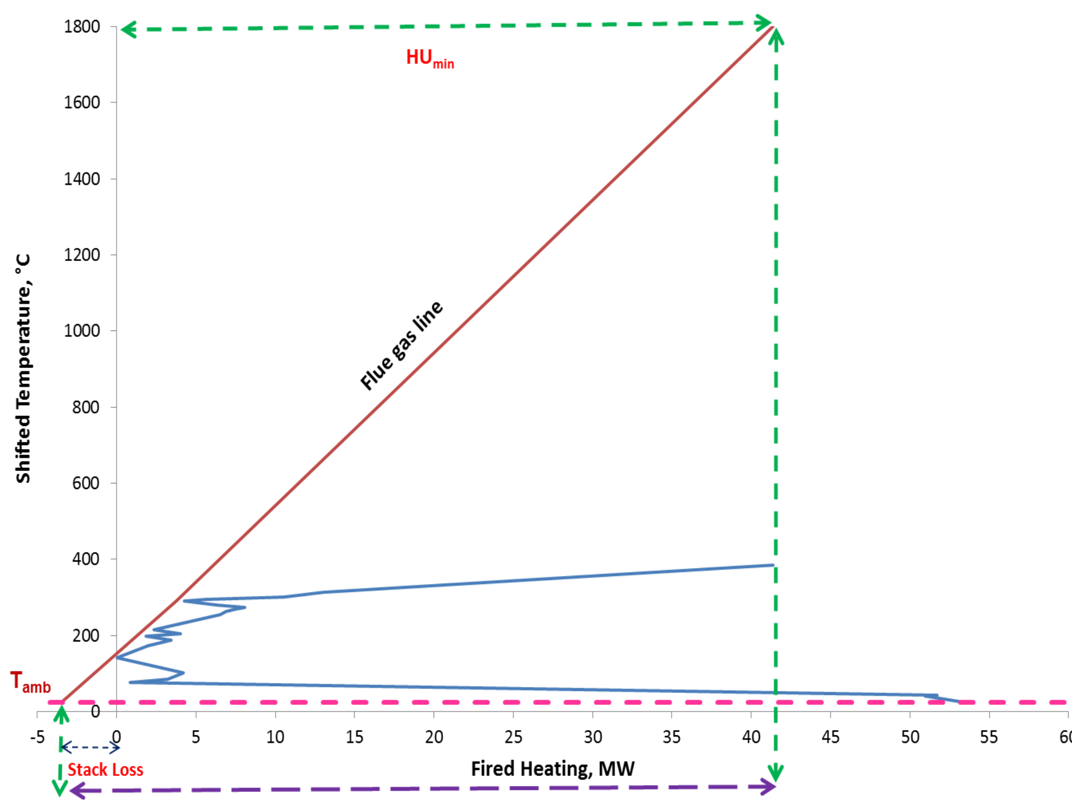

Figure 5.7 Grand composite curve, best direct optimisation result: preflash case.

5.5 Optimisation framework using artificial neural networks

Optimisation of crude oil distillation systems using artificial neural networks is attracting significant research interest due to their facility to be implemented in an optimisation framework to determine the best configuration and operating conditions. Artificial Neural Networks (ANN) have been recognised as a powerful tool for highly nonlinear systems due to its ability to learn complex functional relations, linking input and output data of the system (Osuolale and Zhang, 2016). Moreover, their evaluation is considerably less computationally demanding compared with direct optimisation as presented in Chapter 4 so that they represent a suitable option for optimisation-based design applications.

The methodology developed in this work is extended using a combination of a genetic algorithm and artificial neural networks in the same optimisation framework, to evaluate total fuel consumption in a crude oil distillation system with and without a preflash unit as illustrated in Figure 5.8.

As discussed in Chapter 4, the first step to build an ANN model is to generate samples via rigorous simulations; they are classified into converged and unconverged but only those which lead to a converged simulation in Aspen HYSYS are used to build the ANN model.

The optimisation based-design framework takes into account product and residue flow rate constraints as well as lower and upper bounds for the optimisation variables (10 for the case without a preflash unit and 12 for the case with a preflash unit). A genetic algorithm is used to perform the optimisation in MATLAB R2016a; tuning parameters are population size and number of generations.

The stream data needed to build the grand composite curve is taken from the outputs of the ANN model, as it was explained in Chapter 4. Here, the algorithm (see Section 2.7.5) developed in MATLAB to allow stack loss evaluations is implemented within the optimisation framework in order to evaluate the objective function: minimise fired heating demand of the crude oil distillation system.

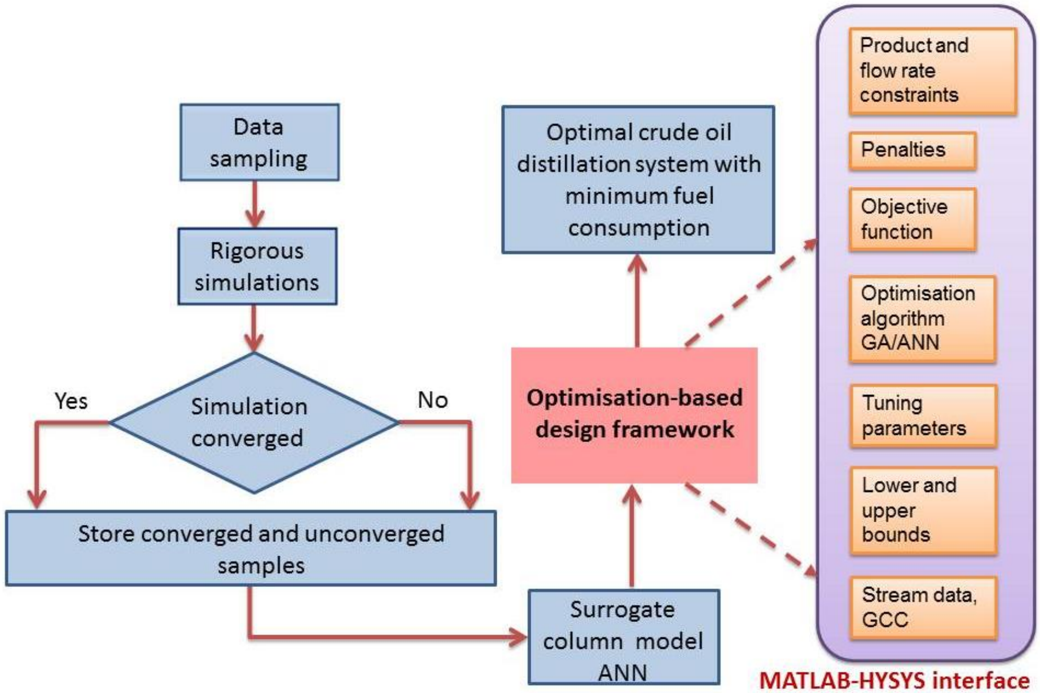

Figure 5.8 Optimisation framework using artificial neural networks.

5.5.1. Crude oil distillation system without a preflash unit

Tables 5.5 and 5.6 summarise optimisation results when optimising both hot utility and fired heating demand in a crude oil distillation system without a preflash unit.

Table 5.5. Summary optimisation results using ANN: no preflash case

	Base Case	**Optimising HU**	**Optimising Fired Heating**
Hot Utility, MW	58.3	44.5	46.5
Cold Utility, MW	64.9	56.1	59.2
Stack Loss, MW	7.1	8.1	5.0
Fired Heating, MW	65.4	52.5	51.5
CPU time,s		96	1395

HU: Hot Utility

Introducing artificial neural networks within the optimisation framework notable reduce the optimisation time required passing from hours as in the direct optimisation to seconds. Fired heating demand decreased in 1 MW when the objective function is to minimise fired heating, while the hot utility demand of the system increased 2 MW. Same trend as it was observed in the previous Section when direct optimisation is applied, confirming the relevance to take into account the complete fuel consumption of the system for a better understanding.

Stack losses are reduced by 3.1 MW so there are more opportunities for heat recovery within the system.

Table 5.6. Degrees of freedom crude oil distillation system without a preflash unit

			GA-ANN optimisation
	Base Case	**Minimising HU**	**Minimising Fired Heating**
PA1 Duty, MW	12.84	6.0	8.6
PA2 Duty, MW	17.89	9.4	8.0
PA3 Duty, MW	11.20	14.0	13.0
ΔT PA1, ºC	30	20.0	20.0
ΔT PA2, ºC	50	29.6	28.8
ΔT PA3, ºC	20	40.0	40.0
Main Steam, kmol h^{-1}	1200	1607	1713
HD Steam, kmol h^{-1}	250	209	188
Reflux Ratio	4.17	4.1	4.1
Column inlet temperature, ºC	365	350	350

PA: pump-around
ΔT: pump-around temperature drop
HU: Hot Utility

It can be seen from Table 5.6 that column inlet temperature is maintained for both optimisation cases; however, the main steam required increased when minimising fired heating improving heat recovery opportunities, as there is mayor liquid and vapour traffic in the column. Pump-around duty 3 increased for both optimisation cases rejecting heat at higher temperatures, thus allowing more heat to be recovered in the heat recovery system.

Figure 5.9 shows the grand composite curve for the best result using artificial neural networks after optimisation is carried out, the flue gas line is limited by a match between process and utility.

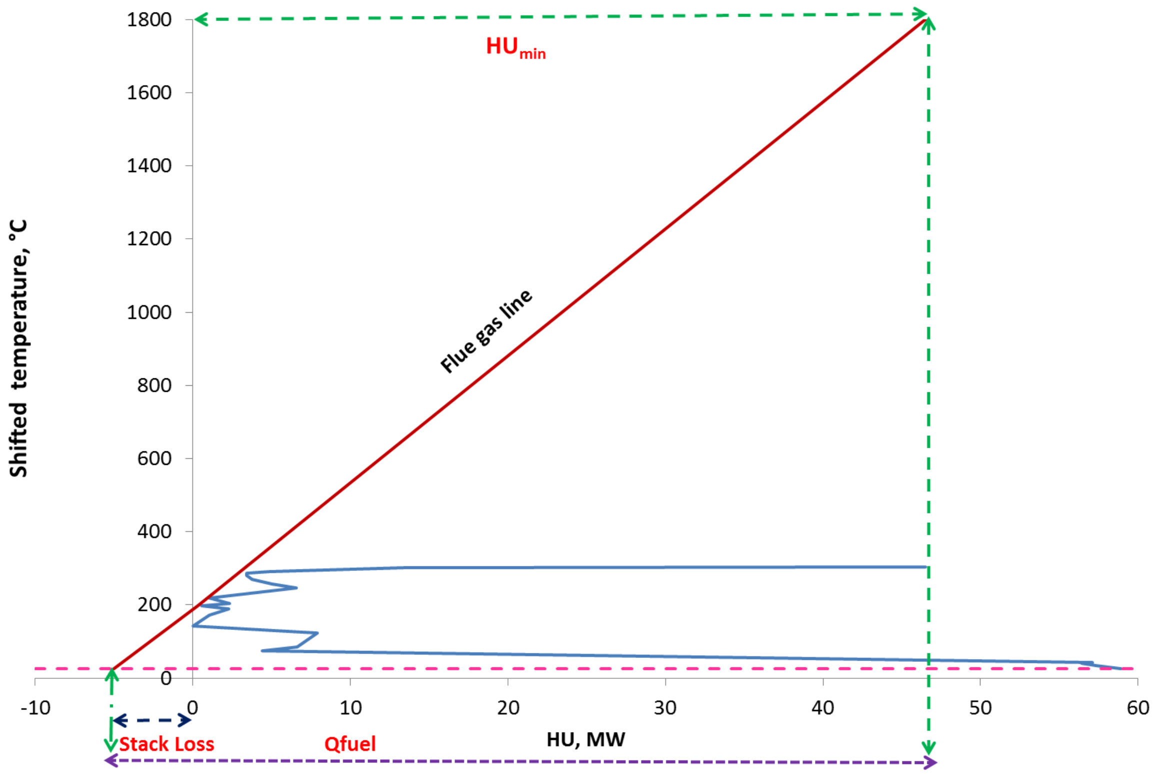

Figure 5.9 Grand composite curve, best optimisation result using ANN: no preflash.

5.5.2. Crude oil distillation system with a preflash unit

Optimisation results

Table 5.7 summarises optimisation results when optimising both hot utility and fired heating demand in a crude oil distillation system with a preflash unit.

Table 5.7. Summary optimisation results using ANN: preflash case

	Base Case	Optimising HU	Optimising Fired Heating
Hot Utility, MW	57.7	38.2	40.8
Cold Utility, MW	64.1	52.5	49.1
Stack Loss, MW	6.4	7.4	3.7
Fired Heating, MW	64.1	47.9	44.5
CPU time,s		103	1379

HU: Hot Utility

Even though the CPU time to perform the optimisation increased, it can be seen from Table 5.7 that again, fired heating demand is reduced when it is optimised, due to the stack loss is reduced in 50% compared with the stack loss calculated for the case when only the hot utility demand is optimised.

Table 5.8 summarises best optimisation results for the degrees of freedom as a result of the optimisation of both hot utility and fired heating demand using artificial neural networks. As can be seen, flash temperature is almost the same for both optimisation cases; reflux ratio is maintained and column inlet temperature increased in 13°C when the objective is to minimise fired heating demand, leading to a reduction in the main steam flow rate. Pump-around duties 1 and 2 were reduced from the base case values in both optimisation cases increasing heat recovery opportunities.

Table 5.8. Optimisation variables: best results optimising with ANN, preflash case

		GA – ANN optimisation	
	Base Case	**Minimising HU**	**Minimising Fired Heating**
PA1 Duty, MW	12.84	6.8	7.8
PA2 Duty, MW	17.89	8.1	6.6
PA3 Duty, MW	11.20	10.5	11.3
ΔT PA1, ºC	30	29.8	30.4
ΔT PA2, ºC	50	30.2	27.5
ΔT PA3, ºC	20	39.3	15.6
Main Steam, kmol h^{-1}	1200	1684	1317
HD Steam, kmol h^{-1}	250	193	264
Reflux Ratio	4.17	3.8	3.8
Column inlet temperature, ºC	365	367	380
Flash temperature, ºC	115	235	236
Vapour feed location (column section)	5	3	3

PA: pump-around
ΔT: pump-around temperature drop
HU: Hot Utility

Figure 5.10 illustrates the best optimisation result using artificial neural networks for the case of adding a preflash unit to a crude oil distillation system. In this case, the flue gas line is limited by a match between process and utility.

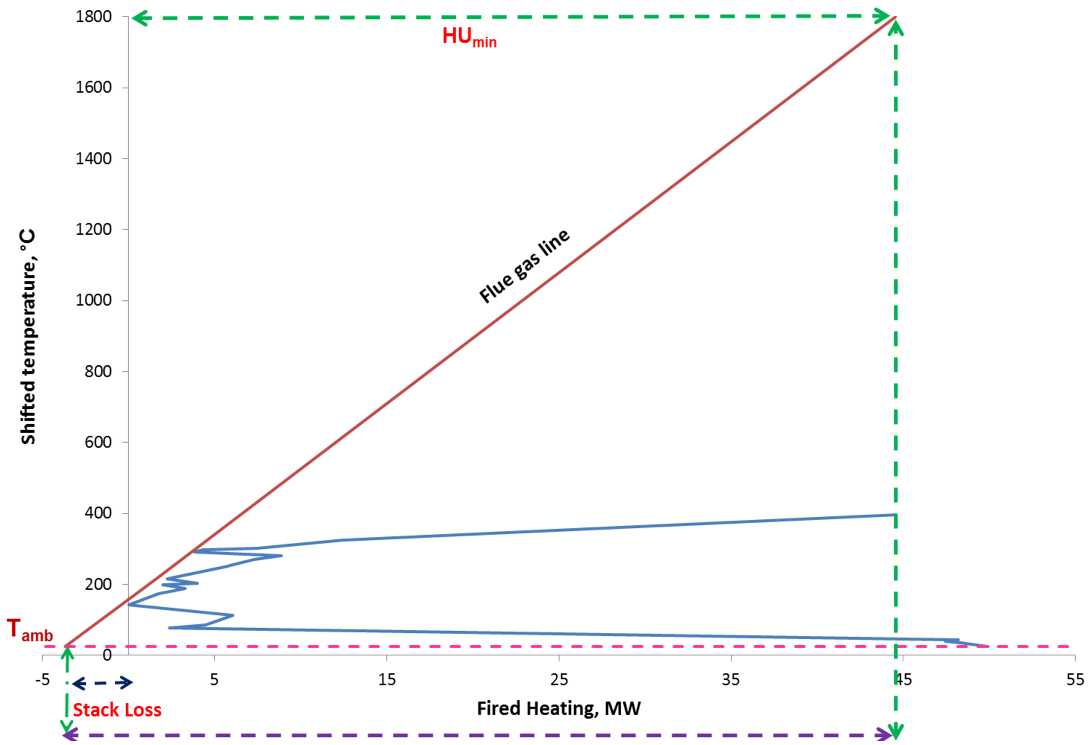

Figure 5.10 Grand composite curve for the best optimisation result using ANN.

5.6 Case study summary

The case study presented in this Chapter demonstrates the capabilities of the methodology developed in this work, extending the scope for the optimisation of fired heating demand applied to a crude oil distillation system with and without a preflash unit. Two optimisation approaches are compared, direct simulation-optimisation and optimisation using artificial neural network models into an optimisation framework with a genetic algorithm.

Tables 5.9 and 5.10 summarise optimisation results for both optimising minimum hot utility demand and optimising fired heating demand. CPU time was notably reduced when using artificial networks models (Tables report the total optimisation time counting data sampling, model training and optimisation).

Direct optimisation of fired heating in a crude oil distillation system without a preflash unit reduced fired heating demand in 1.3 MW (53.0 - 51.7 MW) compared with the case when only hot utility demand is optimised. Similarly, 1 MW (52.5 – 51.5 MW) less was obtained using artificial neural networks. For the preflash case, reductions of 0.5 MW and 3.4 MW of fired heating demand are obtained for the cases when only hot utility is optimised and when fired heating is optimised.

Table 5.9. Optimisation results summary: minimising hot utility demand

	CDU			**Preflash**		
	Base Case	**Direct Opt**	**ANN Model**	**Base Case**	**Direct Opt**	**ANN Model**
HU, MW	58.3	44.8	44.5	57.7	38.1	38.2
CU, MW	64.9	57.6	56.1	64.1	44.6	52.5
Stack loss, MW	7.1	8.1	8.1	6.4	7.3	7.4
Fired heating, MW	65.4	53.0	52.5	64.1	45.4	47.9
CPU time, h		4.1	1.6		6.2	1.6

HU: Hot Utility
CU: Cold Utility
CDU: Crude Distillation Unit

Table 5.10. Optimisation results summary: minimising fired heating demand

	CDU			Preflash		
	Base Case	**Direct Opt**	**ANN Model**	**Base Case**	**Direct Opt**	**ANN Model**
HU, MW	58.3	45.7	46.5	57.7	41.4	40.8
CU, MW	64.9	58.3	59.2	64.1	53.6	49.1
Stack loss, MW	7.1	6.0	5.0	6.4	3.5	3.7
Fired heating, MW	65.4	51.7	51.5	64.1	44.9	44.5
CPU time, h		4.2	1.6		6.7	1.6

HU: Hot Utility
CU: Cold Utility
CDU: Crude Distillation Unit

Figures 5.11 and 5.12 illustrate the optimisation performance of the two approaches presented in this Chapter, direct optimisation (DO) and artificial neural networks (ANN) for the cases without and with a preflash unit respectively. It may be seen from Figure 5.11 that the lowest value for minimum fired heating demand is obtained by direct optimisation; in contrast, optimisation using artificial neural networks provides the lowest value when the objective function is to minimise hot utility demand. However, differences in the lowest values between the two approaches are no greater than 2 MW confirming the accuracy of them.

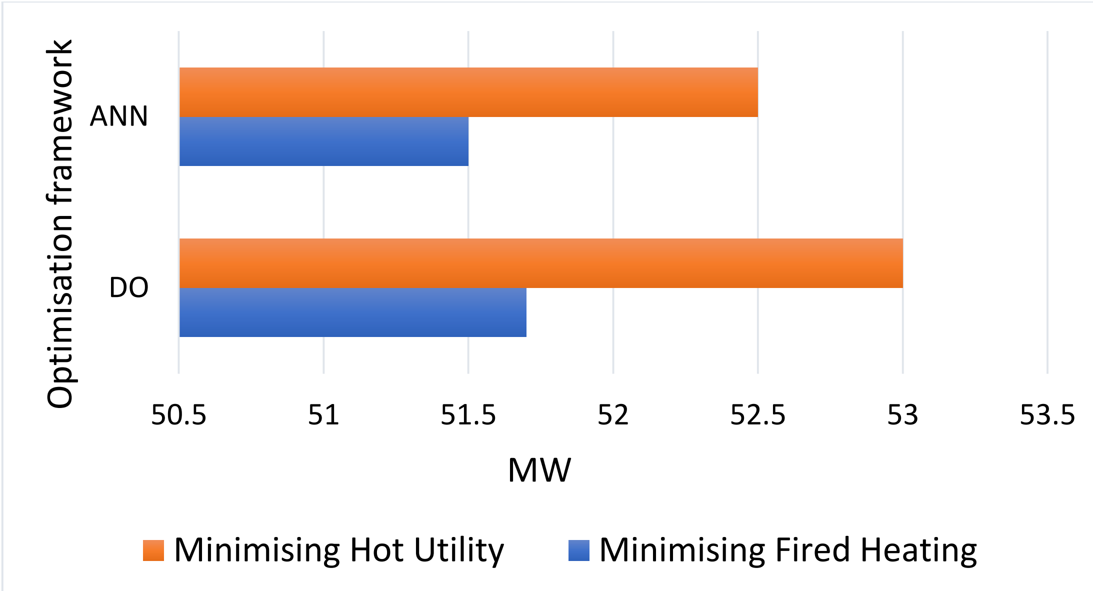

Figure 5.11 Fired heating optimisation performance no preflash case.

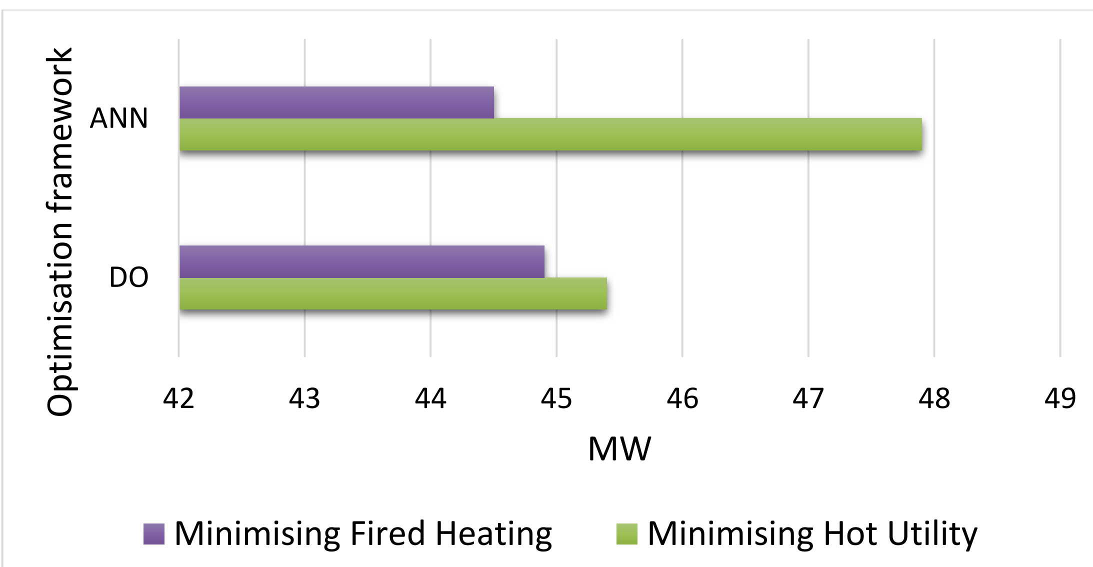

Figure 5.12 Fired heating optimisation performance preflash case.

Figure 5.12 shows the optimisation performance for the case of a crude oil distillation system with a preflash unit. In the case of optimising fired heating, optimisation using artificial neural networks performed better than the direct optimisation approach; while the lowest value when minimising, hot utility is obtained via direct optimisation (See Appendix C for details about optimisation runs).

These results confirm the importance to include calculations regarding to the fired heating demand within an optimisation framework in order to have more realistic results about the about heat recovery opportunities of a crude oil distillation system.

5.7 Conclusions

A systematic design optimisation approach to minimise fired heating demand is proposed for crude oil distillation systems with and without a preflash unit, applying rigorous and artificial neural network models. The methodology accounts for industrially relevant constraints related to product quality and yield.

The case study presented in this Chapter confirms that 1) introducing a preflash unit within a heat-integrated crude oil distillation system bring significant improvements in both hot and fired heating demand, 2) minimising fired heating demand of the system offers a better understanding about the amount of fuel combusted, hence improving opportunities for heat integration in the system. Additionally, impact to the ambient due to stack losses is minimised.

Limitations of the proposed design methodology are that the number of trays in the main column is keep fixed. Future work will have to take into account column design together with different objective functions accounting for capital and energy costs.

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Chapter 6

Overall Summary

This Chapter summarises and link results from case studies presented in Chapters 3, 4 and 5. The base case in each case study (with and without a preflash unit) is outlined, comparing best optimised designs.

In Chapter 3, direct simulation-optimisation of a crude oil distillation system with and without a preflash unit is presented. In the first case study (Case 3.1), main column structure fixed. It is divided into two parts: Case 1, comprise constraints related to product quality only while Case 2, include constraints on both product quality and product flow rates (residue). In the second case study (Case 3.2) the design of the main column is optimised together with the operating conditions of the corresponding flowsheet maintaining constraints in product quality for the residue.

Chapter 4 extends the methodology developed in Chapter 3 implementing artificial neural networks into the optimisation framework with the aim of reducing optimisation time, taking advantage of recent developments in the area[1]. Two optimisation algorithms are evaluated (simulated annealing and genetic algorithms) in terms of performance (objective function value) and

[1] Ochoa-Estopier, L. M. (2014). Optimisation of Existing Heat-Integrated Crude Oil Distillation Systems. PhD Thesis, The University of Manchester. Ibrahim, D. (2018). Optimal Design of Flexible Heat-Integrated Crude Oil Distillation Systems. PhD Thesis, The University of Manchester, Manchester, UK.

optimisation time. Better optimisation results are obtained using genetic algorithms than those generated by the optimisation framework using simulated annealing.

Finally, Chapter 5 introduces a novel optimisation-based design framework for fired heating demand. To allow simultaneous evaluation of minimum hot utility and fired heating demand, an algorithm in MATLAB is developed (See Section 2.9.4 taking into account three different scenarios according to the flue gas line and process limitations (i.e. a pinch point, a match between process and utility and a dew point temperature limit). For optimisation purposes, two approaches are analysed (direct simulation-optimisation and artificial neural networks embedded into an optimisation framework using genetic algorithms) to gain some insight about the complete fuel consumption of the crude oil distillation system with and without a preflash unit.

Table 6.1 shows optimisation results for a crude oil distillation system without a preflash unit and Table 6.2 summarise optimisation results for the case when a preflash unit is added to a crude oil distillation system. In both Tables, optimisation results are presented as follows: the first two columns include the optimisation variables (10 for the case without a preflash and 12 for the case with a preflash) and units, the third column highlight the base case conditions for each crude oil distillation system. Then, the best results obtained for minimising hot utility demand using direct optimisation are presented, including results for the case when the column structure is fixed and when it is optimised simultaneously with the operating variables. Best optimisation results obtained using artificial neural networks and genetic algorithms are shown in the sixth column in both Tables. The last two columns correspond to the best optimisation results when the objective function is to minimise fired heating demand of each system using direct optimisation and a combination of genetic algorithms and artificial neural networks.

As can be seen from Table 6.1, optimisation results related to the minimum hot utility demand of the crude oil distillation system are all less than the base case (no optimised). The best results for minimum hot utility demand and minimum fired heating demand are obtained applying artificial neural networks. Optimisation times are considerably reduced (note that for the ANN optimisation, times reported in Tables are only those needed to reach the lowest objective function value) compared with those required by the direct optimisation (DO).

It was observed that higher column inlet temperatures lead to lower values for main steam flow rates while lower column inlet temperatures require high steam flow rates. Steam helps to reduce the partial pressure of the crude oil components hence their boiling points and thus reducing energy requirements. Steam in side-strippers helps to remove light components.

Pump-around duties 1 and 2 for all cases are below the base case values whereas for pump-around 3, optimised values are in most cases higher than the value for the base case allowing more heat to be available for recovering purposes within the system. In general, pump-arounds are higher level temperature sources helping to increase energy efficiency of crude distillation units.

Reflux ratio values are all around 4.0, close to the initial base case. One of the key roles of reflux ratio is to control the temperature at the top of the distillation column. Higher values of reflux ratio increase the efficiency of separation.

Table 6.1 Optimisation results summary: no preflash case

			Min Hot Utility			Min Fired Heating	
			DO				
Variable	**Units**	**Base Case**	**Column fixed**	**Column optimised**	**ANN/GA**	**DO**	**ANN/GA**
Main Steam Flow Rate	kmol h^{-1}	**1200**	1247	1298	1607	1620	1713
HD Steam Flow Rate	kmol h^{-1}	**250**	188	275	209	264	188
PA1 Duty	MW	**12.8**	7.4	9.3	6.0	10.0	8.6
PA2 Duty	MW	**17.8**	9.8	10.1	9.4	8.5	8.0
PA3 Duty	MW	**11.2**	14.0	10.5	14.0	13.7	13.0
PA1 ΔT	°C	**30**	31.9	23.7	20.0	22.3	20.0
PA2 ΔT	°C	**50**	34.9	36.2	29.6	29.4	28.8
PA3 ΔT	°C	**20**	39.9	39.8	40.0	39.9	40.0
Column Inlet Temperature	°C	**365**	362	363	350	351	350
Reflux Ratio		**4.17**	4.1	4.0	4.1	3.9	4.1
Minimum Hot Utility	MW	**58.3**	**46.6**	**48.4**	**44.5**	**45.7**	**46.5**
Minimum Fired Heating	MW					**51.7**	**51.5**
Optimisation time			4.2h	8.0h	96s	4.2h	1395s

PA: pump-around; ΔT: pump-around temperature drops
ANN: artificial neural networks; GA: genetic algorithm; DO: direct optimisation

Table 6.2 Optimisation results summary: preflash case

			Min Hot Utility			Min Fired Heating	
			DO				
Variable	**Units**	**Base Case**	**Column fixed**	**Column optimised**	**ANN/GA**	**DO**	**ANN/GA**
Main Steam Flow Rate	kmol h^{-1}	**1200**	1195	1262	1684	1672	1317
HD Steam Flow Rate	kmol h^{-1}	**250**	180	209	193	182	264
PA1 Duty	MW	**12.8**	8.5	7.2	6.8	6.6	7.8
PA2 Duty	MW	**17.8**	8.8	8.8	8.1	6.9	6.6
PA3 Duty	MW	**11.2**	13.0	11.9	10.5	8.3	11.3
PA1 ΔT	°C	**30**	38.8	33.4	29.8	39.4	30.4
PA2 ΔT	°C	**50**	31.6	31.1	30.2	26.5	27.5
PA3 ΔT	°C	**20**	21.0	21.3	39.3	20.1	15.6
Column Inlet Temperature	°C	**365**	383	377	367	370	380
Reflux Ratio		**4.17**	3.1	3.3	3.8	4.1	3.8
Preflash temperature	°C	**115**	240	230	235	240	236
Vapour feed location, section		**5**	3	3	3	3	3
Minimum Hot Utility	MW	**57.7**	**37.9**	**38.6**	**38.2**	**41.4**	**40.8**
Minimum Fired Heating	MW					**44.9**	**44.5**
Optimisation time			6.2h	8.5h	103s	6.7h	1379s

Table 6.2 summarises optimisation results for the case when a preflash unit is added to a crude oil distillation system. Initial base case (no optimised) is highlighted. For the case of minimising hot utility demand, again best optimisation result is obtained by using artificial neural networks.

It is worth to mention that several optimisation runs were performed to gain confidence in the reported results. For the case of direct optimisation (DO) three runs were carried out, while for the cases using artificial neural networks, ten optimisation runs are performed (See Appendices A, B and C for further details).

More importantly, Tables 6.1 and 6.2 show different system conditions for each 'best optimised case', pointing out the need to a further analysis i.e. details about the full costing of the system in order to have a solid basis to select the best practical option among the ones presented in this work. However, the detailed analysis performed in this work related to the minimum hot utility demand and minimum fired heating demand of the crude oil distillation system lays the foundation for further analysis. Even though no cost analysis was included in this work, it was demonstrated that including a preflash unit within a crude oil distillation system effectively reduces the hot utility demand of the system which in turn will reduce the overall utilities costs.

Chapter 7

Conclusions and Future Work

7.1 Conclusions

Crude oil distillation systems are the major energy consumers in a refinery. Even a small reduction in their energy demand will have a significant impact in heat recovery opportunities and environmental impact.

In this thesis, a systematic methodology for the design of energy-efficient crude oil distillation systems has been presented. The methodology exploits interactions between the separation units, i.e. crude oil distillation column and preflash unit and the associated heat recovery system applying pinch analysis. An optimisation-based design framework is developed, enabling the selection of key operational and structural variables within the crude oil distillation system whilst accounting for product quality and yield.

In Chapter 3, a direct simulation-optimisation methodology is presented to minimise hot utility demand of a crude oil distillation system (with and without a preflash unit). Optimisation of the system is carried out using an interface between Aspen HYSYS and MATLAB, which facilitates data transfer between the software packages, allowing an easy visualisation of important operational variables using spreadsheets in Aspen HYSYS. The optimisation framework allows a systematic evaluation of hot utility demand of the heat-integrated crude oil distillation system without the need for detailed information about the heat recovery network; instead the grand composite curve is used as a tool to estimate minimum heating and cooling requirements of the system. Case studies presented in Chapter 3 demonstrate the capabilities of the proposed optimisation-based design methodology. Results from the case studies show that adding a preflash unit within a crude oil distillation system can lead to energy savings of 19%. Case study 3.2 addressed the simultaneous design of the main column and optimisation of structural and operating variables. Results show that marginal energy savings (0.5%) are achieved when both the structure of the column and the operational variables are optimised simultaneously. This result suggests that the additional stages and new distribution of stages do not effectively improve the separation performance and heat recovery opportunities simultaneously.

In Chapter 4, artificial neural network models are incorporated into the optimisation-based design methodology proposed in Chapter 3. The aim of this approach is to reduce computational time; direct optimisation runs took around 5 hours for the case without a preflash unit and around 7 hours for the case with a preflash unit. Taking advantage of recent developments in the area (Ochoa-Estopier, 2014; Ibrahim, 2018) a column model was built using samples generated via rigorous simulations in Aspen HYSYS v8.8. The suitability of two stochastic optimisation algorithms – genetic algorithm (GA) and simulated annealing (SA) – is explored using the MATLAB optimisation Toolbox. This approach provided robust results for the case studies analysed, with and without a preflash unit, without compromising model accuracy, column performance, product quality, and product yields. Previous works have not reported the implementation of artificial neural networks into an optimisation framework for a heat-integrated crude oil distillation system with a preflash unit. Therefore, the proposed methodology can benefit current industrial practice by reducing engineering time.

Furthermore, considering only the minimum hot utility demand of a crude oil distillation system may lead to underestimation of the actual energy demand as stack loss associated with fired heaters is not taken into account. To overcome this limitation in the current open literature, Chapter 5 presents a novel optimisation-based design methodology that enables the minimisation of fired heating demand of a crude oil distillation system (with and without a preflash unit). The developed surrogate models (artificial neural networks) are further evaluated by comparing predictions of the minimum hot utility demand and minimum fired heating demand with values obtained from the rigorous model. To date, the literature search has not revealed any studies that consider both the efficiency of the fired heater and design or operation of the crude oil distillation column with a preflash unit. This work extends the methodology presented in Chapters 3 and 4 to account for the efficiency of the fired heater. In order to allow evaluation of the amount of heat released to the ambient (stack losses), an algorithm is coded in MATLAB, and implemented into an optimisation framework enabling the minimisation of fired heating while simultaneously optimising both structural and operating variables of the system, maintaining product qualities and the residue flow rate within allowed ranges of ±10°C and ±1% respectively in line with industrial practice. Results revealed that optimising hot utility demand only does not guarantee that the stack loss will be the minimum so that there is a need for more detailed analysis that reveals further opportunities to recover heat within the crude oil distillation system.

The methodology developed in this work has the merits of using rigorous and surrogate process models, of being systematic, of using robust optimisation techniques and of accounting for configuration as well as operating conditions. Case study results indicate that energy demand can be reduced by introducing a preflash unit within the crude oil distillation system. Heat integration is considered simultaneously using pinch analysis.

7.2 Future Work

The following future work is proposed to extend the methodology presented in this work and to enhance its capabilities:

1. Extend the proposed design methodology to consider the design of crude oil distillation systems with other pre-separation arrangements i.e. a prefractionation column (See Appendix D).

2. Include the vacuum distillation column within the crude oil distillation system extending the methodology presented in this work. Evaluate fired heating demand of the vacuum furnace applying the algorithm developed in MATLAB to complement the analysis of total fuel consumption in the system.

3. The objective function included within the optimisation framework proposed in this work can be extended to capture the trade-offs between yield and energy demand, e.g. by maximising net profit.

4. Stripping steam analysis can be added to the grand composite curve calculations in the MATLAB code. Temperature dependence of fluids can be taken into account during the simulation-optimisation steps enhancing the proposed methodology.

5. In this work, the structure of the main column is maintained fixed, future work could be extended to consider the design of the main column including the number of trays as a discrete variable as it was presented in a case study in Chapter 3.

6. The algorithm developed to allow calculations for the fired heating demand presented in Chapter 5 can be extended to include other limitations for the flue gas line depending on the nature of the process.

7. Full costing study of the crude oil distillation system with and without a preflash unit will complement and help to select the best set of operating conditions for industrial implementation of the methodology developed in this work.

APPENDIX A

Supporting Information for Chapter 3

Table A1 shows the crude oil assay[1] used in the case study presented in Section 3.3.1.

Table A1. Crude oil assay (Venezuelan Tia Juana Light)1

Light ends	**Component name**	**Volume %**
	Ethane	0.04
	Propane	0.37
	i-Butane	0.27
	n-Butane	0.89
	i-Pentane	0.77
	n-Pentane	1.13
TBP Curve	**Temperature, °C**	**Volume %**
	36.1	0
	64.4	5
	100.6	10
	163.9	20
	221.1	30
	278.9	40
	337.2	50
	397.2	60
	463.9	70
	545.0	80

Density: 867.6 kg/m^3

Once the crude oil assay is defined it is cut into 25 pseudo-components generated using the standard oil characterisation procedure in Aspen HYSYS v8.8. Table A2 shows the normal boiling temperature (NBP) in °C, compositions (volume fraction on a 100% basis) and volumetric flow rates (in $m^3\ h^{-1}$) for pure components and pseudo-components.

Table A2. Crude oil characterisation, (Venezuelan Tia Juana Light)[1,2]

Name	**NBP, °C**	**Volume Fraction**	**Vol Flow ($m^3\ h^{-1}$)**
Ethane	-89.0	0.04	0.26
Propane	-42.0	0.37	2.45
i-Butane	-12.0	0.27	1.79
n-Butane	-1.0	0.89	5.90
i-Pentane	28.0	0.77	5.10
n-Pentane	36.0	1.13	7.49
NBP_47	47.1	4.25	28.16
NBP_72	72.4	3.37	22.33
NBP_97	97.5	3.26	21.62
NBP_122	121.8	3.65	24.21
NBP_146	146.2	3.85	25.49
NBP_171	170.6	4.03	26.68
NBP_195	194.9	4.15	27.48
NBP_219	219.2	4.15	27.47
NBP_244	243.7	4.08	27.05
NBP_268	268.2	4.07	26.97
NBP_293	292.6	4.06	26.92
NBP_317	317.0	4.03	26.71
NBP_341	341.5	4.02	26.61
NBP_366	365.8	3.95	26.15
NBP_390	390.3	3.82	25.32
NBP_415	414.6	3.67	24.33
NBP_449	448.6	6.15	40.76
NBP_493	492.7	5.47	36.21
NBP_538	537.8	4.87	32.29
NBP_581	580.7	4.26	28.25
NBP_625	624.8	3.21	21.29
NBP_685	685.5	4.78	31.67
NBP_771	770.9	2.81	18.61
NBP_858	857.7	1.41	9.33
NBP_950	949.8	1.14	7.56
Total		100	662.46

Table A3. Design specifications and variables, crude oil distillation system with a preflash

Variable	Units	Initial Value
Reflux Ratio		4.17
LN Prod Flow	kmol h^{-1}	833
HN Prod Flow	kmol h^{-1}	491
LD Prod Flow	kmol h^{-1}	515
HD Prod Flow	kmol h^{-1}	165
RES Prod Flow	kmol h^{-1}	565
PA1 Duty	MW	12.84
PA2 Duty	MW	17.89
PA3 Duty	MW	11.20
PA1 ΔT	°C	30
PA2 ΔT	°C	50
PA3 ΔT	°C	20
LN T5%	°C	27
HN T5%	°C	143
LD T5%	°C	218
HD T5%	°C	308
RES T5%	°C	363
LN T95%	°C	110
HN T95%	°C	196
LD T95%	°C	300
HD T95%	°C	354
RES T95%	°C	755
Column Inlet Temperature	°C	365
Flash Temperature	°C	115
Vapor Feed Location[a]		5

[a] Section number in main column

PA: pump-around; ΔT: pump-around temperature drop

Table A4. Distribution of theoretical stages in the main column and side strippers (SS).

Column Section	Stage numbers
Section 1	1–9
Section 2	10–17
Section 3	18–27
Section 4	28–36
Section 5	37–41
Section 6 (HN SS)	42–47
Section 7 (LD SS)	48–54
Section 8 (HD SS)	55–59

SS: side-stripper

Table A5. Initial product quality specifications and flow rates, crude oil distillation system.

Product	**Base Case ASTM (°C)**		**Product flow rates ($m^3\ h^{-1}$)**	**Product flow rates ($kmol\ h^{-1}$)**
	T5 %	T95 %		
LN	26	109 [a]	102	833
HN	143	196 [a]	87	491
LD	217 [a]	300 [a]	128	515
HD	308	353 [a]	54	165
RES	363	754	292	565

[a] Specified in HYSYS

Table A6. Process stream data, crude oil distillation system without a preflash (not optimised base case)

Name	Process Stream Temperatures, °C		Duty, MW	ΔT_{min}, °C
	Inlet	Outlet		
Q crude	25.0	185.0	60.1	30
Q heater	185.0	266.0	39.6	30
Q furnace	266.0	365.0	51.9	30
Q HN	190.2	40.0	6.5	30
Q RES	325.1	100.0	46.4	30
Q LD	285.9	40.0	17.6	30
Q HD	270.2	50.0	6.8	30
Q LN	59.0	40.0	0.8	30
Q condenser	93.8	59.0	56.2	30
PA1	147.4	117.4	12.8	30
PA2	238.6	188.6	17.9	30
PA3	310.9	290.9	11.2	30
HN SS reboiler	181.3	190.2	12.8	30
LD SS reboiler	276.5	285.9	5.3	30

PA: pump-around; SS: side-stripper; ΔT_{min}: minimum temperature difference approach

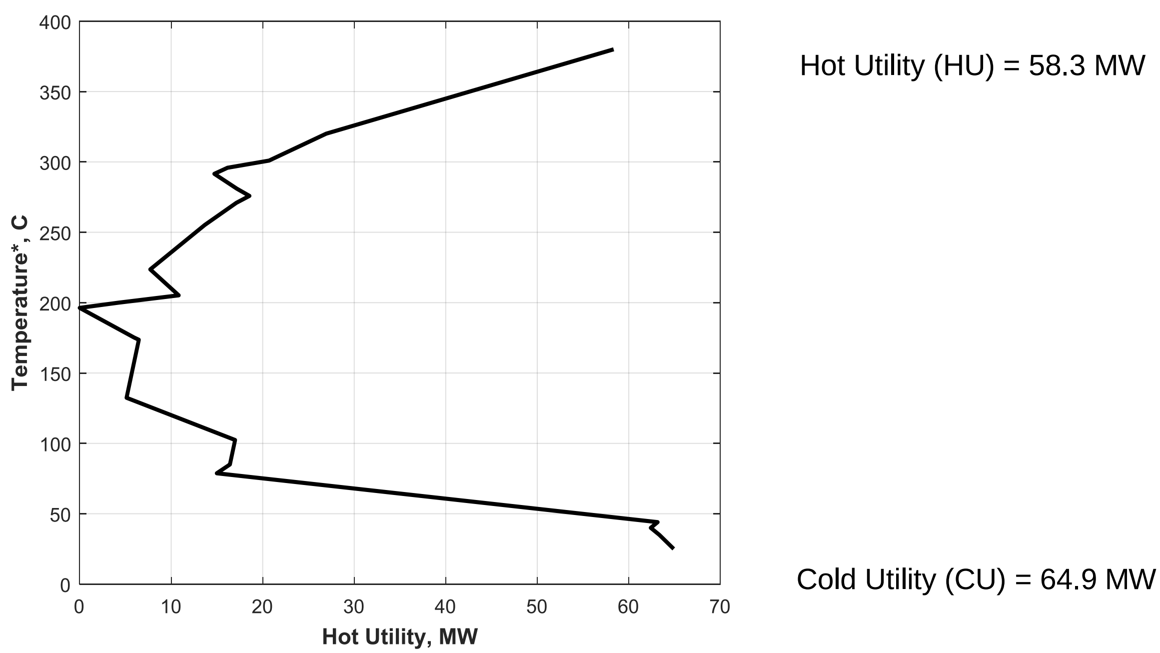

Figure A1. Grand composite curve (base case: crude oil distillation system without a preflash).

Table A7. Process stream data, optimised crude oil distillation system with a preflash: Case 1

Name	Process Stream Temperatures, °C Inlet	Outlet	Duty, MW	ΔT_{min}, °C
Q crude	25.0	230.0	81.7	30
Q heater	230.0	266.0	12.9	30
Q furnace	266.0	354.1	36.3	30
Q HN	188.0	40.0	6.5	30
Q RES	325.1	100.0	45.4	30
Q LD	285.4	40.0	16.9	30
Q HD	265.1	50.0	6.0	30
Q LN	58.6	40.0	0.8	30
Q condenser	91.2	58.6	46.8	30
PA1	155.0	129.5	6.8	30
PA2	223.7	200.6	8.4	30
PA3	303.2	263.9	8.9	30
HN SS reboiler	182.3	188.0	3.0	30
LD SS reboiler	275.0	285.4	7.0	30

PA: pump-around; SS: side-stripper; ΔT_{min}: minimum temperature difference approach.

Table A8. Process stream data optimised crude oil distillation system with a preflash: Case 2

Name	Process Stream Temperatures, °C Inlet	Outlet	Duty, MW	ΔT_{min}, °C
Q crude	25.0	240.0	86.5	30
Q heater	240.0	266.0	8.9	30
Q furnace	266.0	383.4	47.4	30
Q HN	188.2	40.0	6.5	30
Q RES	343.4	100.0	48.2	30
Q LD	285.4	40.0	16.8	30
Q HD	278.0	50.0	7.6	30
Q LN	58.6	40.0	0.7	30
Q condenser	91.6	58.6	47.1	30
PA1	157.1	118.2	8.5	30
PA2	229.0	197.3	8.8	30
PA3	312.7	291.6	13.0	30
HN SS reboiler	182.7	188.2	2.8	30
LD SS reboiler	275.5	285.4	6.2	30

PA: pump-around; SS: side-stripper; ΔT_{min}: minimum temperature difference approach

Table A9. Genetic Algorithm results: Case 1

	CDU without a preflash		CDU with a preflash	
Run	**Objective Function (MW)**	**CPU time (hours)**	**Objective Function (MW)**	**CPU time (hours)**
1	43.4	4.0	35.9	5.8
2	43.9	4.4	36.0	7.4
3	43.8	5.2	36.1	6.0

Population Size: 100; Generations: 500

Table A10. Genetic Algorithm results: Case 2

	CDU without a preflash		CDU with a preflash	
Run	**Objective Function (MW)**	**CPU time (hours)**	**Objective Function (MW)**	**CPU time (hours)**
1	46.6	4.7	38.2	6.4
2	47.2	4.5	38.0	6.0
3	46.6	4.2	37.9	6.2

Population Size: 100; Generations: 500

References:

(1) Watkins, R. N. (1979). *Petroleum Refinery Distillation*, GulfPub.Co., Houston, USA.

(2) Ibrahim, D., Jobson, M., Guillén-Gosálbez, G. (2017). Optimization-Based Design of Crude Oil Distillation Units Using Rigorous Simulation Models. *Ind. Eng. Chem. Res.*, 56 (23), 6728.

Extract of MATLAB Code – Interface between Aspen HYSYS and MATLAB and principal commands used.

```
%   Interface HYSYS v8.8 - MATLAB R2016a
%   Establish link with Aspen HYSYS
hy=actxserver('HYSYS.APPLICATION');
%   Connect to the active HYSYS document
hy_ActiveDoc=hy.ActiveDocument;
set(hy,'Visible',1);
hy.ChangePreferencesToMinimizePopupWindows(0);
%   Connection to the HYSYS solver
hy_Solver=hy_ActiveDoc.Solver;
%   Connection to flowsheet
hy_Flowsheet=hy_ActiveDoc.Flowsheet;
%   Connection to CDU on flowsheet
CDU=hy_Flowsheet.Operation.Item('CDU');
%   Connection to items on CDU Sub-flowsheet
CDU_SubFlowsheet=CDU.ColumnFlowsheet;
%   Connection to streams on Main flowsheet
CDU_MFStream=hy_Flowsheet.Streams;
%   Connection with column specifications
CDU_Specification=CDU_SubFlowsheet.Specifications;
%   Connection to CDU on spreadsheet
CDU1=hy_Flowsheet.Operation.Item('CDU_Results');
% Setting the location of the flashed vapor to the column:
  PF = [1,0,0,0,0;
        0,1,0,0,0;
        0,0,1,0,0;
        0,0,0,1,0;
        0,0,0,0,1];
% Initializing Optimization Variables
% Duty Pump-around 1
  Q_PA1x = y(1);
% Reading variables from HYSYS:
% Pump-around Duties, MW
  Q_PA1 = CDU_Specification.Item('PA_1_Duty(Pa)');

% Product Flow rates:
  LNx = get(CDU_Specification,'Item',1);

% Product quality specifications:
  T5_RESx = get(CDU_Specification,'Item',23);

% Sending Values from MATLAB to HYSYS:
  Q_PA1.Goal.SetValue(Q_PA1x,'MW')

% Read Variables from HYSYS:
% Product Specifications
  T5_RES = T5_RESx.CurrentValue;
```

APPENDIX B

Supporting Information for Chapter 4

Table B1. ANN/GA optimisation runs (Case 4.1)

Run	HU, MW	CPU Time, s	HYSYS validation	Difference
1	**44.5**	**96**	**44.6**	**-0.1**
2	44.6	96	44.9	-0.2
3	44.6	96	44.7	-0.1
4	44.7	96	45.4	-0.7
5	44.7	96	44.9	-0.1
6	44.9	98	45.0	-0.1
7	45.0	96	45.1	-0.1
8	45.3	96	45.5	-0.2
9	45.4	97	45.4	0.0
10	46.1	95	46.2	-0.1

Table B2. SA/ANN optimisation runs (Case 4.1)

Run	HU, MW	CPU Time, sec	Function evaluations	HYSYS validation	Difference
1	46.9	106	19016	46.8	0.1
2	**46.9**	**41**	**7335**	**46.9**	**0.0**
3	47.2	74	14255	47.2	0.0
4	47.5	122	22118	47.6	0.0
5	47.9	60	11993	47.9	0.0
6	48.0	47	9456	48.2	-0.2
7	48.0	76	13253	48.3	-0.3
8	48.4	41	8143	48.3	0.0
9	48.5	43	7516	48.5	0.0
10	49.1	41	7769	49.1	0.0

Table B3. Direct simulation-optimisation runs (Case 4.1)

Run	HU, MW	CPU Time, hours
1	45.0	3.8
2	46.1	4.1
3	**44.8**	**4.1**

Table B4. Error analysis, optimisation results (Case 4.1)

	ANN model GA	Direct opt GA	Absolute error
Product quality ASTM D86, (°C)			
T5% RES	361.4	362.0	0.6
T5% LN	25.0	25.1	0.1
T5% HN	132.5	133.3	0.8
T5% LD	217.5	217.6	0.0
T5% HD	306.4	306.0	0.4
T95% RES	754.3	754.5	0.2
T95% LN	109.7	109.7	0.0
T95% HN	196.0	196.0	0.1
T95% LD	300.1	300.1	0.0
T95% HD	353.5	353.5	0.0
Supply temperatures, (°C)			
HN cooler	187.6	188.4	0.8
RES cooler	320.6	319.9	0.7
LD cooler	285.7	285.7	0.0
HD cooler	270.3	270.7	0.5
LN cooler	58.6	58.7	0.1
Condenser	90.9	90.6	0.4
PA1	157.4	156.5	0.9
PA2	231.6	231.2	0.4
PA3	301.4	300.2	1.2
HN reboiler	182.3	183.1	0.7
LD reboiler	275.9	276.0	0.1

Table B5. Error analysis continuation, optimisation results (Case 4.1)

	ANN model GA	**Direct opt GA**	**Relative error**
Product flow rates, $m^3\ h^{-1}$			
LN	100.7	101.1	0.0
HN	88.8	88.4	0.0
LD	125.9	125.5	0.0
HD	55.1	56.1	0.0
RES	292.1	291.6	0.0
Enthalpy change, MW			
Fired heater	43.7	43.9	0.0
HN cooler	6.5	6.5	0.0
RES cooler	43.2	42.9	0.0
LD cooler	17.4	17.3	0.0
HD cooler	6.9	7.1	0.0
LN cooler	0.8	0.8	0.0
Condenser	59.0	60.6	0.0
HN reboiler	2.5	2.7	-0.1
LD reboiler	5.7	5.6	0.0

Table B6. Validation of ANN results on rigorous model (Case 4.1)

	Rigorous model	**ANN model**	**Difference**
Product quality ASTM D86, (°C)			
T5% RES	361.4	361.4	0.0
T5% LN	25.0	25.0	0.0
T5% HN	132.9	132.5	0.3
T5% LD	217.5	217.5	0.0
T5% HD	306.2	306.4	-0.3
T95% RES	754.4	754.3	0.0
T95% LN	109.7	109.7	0.0
T95% HN	196.0	196.0	0.0
T95% LD	300.1	300.1	0.0
T95% HD	353.5	353.5	0.0
Supply temperatures, (°C)			
HN cooler	187.9	187.6	0.3
RES cooler	320.8	320.6	0.2
LD cooler	285.7	285.7	0.0
HD cooler	269.9	270.3	-0.3
LN cooler	58.5	58.6	-0.1
Condenser	90.8	90.9	-0.1
PA1	157.2	157.4	-0.1
PA2	231.6	231.6	0.0
PA3	301.1	301.4	-0.4
HN reboiler	182.6	182.3	0.3
LD reboiler	276.0	275.9	0.1

Table B7. Continuation validation of ANN model results on rigorous model (Case 4.1)

	Rigorous model	**ANN model**	**Difference**
Product flow rates, $m^3\ h^{-1}$			
LN	100.8	100.7	0.1
HN	88.7	88.8	-0.1
LD	125.7	125.9	-0.2
HD	55.2	55.1	0.1
RES	292.2	292.1	0.1
Enthalpy change, MW			
Fired heater	43.8	43.7	0.1
HN cooler	6.5	6.5	0.0
RES cooler	43.2	43.2	0.0
LD cooler	17.3	17.4	-0.1
HD cooler	7.0	6.9	0.0
LN cooler	0.8	0.8	0.0
Condenser	58.8	59.0	-0.2
HN reboiler	2.4	2.5	-0.1
LD reboiler	5.6	5.7	-0.1

Table B8. GA/ANN optimisation runs (Case 4.2)

Run	**HU, MW**	**CPU Time, sec**	**HYSYS validation**	**Difference**
1	**38.2**	**103**	**40.4**	**-2.2**
2	38.3	102	42.5	-4.2
3	38.4	104	46.8	-8.4
4	38.5	105	41.8	-3.3
5	38.5	105	43.3	-4.8
6	38.5	104	39.2	-0.7
7	38.6	104	40.4	-1.8
8	38.6	103	39.6	-1.0
9	38.7	105	39.9	-1.2
10	38.8	110	40.4	-1.7

Table B9. SA/ANN optimisation runs (Case 4.2)

Run	HU, MW	CPU Time, sec	Function evaluations	HYSYS validation	Difference
1	**39.4**	**118**	**20961**	**39.5**	**-0.1**
2	39.8	73	14065	42.3	-2.5
3	40.2	71	12276	41.6	-1.3
4	40.3	95	16039	40.6	-0.3
5	40.6	71	13285	42.3	-1.7
6	40.8	59	11610	41.0	-0.3
7	44.6	43	7587	44.5	0.1
8	45.4	48	9329	46.1	-0.7
9	45.6	73	13300	47.2	-1.6
10	46.4	38	6647	47.7	-1.3

Table B10. Direct simulation-optimisation runs, preflash

Run	HU, MW	CPU Time, hours
1	39.1	6.1
2	**38.1**	**6.1**
3	38.6	6.5

Table B11. Error analysis optimisation results (Case 4.2)

	ANN/GA	Direct opt GA	Absolute error
Product quality ASTM D86, (°C)			
T5% RES	362.2	361.7	0.5
T5% LN	25.4	25.0	0.4
T5% HN	138.0	134.9	3.1
T5% LD	217.5	217.5	0.0
T5% HD	304.7	303.9	0.8
T95% RES	754.4	754.4	0.0
T95% LN	109.7	109.7	0.0
T95% HN	195.8	196.0	0.2
T95% LD	300.1	300.1	0.0
T95% HD	353.5	353.5	0.0
Supply temperatures, (°C)			
Preheat train 1	235.2	240.0	4.7
HN cooler	189.0	188.2	0.8
RES cooler	326.7	340.8	14.0
LD cooler	285.5	285.5	0.0
HD cooler	274.1	277.9	3.8
LN cooler	58.8	58.6	0.1
Condenser	90.1	91.1	1.0
PA1	152.0	156.0	4.1
PA2	225.9	228.5	2.6
PA3	308.7	312.1	3.4
HN reboiler	182.7	182.6	0.1
LD reboiler	275.2	275.5	0.3

Table B12. Error analysis optimisation results continuation (Case 4.2)

	ANN/GA	Direct opt GA	Relative error
Product flow rates, m^3 h^{-1}			
LN	101.9	101.0	0.0
HN	87.1	88.7	0.0
LD	124.9	123.5	0.0
HD	56.5	57.5	0.0
RES	292.2	292.0	0.0
Enthalphy change, MW			
Preheat train 1	84.5	86.6	0.0
Preheat train 2	11.1	9.0	0.2
Fired heater	41.0	46.6	-0.1
HN cooler	6.5	6.5	0.0
RES cooler	44.1	47.7	-0.1
LD cooler	17.0	17.0	0.0
HD cooler	7.0	7.6	-0.1
LN cooler	0.8	0.8	0.0
Condenser	57.6	47.7	0.2
HN reboiler	4.3	2.9	0.5
LD reboiler	6.4	6.3	0.0

Table B13. Validation of ANN results on rigorous model (Case 4.2)

	Rigorous model	ANN model	Difference
Product quality ASTM D86, (°C)			
T5% RES	361.7	362.2	-0.5
T5% LN	25.4	25.4	0.0
T5% HN	137.4	138.0	-0.6
T5% LD	217.5	217.5	0.0
T5% HD	305.3	304.7	0.7
T95% RES	754.4	754.4	0.0
T95% LN	109.7	109.7	0.0
T95% HN	196.0	195.8	0.2
T95% LD	300.1	300.1	0.1
T95% HD	353.6	353.5	0.1
Supply temperatures, (°C)			
Preheat train 1	235.0	235.2	-0.2
HN cooler	189.7	189.0	0.7
RES cooler	326.5	326.7	-0.3
LD cooler	285.6	285.5	0.0
HD cooler	275.1	274.1	0.9
LN cooler	58.8	58.8	0.0
Condenser	90.2	90.1	0.1
PA1	151.5	152.0	-0.5
PA2	225.8	225.9	-0.1
PA3	307.7	308.7	-1.0
HN reboiler	183.3	182.7	0.6
LD reboiler	275.5	275.2	0.3

Table B14. Continuation validation of ANN results on rigorous model (Case 4.2)

	Rigorous model	**ANN model**	**Difference**
Product flow rates, $m^3\ h^{-1}$			
LN	102.0	101.9	0.0
HN	87.6	87.1	0.5
LD	124.4	124.9	-0.4
HD	56.6	56.5	0.1
RES	292.0	292.2	-0.2
Enthalphy change, MW			
Preheat train 1	84.1	84.5	-0.3
Preheat train 2	10.9	11.1	-0.2
Fired heater	41.2	41.0	0.2
HN cooler	6.5	6.5	0.0
RES cooler	44.4	44.1	0.4
LD cooler	17.1	17.0	0.1
HD cooler	7.3	7.0	0.4
LN cooler	0.8	0.8	0.0
Condenser	57.3	57.6	-0.3
HN reboiler	4.6	4.3	0.3
LD reboiler	6.2	6.4	-0.1

APPENDIX C

Supporting Information for Chapter 5

Table C1. Optimisation runs using ANN model, no preflash

Run	FH, MW	SL	Time,s	Time, h	CU, MW	HU, MW
1	**51.5**	**5.0**	**1395**	**0.39**	**59.2**	**46.5**
2	51.7	6.2	1377	0.38	57.7	45.5
3	51.8	6.3	1333	0.37	56.7	46.1
4	51.8	6.3	1333	0.37	56.7	46.1
5	51.9	5.7	1387	0.39	59.5	46.2
6	51.9	5.7	1331	0.37	59.9	46.2
7	52.2	4.6	1340	0.37	60.4	47.6
8	52.4	6.3	1331	0.37	56.6	46.1
9	52.8	4.7	1342	0.37	60.3	48.1
10	53.6	7.7	1325	0.37	57.4	45.9

Table C2. Optimisation runs direct optimisation, no preflash

Run	FH, MW	SL	Time,h	CU, MW	HU, MW
1	52.07	4.7	4.5	60.0	48.3
2	52.66	4.9	4.2	58.6	48.5
3	**51.19**	**6.0**	**4.2**	**58.3**	**45.7**

Table C3**.** Optimisation runs using ANN model, preflash

Run	FH, MW	SL	Time,s	Time,h	CU, MW	HU, MW
1	**44.5**	**3.7**	**1379**	**0.4**	**49.1**	**40.8**
2	44.6	3.6	1334	0.4	53.5	41.0
3	44.6	4.5	1399	0.4	54.8	40.1
4	44.6	4.8	1346	0.4	50.1	39.8
5	44.6	4.3	1353	0.4	52.4	40.3
6	44.6	3.1	1428	0.4	54.7	41.5
7	44.7	4.5	1420	0.4	52.0	40.1
8	44.7	4.6	1350	0.4	52.5	40.0
9	44.7	4.9	1394	0.4	48.6	39.8
10	44.8	3.6	1476	0.4	50.4	41.2

Table C4. Direct optimisation runs, preflash

Run	FH, MW	SL	Time,h	CU, MW	HU, MW
1	46.2	5.4	6.7	49.3	40.8
2	**44.9**	**3.5**	**6.7**	**53.6**	**41.4**
3	46.2	5.8	6.9	48.8	40.4

Note for all the Tables: FH: Fired heating, SL: Stack loss, CU: Cold utility, HU: Hot utility.

Table C5. Optimisation results product quality– direct optimisation no preflash case

Product	**Base Case ASTM D86 (°C)**		**Fired Heating Direct optimisation ASTM D86 (°C)**	
	T5%	**T95%**	**T5%**	**T95%**
LN	25.6 [b]	109.7 [a]	24.6	109.7
HN	140.2 [b]	196.0 [a]	131.5	196.0
LD	217.5 [a]	300.1 [a]	217.5	300.1
HD	308.5 [b]	353.5 [a]	307.8	353.5
RES	361.6 [b]	754.4 [b]	361.5	754.4

[a] Specified in HYSYS , [b] Specified in MATLAB

Table C6. Optimisation results product flow rates – direct optimisation no preflash case

Product flow rate (m^3 h^{-1})	**Base Case**	**Fired Heating Direct optimisation**
LN	102.4	100.4
HN	86.8	89.1
LD	127.6	126.7
HD	53.7	54.2
RES	292.1 [a]	292.1

[a] Constraint in MATLAB

Table C7. Optimisation results product quality – direct optimisation preflash case

Product	**Base Case ASTM D86 (°C)**		**Fired Heating Direct optimisation ASTM D86 (°C)**	
	T5%	**T95%**	**T5%**	**T95%**
LN	25.6 [b]	109.7 [a]	25.6	109.7
HN	140.2 [b]	196.0 [a]	133.2	196.0
LD	217.5 [a]	300.1 [a]	217.5	300.1
HD	308.5 [b]	353.5 [a]	305.9	353.5
RES	361.4 [b]	754.3 [b]	361.8	754.4

[a] Specified in HYSYS [b] Specified in MATLAB

Table C8. Optimisation results product flow rates – direct optimisation preflash case

Product flow rate ($m^3\ h^{-1}$)	Base Case	Fired Heating Direct optimisation
LN	102.4	101.0
HN	86.8	88.5
LD	127.6	124.7
HD	53.7	56.3
RES	292.1 [a]	292.0

[a] Constraint in MATLAB

Table C9. Optimisation results product quality– ANN model no preflash case

Product	Base Case ASTM D86 (°C)		Fired Heating ANN model ASTM D86 (°C)	
	T5%	T95%	T5%	T95%
LN	25.6 [b]	109.7 [a]	25.0	109.7
HN	140.2 [b]	196.0 [a]	132.5	196.0
LD	217.5 [a]	300.1 [a]	217.6	300.1
HD	308.5 [b]	353.5 [a]	306.7	353.5
RES	361.6 [b]	754.4 [b]	362.0	754.5

[a] Specified in HYSYS [b] Specified in MATLAB

Table C10. Optimisation results product flow rates – ANN model no preflash case

Product flow rate ($m^3\ h^{-1}$)	Base Case	Fired Heating ANN model
LN	102.4	100.6
HN	86.8	89.0
LD	127.6	125.9
HD	53.7	55.6
RES	292.1 [a]	291.5

[a] Constraint in MATLAB

Table C11. Optimisation results product quality – ANN model preflash case

Product	Base Case ASTM D86 (°C)		Fired Heating ANN model ASTM D86 (°C)	
	T5%	T95%	T5%	T95%
LN	25.6 [b]	109.7 [a]	25.2	109.7
HN	140.2 [b]	196.0 [a]	135.3	195.8
LD	217.5 [a]	300.1 [a]	217.5	300.1
HD	308.5 [b]	353.5 [a]	305.8	353.5
RES	361.4 [b]	754.3 [b]	361.9	754.4

[a] Specified in HYSYS [b] Specified in MATLAB

Table C12. Optimisation results product flow rates – ANN model preflash case

Product flow rate (m^3 h^{-1})	**Base Case**	**Fired Heating ANN model**
LN	102.4	101.5
HN	86.8	87.7
LD	127.6	125.2
HD	53.7	56.2
RES	292.1 [a]	292.0

[a] Constraint in MATLAB

APPENDIX D

Prefractionator Design, Simulation and Optimisation

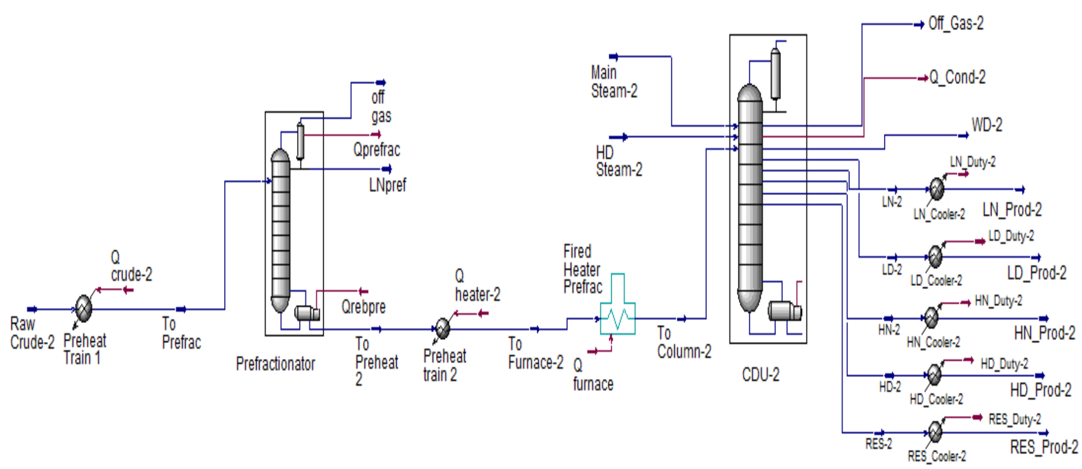

Figure D1 Aspen HYSYS v8.8 screenshot: crude oil distillation system with a prefractionator.

Proposed optimisation-based design methodology:

1. Prefractionator design:
   a. Number of stages
   b. Feed stage
   c. Reflux ratio
   d. Prefractionator temperature
   e. Column specifications – distillate flow rate to further processing

2. Sensitivity studies: understanding operational variables ranges.

3. Integrate prefractionator into the crude oil distillation system – converged simulation in HYSYS.

4. Update stream information for the grand composite curve, to allow minimum hot utility demand, HU and minimum fuel consumption calculations - include Qcond prefractionator.

5. Perform direct optimisation of the system using genetic algorithms, GA – update MATLAB code.

6. Perform optimisation using surrogate models, in particular, artificial neural networks:

   a. Generate samples – rigorous simulations in Aspen HYSYS v8.8.

   b. Create ANN functions and parity plots.

7. Integrate ANN model into an optimisation framework.
8. Evaluate and compare optimisation results for minimum hot utility demand and total fired heating of the system.

APPENDIX E

Publications and Conference Presentations

Published Journal paper

Ledezma Martínez, M., Jobson, M., Smith, R. (2018a). Simulation-optimization-based Design of Crude Oil Distillation Systems with Preflash Units. *Industrial & Engineering Chemistry Research*, *57*(30). doi.org/10.1021/acs.iecr.7b05252

Conference peer reviewed papers

1. Ledezma Martínez, M., Jobson, M., Smith, R. (2017). Simulation-optimisation-based Design of Crude Oil Distillation Systems with Preflash Units. In *Proceedings of the 27th European Symposium on Computer-Aided Process Engineering (ESCAPE-27)* (Computer Aided Chemical Engineering). doi.org/10.1016/B978-0-444-63965-3.50139-2.

2. Ledezma-Martínez, M., Jobson, M., Smith, R. (2018b). A new optimisation-based design methodology for energy-efficient crude oil distillation systems with preflash units. *Chemical Engineering Transactions*, *69*, 385-390. doi.org/10.3303/CET1869065.

27th European Symposium on Computer-Aided Process Engineering (ESCAPE-27),
Computer Aided Chemical Engineering – Barcelona, Spain 2017.

Simulation-optimisation-based Design of Crude Oil Distillation Systems with Preflash Units

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Abstract

Crude oil distillation systems are energy intensive processes. A crude oil distillation system typically comprises a preheat train, a preflash unit and an atmospheric distillation unit. Preflash units in a crude oil distillation system create opportunities to reduce demand for fired heating. This work aims to develop a new design approach to enhance production and to reduce energy consumption and operating cost. Existing design methodologies do not allow systematic design optimisation of crude oil distillation systems with preflash units. Thus, a systematic approach is proposed that exploits interactions between the separation units and the heat recovery system, while meeting product quality specifications. The optimisation framework applies a stochastic optimisation algorithm (simulated annealing) to minimise utility consumption by selecting optimal values for operational variables: stripping steam, pump-around duties, pump-around temperature drops, column feed inlet temperature and preflash temperature. An interface between Aspen HYSYS v8.6 and MatLab R2016a facilitates integration of modelling and optimisation. Heat recovery is systematically evaluated using pinch analysis (grand composite curve) to account for the impact of operational variables on energy demand. A case study demonstrates the capabilities of the approach and illustrates that implementing preflash units can reduce hot utility demand.

Keywords: energy consumption, heat integration, grand composite curve.

1. Introduction

Crude oil distillation systems play a central role in petroleum refining. A typical crude oil distillation system comprises a preheat train, crude oil distillation units with side strippers and pump-arounds and sometimes pre-separation units, such as flash units and prefractionation columns. These systems are energy-intensive: it is estimated that 7 to 15 % of the crude oil input is consumed in refinery processes, of which 35 to 45 % is used for crude oil distillation (Szklo and Schaeffer, 2007). Preflash units are useful for reducing the fired heat demand for crude oil preheating prior to distillation. The preflash unit removes some light components and some of light naphtha; the vapour stream bypasses the fired heater, helping to reduce its fuel consumption. The vapour stream can then be mixed with the stream leaving the furnace or be fed to the main column at a suitable location.

Research studies have investigated the design and optimisation of crude oil distillation systems to maximise the benefits of including preflash units. Golden (1997) provides useful insights into how key parameters, such as flash temperature and flashed vapour feed location, affect the performance of the main distillation column. Ji and Bagajewicz (2002) present a rigorous analysis for setting the inlet and outlet conditions for the design of a crude oil distillation unit with preflash units. Preflash temperature and feed location of preflash vapour in the main column are addressed; pinch analysis is applied to assess minimum utility requirements. Errico et al. (2009) compare the performance of columns with preflash units, considering product flow rates, product quality and potential for energy savings. One disadvantage of this study is that column operating conditions and the preflash temperature are constant. Wang et al. (2011) apply thermodynamic metrics to select the best pre-separation scheme for heavy crude oils. Nine predistillation arrangements are explored, and the option with two preflash units is found to perform best. Details of hot utility demand and product quality specifications are not reported, however. Benali et al. (2012) demonstrate that preflash units can bring benefits in terms of exergy destruction, although their methodology for adjusting the column operating conditions and for analysing the impact of the process changes on heat recovery opportunities is not discussed.

Other researchers explore using optimisation to improve the performance of the crude oil distillation system using preflash units. Al-Mayyahi et al. (2014) utilise multi-objective optimisation techniques to study the effects of single and multiple preflash units on both energy consumption and yield. Their study investigates the vapour feed location and considers heat integration with and without preflash units. The optimisation variables varied include the steam flow to the main column and the furnace outlet temperature, as well as the vapour fraction from each flash unit; significantly, pump-around duties and temperature drops are not considered. Wang et al. (2016) present a simulation-optimisation study in the context of an existing crude oil distillation processes for two different feedstocks. The study addresses a three-column system (i.e. prefractionation column), where the grand composite curve is used to evaluate energy consumption and CO_2 emissions. Pump-around duties and temperatures are varied, while the inlet temperatures to the three distillation units and stripping steam flow rates are maintained as constants. Enríquez-Gutiérrez (2016) applies a simulation-optimisation strategy to explore the option of installing a preflash unit as a retrofit option in a crude oil distillation system when increasing capacity. This study confirms that installing a preflash unit can help to alleviate hydraulic constraints in the column (Fraser, 2014), thus avoiding the need to replace column internals.

None of the methodologies discussed above provide a systematic design methodology for optimisation of crude oil distillation systems with preflash units that accounts for an extensive set of operating variables, heat integration and product quality.

2. Methodology

The aim of this work is to develop a systematic approach to design cost-effective, energy-efficient crude oil distillation systems with preflash units, accounting for product quality and heat integration. The approach builds on the simulation–optimisation technique of Caballero et al. (2005) for the design of distillation columns facilitated by an Aspen HYSYS–MatLab interface. A comprehensive set of degrees of freedom is used – including pump-around duties and temperature drops, stripping steam flow rates, the column feed inlet temperature and the preflash temperature. Rigorous simulation of the column is carried out within Aspen HYSYS v8.6. Product quality specifications are constrained, either within the simulation process or within the optimisation, using a penalty function. Heat integration is addressed by applying pinch technology: the grand composite curve is used to assess the minimum utility demand, i.e. for fired heating.

The crude oil distillation process is modelled using Aspen HYSYS; the crude oil models are well established in industrial practice and the rigorous distillation models have demonstrated their potential to provide highly accurate representations of this complex process. The models require both the process and column configurations to be fully defined. Using heater and coolers, rather than heat exchangers, allows the process simulation and the heat recovery analysis to be decoupled, which simplifies the simulation without compromising the evaluation of minimum utility consumption. For the configuration with a preflash unit, heating of the crude oil is modelled using two heaters – one representing the heating upstream of the preflash unit and the other representing the preheating of the flash liquid by heat recovery and fired heating.

The simulation model in Aspen HYSYS is linked to MatLab R2016a via an ‘automation’ interface that allows the user to send inputs to and collect outputs from the simulation package (AspenTech, 2010). Pinch analysis is carried out within MatLab given stream data (supply and target temperatures and duties). In this way the minimum utility targets can be re-calculated as column operating conditions are optimised.

Before the process is optimised, an initial converged simulation is required. Sensitivity studies facilitate understanding of trends in the system behaviour with respect to each design or optimisation variable. Optimisation bounds are defined using results of these sensitivity studies. Once the simulation model and the HYSYS–MatLab interface are set up, optimisation is carried out using embedded algorithms in MatLab and iterative updating of simulation results.

This study considers a fixed column design and a given set of products. The focus is on reducing the fired heat demand of the system. Optimisation variables are pump-around duties and temperature drops, stripping steam flow rates, column feed temperature and the preflash temperature. The objective function is the minimum hot utility demand, where the minimum hot utility demand is calculated using pinch analysis. Thus how operational variables impact on energy demand is systematically accounted for.

For the case with a preflash unit, the flash temperature is an important degree of freedom. Higher temperatures allow more vaporised crude oil to bypass the fired heater, increasing opportunities for heat recovery. In this work, the vapour is assumed to be mixed with the crude oil leaving the fired heater; future work will also consider the option of the vapour being introduced elsewhere in the column.

Product specifications are set within the simulation package. As there are insufficient degrees of freedom with the simulation to ensure that all product specifications are met, additional product quality specifications are defined as inequality constraints; the objective function is penalised if these constraints are violated.

Experience showed that non-linear optimisation techniques (such as fmincon in MatLab) frequently led to the optimisation reaching a local optimum. Therefore, stochastic optimisation is applied: simulated annealing is implemented in the MatLab R2016a Global Optimisation Toolbox as simulannealbnd. The simulated annealing algorithm requires the user to specify the initial annealing temperature and to choose an annealing function. The termination criteria for the optimisation are the maximum number of iterations and a tolerance in the objective function.

If an Aspen HYSYS simulation does not converge within a certain number of iterations, this can interrupt the optimisation process and significantly increase CPU time. Therefore, following the approach of Enríquez-Gutiérrez (2016), a penalty is applied to the objective function, identifying that particular simulation as having very poor results. Aspen HYSYS is then reset to the base case and optimisation continues.

3. Case Study

The case study is based on data in Watkins (1979). Figure 1 illustrates the crude oil distillation system. The crude oil system comprises an atmospheric distillation unit with a condenser, three pump-arounds and three side strippers and a preflash unit. The system processes 100,000 bbl day^{-1} (662.4 m^3 h^{-1}) of Venezuelan Tia Juana light crude oil. The unit produces five products: Light Naphtha (LN), Heavy Naphtha (HN), Light Distillate (LD), Heavy Distillate (HD) and Residue (RES). The unoptimised base case design is derived from a study by Chen (2008). Vapour leaving the preflash unit is mixed with the stream leaving the fired heater; the mixture is sent to the feed stage in the main column. Steam is utilised as a stripping agent in the main column and in the HD stripper. The HN and LD strippers use reboilers, rather than live steam. Product specifications are expressed in terms of ASTM T5 % and T95 % (in °C).

The optimisation is carried out as described in Section 2. The maximum number of iterations is specified to be 300 and the function tolerance is 1×10^{10}. The initial annealing temperature is 200 °C, and the annealing Boltzmann function is used.

A summary of optimisation results and bounds for operational variables obtained for the crude oil distillation system with and without a preflash unit is presented in Table 1. Optimisation runs took around 23 seconds of CPU time on an HP desktop PC with intel(R) Core i5 processor running at 3.20 GHz and 8 GB of RAM.

Table 2 presents results related to product quality in terms of ASTM T5 % and T95 % (in °C) for the crude oil distillation system with and without a preflash unit. It may be seen that the product quality constraints are all met within the allowed range of temperatures (±10 °C). Table 3 shows the results for the product flow rates in the two optimised cases. These results show that the product yields change relatively little, which is a consequence of the product quality being constrained. The hot utility demand of the crude oil distillation system decreases from 47 MW for the optimised based case to 45 MW for the optimised system with a preflash.

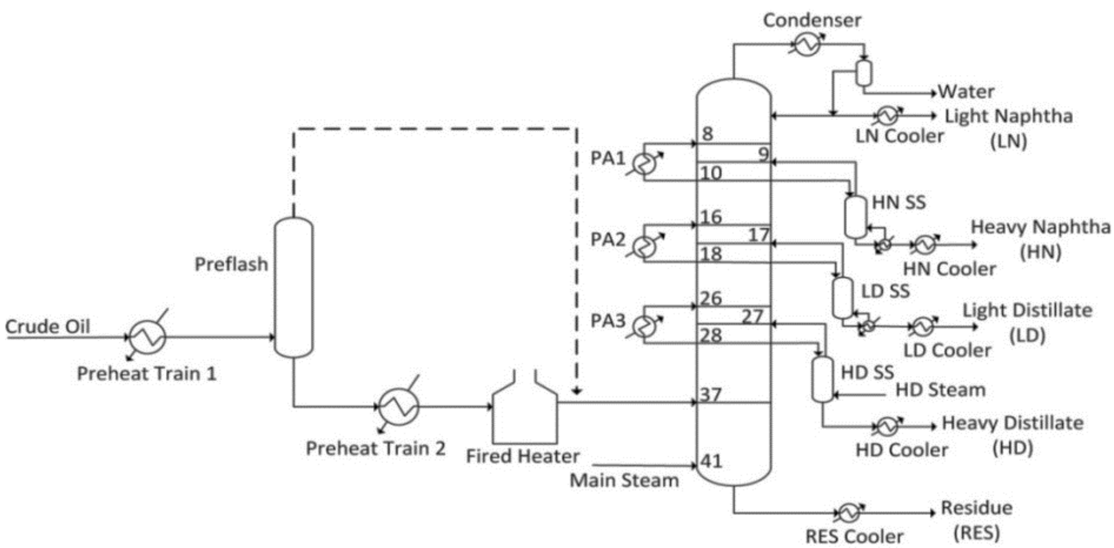

Figure 2 Crude oil distillation system with a preflash unit

Table 4 Summary of optimisation results and bounds for crude oil distillation system

Variable	**Units**	**Base Case**	**Lower Bound**	**Upper Bound**	**Optimisation Results**	
					No Preflash	With Preflash
Main Steam	kmol/h	1200	900	1800	1213	1194
HD Steam	kmol/h	250	200	375	245.8	264.7
PA1 Duty	MW	12.8	14	6	6.6	6.1
PA2 Duty	MW	17.8	18	6	11.3	8.3
PA3 Duty	MW	11.2	12	6	9.0	8.6
PA1 ΔT	°C	30	20	50	22.9	25.2
PA2 ΔT	°C	50	15	60	38.2	42.0
PA3 ΔT	°C	20	10	40	36.5	28.2
Column Inlet Temperature	°C	365	350	385	352.3	365.9
Flash Temperature	°C	185	180	230	–	199.8

Table 5 Product quality specifications

Product	Base Case ASTM (°C)		Optimisation Results No Preflash ASTM (°C)		Optimisation Results With Preflash ASTM (°C)	
	T5 %	T95 %	T5 %	T95 %	T5 %	T95 %
RES	363	754	359	753	355	752
LN	26	109*	25	109	25	109
HN	143	196*	133	196	133	196
LD	217*	300*	217	300	217	300
HD	308	353*	308	353	306	353

* Specified in HYSYS

Table 3 Product flow rates (in $m^3\ h^{-1}$)

Product	Base Case	Optimised No Preflash	Optimised With Preflash
RES	292.1	295.2	299.1
LN	102.4	100.9	100.9
HN	86.8	88.5	88.6
LD	127.6	127.3	126.2
HD	53.7	50.8	47.7

4. Conclusions

A systematic design optimisation approach is proposed for a crude oil distillation system with a preflash unit, starting with rigorous simulations and using the grand composite curve as a tool to estimate hot utility demand of the system. Results of adding a preflash within the distillation system demonstrate that the simulation-optimisation methodology proposed in this work is capable of reducing energy consumption in comparison with the base case, while maintaining product quality specifications. In future work, the simulation-optimisation design methodology will consider the vapour feed location in the main column, the column design and capital-energy trade-offs. The proposed methodology will be extended to consider design of crude oil distillation systems with other pre-separation arrangements, including more than one preflash unit or a prefractionation column.

Acknowledgement

The authors thank the Mexican National Council of Science and Technology (CONACyT) for the financial support granted for the development of this work.

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International Conference Presentations

1. European Symposium on Computer-Aided Process Engineering, ESCAPE-27, Barcelona, Spain, October 2017, oral presentation
2. 17th AIChE Annual Meeting, Minneapolis, USA, October 2017, oral presentation
3. 11th International Conference on Distillation and Absorption, Florence, Italy, September 2018.

National Conference Presentations

1. ChemEngDay UK 2015, University of Sheffield – poster presentation
2. CEAS PGR Conference 2015 – poster presentation
3. Process Integration Research Consortium, 2015 - poster presentation
4. ChemEngDay UK 2016, University of Bath –poster presentation
5. CEAS PGR Conference 2016 – poster presentation
6. Process Integration Research Consortium, 2016 – poster presentation
7. ChemEngDay UK 2017, University of Birmingham – poster presentation
8. CEAS PGR Conference 2017- oral presentation
9. Manchester Energy Conference 2017 - oral presentation
10. XV Symposium of Mexican Studies and Students in the UK 2017, University of Durham - oral presentation
11. Process Integration Research Consortium, 2017 – oral presentation
12. University of Yucatan Mexico, January 2018 – oral presentation
13. Process Integration Research Consortium 2018 – poster presentation

Prizes and awards:

- Best poster, Modelling and Simulation topic in 11th International Distillation & Absorption Conference 2018, Florence, Italy.

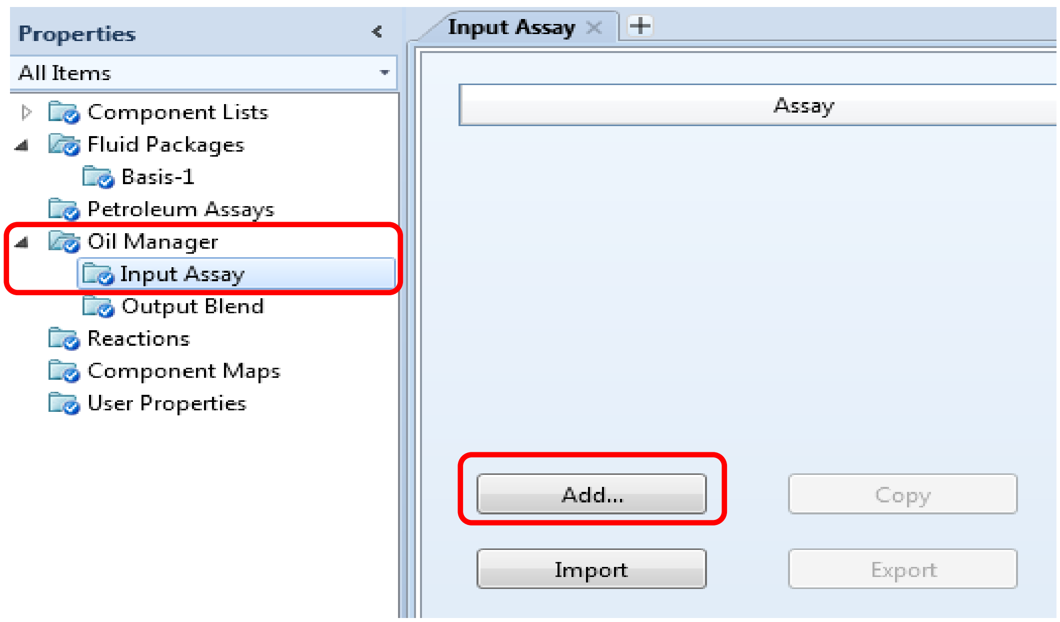
APPENDIX F

Crude Oil Characterisation Step by Step

Characterise the Assay

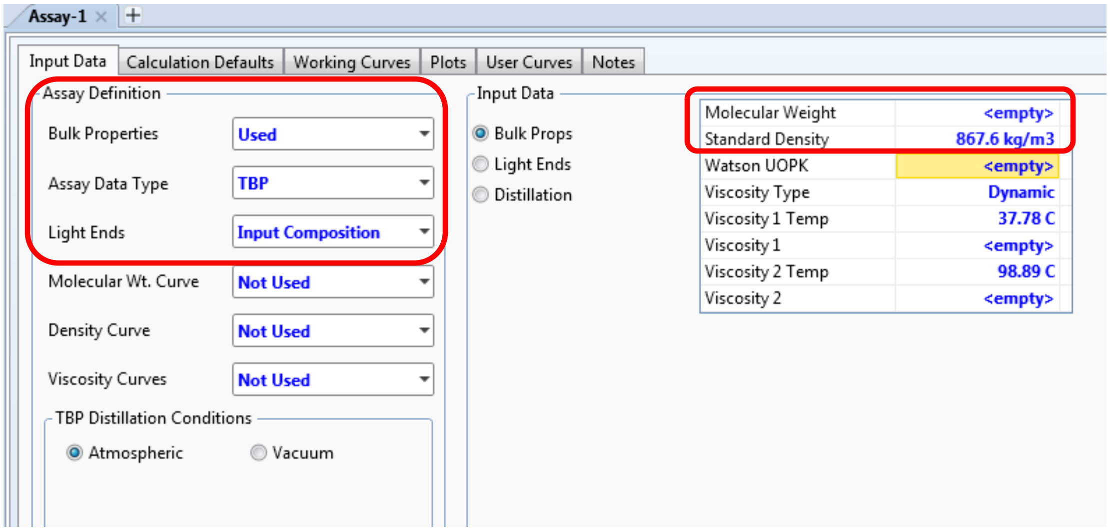
The assay contains all of the petroleum laboratory data, boiling point curves, light ends, property curves and bulk properties. HYSYS uses the Assay data to generate internal TBP, molecular weight, density and viscosity curves.

Step 1: Provide the Assay Data. Click on the Oil Manager tab to display the Input Assay and Output Blend folders. Click on the Add button.

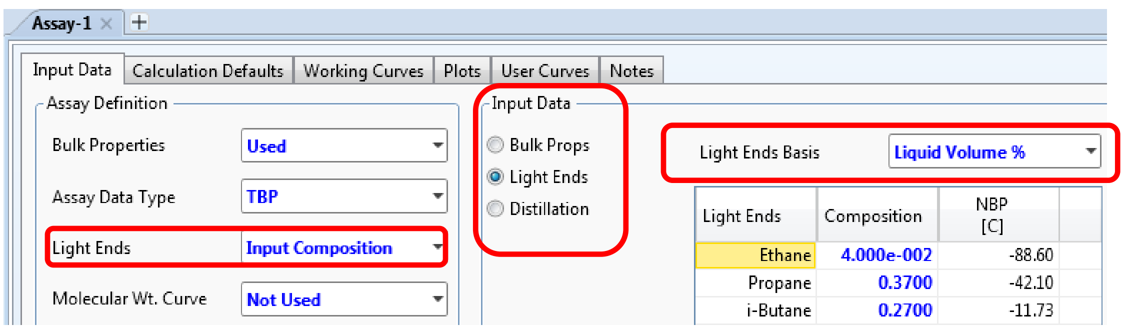


Step 2: Enter the values for Standard Density, Light Ends and data for the TBP curve.

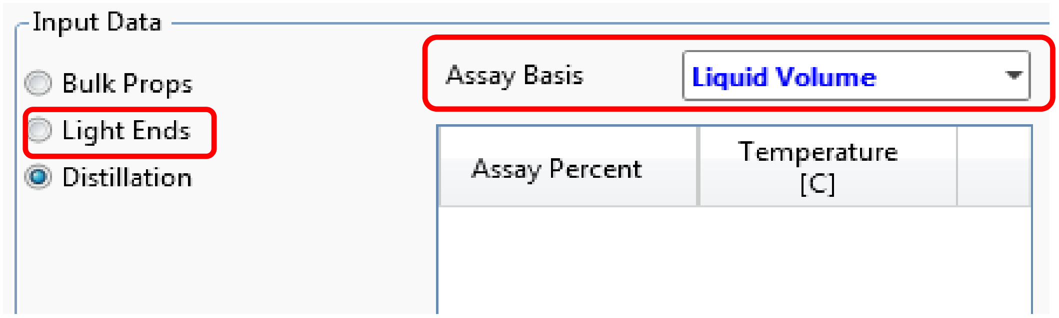
- Select the Assay Data Type as "TBP".

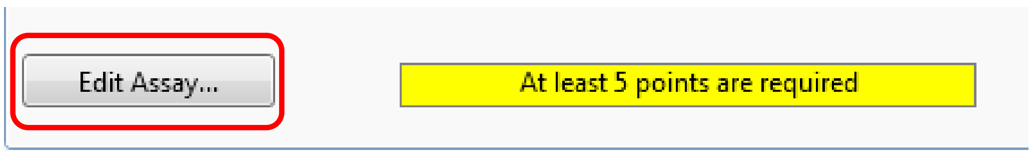


- **Light Ends:** Select "Input composition" within the Assay Definition Tab. Click on the ribbon for "Light Ends" in the Input Data group. Choose the Light Ends Basis as "Liquid Volume %". Finally, input the Light Ends data.

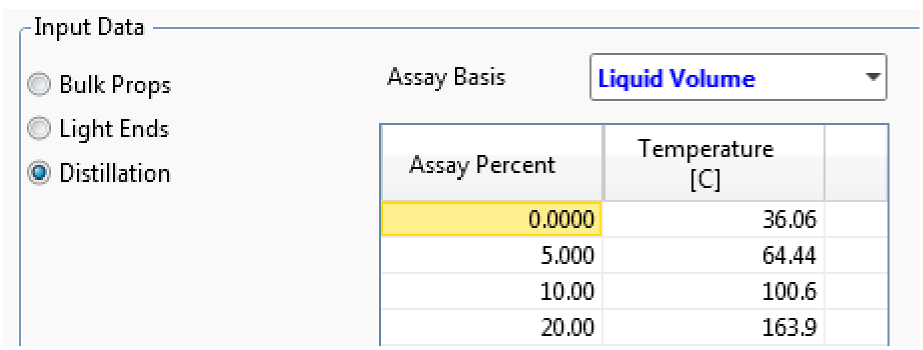


- **Distillation input** – in this part, enter the TBP data. To start, select the Assay Basis as Liquid Volume. Click on the Edit Assay Button.

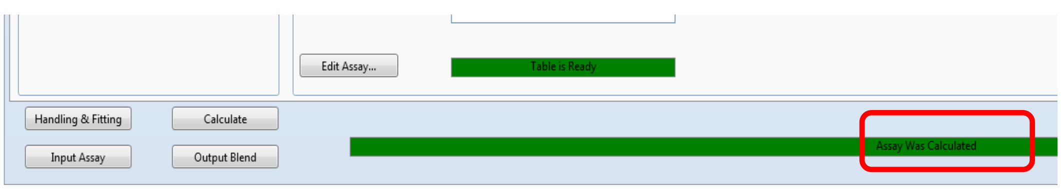




- Input the TBP information needed for the Assay:

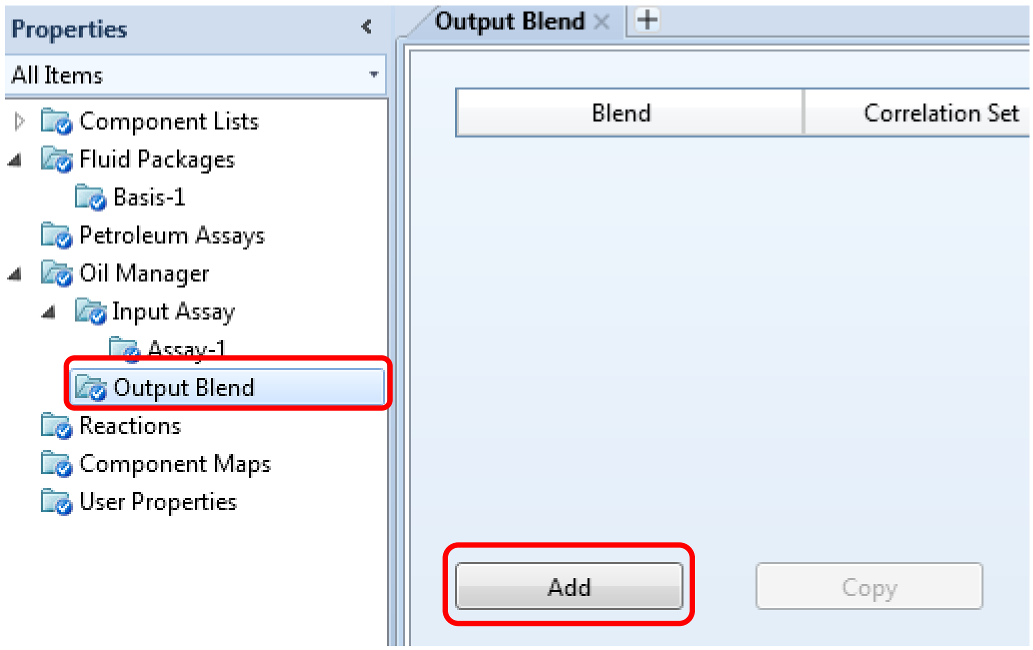


- Click the Calculate button. The status message at the bottom of the Assay view will change from “yellow” to “green” with the legend Assay Was Calculated.

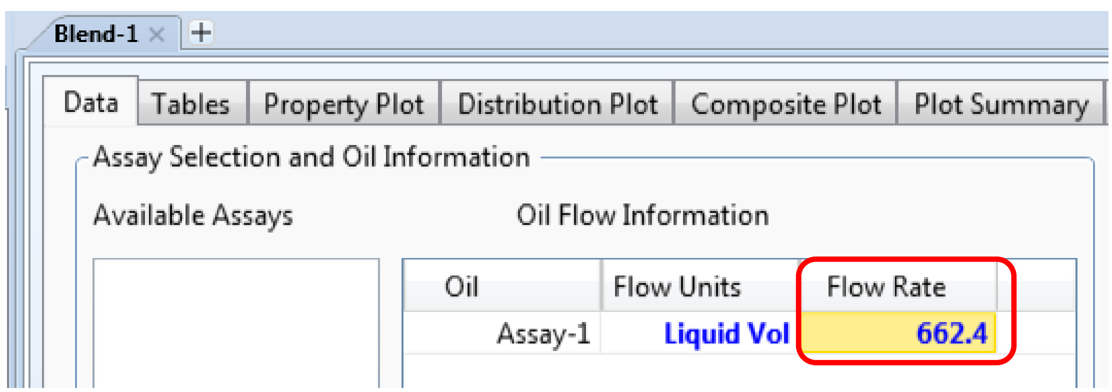


- Once the Assay is calculated, the working curves are displayed on the Plots and Working Curves tabs.

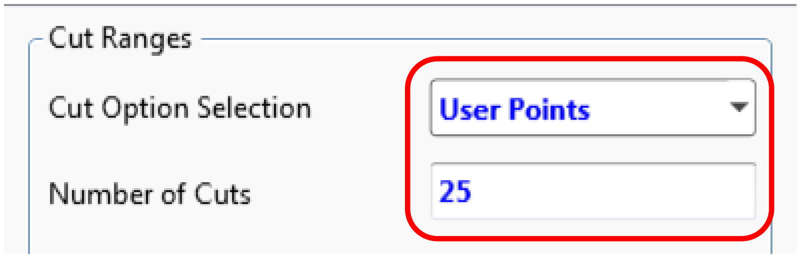
Step 3: Create a Blend to cut the Assay. The Output Blend characterisation in HYSYS splits the internal working curves for the assay into pseudo-components. To start, click on the Output Blend Tab then, click the Add button.



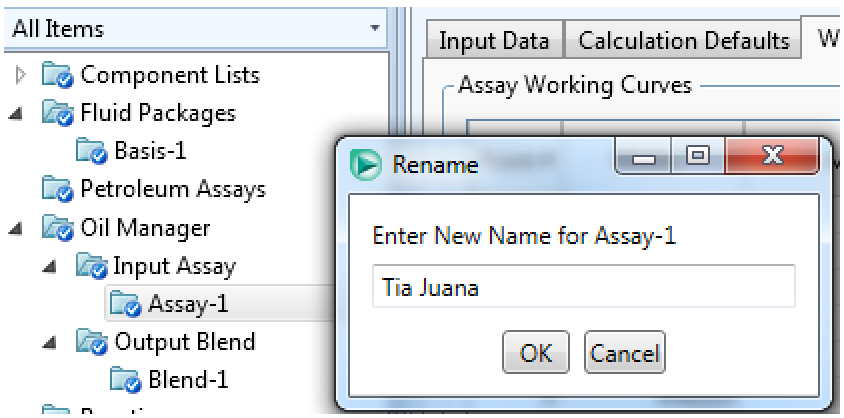
- Input the flow rate value:



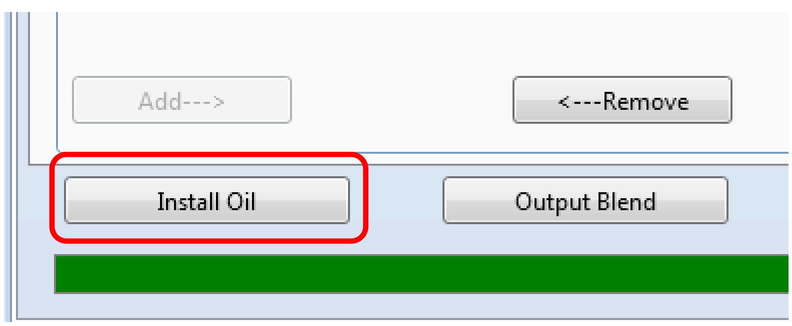
- Select User Points as a Cut Option Selection, and the Number of Cuts as follows:



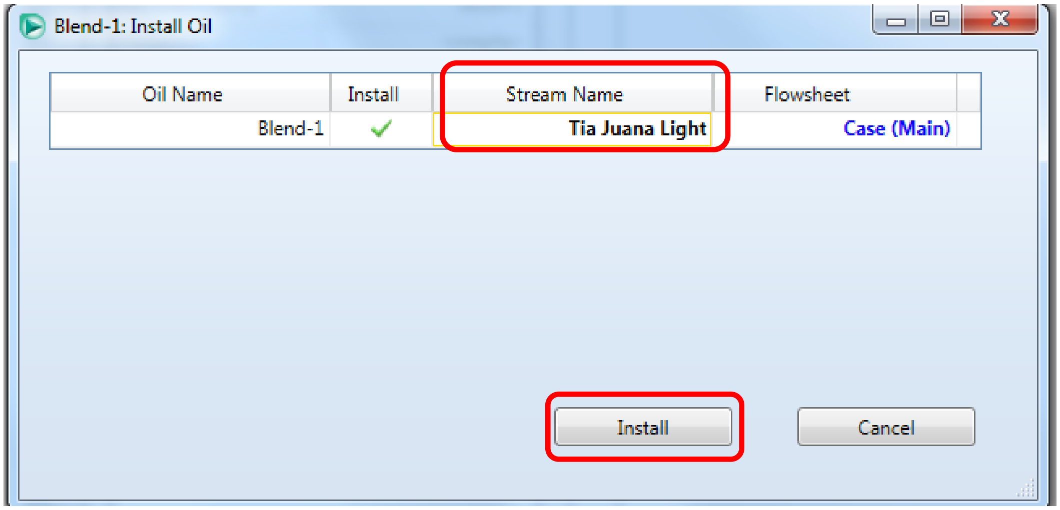
Results of the calculation can be viewed on the Tables and Property Plot Tabs. To rename the Assay, right click on the Assay-1 folder. Type the name for the Assay.



The final step of the characterisation is to install the pseudo-components in the Fluid Package. To install the oil in the simulation environment, click on the Install Oil Button.



In the Stream Name column, enter the name Tia Juana Light to which the oil composition will be transferred.



Aspen HYSYS will assign the composition of the calculated Oil and Light Ends into this stream, completing the characterisation process.

Reference:

AspenTech documentation (2007). Refining Tutorial. Aspen Technology Inc.: Burlington, MA.