DOCTORAL PROGRAM IN REFINING, PETROCHEMICAL AND CHEMICAL ENGINEERING (ENGIQ)

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ENERGY OPTIMIZATION OF MATOSINHOS REFINERY'S AROMATICS PLANT

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Dear Student,
Before you overthink,

"Your mind is lying to you.

You are about to hear a strange but true story.

Legend has it, Harry Houdini, the master magician once claimed that he could break out of any jail cell in the world. All he had to do was walking into that jail cell with his street close on. He said: "I´ll be out of there in one hour. No problem." Well, a very old jail, down South, heard about Houdini's claims and they accepted his challenge.

On the day of the event, many people gathered outside. Very confidently, Houdini walked right into the jail and into the cell and they shut the metal doors behind him. The first thing Houdini did was he took of his coat. Then, very strangely he took of his belt. Secretly hidden in Houdini´s belt was a ten inch piece of steel, very tough and very flexible and Houdini started working. In about 30 minutes, that confident expression Houdini had when walked in, disappeared. In one hour he was bathed in sweat. And at the end of two hours, Houdini in defeat collapsed against the door, which then opened.

It opened because you see, that door had never been locked. But that´s not entirely true, is it? That door was locked. It was firmly and thoroughly locked in Houdini´s mind. Which meant it was locked as if the best locksmith in the world had put his lock on it.

The mind his powerful. How many doors in your life do you think are locked but aren´t? How many times have you been stuck in the mental prison of overthinking? Something that really had a simple solution.

There is an ancient African proverb that says "when there is no enemy within, the enemy outside can do us no harm". Your mind is the most powerful force you will ever face. It will tell you lies. It will tell you can´t do that. You´re not meant for that. You´re not good enough for that. You can´t go on anymore. You don´t have the energy. You must thank for its opinion and carry on. Because like Houdini showed us, the only locked doors that exist are in your own mind. The doors in reality are open and all you have to do is walked through."

By Prince Ea
Motivational Speaker

Don´t let others opinions become your reality.
Vanessa Araújo

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At last but not the least, I would like to give a special thanks to my family for supporting me spiritually and mentally throughout this PhD road and for keeping me motivated and resilient until the end.

Abstract

The present work entitled "Energy Optimization of Matosinhos Refinery's Aromatics Plant" is integrated in the Doctoral Program in Refining, Petrochemical and Chemical Engineering (EngIQ) which started in the academic year 2014-2015. This PhD project was developed in the Aromatics Plant of Galp energia Matosinhos Refinery. Due to the energy intensive consumption of the several processes that comprise the Aromatics Plant, some reformulations are evaluated to achieve higher energy efficiency without changing operating processes or its respective operating conditions.

Pre-Distillation and Arosolvan Units are the two main process units of the Aromatics Plant that are analyzed in terms of energy savings. For this purpose, data was extracted from two years of operations, considering only the variables with direct influence on heat exchanger networks and from each process unit. Missing and incoherent data, including outliers, were removed from the data sets. A cluster analysis technique was then applied to each data set with the goal of identifying different clusters which describe process operational data in terms of representative operational scenarios. A global scenario considering the overall mean values of the extracted data was also considered. For all these scenarios, a process-level Pinch Analysis was performed to evaluate the potential of energy savings. These potentials were compared concluding that there is no significant difference in terms of energy savings and thus, only global scenario was considered for further analysis.

A site wide energy performance analysis was also performed considering direct and indirect heat integration tools. Through direct heat integration, a single grand composite curve comprising both process units as one single unit was constructed to estimate energy targets without taking into consideration intra-process heat integration. Total Site Analysis using total site profiles was then applied to evaluate indirect heat integration using intermediate utilities to evaluate heat recovery opportunities after intra-process heat integration has taken place within each process unit. The overall results obtained with both approaches were considered unworthy and do not justify being considered in further analysis to find retrofit solutions due to the investment costs involved to overcome the drawbacks of battery limits and the distance between the process units.

Retrofit methods using heuristic rules and a hybrid methodology, combining Pinch Analysis and mathematical programming tools, were applied to eliminate the inefficient zones of energy consumption of the heat exchanger networks in both process units. The retrofit solutions were compared and the best solution was selected based on total capital cost and payback period.

Key Words: Aromatics Plant, Heat Process Integration, Pinch Technology, Total Site Heat Integration, Retrofit Methods, Heuristic Rules, Hybrid Methodology.

Resumo

O presente projeto aborda o tema "Otimização Energética da Fábrica de Aromáticos da Refinaria de Matosinhos", integrado no Programa Doutoral em Engenharia da Refinação, Petroquímica e Química (EngIQ) iniciado no ano académico 2014-2015. Este projeto foi desenvolvido na Fábrica de Aromáticos da Refinaria de Matosinhos da Galp energia, que é consumidora intensiva de energia devido aos seus processos envolvidos, sendo por isso necessário implementar estratégias de melhoria e avaliar reformulações para reduzir os consumos energéticos e custos operatórios.

A Unidade de Pré-Distilação e a Unidade Arosolvan são as unidades da Fábrica de Aromáticos que serão analizadas em termos de poupanças energéticas. Para este efeito, efetuou-se a extração de dados operacionais em média diária de ambas as unidades processuais referente a um período de dois anos. Estes dados operacionais incluem as variáveis que directamente influenciam a rede de permutadores de calor. Para cada matriz de dados foi aplicada uma técnica de análise de agrupamentos com o objectivo de identificar diferentes grupos de dados operacionais (agrupamentos) que representem possíveis diferentes cenários de operação. Um cenário global representado pela média global dos dados extraídos foi igualmente considerado. Para todos estes cenários efetuou-se uma Análise do Ponto de Estrangulamento ao nível processual para avaliar os potenciais de poupança energética. Da comparanção destes potenciais entre todos os cenários resultou uma diferença pouco significativa e, por isso, apenas o cenário global foi considerado nas análises seguintes do estudo.

Uma análise do desempenho do consumo energético considerando a integração de calor directa e indirecta das duas unidades processuais foi igualmente efectuada utilizando as ferramentas adequadas para cada método. Para uma avaliação da integração de calor direta, considerando as duas unidades processuais como uma única unidade, foi analisada uma única grande curva composta para estimar os consumos mínimos de utilidades sem considerar a integração energética intra-processual. Mais ainda, uma análise de integração de calor indireta por utilização de fluídos intermédios foi efetuada para identificar oportunidades de recuperação de calor após considerar a integração energética intra-processual. Os resultados obtidos por ambas as abordagens demonstraram serem pouco significativos em termos de poupança energética, não justificando uma progressiva análise de melhorias de modificações das redes de permutadores de calor devido aos custos de investimento envolvidos nos novos equipamentos e tubagens para utlrapassar as limitações das fronteiras das unidades processuais, bem como as distâncias a abranger entre as mesmas.

Por conseguinte, métodos de reformulação considerando regras heuristicas e uma metodologia híbrida, combinando a Análise do Ponto de Estrangulamento e a metodologia sequencial de modelos de programação matemática, foram aplicados para eliminar as zonas ineficientes de consumo de energia das redes de permutadores de calor das duas unidades processuais. As soluções de reformulação encontradas foram comparadas entre si utilizando o custo total de capital e o período de retorno do investmento como critérios económicos.

key Words: Fábrica de Aromáticos, Integração de Calor de Porcessos, Análise do Ponto de Estrangulamento, Integração Global, Metodos de Refomulação, Regras Heurísticas, Metodologia Híbrida.

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Nomenclature

Symbol	Description	Units
A	Heat Transfer Area	m^2
A_{MIN}	Minimum heat transfer area	m^2
BI	Bromine Index	
BT	Benzene, Toluene	
BAT	Best Available Techniques	
BTX	Benzene, Toluene, Xylenes	
cp	Heat capacity	kJ/(kg.ºC)
C_p^0	Purchase cost of new equipment	€
CC	Composite Curve	
CS	Carbon Steel	
CCC	Cold Composite Curve	
CAPEX	Capital Cost	€/year
CCRU	Continuous Catalyst Regeneration Unit	
CEPCI	Chemical Engineering Plant Cost Index	
COLO	Coke Oven Light Oil	
DBC	Davis-Bouldin Criterion	
CBM	Bare Module Cost	€
DWC	Divided-wall Column	
CP	Cold process streams	
CW	Cooling Water	
CU	Cold utilities	
EB	Ethylbenzene	
ED	Extractive Distillation	
EMAT	Exchange Minimum Approach Temperature	ºC
F	Mass Flowrate	kg/hr
F_P	Factor Pressure	
FCC	Fluid Catalytic Cracking	
GCC	Grand Composite Curve	
GGE	Green Gas Emission	
GAMS	General Algebraic Modelling System	
H	Enthalpy	MW
h	Individual heat transfer coefficient	kJ/(m^2.hr.ºC)
HI	Heat Integration	
HP	Hot process streams	
HU	Hot utilities	
HP Steam	High pressure steam	
HCC	Hot Composite Curve	
HDA	Hydrodealkylation	
HEN	Heat Exchanger Network	
HRAT	Heat Recovery Approach Temperature	ºC

IEA	International Energy Agency	
$K_{optimal}$	Optimal number of clusters	
LP	Linear Programming	
LP Steam	Lower-pressure steam	
LLE	Liquid-liquid extraction	
LNG	Liquified Natural Gas	
LPG	Liquified Petroleum Gas	
LMTD	Logarithmic Temperature Difference by Patterson approximation	ºC
m	massic flow	kg/hr
MD	Mahalanobis Distance	
MP Steam	Medium pressure steam	
MX	Methaxylene	
MCp	Heat Capacity Mass Flowrate	kJ/(kg.ºC)
MER	Maximum Energy Recovery	MW
MEG	Monoethylene Glycol	
MILP	Mixed-Integer Linear Programming	
MINLP	Mixed-Integer Nonlinear Programming	
N_{MIN}	Minimum number of heat exchangers	
NHT	Naphtha Hydrotreatment	
NFM	N-formyl-morphylane solvent	
NLP	Nonlinear Programming	
NMP	N-methyl-pyrrolidone solvent	
OX	Orthoxylene	
OPEX	Operating Cost	€/year
PI	Process Integration	
PBP	Payback Period	years
PFD	Process Flowsheet Diagram	
P&ID	Process and Instrumentation Diagrams	
Pygas	Pyrolysis gasoline	
PNA	Paraffins, Naphthenes, Aromatics	
PONA	Paraffins, Olefins, Naphthenes, Aromatics	
PTA	Problem Table Algorithm	
PX	Paraxylene	
Q	Heat Load	MW
$Q_{C,\ min}$	Minimum cold utility	MW
$Q_{H,min}$	Minimum hot utility	MW
QS	Heat Load of Hot Utility	
QW	Heat Load of Cold Utility	
R_k	Heat residual heat load	MW
SVC	Silhouette Value Criterion	
SSSP	Site Source-Sink Profiles	
T	Temperature	ºC
TI	Temperature Interval	ºC

T_{INLET}	Inlet Temperature of a Stream	ºC
T_{OULET}	Outlet Temperature of a Stream	ºC
TAC	Total Annualized Cost	€/year
TSP	Total Site Profiles	
$T_{DEWPOINT}$	Dew point temperature	ºC
$T_{BUBLEPOINT}$	Buble point temperature	ºC
TA	Transalkylation	
TIAT	Temperature Interval Approach Temperature	ºC
TDI	Toluene Diisocyanate	
TDP	Toluene disproportionation	
T-H	Temperaute - Enthalpy diagram	
THDA	Thermal Hydrodealkylation	
ToAlk	Toluene alkylation	
TSHI	Total Site Heat Integration	
VOC	Volatile Organic Compounds	
U	Global Heat Transfer Coefficient	W/(m^2.ºC)
ΔT_{LM}	Logaritmic temperature difference	ºC
ΔT_{min}	Minimum temperature difference	ºC
ʎ	Enthalpy of vaporization or condensation of a phase change	kJ/kg

Chapter 1: Project Introduction and General Framework

The present PhD project, entitled "Energy Optimization of Matosinhos Refinery's Aromatics Plant", is integrated in the Doctoral Program in Refining, Petrochemical and Chemical Engineering (EngIQ). The project was developed in Matosinhos Refinery's Aromatics Plant of Petrogal S.A., Galp energia. The Aromatics Plant handles several processes that require high energy demands. An evaluation of potential of energy savings and the required reformulations is performed to improve processes energy efficiency and operating costs.

1.1. Galp energia - Matosinhos Refinery of Petrogal S.A.

Galp energia is a portuguese Oil & Gas company focused on crude oil exploration and production, refining and treatment processes, and also manufacturing process units. As shown in Figure 1.1, Galp energia is present worldwide in four continents: Europe (Portugal and Spain), South America (Brazil, Uruguay, and Venezuela), South Africa (Angola, Mozambique, Cape Verde, Guinea-Bissau, Swaziland, Gambia, and Equatorial) and Asia (East Timor) (Galp energia, 2014).

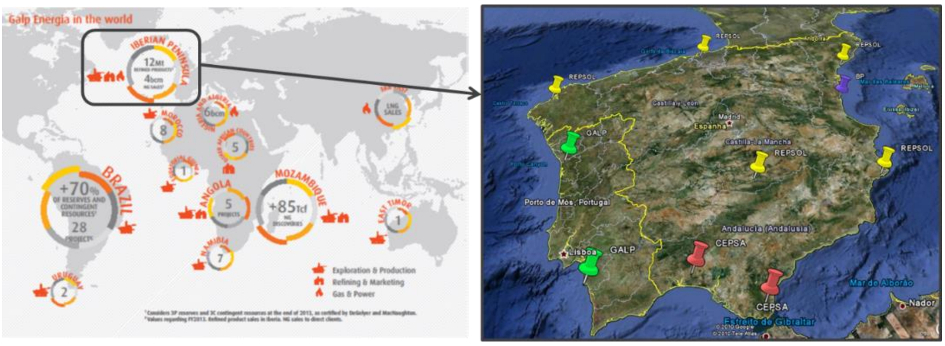


Figure 1.1: Galp energia worldwide (Galp energia, 2014).

In the oil industry, the process value chain of transitioning and transforming raw materials into valuable final products is divided in three steps: upstream, midstream and downstream. Upstream is the part of the process responsible for exploring, extracting and producing crude oil and natural gas from the reservoirs. Exploration and production activities are located in three core countries: Brazil, Angola and Mozambique. Midstream is a combination of crude refining processes for transforming crude oil into sub-products that can be used for many activities. Galp energia has two refineries in Portugal, as shown in Figure 1.1, one in Oporto and another one in Sines. Downstream is the process of marketing and distribution of refined products to consumers (Galp energia, 2014).

Matosinhos Refinery of Petrogal S.A. is located in Oporto city, Portugal, and it started operating in 1961. Since then has been upgraded to keep up with technology and market developments. It has a total annual capacity to refine 5.5 million tonnes per year of crude oil. Crude oil is a complex mixture of hydrocarbons associated with certain impurities (sulphur compounds, nitrogen compounds, oxygen compounds) that must be removed to obtain the different products with market value such as fuels, base oils, lubricating oils, petroleum waxes, paraffins, bitumens and the main raw materials for the petrochemical industry. The production capacity of the different products are presented in Table 1.1 (Galp energia, 2013, 2015).

Table 1.1: Production capacity or treatment of Matosinhos Refinery (Galp energia, 2013, 2015).

Product	Production Capacity (tonnes/year)
Fuels	3,700,000
Based Oils	150,000
Aromatics and Solvents	440,000
Bitumens	150,000
Petroleum waxes	12,000
Lubricants	26,350
Sulphur	10,000

The characteristics of the different crude oils are directly related to its origin and composition, which have a great impact in the refinery production management to respect quantitative and qualitative demands of the market. The industrial complex can be summed up into three sections: Refining and Treatment Processes, Manufacturing Process Units and Utilities Production System.

Refining and Treatment Processes are very complex and dictate the diversity and characteristics of the different products. There are three main groups of processes, which dictate the diversity and characteristics of the different products:

- Separation processes that allow physical separation of products, based on differences in their boiling points, densities and solubilities (distillation, fractionation and extraction with solvents);
- Chemical reactions occurring at certain temperature and pressure, that allows the molecular transformations needed to obtain the desired products with specific characteristics, and using catalysts to accelerate the process;
- Chemical and/or physical treatments, which are used to improve the quality and purity of the final products by eliminating its impurities.

Manufacturing Process Units integrate the production processes needed to obtain the final products. There are four main industrial complexes: the fuels plant, the base oils plant, the aromatics plant and, completing the productive line of the refinery industrial complex, the lubricants plant where the main operation is the stocking (mixing) of components.

Refining and Treatment Processes, as well as Manufacturing Process Units, are sustained by a common Utilities Production System that is responsible for the production and distribution of different utilities and types of energy. This installation is responsible for running process equipment, for generating steam, and for supplying heating to the different process units.

The Aromatics Plant of Matosinhos Refinery is one of the Manufacturing Process Units integrating the chemical complex, and provides basic molecules to be used by the petrochemical industry, namely benzene, toluene and xylenes. Besides increasing business competition in terms of valuable final products in the national and worldwide market, Galp energia promotes innovation, investigation and development of technology for increasing the sustainability, energy efficiency of process units and for reducing their environmental negative impact.

1.2. Aromatics as Building Blocks of Petrochemical and Chemical Industries

Aromatics are intermediate products used as basic building blocks of petrochemical industry, being the most important the benzene, the toluene and the xylenes (BTX). Three types of feedstocks are used to produce aromatics (Figure 1.2): pyrolysis gasoline (pygas), which is a co-product of ethylene plants, reformate from petroleum naphthas, obtained through catalytic reforming processes used in gasoline production, and light oil from coke oven plants (COLO). From these three types of raw materials, reformate or reformed naphtha accounts for 70 % of total world aromatics supply. Paraffins, olefins, naphthenes and aromatics (PONA) with 6-12 carbon atoms, generally compose heavy naphtha distillate fraction. The percentage of PONA in heavy naphtha depends on the type and origin of crude oil (Forzatti, 2006; Johnson, 2004; Jones, 2006; Matar and Hatch, 2000).

The main difference between these feedstocks is in its composition relative to a specific aromatic. The composition of pygas changes widely with the type of its feedstock. Liquefied natural gas (LNG) produces a pygas that is rich in benzene but poor in xylenes, while pygas from ethylene plants, processing naphta and heavier feedstocks, has substantial amounts of xylenes. Also, pygas provides higher amounts of benzene than reformate and thus it is an important source for benzene production. Moreover, pygas can also be combined with reformate before being fed to an aromatics complex. On the other hand, reformate obtained from heavy naphtha is richer in xylenes than pygas and thus para-xylene production is based on reforming petroleum naphtha. Hydrocraked naphtha is produced in the refinery by cracking heavier streams in the presence of hydrogen. This hydrocraked naphtha is rich in naphthenes, which makes it an excellent reforming feedstock. Straight-run naphthas are more available in the market than hydrocracked naphtha, but are thoroughly hydrotreated before being used as feedsources in aromatics complexes. However, this pretreatment is not as severe as the pygas pretreatment (Johnson, 2004). In some regions of the world, there is no sufficient heavy naphtha and thus non-traditional sources for aromatics production are used. Among the non-traditional sources are condensate from gas field, methanol from liquid petroleum gas (LPG), fluid catalytic cracking (FCC) gasoline fractions, and olefins fraction of FCC gasoline. Nowadays, some of these non-traditional feeds are becoming more competitive relative to the traditional ones (Gentry, 2015).

Products derived from benzene, toluene and xylenes are discriminated in Figure 1.2. These colourless liquids with a characteristic smell are hydrocarbons with one or more benzene rings used as important chemical precursors that can be converted into many products of our daily basis such as clothing, packaging, paints, adhesives, computers, compact discs and sports products (CEFIC, 2014).

Benzene, besides being extracted from the three mentioned main sources, can also be derived from toluene and heavy aromatics conversion processes. The largest derivative from benzene, with a 45 % share (Figure 1.2), is ethylbenzene, which is an intermediate used in the production of styrene that is further converted into materials such as polystyrene. Cumene is the second most important derivative from benzene, with a 20 % share, and is the main precursor of phenol.

Xylenes are a mixture of xylene isomers (para-xylene (PX), ortho-xylene (OX), and meta-xylene (MX)) extracted or distilled from gasoline refining. Mixed xylenes can be used as solvents and in the printing, rubber, and leather industries. They are also a desirable gasoline component, but are blended less often than toluene because there is greater demand and higher value in their chemical applications.

Xylene is mainly supplied as a mixed stream but there are several processes used to separate the individual isomers for specific end-uses. Para-xylene is used as a feedstock for terephthalic acid, a key component in polyethylene terephthalate (PET) resins. Ortho-xylene is used in plasticisers, medicines, and dyes.

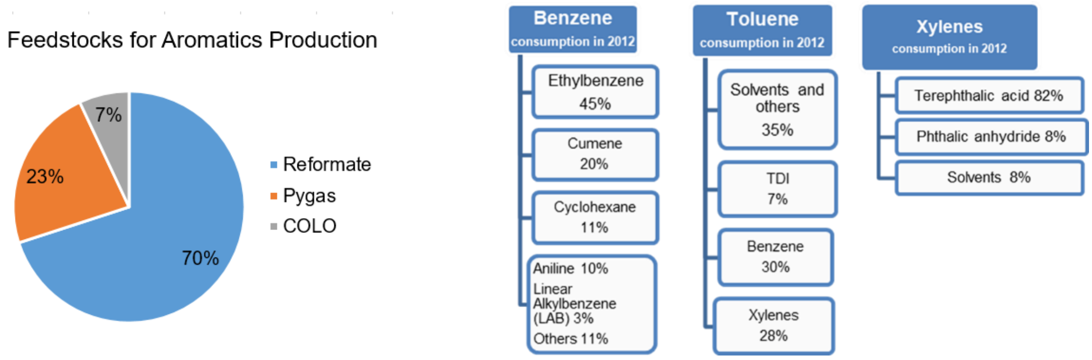


Figure 1.2: Main feedstocks for aromatics production and main derivative products from benzene, toluene and xylenes (Bender, 2013; European Commission, 2003).

Toluene obtained from gasoline manufacturing streams is used to produce one of three grades of purity in very large quantities: toluene diisocyanate (TDI) grade, nitration grade and commercial grade. TDI grade toluene is used to produce isocyanates, which are mixed with polyols in the manufacture of polyurethanes. In turn, polyurethanes are used in a wide variety of consumer goods. Nitration grade toluene is used as solvent and also in the production of phenol. Both nitration and commercial grades are used as feed in the hydrodealkylation process to convert toluene into benzene and in the disproportionation process to convert toluene into both benzene and xylenes. Although benzene and xylenes market demands are higher than for toluene, it is toluene that is produced in higher quantities. Therefore, toluene is becoming a valuable source for additional production of benzene and xylenes through conversion processes. In addition, the low volatility of toluene makes it a good octane-enhancer for gasoline blending (Bender, 2013; European Commission, 2003; Fahim *et al.*, 2010).

1.3. Aromatics Market Overview

BTX (benzene, toluene and xylenes) are among the major chemicals produced and marketed by Galp energia, which is the leader of national market. Regarding the production profile of Galp energia, diesel and gasoline continue to be the products with the highest production (38 % and 23 %, respectively) and aromatics the lowest production with 3 %, as shown in Figure 1.4. The production of aromatics has its ups and downs as described through Figure 1.5. The aromatics market is directly driven by the demand of manufacturer industries such as petrochemical and chemical industries demands (Galp energia, 2013, 2015, 2017).

The global aromatics market is expected to grow at moderate annual increment and manufacturing is increasingly shifting towards Asia Pacific region. China is the largest contributor and currently accounts for nearly half of the global production of aromatics. While the production growth has been very high in Asia Pacific region, global consumption is expected to slow down due to economic slowdown of many developing and developed countries. Thus, aromatics operating rates might decline in the future leading to lower margins and pressure on higher cost producers.

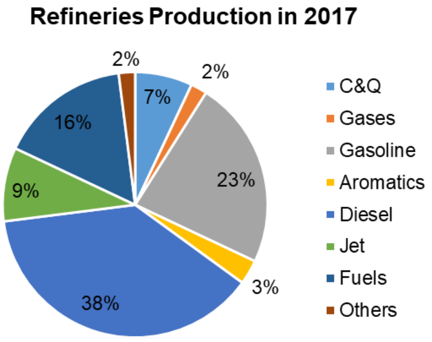


Figure 1.3: Refineries production (Galp energia, 2017).

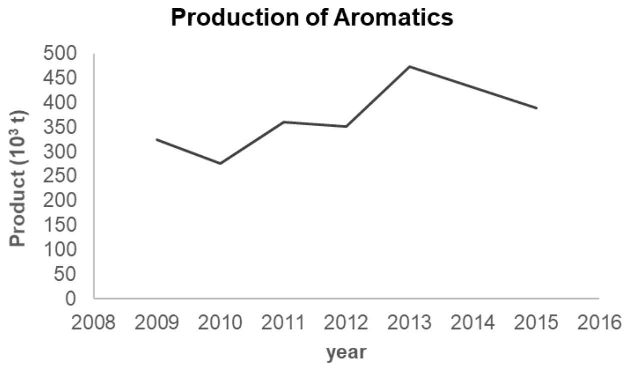


Figure 1.4: Production of aromatics in Matosinhos Refinery (Galp energia, 2013, 2015).

Asia has become the leader of the aromatics market, as well illustrated by the charts of Figure 1.5. In 2013, Asian producers have a benzene market share of more than 40 % (Figure 1.6, left). Asia and China in particular are also leaders on the demand side, being expected an increase of 19 million tonnes of PX demand in China (more than 63 % of the global expected demand increase, which is 30 million tonnes). On the contrary, benzene global production and Western Europe production have decreased along the years. PX demand is expected to be approximately constant in Europe until 2024 (CEFIC, 2014; Guangdong, 2014; Hodges, 2014).

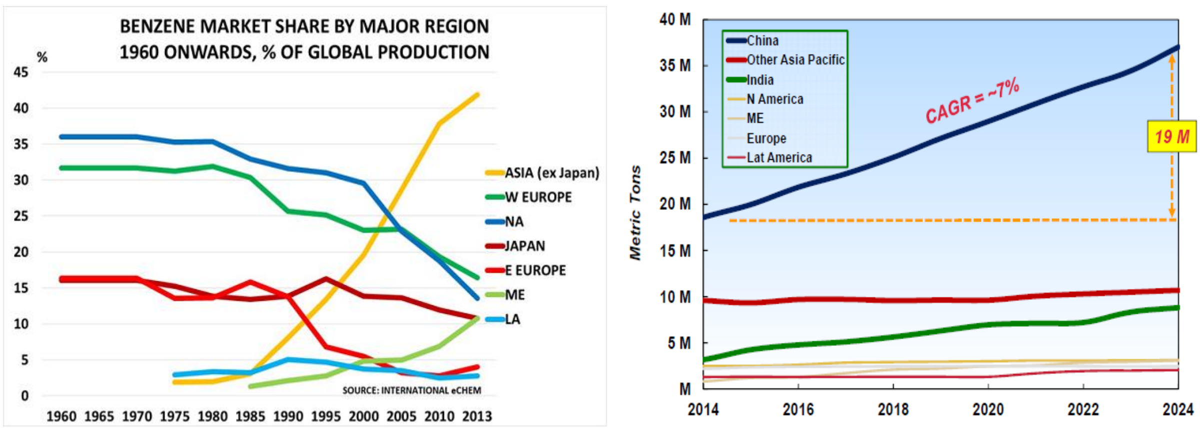


Figure 1.5: Benzene global market share by region (left) and para-xylene demand prediction (right) (Guangdong, 2014; Hodges, 2014).

Global aromatics market forecasted for 2027 indicate that Eastman Chemical, Ashland, BASF SE, Huntsman Corporation, Celanese Corporation, Petrochem Carless, INEOS AG, ExxonMobil, Royal Dutch Shell and Honeywell are and will be prominent players at the forefront of competition in the global aromatics market. The rapid growth in major economies and demand from the petrochemicals sectors have contributed to an increase in world oil demand. An increase of 1.6 % (or 1.5 million barrels a day) in 2017 in world oil demand was noted, a rate that is higher than the annual average of 1 % seen over the last decade (IEA, 2017).

1.4. The role of Energy Efficiency in Refining and Petrochemical Industry

Energy consumption is driven by the demands of the manufacturing industries and it has a global increase of 2.1 % in 2017, which is more than twice the growth rate noted in 2016, being China and India responsible for 40 % of this growth. Together, global energy-related CO_2 emissions grew by 1.4 % in 2017, achieving the highest value of 32.5 gigatonnes, a resumption of growth after three years of global emissions remaining constant.

The increase in world energy demands leads to an increase in efforts and investments in order to improve the efficiency of energy use in process industries. Even in the most energy efficient refineries, energy consumption is responsible for more than 55 % of operational costs. However, due to a weaker improvement in efficiency policies coverage, as well as to lower energy prices, energy efficiency was neglected and improvements slowed down dramatically in 2017. Global energy intensity (defined as the energy consumed per unit of economic output) only decreased 1.7 % in 2017, compared with an average of 2.3 % over the three previous years, and half of what is required to remain on track with the Paris Agreement (Figure 1.6).

Energy intensity and carbon intensity (defined as CO_2 emitted per unit of energy consumed) are the two drivers of carbon emissions. While global carbon intensity declined less in 2017 than in 2016, the rate remains similar to the average rate of improvement in 2014-16, due to the increasing expansion of renewables. However, the slower improvement in energy intensity in 2017 was not sufficient to counteract the effect of higher economic growth, leading to the increase in global energy related carbon emissions in 2017 (IEA, 2017).

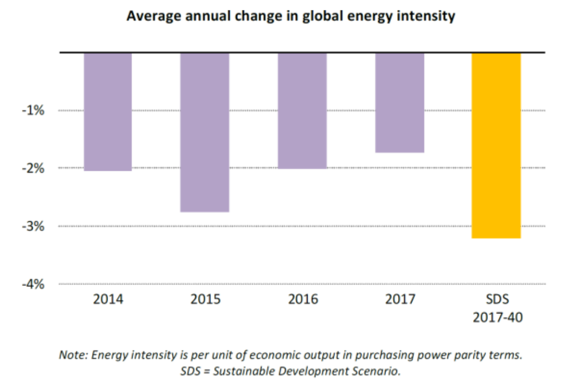


Figure 1.6: Average annual change in global energy intensity (IEA, 2017).

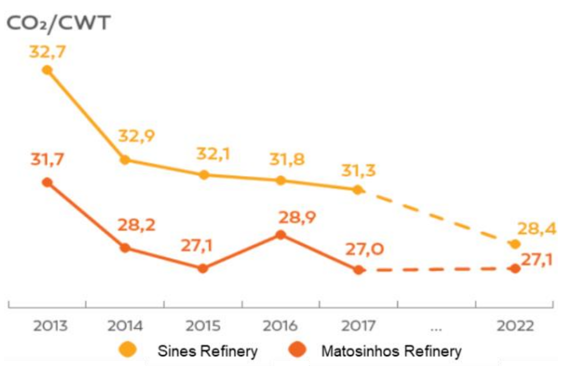


Figure 1.7: Carbon emissions (CO_2) per complexity weighted tonne (Galp energia, 2013).

Integrated in the world energy intensity panorama, Galp energia invests in innovation, technology and development to achieve high-energy efficiency in its process operations by using energy in a more sustainable way. Galp energia works to reduce the carbon intensity in refining as shown in Figure 1.7. The Matosinhos Refinery has been in the first reference quartile Solomon since 2015 in energy efficiency. By 2020, Galp investments in eco-efficiency projects will result in a 25 % reduction in carbon intensity at the Sines Refinery and 15 % reduction at the Matosinhos Refinery, compared to 2013.

1.5. Objectives and Methodology

Any Aromatics Plant is an energy intensive consumer as it handles processes that require high energy demand. These processes have auxiliary equipment, such as heat exchanger networks, that enhance heat transfer and energy consumption. Energy consumption will also depend on the extent of heat integration and technology being used. Therefore, it is important to create innovative solutions, to adapt advanced technologies and implement optimization strategies to reduce energy consumption.

This PhD project aims to evaluate possible reformulation scenarios of Matosinhos Refinery's Aromatics Plant to increase its energy efficiency and to achieve higher performance, in terms of energy consumption and operating costs. The Matosinhos Refinery's Aromatics Plant comprises two process units (Pre-Distillation Unit and Arosolvan Unit) that are here subjected to an energy performance evaluation and energy optimization studies through the application of different methodologies with the aim to minimize energy consumption and to improve energy efficiency of the process units. These methodologies comprise different areas such as process modelling, simulation and optimization.

To evaluate the behaviour of the two process units in terms of energy consumption, the required data is extracted and pre-treated removing mainly missing data and possible outliers using SPSS Software. A multivariate statistical technique in the group of clustering analysis coupled with optimal clusters evaluation criteria is applied using MATLAB Statistical Toolbox to identify different operational scenarios (clusters or groups) within each process unit to be used in further energy performance evaluation and to determine the potential of energy savings. These potentials are obtained comparing the actual energy consumption and the minimum energy consumption for each operational scenario considered (clusters).

One of the strategies included in this work for an accurate energy performance evaluation is Heat Process Integration using Pinch Technology to achieve a more efficient way to use energy resources. This strategy not only focus on energy integration, but includes a group of other strategies to configure and integrate the different processes. A process-level Pinch Analysis is carried out to estimate the minimum energy requirements (energy targets) for each process unit considering the different operational scenarios and using Pinch Analysis graphical tools obtained through Aspen Energy Analyzer. These energy targets will be compared to the actual energy consumption within each process unit that are also estimated for the different operational scenarios through process modelling and simulation using Aspen Plus. Established the maximum heat recovery that it is possible to be achieved, and determined by energy savings, both process units will go through a heat process integration applied in heat exchangers networks to reduce external utilities consumption and thus, achieve a heat exchanger network with minimum energy requirements. For this purpose, the inefficient zones of energy consumption within heat exchanger networks of each process unit are identified and eliminated through the implementation of different retrofit methods to achieve maximum heat recovery. The energy evaluation study is then extended to a site wide heat recovery evaluation by considering the whole site of the Aromatics Plant and thus, integrating both process units. Total Site Heat Integration strategies are applied to determine the maximum heat that is possible to be recovered by considering the two process units as a single unit or through the use of intermediate fluids.

An energy optimization study using mathematical programming tools are also applied in this work with the aim to obtain heat exchanger networks with minimum energy requirements (operating costs) and with minimum investment costs. Mathematical programming tools are here considered as an alternative approach to implement retrofit methods and obtain different network structures with minimum investment costs considering energy consumption the dominant factor.

An economic evaluation of the different retrofit design solutions obtained through thermodynamic methods (Pinch Technology) and optimization methods (mathematical programming tools) is carried out to rank the retrofit solutions according to some economic criteria, such as capital cost and payback period, to evaluate and determine the best solution found for fixed energy targets.

In pursuit of a good energy performance, coupled with small modifications with small associated energy gains, an evaluation and optimization project for structural changes in Aromatics Plant will be carried out to evaluate energy savings in the consumption of the process units. The rationalization of energy consumption is a concern for the Aromatics Plant, whose energy performance has been shown in benchmarking, lower than its competitors of equal capacity.

1.6. Thesis Structure

The present PhD thesis includes 7 chapters which comprises different methodologies for an accurate energy performance evaluation of Matosinhos Refinery's Aromatics Plant that are schematically summarized and represented in Figure 1.8, which also functions as a graphical abstract of the thesis.

A detailed description of the Aromatics Plant is presented in Chapter 2. Two process units of the Aromatics Plant are considered in this work: Pre-Distillation Unit and Arosolvan Unit. Pre-Distillation Unit is the "front end" of the Aromatics Plant that receives reformate and converts it into different fractions through subsequent unit operations. Arosolvan Unit receives benzene and toluene mixture processed in Pre-Distillation Unit to recover and purify benzene and toluene into individual final products. In this chapter, it is also presented a brief comparison between current processes being used in the Aromatics Plant in study with new and more advanced processes not only in terms of process efficiency improvement but also in terms of achieving higher energy efficiency. Moreover, past reformulations and process integration studies that were carried out within the aromatics plant are identified.

In Chapter 3, to perform an energy evaluation of the Aromatics Plant, operational data is extracted based on the instrumentation and control system, identified through the Process Flow Diagrams (PFD) and Process and Instrumentation Diagrams (P&ID). Data from two years of operation is extracted and pre-treated to remove gross errors, missing data and possible outliers. It is proposed a cluster analysis method to partition operational data into clusters (groups) with the aim to identify different operational scenarios for subsequent energy optimization studies.

In Chapter 4, a process-level Pinch Analysis is performed and thus energy targets are calculated for each process unit, and considering each operational scenario (each cluster) previously identified in Chapter 3 and also the global scenario (overall mean values). Then, actual energy consumptions (for each process unit and each scenario) are estimated through Aspen Plus simulations of the installed heat exchanger networks. Pinch Analysis tools, such as composite curves and grand composite curves, are then applied to estimate energy targets for a given minimum temperature difference to run the process units. Energy targets, calculated through Aspen Energy Analyzer, are compared to actual energy consumption to evaluate potential of energy savings, which traduces the heat that could be possibly recovered within each process unit through Heat Process Integration. An economic evaluation is performed for the different retrofit design solutions and ranked according to some economic criteria.

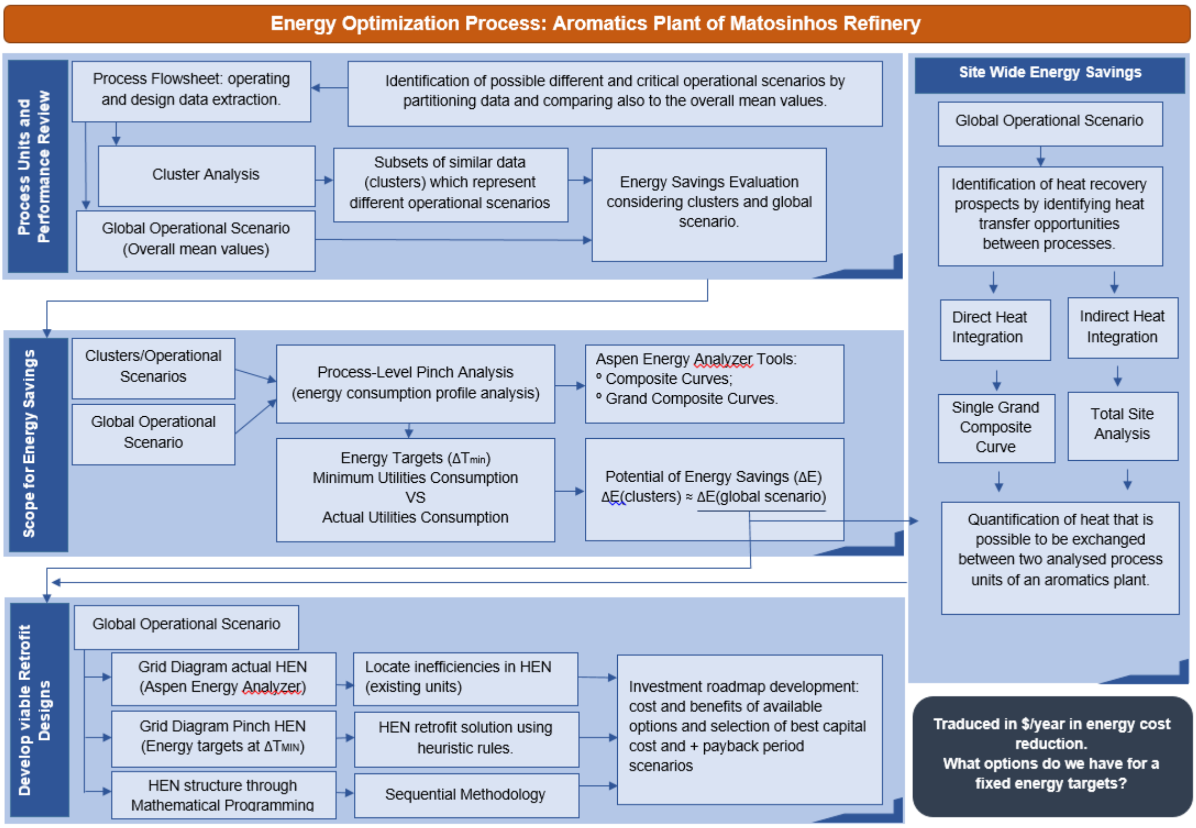


Figure 1.8: Graphical abstract of PhD project.

In Chapter 5, a site wide energy performance analysis considering the overall operational scenario is carried out using a total site heat integration (TSHI) methodology. Maximum heat recovery are here evaluated considering direct and indirect heat integration. In direct integration, Pre-Distillation and Arosolvan Units are integrated as a single unit and energy targets are estimated. Indirect heat integration using intermediate fluids is evaluated through Total Site Analysis to estimate heat recovery prospects by identifying heat transfer opportunities across the two process units, which are linked through a central utility system. The utility system works as an intermediate energy carrier across the two process units. The methodology is based on the construction of total site profiles, which are a representation of Site Sink and Site Source profiles, giving the overall heating and cooling demands for the whole site.

In Chapter 6, process units are subjected to a heat integration and optimization study to maximize heat transfer efficiency and thus, reduce operating costs. The methodology developed has the main objective to redesign and improve the two process units individually by finding an optimal retrofit solution that allows a more efficient and economic use of energy. For this purpose, a hybrid methodology, combining pinch analysis and mathematical programming tools, is developed for the retrofit of heat exchanger networks with minimum investment cost for fixed energy targets. A grid diagram is used to represent the current network and to locate inefficient zones of heat integration. The inefficient zones are then removed using mathematical programming tools through the implementation of the sequential methodology considering retrofit design methods with maximum reuse of the existing heat exchangers. Mathematical programming methods are based on optimization formulations, which are developed from a HEN superstructure. This represents a set of alternative retrofit designs in which the optimization algorithm searches for the optimal network satisfying energy/cost requirements. The solutions obtained will be compared to each other and to the ones obtained with Pinch Analysis and retrofit methods based on heuristic rules. The best solution found correspond to the lowest total investment cost and payback period.

In Chapter 7 are presented the main conclusions regarding the developed studies and suggestions for future works.

Chapter 2: Aromatics Plant

Abstract

Matosinhos Refinery's Aromatics Plant description is here presented in detail. Aromatics plant integrates two main process units. Pre-Distillation Unit processes reformate into different fractions: light gasoline, a mixture of aliphatic and aromatics, a mixture of xylene isomers and heavy aromatics for solvents production. Arosolvan unit receives the mixture of aliphatic and aromatics, mainly benzene and toluene, which are the ones to be recovered and purified into its individual final products. In addition, a comparison between current processes and the new and more advanced processes is addressed not only in terms of process efficiency improvement but also in terms of achieving higher energy efficiency. Moreover, past reformulations and process integration studies that were carried out within the aromatics plant are mentioned.

Key words: Matosinhos Refinery, Aromatics Plant, Process Units, Products

2. Introduction

A typical aromatics plant is a combination of process units that convert naphtha into basic BTX intermediate products. Its configuration will depend on feedstocks used, desired products and available capital investment. An example of a modern configuration plant is presented in Figure 2.1 (Johnson, 2004; Peng, 2012). The increase in demand for benzene and PX has driven the expansion and reconfiguration of traditional plants, with new processes to convert toluene and xylenes into more benzene and PX. In general, an aromatics plant incorporates three main process groups:

- Aromatics generation processes - BTX are produced by catalytic reforming or thermal cracking naphtha processes where a group of reactions takes place to convert naphtha into BTX. For example, reformate splitter which separates benzene and toluene mixture from xylenes and heavy aromatics mixture for further purification;
- Aromatics conversion processes - Auxiliary processes convert a specific aromatic into other aromatics to supplement market demands. For example, toluene, which is produced in higher quantities but has lower market demand, is converted into additional benzene and PX with higher markets demands. Moreover, after extracting PX, other isomers can be converted into additional PX. Two examples are toluene transalkylation and disproportionation conversion processes to increase benzene and PX production and xylenes isomerization to increase PX production;
- Products recovery and purification processes - Different aromatics are separated, recovered and purified into individual products. For example, BT extraction to separate and purify benzene and toluene into individual and final products and xylenes fractionation to extract xylenes mixture and separate different isomers such as PX (Gentry, 2015).

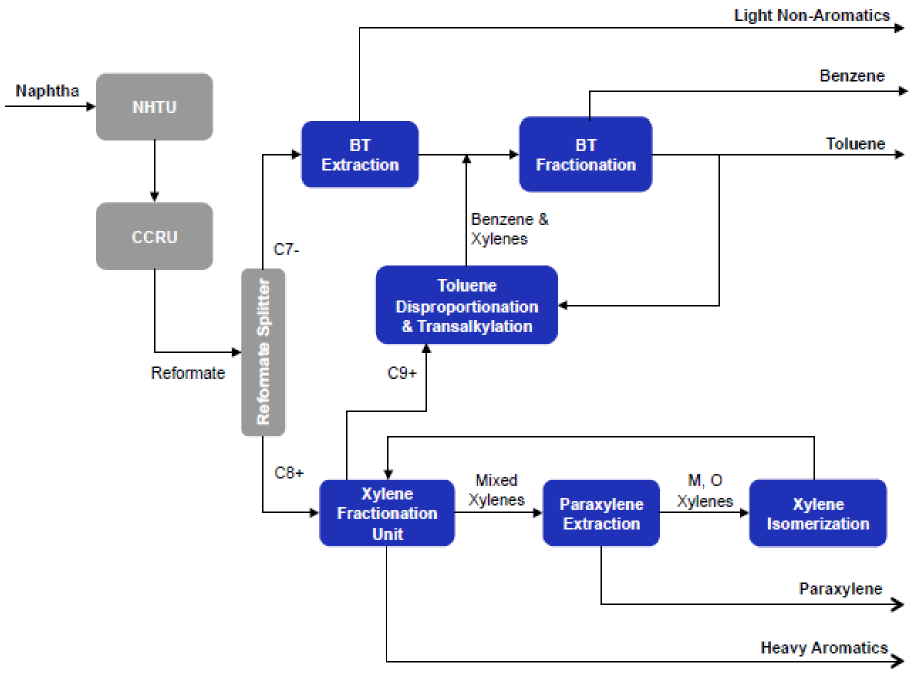


Figure 2.1: Modern plant configuration to produce mainly benzene and p-xylene (Johnson, 2004; Peng, 2012).

Aromatics Plant of Matosinhos Refinery started operating in 1981, with a capacity to process 850,000 tonnes/year of reformate to produce aromatics, being the currently annual output of aromatics plant of 440,000 tonnes. Its location is downstream of Fuel Plant from which receives crude naphtha to complement refining process using semi-continuous regenerative catalytic and continuous regenerative catalytic reforming processes (aromatics generation processes). Naphtha is the only feedstock used by the refinery to produce aromatics. The resulting homogenised reformate mixture is sent to aromatics plant where it is processed into different aromatics cuts as exemplified through the production process diagram of Figure 2.2.

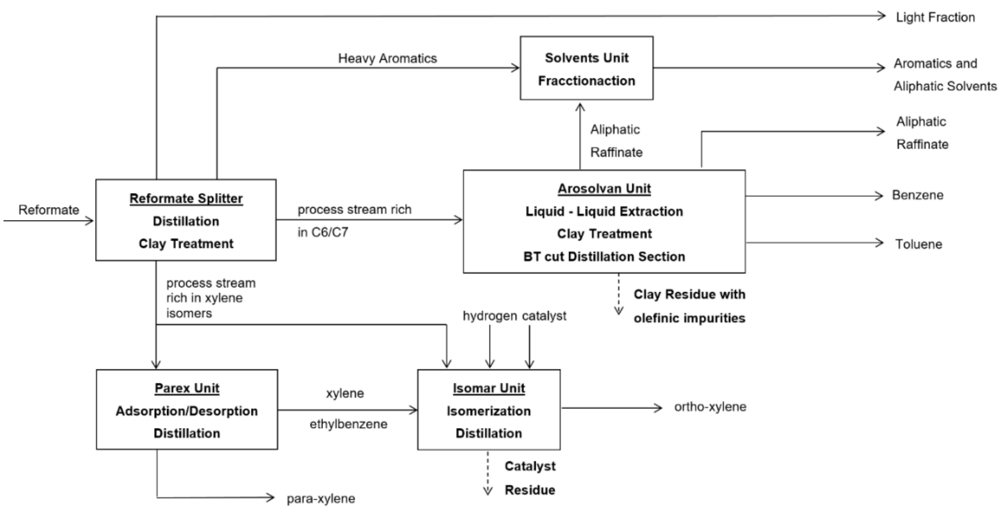


Figure 2.2: Production Process Diagram of aromatics compounds of Matosinhos Refinery (Galp energia, 1996, 2015).

The aromatics plant was projected considering a modern configuration to produce mainly benzene and para-xylene. The initial plant project incorporated five main process units: i) Pre-distillation Unit (U100), which operates as a reformate splitter unit to obtain different fractions; ii) Arosolvan Unit (U200), to produce mainly benzene and toluene as final products; iii) Parex Unit (U300), to produce xylene isomers and extract para-xylene (PX) from the mixture; iv) ISOMAR Unit (0400), to isomerize xylene isomers into PX to increase its yield and to separate ortho-xylene (OX); v) Solvents Unit (0500), to produce different solvents for the market (Galp energia, 1996, 2015). However, since 2015, PAREX and ISOMAR units were shutdown, being Pre-Distillation, Arosolvan and Solvents Units the only three operating today. Pre-Distillation and Arosolvan Units are the ones considered in this developed energy integration and optimization study to achieve maximum energy efficiency. A brief description of both units are described as follows based on the manuscripts of Galp energia (Galp energia, 1996).

2.1. Pre-Distillation Unit (U100)

In the "front end" of aromatics plant is Pre-Distillation Unit (U100), or reformate splitter unit, which processes reformate to obtain different fractions as indicated in Table 2.1 for subsequent units. A generalized scheme is represented in Figure 2.3. A more detailed process flow diagram is presented in Figure 2.4. Three towers, a furnace, a clay treatment and a heat exchanger network compose the unit. The identified heat exchangers of its network are presented in Annex I.

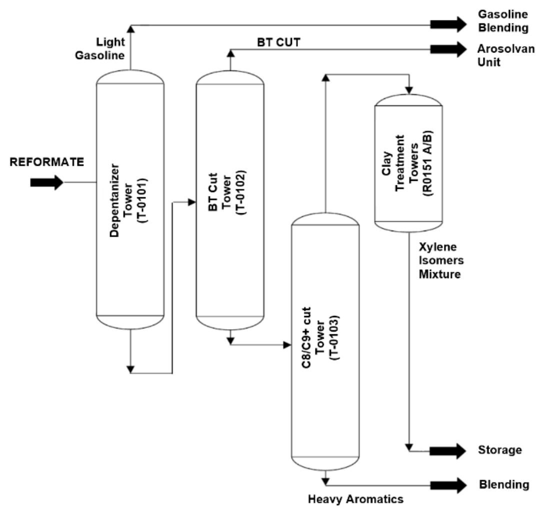


Figure 2.3: Simple schematic representation of Pre-Distillation Unit.

Table 2.1: Main fractions obtained from reformate processed in Pre-Distillation Unit.

Pre-Distillation Process Units main Fractions	
Light Gasoline	Light fraction ($C5^-$ cut) is used in gasoline blending
BT cut	A mixture of benzene and toluene (C6/C7 cut) to be processed and separated into benzene and toluene as pure individual products in Arosolvan Unit.
Xylene Isomers Mixture	A xylenes fraction (C8's cut) to be stored and sold.
Heavy Aromatics Fraction	A $C9^+$ cuts is used or in the production of solvents in Solvent unit or used in gasoline blending.

2.1.1. Depentanizer Tower (T0101)

Depentanizer tower (T0101) is a simple fractionation (distillation) process in which light components or light gasoline ($C5^-$ cut) are fractionated and separated from aromatics and non-aromatics mixture ($C6^+$ cut) by taking advantage of boiling points difference between both cuts. This is done because light components cannot be converted into aromatics. Tower's representative process diagram and design data is shown in Figure 2.5 and in Table 2.2, respectively.

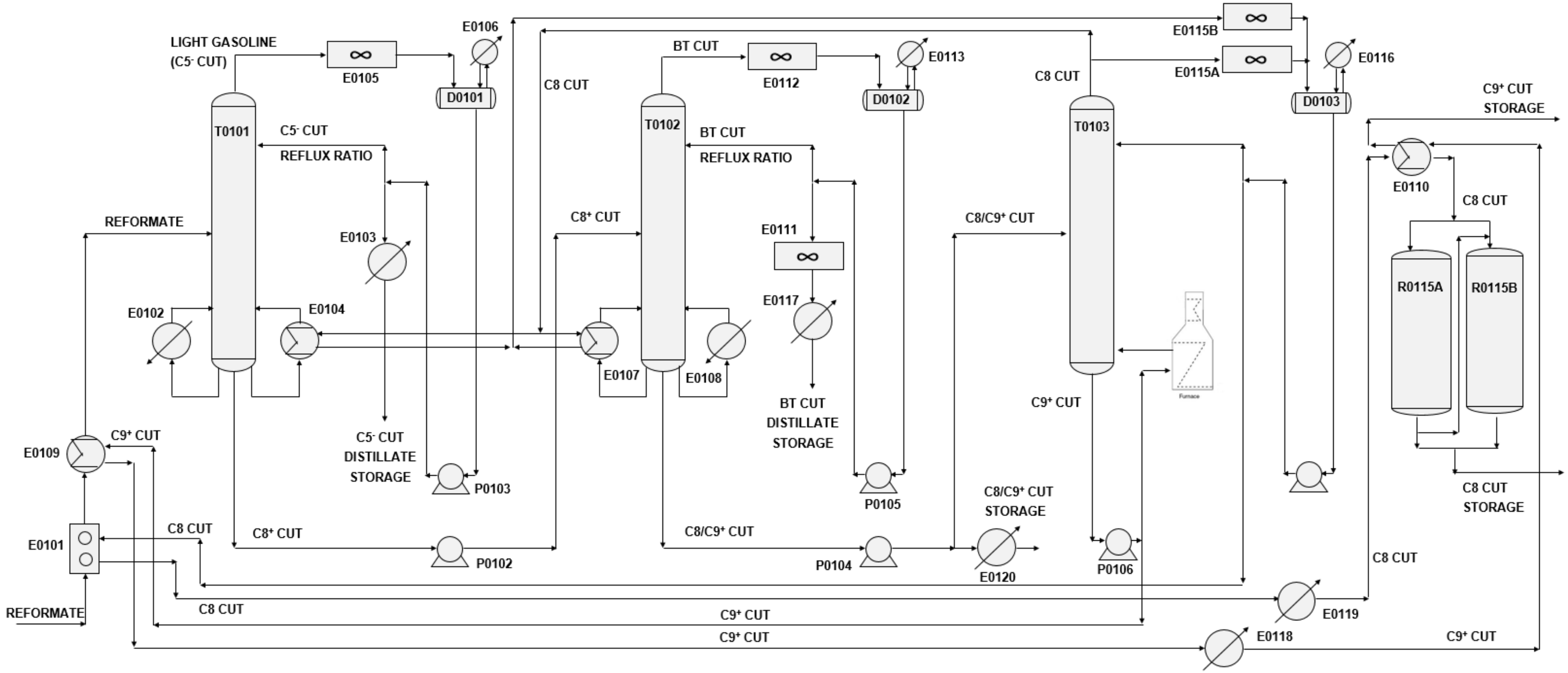


Figure 2.4: Process Flow Diagram of Pre-Distillation Unit (U100) of Matosinhos Refinery´s Aromatics Plant.

Reformate is fed to tower T0101 through tray number 12. Before being fed, reformate is pre-heated successively in two heat exchangers (E0101 and E0109) using as heating source two output processes streams (xylenes cut and heavy aromatics cut) from the subsequent heavy aromatics tower (T0103). Pre-heat process allows to increase its temperature closed to tower's operating temperature (70ºC) and, thus, it minimizes the required supplied energy in the reboilers to run the tower.

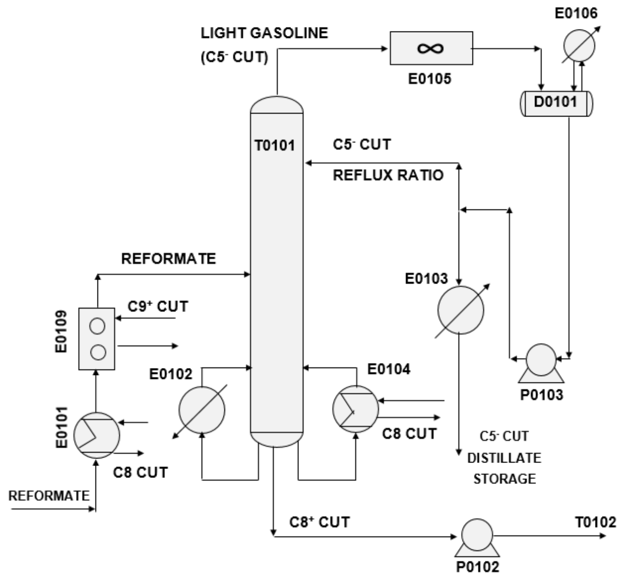


Figure 2.5: Simple process diagram of dependentanizer Tower (T0101).

Table 2.2: Design Data of Depentanizer Tower.

	Tower		T0101
Design	Capacity (m^3)		132.5
	Diameter Top (mm)		1730
	Diameter Bottom (mm)		2540
	Heigh (mm)		39200
	No of trays		53
	Feed tray No		12
	Pressure (kg/cm^2g)		4.5
	Temperature (°C)		190
Operating Conditions	Feed	Product	Reformate
		Pressure (kg/cm^2g)	7.4
		Temperature (°C)	90
	Top Product	Product	Light Gasoline
		Pressure (kg/cm^2g)	2.3
		Temperature (°C)	70
	Bottom Product	Product	$C6^+$ Cut
		Pressure (kg/cm^2g)	2.7
		Temperature (°C)	157

As it has lower boiling point, light gasoline ($C5^-$ cut) is separated from the top of tower T0101 as vapour stream. The fraction then enters in the tower's overhead condenser (air cooler E0105) in which occurs total condensation. The condensed stream is sent to tower's reflux drum (D0101) to hold the condensed vapour from the top of T0101 so that liquid (reflux) can be recycled back to T0101. Some of this liquid is recycled back to the top of T0101 (top reflux) and some is removed from the system (distillate or top product) through Pump P0103. The distillate is sent to a second cooling process using cooling water (cooler E0103) as external cold utility and then mixed with an output process stream (raffinate) from Arosolvan unit to decrease its vapour pressure and be used in gasoline blending.

Heavy fraction ($C6^+$ cut) is separated from the bottom of T0101 and directly pumped (P0102) to subsequent BT cut tower (T0102). Two thermo-syphon reboilers are coupled to distillation column to provide the necessary vaporization for the process. Some of the liquid from the bottom of the column is heated through an output process stream of tower T0103 (E0104) and through medium pressure steam at 195 ºC as hot utility (E0102). Tower's operational temperature is controlled by steam flowrate.

2.1.2. BT Cut Tower (T0102)

The heavy fraction ($C6^+$ cut) obtained through T0101 is a mixture of aromatics and non-aromatics. The mixture is fed to BT cut tower (T0102) in which it is separated in two aromatics mixtures: a BT cut mixture composed by benzene, toluene and non-aromatics, and a mixture of xylenes and heavy aromatics (C8/C9$^+$ cut). Tower's representative process diagram and design data is shown in Figure 2.6 and in Table 2.3, respectively.

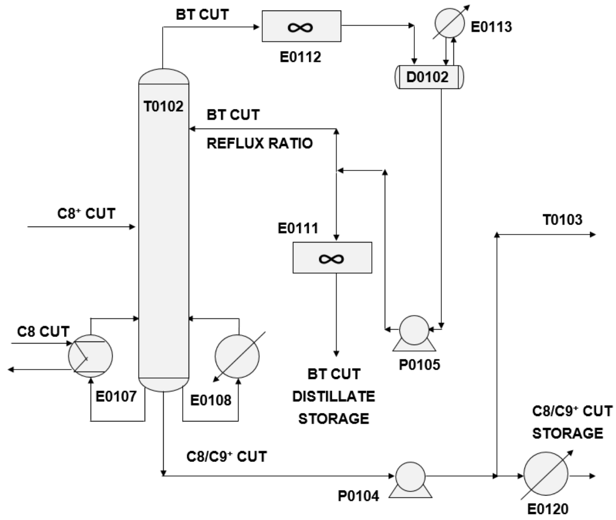


Figure 2.6: Simple process Diagram of BT cut tower (T0102).

Table 2.3: Design Data of BT cut tower (T0102).

Tower			T0102
Design	Capacity (m^3)		487.5
	Diameter (mm)		3800
	Heigh (mm)		39800
	No of Plates		53
	Feed Plate Nº		27
	Pressure (kg/cm^2g)		3.5
	Temperature (°C)		230
Operating Conditions	Feed	Product	C6$^+$ Cut
		Pressure (kg/cm^2g)	4.62
		Temperature (°C)	157
	Top Product	Product	BT Cut
		Pressure (kg/cm^2g)	0.3
		Temperature (°C)	103
	Bottom Product	Product	C8$^+$ cut
		Pressure (kg/cm^2g)	0.7
		Temperature (°C)	174.7

BT cut separated from the top of T0102 as vapor stream enters in the tower's overhead condenser (air cooler E0112) in which occurs total condensation. The condensed stream is sent to tower's reflux drum (D0102) to hold the condensed vapor from the top of T0102. Some of this liquid is recycled back to the top of T0102 (top reflux) and some is removed from the system (distillate or top product) through Pump P0105. The distillate is sent to a second cooling process using air as external cold utility (air cooler E0111) and then sent to storage tank. The storage of this mixture has the main purpose to stabilize its composition, although it is a highly energetic and disadvantage procedure.

The mixture of xylenes and heavy aromatics (C8/C9$^+$ cut) is separated from the bottom of the tower and it is pumped to subsequent C8/C9$^+$ cut tower (T0103). Two thermo-syphon reboilers are coupled to distillation column to provide the necessary vaporization for the process. Some of the liquid from the bottom of the column is heated through an output process stream of tower T0103 (E0107) and through medium pressure steam at 195 ºC as hot utility (E0108). Tower's operational temperature is controlled by steam flowrate. In maintenance periods, the bottom product of tower T0102 is fractionated and sent to storage tank, after being cooled using cooling water (E0120).

2.1.3. C8/C9$^+$ Cut Tower (T0103)

Xylenes and heavy aromatics mixture (C8/C9$^+$ cut) is fed into distillation tower (T0103) in which the mixture is fractionated into main xylene isomers stream (C8's cut) and a mixture of heavy aromatics (C9$^+$ cut). Tower's representative process diagram and design data are shown in Figure 2.7 and in Table 2.4, respectively.

Xylene isomers cut is separated from the top of the T0103 as vapor stream. Part of the stream (Stream A) enters in one of the tower's overhead condenser (air cooler E0115A) in which occurs total condensation. The other part of the xylene isomers vapor stream is sent to the reboilers of towers T0101 (reboiler E0104) and T0102 (reboiler E0107) in which the condensation heat of the process stream is used as heating source to vaporize the bottom streams of the respective columns. After total condensation in the reboilers, the stream is cooled in another tower's overheads cooler using air cooling as cold utility (air cooler E0115B). After cooling process, both streams are mixed and xylenes isomers mixture is sent to tower's reflux drum (D0103) to hold the condensed vapor from the top of T0103. Some of this liquid is recycled back to the top of T0103 (top reflux) and some is removed from the system (distillate or top product) through Pump P0106. The distillate is used as heating source to pre-heat reformate (E0101) and then cooled again using cooling water (cooler E0119) for storage tanks.

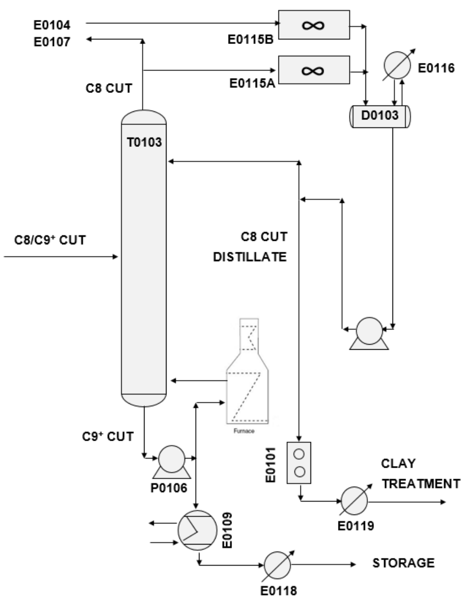


Figure 2.7: Simple process diagram of C8/C9$^+$ cut tower (T0103).

Table 2.4: Design Data of C8/C9$^+$ cut tower (T0103).

Tower			T0103
Design	Capacity (m^3)		858.8
	Diameter (mm)		3900
	Heigh (mm)		70130
	No of Plates		100
	Feed Plate Nº		51
	Pressure (kg/cm^2g)		6.3
	Temperature (^oC)		275
Operating Conditions	Feed	Product	C8$^+$ cut
		Pressure (kg/cm^2g)	13.17
		Temperature (^oC)	174.7
	Top Product	Product	C8's cut
		Pressure (kg/cm^2g)	3.7
		Temperature (^oC)	207
	Bottom Product	Porduct	C9$^+$ cut
		Pressure (kg/cm^2g)	4.5
		Temperature (^oC)	246

The mixture of heavy aromatics (C9$^+$ cut) is used as heating source in the second pre-heat process of reformate (E0109) and then cooled using cooling water (cooler E118) before being sent to storage tank. Heavy aromatics are used in the production of several solvents.

2.1.4. Clay Treatment Towers (R0151 A/B)

Xylene isomers mixture are sent to clay treatment towers (R0151 A/B) with the main purpose to remove small quantities of di-olefins and heavier unsaturated non-aromatics products. The level of contamination by these impurities are measured by bromine index, which specifies the olefins content in the mixture and the degree of unsaturation. A disturbance in this index indicates that xylene isomers mixture does not respect the required specifications (value higher or equal to 20). The clay acts as a catalyzer and accelerates the polymerization of those impurities producing heavier products, which are retained by the clay. Tower's datasheet and design data is shown in Figure 2.8 and in Table 2.5, respectively.

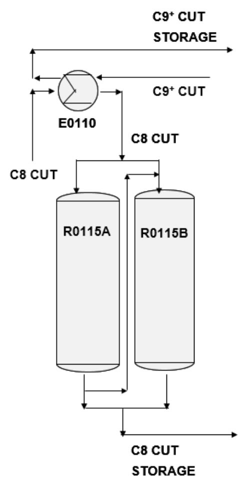


Figure 2.8: Simple process diagram of clay treatment towers (R0151 A/B).

Table 2.5: Design data of clay treatment towers (R0151B).

Towers	R0115A	R0115B
Feed Type	C8 cut	C8 cut
Feed (kg/h)	52835	52835
Feed temperature (°C)	206	206
Feed pressure (kg/cm^{2}g)	12.4	12.4
Bottom product	C8 cut	C8 cut
Top operating pressure, Pop (kg/cm^{2}g)	12.1	12.1
Bottom Operating pressure, Pop (kg/cm^{2}g)	10.1	10.1
Operating Temperature (ºC)	176 - 205	176 - 205
Number of trays	fixed bed	fixed bed
Feed tray number	top	top
Height (mm)	11000	11000
External Diamiter (mm)	3100	3100
Material	CS BLR	CS BLR

The system consists of two towers (R0151 A/B) which work in series. The pre-heated feed at desired temperature is fed at the top of tower R0151A, where it occurs the first treatment. The bottom product is fed to the top of tower R0151B where the second treatment occurs. The final product obtained from the bottom of R0151B is storage to be sold and processed outside the refinery. A heat exchanger (E0110) is placed to pre-heat the feed before the treatment to set the bromine index value higher or equal to 20, by managing the feed temperature when it is required.

In the beginning of the clay's life cycle, the operating temperature is as lower as possible, increasing with the decrease of its efficiency, which is affected directly by the impurities accumulated in the clay bed. The operating temperature is increased periodically through the heat transfer in E0110 with heavy aromatics ($C9^+$ cut). Depending on clay's characteristics, its life cycle is around three years.

When operating, the towers need little attention. The operating system is controlled by measuring the bromine index of the effluent and compared to the one measured from the feed. Along with the decrease in efficiency, feed temperature is gradually increased before clay`s activities is degraded and aromatics products are out of required specifications. When this happens, R0151B is shutdown to change clay bed while R0151A keeps operating. After changing clay bed, R0151B starts to operate in parallel with R0151A until it is established an equilibrium in temperatures. After that, both towers start operating in series again.

2.2. Arosolvan Unit

Arosolvan Unit (U200) was projected to produce benzene and toluene with high purity from BT cut mixture obtained from the top of tower T0102 of Pre-Distillation Unit. It integrates three main sections: aromatics extraction section, washing treatment section and BT distillation section. The identified heat exchangers of overall heat exchanger network are presented in Annex II.

2.2.1. Aromatics Extraction Section

Aromatics extraction section is based on Arosolvan process developed by Lurgi licensed company, which is a liquid-liquid extraction (LLE) process combined with conventional distillation process to recover benzene and toluene from BT cut mixture. An extractor, an extract recycle tower and a solvent recovery tower integrate this section. A process diagram of aromatics extraction section is shown in Figure 2.10. LLE unit has the following steps: i) extractor, where the mixture is brought into contact with the solvent (T0201); ii) extractive stripper, where the non-aromatics that also have been extracted are stripped off (T0202); iii) solvent stripper, where the aromatics are separated from the solvent (T0203); iv) and raffinate and extract washing column (T0205 and T0206, respectively), for the recovery and regeneration of the solvent residue which has been dissolved in the raffinate (Emmrich *et al.*, 2001).

Extractor and Liquid-Liquid Extraction Process (T0201)

BT cut mixture, the liquid stream (carrier) containing the components to be recovered (benzene and toluene), is fed to the extractor tower (T0201), where it contacts an organic solvent. The data sheet and design data is shown in Figure 2.9 and in Table 2.6. The solvent is a mixture of N-methylpyrrolidone (NMP) and monoethylene glycol (MEG). The two liquids must be immiscible or slightly miscible to allow forming a dispersion with one liquid dispersed as droplets in the other. Mass transfer occurs between the droplets (dispersed phase) and the surrounding liquid (continuous phase). The separation of the two liquids occurs only if they have different densities. The boundary between continuous phase and dispersion phase is called interface and it can occur at the top or at the bottom of the extractor.

Extraction is performed continuously operating in counter-current mixing and following a mixer-settle principle. This configuration doesn`t limit the number of stage units per extraction allowing multiple stages per unit. According to the density of the solvent relative to BT cut mixture, the solvent can be fed into the extractor from its bottom or from its top. In this case, as the solvent has higher density than the mixture, it enters through the top of the extractor and the mixture is carried downward to the bottom of the extractor, being the carrier stream removed from the top. Light phase or aliphatic raffinate, composed by non-aromatics and solvent residue, is removed from the top of the extractor and sent to raffinate washing tower (T0205). Extract composed by a mixture of solvent, aromatics and nonaromatics, with low boiling points, is obtained as bottom product and sent to extract recycle tower (T0202).

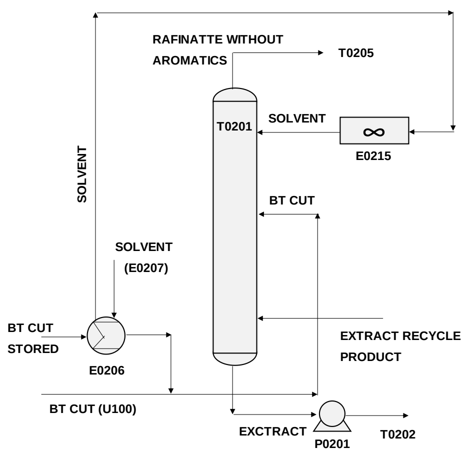


Figure 2.9: Simple process diagram of extractor operating in counter-current (T0201).

Table 2.6: Design data of the extractor (T0201).

Tower			T0201
Design	Capacity (m^3)		380
	Diameter (mm)		4470
	Heigh (mm)		22700
	Feed Plate Nº		8,6,1
	Pressure (kg/cm^2g)		3.5 - 4.5 FV
	Temperature (^oC)		100
Operating Conditions	Feed	Product	BT Cut
		Pressure (kg/cm^2g)	4.5
		Temperature (^oC)	60
	Top Product	Product	Raffinate
		Pressure (mmHg)	0.3
		Temperature (^oC)	60
	Bottom Product	Product	Extract
		Pressure (kg/cm^2g)	2.5
		Temperature (^oC)	60

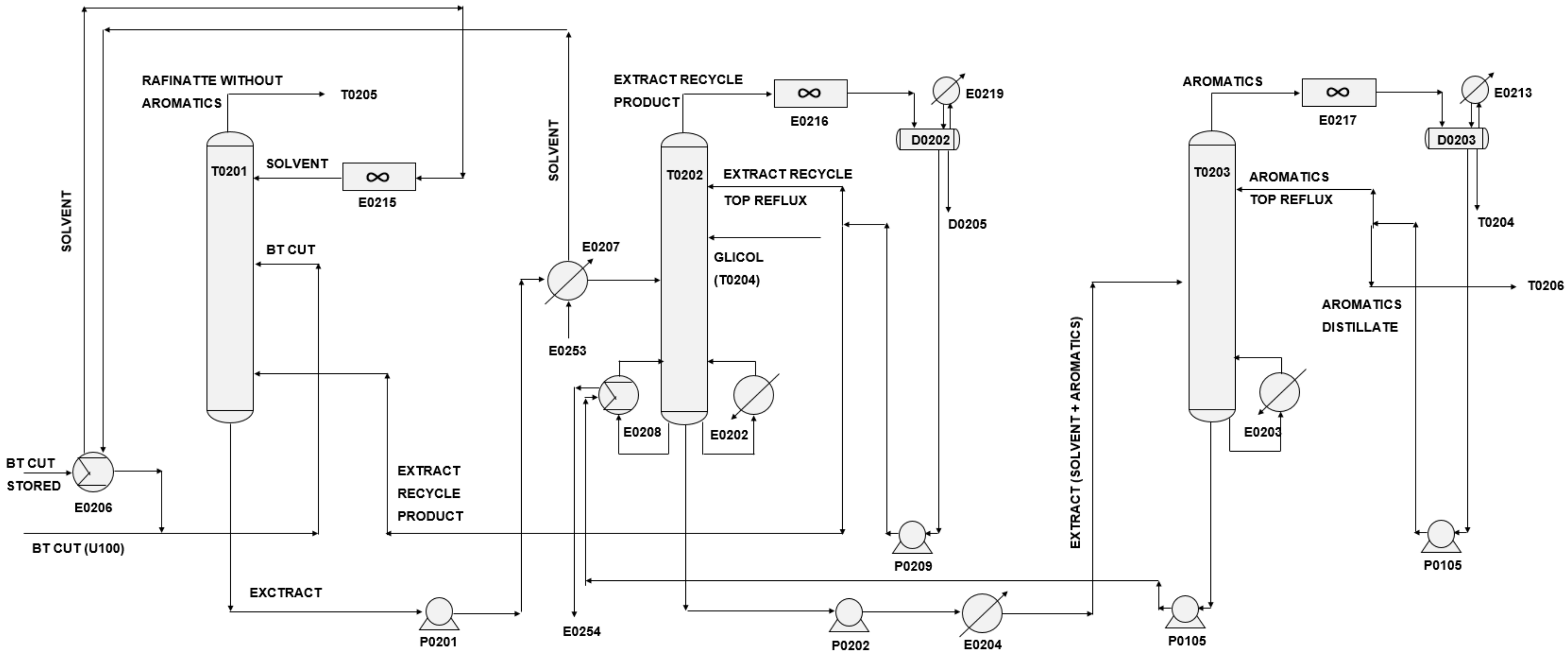


Figure 2.10: Schematic process diagram of aromatics extraction section of Arosolvan Unit.

The operating temperature and pressure of the extractor is 60 ºC and 1 atm, approximately. It is important that the extractor operate at optimal pressure, as the pressure at the top of the extractor must be constant and equal to 1.2 kg/cm^2 abs or the nonaromatics with low boiling points may vaporize.

A three-step approach is required to recover pure aromatics fraction from the extract: i) remove extract recycle product in the extractor (T0202); ii) remove the solvent in solvent recovery tower (T0203); and iii) eliminate small quantities of solvent in the extract washing column (T0206) in the washing treatment section.

Extract Recycle Tower (T0202)

The extract from the bottom of the extractor tower is pumped (P0201) and pre-heated using solvent as an output stream recovered from solvent stripper. Extract enters in the extract recycle tower (T0202) in which is performed an extractive distillation process. This process takes the advantage of the boiling points of the different components of the mixture. The solvent has the higher boiling point while aromatics and nonaromatics have similar boiling points. The boiling point of the solvent alters the volatilities of the components in the mixture, avoiding the formation of new azeotropes and ensures that the solvent does not vaporize in the distillation process. This way, the separation of aromatics from the extract is possible. The absence of azeotropes plus the fact that the solvent can be recovered by simple distillation makes extractive distillation a less complex and more widely useful process than azeotropic distillation. The data sheet and design data is shown in Figure 2.11 and in Table 2.7.

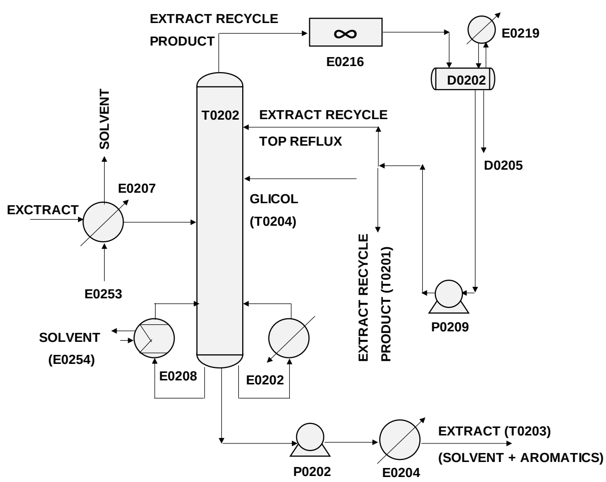


Figure 2.11: Simple process diagram of extract recycle tower (T0202).

Table 2.7: Design data of extract recycle tower (T0202).

Tower			T0202
Project Design Data	Capacity (m^3)		171
	Diameter (mm)		2800
	Heigh (mm)		31700
	No of Plates		50
	Feed Plate Nº		40
	Pressure (kg/cm^{2}g)		3.69
	Temperature (ºC)		210
Operating Conditions	Feed	Product	Extract
		Pressure (kg/cm^{2}g)	9.4
		Temperature (ºC)	170
	Top Product	Product	Extract Recycle
		Pressure (mmHg)	662
		Temperature (ºC)	66
	Bottom Product	Porduct	Extract
		Pressure (kg/cm^{2}g)	0.2
		Temperature (ºC)	145

Light nonaromatics residue is separated from the extract from the top of the extract recycle tower. Light phase of this process is a mixture of light non-aromatics with small quantities of benzene and water. This fraction enters in the top overheads condenser (air cooler E0216) in which occurs total condensation. Then, the condensed process stream is sent to a tower's reflux drum (D0202) to hold the condensed vapor from the top of the column. The water, which might be in the top product, is here purged. Part of this stream is recycled back to the top of the column (top reflux) and another part is removed from the system (distillate or top product) through Pump P0209. The distillate is directly fed to the bottom of extractor tower (T0201) to promote the saturation of light nonaromatics. This way, heavy nonaromatics are prevented to get to extract recycle tower where they won't be able to be removed.

The extract without nonaromatics, which is obtained from the bottom of the extract recycle tower, is used as a heating source to vaporize the bottom product of water distillation tower (T0204), suppling heat to run the equipment through the reboiler (E0204), before being fed to extract stripper tower (T0203). Two thermo-syphon reboilers are coupled to extract recycle column to provide the necessary vaporization for the process. Some of the liquid from the bottom of the column is heated through an output process stream of solvent stripper tower T0203 (E0208) and through medium pressure steam at 215 ºC as hot utility (E0202).

Solvent Stripper Tower (T0203)

Extract without nonaromatics is fed to the solvent stripper tower (T0203), which operates in vacuum produced by a vacuum pump to fully strip away the solvent without overheating the product. The main purpose of this process is to recover the solvent to be used again in the process. The data sheet and design data is shown in Figure 2.12 and in Table 2.8.

The aromatics are stripped from the top of the tower (top product) with a small quantity of solvent MEG and then, the stream is sent to the solvent stripper overheads condenser (E2017) in which total condensation occurs using air as external cold utility. After total condensation, aromatics are received by solvent stripper's reflux drum (D0203) to hold the condensed vapor from the top of the column. Part of this stream is pumped (P0212) back to the top of the column (top reflux) and another part is removed from the system (distillate or top product). The distillate is fed to extract washing tower (T0206).

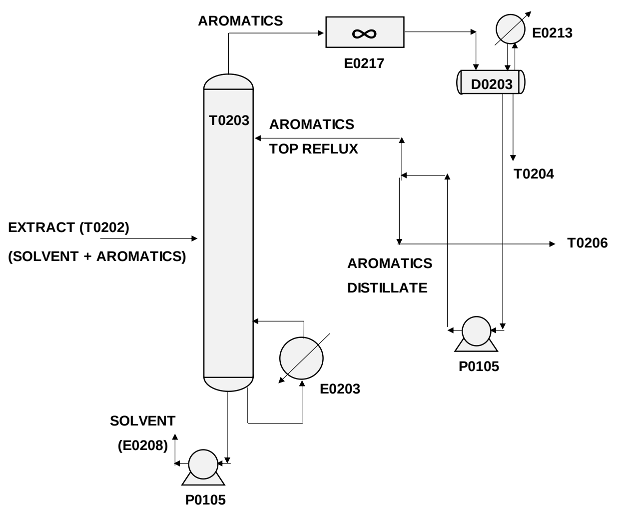


Figure 2.12: Simple process diagram of solvent stripper.

Table 2.8: Project design data and operating conditions of tower (T0203).

Tower			T0203
Project Design Data	Capacity (m^3)		234
	Diameter (mm)		3500
	Heigh (mm)		24100
	No of Plates		35
	Feed Plate Nº		20
	Pressure (kg/cm^2g)		3.5
	Temperature (°C)		290
Operating Conditions	Feed	Product	Extract
		Pressure (kg/cm^2g)	3.1
		Temperature (°C)	250
	Top Product	Product	Extract
		Pressure (mmHg)	169
		Temperature (°C)	76
	Bottom Product	Product	Solvent
		Pressure (mmHg)	294
		Temperature (°C)	170

The solvent is fully stripped from the bottom of the tower as bottom product and it is used as heating source to pre-heat the extract from the bottom of the extractor (T0203) before being fed to extract recycle tower (T0202). Then, the regenerated solvent is sent back to the extractor where is mixed with fresh solvent. The bottom product of the tower is vaporized in the reboiler (E0203) using medium pressure steam at 215 ºC to supply the required heat to the process.

2.2.2. Washing Treatment Section

Arosolvan Unit has a washing treatment section incorporated with the main purpose to clean the raffinatte obtained from the extractor to be later used in gasoline blending and to clean aromatics before being sent to benzene and toluene distillation section that follows. A schematic representation of its process diagram is shown in Figure 2.13.

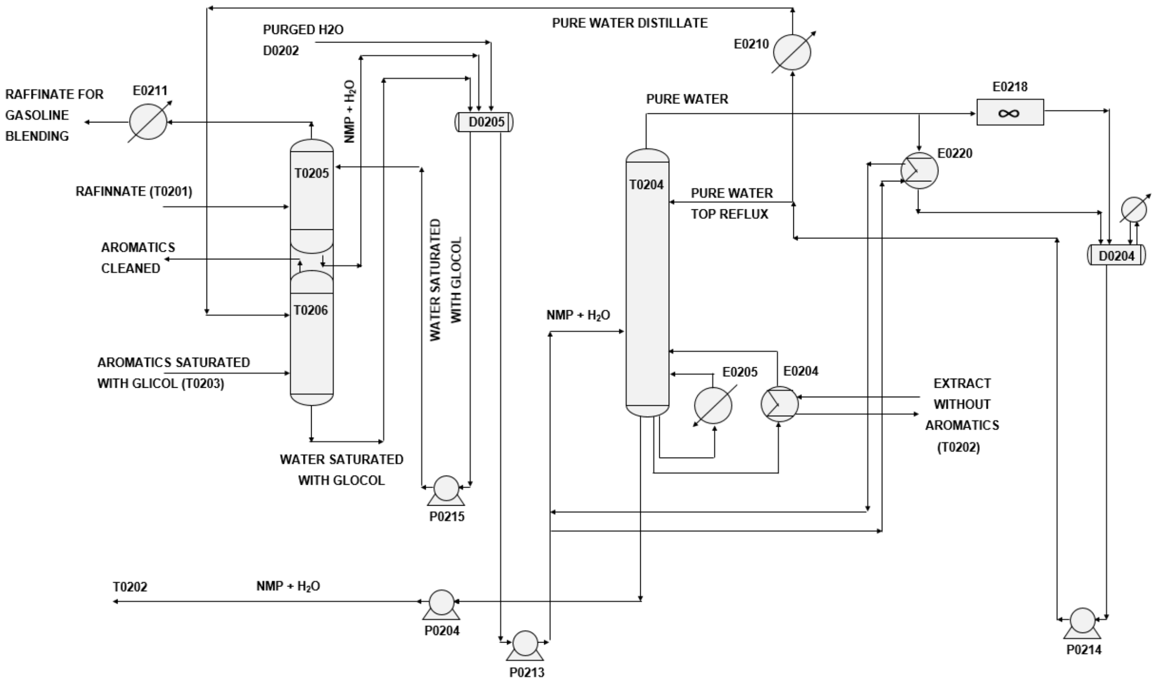


Figure 2.13: Washing treatment section of Arosolvan Unit.

Raffinate and extract washing processes occur inside the same tower. One single column is divided into two sections in which one is the raffinate washing tower (T0205) and the other is the extract washing tower (T0206). A simple process diagram and design data are shown in Figure 2.14 and in Table 2.9.

Raffinate washing tower (T0205) operates with constant feed and high separation velocities. This tower receives the aliphatic raffinate, obtained from the top of the extractor (T0201) containing nonaromatics and NMP solvent residue. In this tower, NMP solvent saturated with water is recovered and regenerated from aliphatic raffinate using water purified in water distillation tower (T0204). The NMP solvent saturated with water is sent to raffinate washing tower's reflux drum (D0205) in which some of the water is separated from the solvent and purged. This process is performed twice. In the first washing process, the effluent obtained as bottom product from the extract washing tower (T0206) is used and then, it is pumped back to water distillation column. The second washing treatment is performed using pure water obtained from the top of water distillation column.

Extract washing tower (T0206) is the last step of aromatics purification and it receives the aromatics stripped off from solvent stripper tower (T0203) saturated with MEG solvent. In extract washing tower, fresh water is fed at the top of the tower and the aqueous effluent saturated with MEG solvent obtained from the bottom of the extract washing tower is sent to washing towers' reflux drum (D0205) in which water is separated from MEG. Both water streams resulting from both raffinate and extract washing processes are used in the first raffinate washing treatment in raffinate washing tower (T0205).

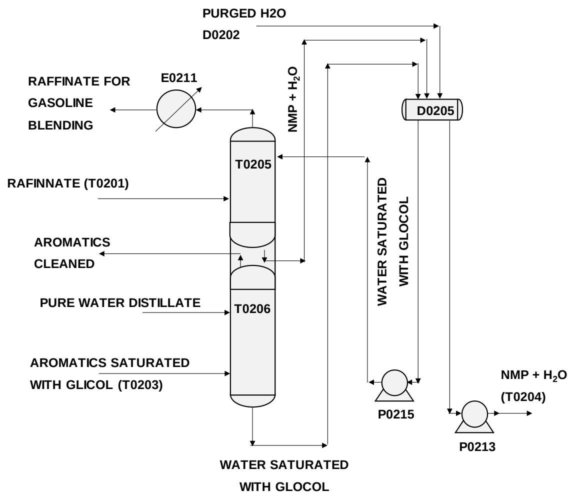


Figure 2.14: Simple process diagram of Raffinate and Extract washing towers (T0205 and T0206).

Table 2.9: Design data raffinate and extract washing towers (T0205 and T0206).

Tower			T0205	T0206
Project Design Data	Capacity (m^3)		25	26
	Diameter (mm)		2175	2175
	Heigh (mm)		6000	6400
	No of Plates		6	6
	Feed Plate Nº		1	1
	Pressure (kg/cm^{2}g)		11 FV	15.8 FV
	Temperature (^{o}C)		100	100
Operating Conditions	Feed	Product	Raffinate	Extract
		Pressure (kg/cm^{2}g)	8.87	12.85
		Temperature (^{o}C)	60	48
	Top Product	Product	Raffinate	Extract
		Pressure (mmHg)	8.2	12.2
		Temperature (^{o}C)	60	50
	Bottom Product	Product	Mixture (NMP + Water)	Mixture (MEG + Water)
		Pressure (kg/cm^{2}g)	9.1	12.4
		Temperature (^{o}C)	60	48

A reflux drum (F0251) receives the aromatics saturated with water where the water is separated and recovered from the aromatics. Purified aromatics are heated and then, it is sent to a clay treatment process (R0251A/B). Purified aromatics are then sent to BT distillation section to obtain benzene and toluene with high purity and as individual final products. Pure water required for the operation of the washing towers of aromatics and raffinate (T0206 and T0205) is recovered as top product in water distillation tower (T0204). A simple process diagram and design data is shown in Figure 2.15 and in Table 2.10.

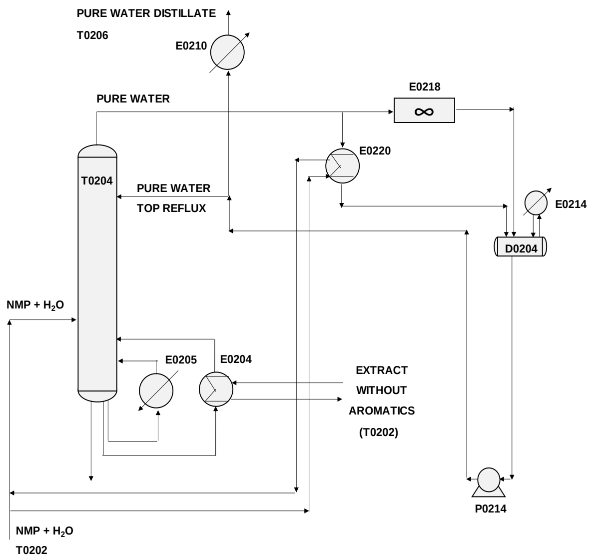


Figure 2.15: Simple process diagram of water distillation tower (T0204).

Table 2.10: Design data water distillation tower (T0204).

Tower			T0204
Project Design Data	Capacity (m^3)		26.4
	Diameter (mm)		1850
	Heigh (mm)		16300
	No of Plates		20
	Feed Plate Nº		Lower than 1
	Pressure (kg/cm^{2}g)		3.5
	Temperature (^{o}C)		190
Operating Conditions	Feed	Product	Mixture (NMP, MEG, H_2O)
		Pressure (kg/cm^{2}g)	2.31
		Temperature (^{o}C)	60
	Top Product	Product	Water
		Pressure (mmHg)	0.2
		Temperature (^{o}C)	104
	Bottom Product	Product	Mixture (Solvent + Water)
		Pressure (kg/cm^{2}g)	0.3
		Temperature (^{o}C)	131

2.2.3. BT Distillation Section

BT distillation section integrates a clay treatment process and two main distillation processes to obtain benzene in benzene distillation tower (T0251) and toluene in toluene distillation tower (T0252) as individual final products with high purity. A schematic representation of BT distillation section is represented in Figure 2.17.

As in Pre-Distillation Unit, the purpose of clay treatment is to remove the small quantities of di-olefins and unsaturated non-aromatics that might exist in aromatics stream and might influence the specifications value of benzene, which is produced up-front in the distillation section. The operating system is the same, although in this case, only one of the columns is operating while the other is being changed or maintain in reserve. Purified Aromatics obtained in previous aromatics extraction section are a simple mixture of benzene and toluene. The mixture is fed to benzene distillation tower (T0251) where the separation of benzene from the mixture occurs. A simple process diagram and design data is shown in Figure 2.16 and in Table 2.11.

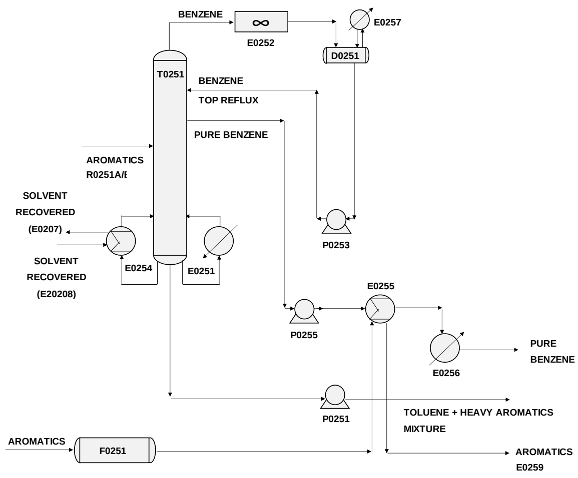


Figure 2.16: Simple process diagram of benzene distillation tower (T0251).

Table 2.11: Design data of benzene distillation tower (T0251).

Tower			T0251
Project Design Data	Capacity (m^3)		130
	Diameter (mm)		2000
	Heigh (mm)		38600
	No of Plates		60
	Feed Plate Nº		24
	Pressure (kg/cm^2g)		3.5 FV
	Temperature (°C)		180
Operating Conditions	Feed	Product	Extract
		Pressure (kg/cm^2g)	3
		Temperature (°C)	120
	Top Product	Product	Benzene
		Pressure (mmHg)	0.45
		Temperature (°C)	93
	Bottom Product	Product	Toluene + C9's
		Pressure (kg/cm^2g)	0.79
		Temperature (°C)	135

Benzene in vapour phase is obtained from the top of the distillation column as top product and then, it is sent to benzene distillation tower's overheads condenser (air cooler E0252) promoting its total condensation. Then, condensed benzene is sent to a reflux drum (D0251) to hold the condensed vapor from the top of the column. The top reflux is pumped back to the column (P0253). Depending on the purity of benzene required, some top condensate can be sent back to extractor tower of Arosolvan process or to reflux drum D0202. The extract feed to the tower contains saturated water, which is detected at the bottom of the reflux drum (D0251). This water is sent back to the reflux drum D0202 to avoid negative environmental impacts.

Pure benzene is removed from plate 55 of the tower, which is cooled before sent to storage. The tower is heated through two reboilers: E0254 in which bottom fluid exchanges heat with solvent and E0251 in which bottom fluid exchanges heat with medium pressure steam.

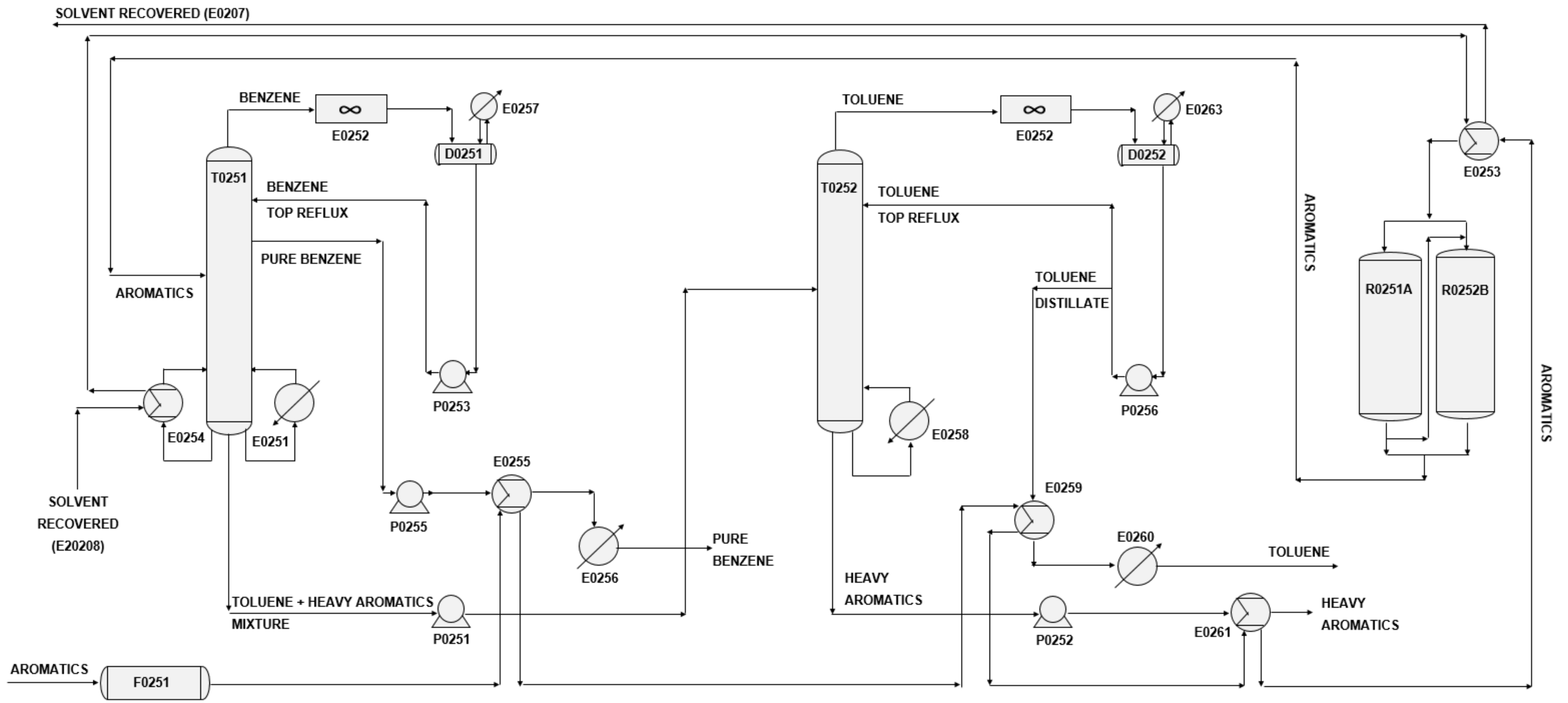


Figure 2.17: Schematic representation of BT distillation section of Arosolvan Unit.

The bottom product of tower T0251 is a mixture that contains toluene and small quantities of xylene isomers. Toluene is recovered as top product of Toluene Distillation Tower (T0252). A simple process diagram and design data is shown in Figure 2.18 and in Table 2.12.

After condensing in an air cooler (E0264) and received by reflux drum (D0252), it is sent to storage after exchanging heat until the required temperature (E0259 and E0258). The column is heated in the reboiler E0258 through an external hot utility. The bottom product of tower T0252 is a mixture of C8's cut and small quantities of toluene and polymers to storage.

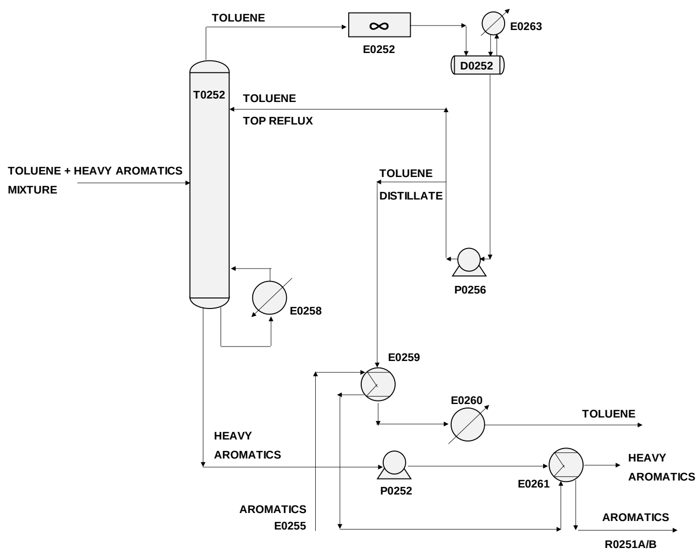


Figure 2.18: Simple process diagram of toluene distillation tower (T0252).

Table 2.12: Design data of toluene distillation tower (T0252).

	Tower		T0252
Project Design Data	Capacity (m^3)		98
	Diameter (mm)		1900
	Heigh (mm)		33800
	No of Plates		50
	Feed Plate Nº		25
	Pressure (kg/cm^2g)		3.5 FV
	Temperature (°C)		220
Operating Conditions	Feed	Product	Toluene + C9's
		Pressure (kg/cm^2g)	4.01
		Temperature (°C)	135
	Top Product	Product	Toluene
		Pressure (mmHg)	0.8
		Temperature (°C)	135
	Bottom Product	Product	C9's cut
		Pressure (kg/cm^2g)	1.18
		Temperature (°C)	168

2.3. Current level of Aromatics Plant of Matosinhos Refinery

Analyzing the whole site, it is possible to verify that Matosinhos Refinery`s aromatics plant does not take advantage of toluene and heavy aromatics conversion processes for additional benzene and para-xylene production. It is also important to know that the current scenario in terms of energy consumption of Matosinhos Refinery`s aromatics plant does not take into consideration the whole site integration but only process-level integration. In addition, due to the location of both reforming processes, they will not be considered in the energy optimization study. Moreover, in 2015, PAREX and ISOMAR units were shutdown, not taking advantage of the production of para-xylene anymore.

Main modifications were performed in Pre-Distillation unit since the aromatics plant started. One of the modifications was the layout of the feed of the clay treatment. Initially, xylenes and heavy aromatics mixture (C8/C9$^+$ cut) was directly fed to the clay treatment columns (R0115 A/B). However, as heavy aromatics components (C9$^+$ cut) saturated clay fixed bed fast due to its impurities, and thus shortening its life cycle usage, the layout of the plant was changed sending only xylenes isomers cut (C8's cut) to clay treatment.

Another modification in the plant done through the years was the addition of the second column of Benzene in Arosolvan Unit to increase operation and production flexibility in terms of the amount of benzene produced towards toluene. The bottleneck of the unit is located in the extraction section. The unit was initially projected with an aromatics load to the extractor to be constantly 190,000 tonne/year. This new configuration allowed an increasing in production of benzene and, consequently, decreasing the production of toluene. Meanwhile, the column was shutdown.

For this reasons, a new energy consumption evaluation and an improvement in the current configuration of the aromatics plant is required to increase its efficiency in terms of process, energy consumed and operating costs.

2.4. Novelties in Aromatics Production Process Technology

Reformate contains in its components a mixture of aromatics and non-aromatics. As mentioned before, aromatics and non-aromatics have closed boiling points, which makes its separation very difficult by simple distillation. Here, the choice of the technology is balanced by comparing the advantages of process type and solvent type. As for the process, it is possible to choose between LLE and extractive distillation (ED) only, which is a more advanced process. In cases of existing LLE units, a hybrid process combining the best features of both technologies can be economically favorable (Emmrich *et al.*, 2001; Lee, 2000; Stoodt and Negiz, 2004). Another possibility, UOP have licensed an industrial process to extract aromatics from naphtha using ionic liquids as solvents. Ionic liquids as extraction agents are accepted in industry due to their negligible vapor pressure, requiring fewer process steps and less energy consumption than extraction processes with conventional solvents (Ferro *et al.*, 2015).

An extractive process unit for aromatics recovery must be configured considering the following factors: new *versus* revamped equipment, cost of utilities, feed composition (boiling range, content in non-aromatics and presence of impurities) and product specifications (Emmrich *et al.*, 2001).

Comparatively to benzene and xylenes production and market demand, toluene is largely produced in higher quantities, but its market demand is the lowest. Therefore, besides toluene application in solvents, toluene became an important feed source to supplement PX and/or benzene production through certain conversion processes (which nowadays occurred combined in the process): Hydrodealkylation (HDA) process, transalkylation (TA); Toluene disproportionation (TDP) or selective toluene disproportionation (STDP) processes; Toluene alkylation (TolAlk or TM) process (Gentry, 2015).

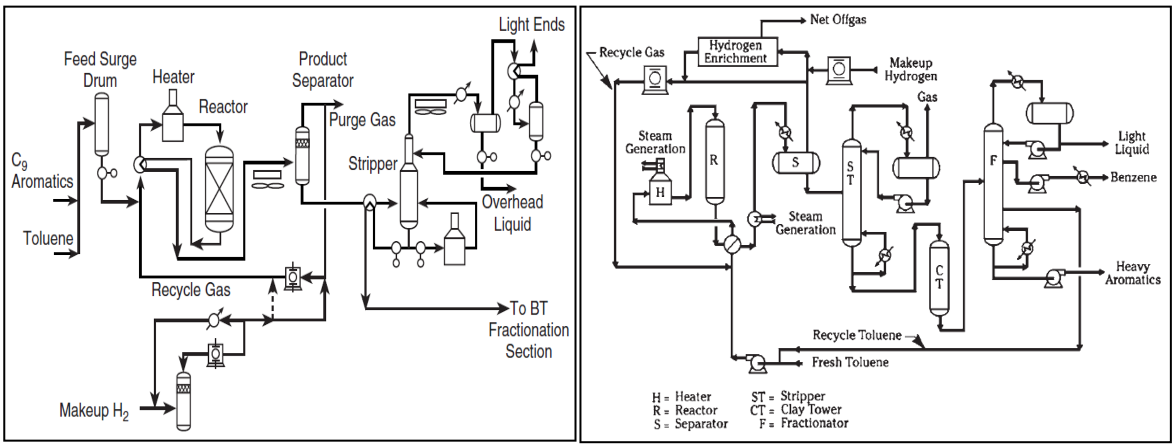


Figure 2.19: Tartoray process flow diagram (left) and THDA process flow diagram for benzene production (right) both licensed by UOP (Stood and Negiz, 2004).

The first industrial implementation was in a toluene recovery (from COLO) plant of Aral Aromatics GmbH in Germany based on improved single-column Morphylane process. It was proved that this new concept is able to reduce energy consumption, to increase product yield and purity and to diminish equipment size and space required. This technology is applicable to benzene, toluene and/or xylenes recovery from any feedstocks (reformate, pygas and COLO), offering flexibility to produce according to market demand (Diehl *et al.*, 2006). Further studies are being made to intensify ED technology into Reactive ED technology, being CDTECH and Sulzer Chemtech the technology providers. CDTECH provides an application in selective hydrogenation using catalytic distillation in benzene reduction and reformate streams (Harmsen, 2007). However, this application is not well defined yet.

2.5. Novelties in Process Development to Increase in Energy Efficiency

Refinery and petrochemical industries are energy intensive consumers, accounting for 25 % of total energy consumption. Operating costs of a process unit are correlated to the energy inputs required to run the process and some type of processes as the ones found in aromatics production complexes require a high energy demand. The energy consumed in an industrial plant is related to economic activity and technological development currently considered. All energy-related processes must operate with maximum efficiency and minimum energy input (Devakottai, 2015; E.I.A, 2013). Therefore, some process improvements to enhance process and energy efficiency have been developed.

At the front end of an aromatics plant, it is encountered a fractionation process to obtain the different fractionation cuts from reformate which some contain aromatics to be separated, converted and recovered in posterior process units. For this purpose, it is used a reformate splitter, which is a fractionation process that transforms reformate into two main fractions: light gasoline ($C5^-$ cut) and aromatics ($C6^+$ cut). Then, a sequence of separation processes are applied to obtain cuts with a composition of a certain aromatic, such as BT cut, Xylene isomers and heavy aromatics. To intensify this sequence of process into a shorter one with less energy consumption, a Divide Wall Column (DWC) was developed to perform these several separation tasks of conventional columns in one single step.

In DWC technology, a pre-fractionator is integrated within the shell of the main reformate splitter by dividing vertically a conventional distillation column with a gas and liquid-sealed wall in the middle section of the column, which separates the main column and the side column. The reformate feed enters the main column where a cut between low and higher boiling points of different components takes place in which C5 fraction is the top product and the side draw consists of a benzene/toluene fraction which is forwarded to an extractive distillation process. DWC requires less energy consumption and less investment costs comparing to conventional fractionation process with two column-systems and it is simple to implement in existing facilities. DWC is also useful for the recovery of high pure benzene in pygas units, which separates low benzene gasoline fraction and benzene containing C6 fraction (Dejanovica *et al.*, 2011; Dejanovica *et al.*, 2010; Ennenbach *et al.*, 2001; Townsend and Singh, 2011). A representation of DWC is shown in Figure 2.20.

This technology allows to separate more than four products in one DWC. To achieve so, different positions of the diving wall were considered in DWC configuration studies. There are two DWCs possible configurations for four products separations that were studied to separate aromatics: Kaibel column and fully extended Petlyuk configurations. Furthermore, the application of DWC was also extended to extractive distillation process (Dejanovica *et al.*, 2011; Dejanovica *et al.*, 2010; Kumar *et al.*, 2018; Yildirim *et al.*, 2011).

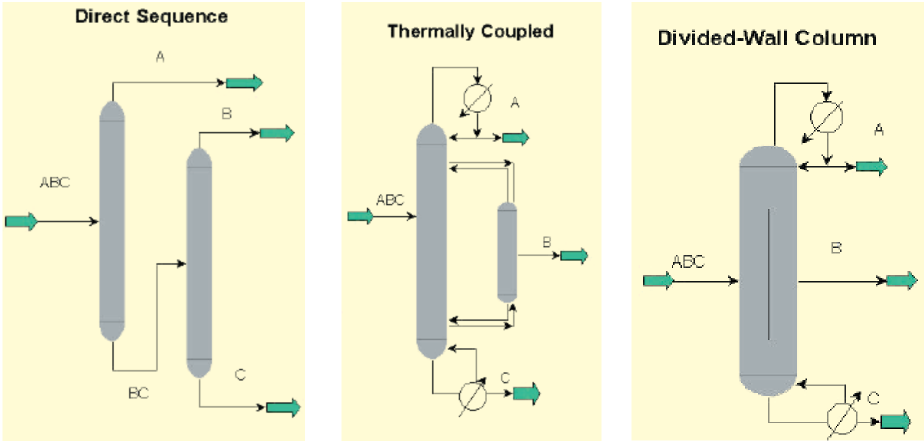


Figure 2.20: Hydrocarbon mixture separation options using fractionation process (Ennenbach *et al.*, 2001).

In March 2011, KBR announced the successful start-up of its DWC tower design for Valero Energy at three of US-based refineries as a way of removing benzene from gasoline streams (Townsend and Singh, 2011). GTC Technology licenced GT-DWCSM for a second DWC at the DTA Refinery in Jamnagar, India. The project involved the substitution of two naphtha splitting towers to one single column with a payback period of less than six months (GTC Tecnhology, 2017b). Moreover, GTC Technology implemented a DWC with two separate sets of condensing systems and offers significant flexibility in terms of producing different levels of hexane in the light naphtha isomerization unit of Bharat Petroleum Corporation, Ltd. (BPCL) refinery in Mumbai, India (GTC Tecnhology, 2017a).

Although DWC technology provides excellent advantages to save energy and other costs, it may bring practical difficulties, such for example an unattractive payback period when the plant lifetime is not long. As an alternative, thermally-coupled distillation sequence also allows lower energy requirements compared to existing conventional column sequences, as well an easy design and small modifications.

To add advantage to both technologies, a heat pump can be coupled with the columns. Heat pumps utilize condensation heat released at the condenser to be used for evaporation in the reboiler allowing energy conservation when temperature difference between the overhead and the bottom of the distillation column is small and the heat load is high. A side heat pump can increase the area utilization bellow the side heat pump by reducing vapour and liquid traffic on the trays above the side heat pump and increasing the vapour and liquid traffic bellow the side heat pump. The application of a side heat pump in DWC has recently been studied. Its application is currently used by combining a side heat pump with thermally-coupled distillation columns to reduce operating costs and to debottleneck the columns (Long and Lee, 2015).

Energy consumption can also be reduced by using more thermal efficient heat exchangers. Compact heat exchanger is a heat exchanger alternative for shell-and-tube heat exchangers without sacrificing quality, longevity and suitability for the most demanding applications. This new welded plate heat exchangers technology is smaller, lighter and less expensive than shell-and-tube heat exchangers.

These heat exchangers can incorporate many streams simultaneously, can increase production, can yield energy savings and also can reduce capital and installation costs. The payback periods are also lower, even at much lower energy price levels (Klemeš et al., 2011; Stankiewicz and Moulijn, 2004). In terms of energy savings, compact heat exchangers can reduce 50 % of energy consumption by only substituting shell-and-tube heat exchangers. Thus, less energy is wasted and more energy is recovered and put back to use. The efficiency in recovering heat of a heat compact exchanger is five times higher than a shell-and-tube heat exchanger (the yield heat recovering is 25 % higher). The high efficiency means that this technology can exploit temperature differences as low as 3 ºC. This thermal efficiency is the result of the turbulence and counter-current flow of the compact exchanger, which also allows reducing fouling and maintenance (Matsufugi, 2012).

Chapter 3: Cluster Analysis of Process Unit Operational Data to Identify Operational Scenarios for an Evaluation of Energy Savings

Abstract

An energy performance of Pre-Distillation and Arosolvan Units of the aromatics plant will be carry out through Pinch Analysis. For this purpose, data was extracted from both process units and a pre-treatment was applied to remove missing data, incoherent data and possible outliers. Cluster analysis using k-means algorithm was applied to data from two years of operation, with the goal of identifying different clusters. The methodology showed potential to describe process operational data in terms of representative operational scenarios (clusters) that may be a useful input for subsequent energy integration and optimization studies. Two cluster evaluation criteria simplified the procedure to achieve the optimal number of clusters when using k-means clustering algorithm. Final results showed that, for Pre-Distillation Unit with a 706x55 matrix dimension, it was identified 6 clusters, while for Arosolvan Unit with a 620x86 matrix dimension, it was identified 3 clusters. Pinch Analysis will further be performed for each operational scenario and results compared with those obtained using the overall mean values (global scenario).

Key words: Cluster Analysis, k-means clustering, Aromatics Plant, Pinch Analysis.

3.1. Introduction

Statistical data analysis is applied in many scientific fields such as biology, economics, engineering, psychology, medicine, marketing, etc. Data can be a complex set of information and size representing all characteristics of a certain scientific goal study, and thus, its structure cannot be defined directly. Therefore, specific data processing methods are required to analyse, explore and synthesize results to improve the knowledge of a field. Multivariate statistical analysis has different techniques for that purpose. However, it is difficult to establish which one is the most appropriate, being its choice determined by the main objectives of the study (Jambu, 1991; Johnson & Wichern, 2007; Myatt, 2007).

Multivariate data analysis can be divided in exploratory data analysis followed by confirmatory data analysis. Exploratory data analysis (data mining) applies methods to recognize data structure and to generate hypotheses for further studies. Such techniques are characterized by visual displays and graphical representations and by the lack of associated statistical significance tests of the results. After defining hypothesis, a confirmatory analysis is performed to test its veracity using a type of statistical significance test. Multivariate methods are then applied essentially to search for data structure or patterns which may be reflected by correlations between several variables or by similarities of subjects as reflected by their multivariate profiles. The aim is to find similarities between the variables and/or similarities between observations in the data set. This analysis arises from the fact that it may exist measurements on similar groups of subjects. The analysis is performed to know what these groups are, how many there are and which subject belongs to each group. This type of analysis is called unsupervised pattern recognition and includes multivariate techniques such as principal component analysis (PCA), multidimensional scaling (MDS) and cluster analysis (CA). In case where the groups are known, it is important to verify how multivariate profiles might discriminate between groups by applying supervised pattern methods such as discriminant analysis or generalized linear model. Another alternative is to find sets of variables that appear to be highly correlated and demonstrate that the similarity between variables arise from the fact that they appear to be indicators. In this case, exploratory factor analysis is a more appropriate method. Confirmatory factor analysis could also be applied to verify which variables are the indicators before carrying out any analysis to test whether data are consistent with such a measurement model. Another way to find correlation between variables is the exploration of patterns of association between sets of multivariate measures with methods such as multiple regression, covariance structure modelling or structural equation modelling (Everitt & Dunn, 2001).

The objectives of multivariate data analysis include the following: i) data extraction and pre-processing or structural simplification without losing valuable information; ii) finding groups in data where similar objects or variables are grouped based on measured characteristics; iii) investigation of the dependence among variables to evaluate the relationships between two or more variables; iv) prediction of values through the relationships between variables and on the basis of observations on those variables; v) hypothesis formulation and testing in terms of parameters of multivariate population to validate the assumptions or reinforce convictions (Johnson & Wichern, 2007; Myatt, 2007).

3.1.1. Data Sets Extraction and Pre-Processing

Data extraction and pre-processing is important prior to any statistical study to expose the essential information. When extracting data, it may be incomplete or containing aggregate data. Data may also contain outliers and/or be inconsistent containing discrepancies in attributes. In cases where there are heterogeneous sources, data integration process is required to become a unique source. Finally, some applications involve particular constraints like ranges for data features which may imply the normalization or transformation of the data distribution features. Data pre-processing involves the following main tasks: data integration, data filtering and cleaning (missing data and outliers removal), discretization, data transformation, and data reduction (García et al., 2015; Myatt, 2007).

As data can be obtained from different sources, it is necessary a properly data integration to decrease redundancies, inconsistencies and duplicates, so it won`t have a negative impact on the analysis. An essential part of this process is to build a data set that establishes a common structure to present a real world example. Processing data extracts and gathers the information to an external file so that processing and modelling can be faster (García et al., 2015). Moreover, missing data and outliers may also be a problem. Methods to remove and eliminate outliers from data sets will be approached further. Missing values are values that are not captured as, for example, data may not be available due to equipment malfunction, be inconsistent with other recorded data and thus deleted, data not entering due to misunderstanding, certain data may not be considered important at the time of entry, not register history or data changes. There are some tools that ignore missing values or use some metric to fill in replacements removing information from the data set and reduce the negative influence in the results (Hair et al., 2010). However, no matter the technique applied, the further away the dataset becomes from the real data, the lower its accuracy (García et al., 2015; Hand et al., 2001).

The prepared data set may not be useful enough for future analysis because some selected attributes may be considered raw data that have a meaning in the original domain from where they were obtained but are not good enough to obtain accurate predictive models. Therefore, some data manipulation is performed to transform the original attributes or to generate new ones with better properties that will improve the efficiency of further analysis. Examples of data transformation methods are discretization, normalization and/or reduction (Aggarwal, 2013; García et al., 2015; Myatt, 2007). Discretization process is a data reduction mechanism with the main purpose to divide the range of a continuous attribute into intervals as some classification algorithms only accept discrete attributes. Data normalization is another important step that may be required to adapt the ranges of the attributes or their distributions to the algorithms being applied in future analysis (Aggarwal, 2013; Hand et al., 2001; Rencher, 2002). In other cases, data reduction may be required to remove or group the high amount of data through the two main dimensions, examples and attributes, simplifying data domain and reducing the time of analysis. Typical methods can be found in Myatt (2007) and García et al. (2015).

3.1.2. Outlier Detection Models for Multivariate Data

According to Ben-Gal (2005), outlier definition often depends on assumptions regarding data structure and on applied detection method. However, some definitions are general enough to cope with various types of data and methods. Different definitions of outliers can be found in the literature: Hawkins (1980) defined outliers "as an observation that deviates so much from other observations as to arouse suspicion that it was generated by a different mechanism". Barnet and Lewis (1994) designated that "an outlying observation, or outlier, is one that appears to deviate markedly from other members of the sample in which it occurs". Rousseeuw and Zomeren (1990) defined outliers as "observations that deviate from the model suggested by the majority of the point cloud, where the central model is a multivariate normal". Singh and Upadhyaya (2012) presents a review of types of outliers and the main difficulties in detecting them in multivariate data. In this work, it will be considered the outliers definition of Aggarwal (2013) who defined outliers as values in the data that are significantly different from the remaining data and are out of range which may impact the accuracy of the multivariate analysis.

Some difficulties are found when handling outliers in multivariate data. A confusion with extreme values are very common since extreme values are a very specific kind of outliers in which it is assumed that too large or too small values are outliers. There are some probabilistic models that quantify the probability that a data point is an extreme value. However, it is possible to generalize the extreme value analysis to multivariate data by determining the points at the multidimensional outskirts of the data (Aggarwal, 2013). In addition, when handling outliers, it is possible to be subjected to masking and swamping effects. Masking effect occurs when one outlier masks a second outlier, if the second outlier can be considered as an outlier only by itself but not in the presence of the first outlier. Masking occurs when a cluster of outlying observations skews the mean and covariance estimates toward it, and the resulting distance of the outlying point from the mean is small (Kannan & Manoj, 2015; Majewska, 2015). Swamping effect occurs when an outlier swamps a second observation, if the observation can be considered an outlier in the presence of the first outlier. After deleting the first outlier, the second observation becomes a non-outlier. This effect occurs when a group of outliers skews the mean and the covariance toward it and away from other non-outlying instances, and the resulting distance from these instances to the mean is large, making them look like outliers (Majewska, 2015).

To eliminate possible outliers in multiple variables, some detection algorithms may be applied, creating a data normal pattern model and then compute an outlier score of a given data point on the basis of the deviations from these patterns. Outlier detection models are chosen based on several important factors such as data type, data size, availability of relevant outlier examples, and the need for interpretability in a model. The last factor is a very important one because it is often desirable to determine if a particular data point is an outlier in terms of its relative behaviour with respect to the remaining data. The interpretability level is dependent on the type of outlier detection model that is being applied. For instance, models that work with original attributes and use fewer data transformation on the data have higher interpretability. Data transformation may enhance the contrast between outliers and normal data but are performed at the expense of interpretability. Examples of generative models are the Gaussian mixture model, a regression-based model, or a proximity-based model. These models make different assumptions about "normal" behaviour of the data and then an outlier score of a data point is computed by evaluating the quality of the fit between the data point and the model. The best choice of a model is often data set specific which requires a good understanding of the data itself before choosing the model (Aggarwal, 2013; García et al., 2015; Hand et al., 2001; Rencher, 2002). Example of outlier detection methods can also be found in books of Rousseeuw and Leroy (1987), Hawkins (1980), Barnet and Lewis (1994) and Aggarwal (2013). The main advantage and disadvantage of these techniques can be found in Petrovskiy (2003). In Ben-Gal (2005) work is presented a good review of different methods for outlier detection for univariate analysis and for multivariate analysis, being demonstrated the importance of using estimators in the presence of outliers. In this work, Mahalanobis Distance as proximity-based method is the main focus.

3.1.3. Mahalanobis Distance as Proximity-based Method

In proximity-based methods, outliers are modelled as points which are isolated from the remaining data. This can be done using three different methods: cluster-based analysis, density-based analysis or nearest neighbour analysis. In the first two methods, the data is pre-aggregated before outlier analysis by either partitioning the points as in cluster-based methods or the space as in depth-based methods, and consequently, data dense regions are formed and outliers are the points out of those regions. In the third method, the distance of each data point to its nearest neighbour is determined. According to Aggarwal (2013), the distance of a data point to its k-nearest neighbour is used in order to define proximity, being the points with large k-nearest neighbour distances considered outliers. In other words, the identified points that are closed together but far from the remaining data are considered outliers. Distance-based methods will be the main focus in this work because compared with the other two methods, it provides more detailed granularity at which the analysis is performed. Depending on the data type and size, distance-based methods can be an advantage or a disadvantage. When the dataset is large, the distance determination can be slow. For smaller datasets, this method can provide more detailed and accurate results (Petrovskiy, 2003).

Clusters and outliers have a complementary relationship as every data is either a member of a cluster or an outlier. In clustering, the aim is to partition the data into groups of dense regions while in outlier detection, the aim is to determine the points that do not fit in any of these dense regions. However, when clustering, the outliers detected can be weak outliers or noise. For example, a data point which is located at the fringes of a large cluster is very different from a point which is completely isolated from all the other clusters. In addition, all data points in very small clusters may wrongly be considered outliers. Therefore, a more accurate distance method can be used to detect outliers in terms of clusters proximity which is called Mahalanobis Distance (Aggarwal, 2013; Hair et al., 2010; Maesschalck et al., 2000).

Mahalanobis Distance using different parameter estimators has been applied in many works. Peña and Prieto (2001) presented a simple multivariate outlier detection procedure using covariance matrix as a robust parameter estimator and kurtosis coefficient of the projected data, comparing estimator properties with others described in literature which showed positive results in practice. Hardin and Rocke (2005) provided an F-test that gives the accurate outlier rejection points for various sample size applying Mahalanobis distance which have an asymptotic chi-squared distribution. Atkinson and Riani (2007) described a procedure based on robust Mahalanobis Distance to identify and conform separated and overlapping clusters in multivariate normal data in relation to outlier detection. Riani et al. (2007) provided a new multiple outlier test using forward search and robust Mahalanobis Distance to detect outliers in a sample of multivariate normal data. The main purpose was to compare the sizes and power obtained with the new test with the ones obtained with best existing tests. The comparisons of the new procedure with tests using other robust Mahalanobis Distance showed good size and high power of the new procedure. Todeschinia et al. (2013) presented a new measure of Mahalanobis Distance in which covariance matrix is centred on each sample instead on data centroid as in the classical covariance matrix, obtaining a new distance matrix with more interesting information for outlier detection. The authors used two parameters called remoteness and isolation degree to evaluate the outliers` features facilitating a better identification of a typical samples isolated from the rest of the data and thus, reflecting the potential application towards outlier detection.

3.1.4. Selection of Multivariate Statistical Analysis Techniques

Multivariate statistical analysis are used to analyse data with two or more measurements on each variable and the variables are analysed simultaneously focusing upon the degree of relationships (correlations and covariance) among these phenomena (Hair et al., 2010; Reis, 1997). They can be classified as dependence techniques, which are applied when one or more variables can be identified as dependent variables (criterion) while the remaining variables are independent (predictor), or inter-dependence techniques, when the variables are not classified as dependent or independent but the whole set of interdependent relationships is analysed (Hair et al., 2010).

Dependence statistical techniques can be characterized according to the number and the type of measurement scale of dependent variables. Considering the number of dependent variables, the techniques to be applied will depend if the variables have a single dependent variable, several dependent variable or several dependent and independent relationships. According to the type of scale, the dependence techniques to be applied will also depend if the variables are either metric (quantitative/numerical) or nonmetric (qualitative/categorical). For example, if the analysis involves a single dependent variable in metric scale, the dependence technique that best fits the data is multiple regression analysis or conjoint analysis. On the other hand, if the single dependent variable is nonmetric, the best technique to be used is multiple discriminant analysis and linear probability models. In cases where several dependent variables are being studied, other dependence techniques must be applied. If the variables are metric, then they must be analysed as independent variables. Depending if those variables are metric or non-metric, the best technique to be applied is multivariate analysis of variance (MANOVA) or canonical analysis with variables transformation to dummy variables, respectively. If it exists several dependent and independent variables relationships, then equation modelling is the appropriate technique (Hair et al., 2010).

As for interdependence techniques, the variables cannot be classified into dependent or independent variables but are analysed simultaneously to find a structure to the entire set of variables. When the structure of the data is the main focus of the analysis, factor analysis or confirmatory factor analysis are the appropriate techniques. If cases or respondents are to be grouped to represent structure, then cluster analysis is the best technique to be applied. When the aim is the analysis of the structure of objects, then the perceptual mapping technique should be used. As in dependence variables, when objects are the aim, the measurement properties of the techniques should be considered. For example, factor analysis and cluster analysis are considered to be metric interdependence techniques, and in cases when nonmetric data is being analysed, they must be transformed into dummy variables so these techniques can be applied correctly. In case objects are being analysed, being metric or non-metric, multidimensional scaling can be applied in both cases while correspondence analysis is only appropriate for non-metric scales (Hair et al., 2010). In this work, the main multivariate statistical analysis techniques to be described are interdependence statistical techniques with the main focus on cluster analysis.

3.1.5. Cluster Analysis

Clustering is an unsupervised multivariate analysis technique that can be used for several purposes since clustering can be considered as a form of summarization and outliers analysis or as a way to find similarities between variables. Books of Anderberg (1973), Hartigan (1975), Jain and Dubes (1988), kaufman and Rousseeuw (1990), Everitt et al. (2011) and Aggarwal and Reddy (2014) approach clustering techniques main applications in different science fields and are considered a good literature review.

Clustering techniques are based on the partition of a set of observations into a distinct number of unknown groups (clusters) in a way that all observations within a group are similar between each other and not similar to other groups' observations. It is assumed that some observations have very distinct features from others that would allow to distinguish groups with different characteristics (Johnson & Wichern, 2007; Rencher, 2002). The first step of cluster analysis is to choose the best way to represent the objects to be clustered. However, there isn't a single unique technique that is appropriately applied to all study cases for finding all varieties of groupings that can be represented by multidimensional data. Therefore, different clustering methods as indicated in Figure 3.1 should be applied on a given data set to analyse what patterns emerge (Martinez & Martinez, 2005).

Clustering algorithms can be divided into two classical methods: hierarchical methods and partition methods (non-hierarchical). In any of them, to determine the groups in the dataset, a proximity measure or measure of nearness is defined to evaluate the degree of distance or "dissimilarity" and the degree of association or "similarity" between groups. The proximity measure is chosen based on the subject matter, scale of measurement and type of variables involved in the dataset (Everitt et al., 2011; Hartigan, 1975; Martinez & Martinez, 2005).

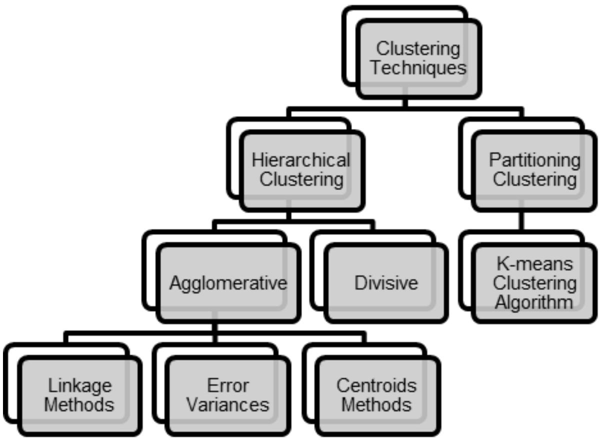


Figure 3.1: Cluster analysis types of methods (Everitt et al., 2011).

Cluster Analysis is also known as unsupervised learning technique due to the fact that it is unknown how many groups are represented by the data, what the group membership or structure is, or even if there are any groups in the first place. Most of the mentioned techniques will find some desired number of groups but what is desirable is some meaningful clusters that represent the true phenomena. Thus, resulting groups must be evaluated to determine whether or not they aid in understanding the problem. The general procedure is given in Table 3.1 (Everitt et al., 2011; Martinez & Martinez, 2005).

Clustering methods require a measure of similarity or proximity, which is expressed as a distance to define the combination of data points to be clustered. Similarity measures can be determined using direct methods or indirect methods, being the latter the most common. The most well-known similarity/dissimilarity indices are correlation indices, distance measures, association coefficients, and probabilistic similarity measures. The relations of similarity between the observations are translated into geometric distances, that is, the observations are points in a given space of coordinates so that the dissimilarities between them correspond to the metric distances between the respective points. The measures of similarity/dissimilarity are several and these must respect certain metric properties that can be found in Reis (1997) and Everitt et al. (2011).

The measures interact as criteria with cluster analysis, as some give the same results with one criterion and different results with another, depending also on the type of data and variables. The choices of variables, data transformation (normalization), and similarity measures are the combination steps for data clustering (Anderberg, 1973). Proximity measures are used to represent the nearness of two objects determining how close data points are to each other or how far apart they are. If a proximity measure represents similarity, the value of the measure increases as two objects become more similar.

Alternatively, if the proximity measure represents dissimilarity, the value of the measure decreases in value as two objects become more similar (Everitt et al., 2011; Reis, 1997).

Table *3*.1: Cluster analysis general procedure (Martinez & Martinez, 2005).

1. Pattern Representation	• Initial preparation of the procedure: i) choosie the number of clusters, ii) choose the distance measures to use (feature selection), iii) determination of how many observations to process, and iv) choose the scaling or other transformations of the data (feature extraction).
2. Pattern proximity measure	• Clustering methods require a measure of distance (proximity) between observations and between clusters. Different distances lead to different partitions of the data.
3. Grouping	• Partitioning the data into clusters using a clustering technique. The grouping can be hard, which means that an observation either belongs to a group or not. In contrast, it can be fuzzy, where each data point has a degree of membership in each of the clusters. It can also be hierarchical, where we have a nested sequence of partitions.
4. Data abstraction	• This is the optional process of obtaining a simple and compact representation of the partitions, such as the centroid of the cluster.
5. Cluster Assessment	• Assessment of the data to see if it contains any clusters. It means an examination of the output of the algorithm to determine whether or not the clusters are meaningful.

The most applied dissimilarity measure is the Euclidean distance between two objects which is the distance to be considered in this work. All these measures assume a degree of commensurability between different variables in a way that it would be more effective if all the variables of the given data set had the same units, such for examples length (meters) or weight (grams). However, in most data sets not all the variables have the same units and therefore altering the choice of units might be a good option so that they are all regarded as equally important. This can be performed using data standardization by dividing each of the variables by its sample standard deviation to provide an equally importance to all the variables. Nevertheless, it is important to stand out that this does not overcome completely the problem since treating the variables as equally important still is an arbitrary assumption and in some cases some variables are most important than others as they must have a higher weight. In addition, for some methods such as scale-invariant cluster analysis that are to be employed for the analysis of continuous data, the problem of standardization becomes irrelevant (Everitt et al., 2011; Hand et al., 2001).

3.1.5.1. Cluster Analysis using Hierarchical Clustering Methods

The hierarchical methods can be classified into agglomerative and divisive methods depending on how cluster solutions are generated. The first type generates a sequence of cluster solutions starting with a cluster with a single solution followed a combination of objects until all objects form a single cluster. The procedure uses linkage methods (single, complete or average linkage), variance methods (ward method) and centroid methods. The divisive hierarchical methods start with a single cluster where all objects are included and splits the objects successively to form clusters until single objects. In both types of methods a tree diagram called dendrogram can be constructed to represent clusters solutions as a map of the process (Everitt et al., 2011; Martinez & Martinez, 2005).

However, it is possible to understand that none of them requires to know ahead the number of groups to determine the number of clusters. The process consists of a sequence of steps where two groups are either merged (agglomerative) or divided (divisive) according to some optimality criterion. Each of these hierarchical methods have *n* observations in their own group (*n* total groups) at one end of the process and one group with all *n* data points at the other end. The two main difficulties dealing with hierarchical clustering is that once points are grouped together or split apart, the step cannot be undone and how many clusters are appropriate to consider after performing the procedure.

An advantage of divisive over agglomerative methods is that most of data set have small number of clusters and that structure would be revealed in the beginning of a divisive method while with agglomerative method this does not happen until the end of the process (kaufman & Rousseeuw, 1990). Agglomerative clustering requires several choices, such as how to measure the proximity (distance) between data points and how to define the distance between two clusters. Determining what distance to use is largely driven by data type, as well as what aspect of the features wants to emphasize. Some of the agglomerative methods can be found in Martinez and Martinez (2005), Everitt et al. (2011) and Aggarwal and Reddy (2014).

One of the disadvantage of hierarchical clustering is how to choose the number of clusters. There are a variety of methods to estimate the optimal number of clusters in both hierarchical clustering and optimization methods (non-hierarchical clustering) which will be described next. However, one way to determine the number of cluster in hierarchical clustering is to select one of the solutions in the nested sequence of clustering that comprise the hierarchy by cutting the dendrogram at a particular height (term best cut) defining the partition such that clusters below that cut are distant from each other by at least that amount and the dendrogram can suggest the number of clusters (Aggarwal & Reddy, 2014; Everitt et al., 2011; Martinez & Martinez, 2005).

Some recent examples of hierarchical clustering applications can be found in literature. Gu et al. (2016) developed a new model combining hierarchical clustering and principal component estimate with the purpose of adapting recycled plastic in more demanding industrial applications. Zhang et al. (2016) researched the major air pollutants in several cities of China, having in consideration seasons factor to evaluate air quality, which has a significant negative impact from several industries. Jiang et al. (2015) applied principal component analysis and hierarchical analysis to investigate the presence of arsenic in groundwater distribution and to evaluate the factors that contribute to high arsenic concentrations to further implement chemical processes controlling occurrence. Bayo and López-Castellanos (2016) carried out a process performance and operation of wastewater treatment plants applying a hybrid method, combining principal factor analysis and hierarchical cluster analysis to ensure their compliance with legislative requirements imposed by European Union.

3.1.5.2. Cluster Analysis using K-means Clustering Algorithm

Non-partitioning (non-hierarchical) methods consist of techniques that optimize some criterion in order to partition the observations into a predetermined number of groups. These methods differ in the nature of objective function as well as the optimization algorithm used to obtain the final clustering. They aim at partitioning a given data set into different subsets (clusters) so that specific clustering criteria are optimized. These criteria are square distances, which are computed for each point from the corresponding cluster center and then takes the sum of these distances for all points in the data set. This algorithm groups the data by minimizing the squared distance between the centroid (mean of the points in the cluster) and the points in the cluster. One of the most commonly used methods is k-means clustering algorithm due to its simple and flexible framework (Likas et al., 2003; MacQueen, 1967; Rencher, 2002). Later, Kanungo et al. (2002), Fahim et al. (2006), Zalik (2008) and Nazeer and Sebastian (2009) contributed for the development of more accurate and efficient enhanced k-means clustering algorithms.

An overview of this clustering technique can be found in Jain et al. 2010. A literature review shows that k-means clustering has many applications, being increasingly applied in industrial fields. As examples, k-means clustering technique was applied by Pyun et al. (2011) to define operating modes of LNG plant systems and thus improve their monitoring and diagnosis. Mandel et al. (2015) evaluated water quality in water distribution networks. Cremaschi et al. (2015) introduced a systematic approach that reduces model-prediction discrepancy for threshold-velocity estimation of fluid-flows to ensure particle transport which is difficult to estimate due to complex nature of fluids physical properties. This is an important research for oil and gas production.

In implementing non-hierarchical cluster methods, one may vary the method for selecting k clusters and the criterion for reallocating observations to clusters for higher stability. To initiate the method, one first selects k centroids. Bradley and Fayyad (1998) demonstrated that refined initial starting points indeed lead to improved solutions of these interactive techniques. The centroids may be the first k observations at some defined level of separation that may be replaced based upon some replacement algorithm, and other variations. Once centroids are selected, each of the observations are evaluated for assignment or reassignment based upon some convergence criterion such as multivariate statistics that involve the determinant and trace of the within-cluster and between-cluster variability. Contributions to overcome the drawbacks of cluster centre initialization can be found in the works of Khan and Ahmad (2004) and Erisoglu et al. (2011).

As it is possible to understand, the difference between hierarchical clustering and k-means clustering resides in the pre-specification of the number of clusters. In the first method the number of clusters is unknown and a dissimilarity proximity matrix is used to initialize the clustering process not allowing the reallocation of the assigned object. K-means clustering is initiated using data matrix and not a dissimilarity matrix by knowing a priori the number of clusters. Observations are reassigned using some criterion with reallocation terminating based upon another criterion (Aggarwal & Reddy, 2014; Everitt et al., 2011; Martinez & Martinez, 2005).

Pelleg and Moore (2002) approached three main drawbacks of K-means clustering: it scales poorly computationally; the number of cluster K has to be pre-specified; and it searches for local minima. It is presented solutions by applying Bayesian Information Criteria and Akaike Information Criteria measures to search the space of clusters locations and the number of clusters to obtain faster and more accurate results. Pham et al. (2005) approached one of the drawbacks of K-means clustering algorithm which is the requirement for the number of clusters to be specified before the algorithm is applied. The author also presents a review of existing methods to overcome the interactive process presenting also a new procedure for this purpose avoiding the need for trial and error. Fang and Wang (2012) developed an estimation scheme to determine the number of clusters based on bootstrap method to increase clustering stability. The authors compared to the work of Wang (2010) who approach clustering stability through cross-validation method. Ortega et al. (2009) presented a paper in which are approached the main issues found when applying K-means algorithm using MATLAB, analysing for example, the convergence of algorithm to a local optimum rather than a global optimum, the algorithm efficiency, the sensibility to the presence of outliers and its limitation as it is only applied to numerical variables. Works of Fischer (2011), Scitovski and Sabo (2014), Fujita et al. (2014) and Amorim and Hennig (2015) also contribute to overcome this drawback.

Former clusters obtained with the application of k-means clustering algorithms can be evaluated using several cluster validity indexes to evaluate the algorithm results and to evaluate the optimal number of clusters to be used in the clustering technique.

3.1.6. Cluster Validation and Number of Clusters Estimation

As discussed, clustering methods require an iterative process to determine the optimal number of clusters. As it is an unsupervised technique, it is important to verify the goodness of partitions after clustering before using its results. Since the algorithm converges to a local minimum, different clusters can be obtained from different initializations. To overcome local minima, k-means algorithm is usually run for a given k with different initial partitions and the best solution found is then selected (Jain, 2010). Calinski and Harabasz (1974) applied variance ratio criterion to determine the optimal number of clusters, which has proven to work well in other situations (Milligan & Cooper, 1985). Halkidi and Vazirgiannis (2001) developed a new cluster validity index (S_Dbw) to evaluate k-means clustering partition and compared to other validity indices, demonstrating good results even when compared to cases in which indices failed to aim cluster stability. Legány et al. (2006) presented a short clustering techniques review and approached the problem of clustering validity by applying the most commonly used cluster validity indices such as validity index of Halkidi and Vazirgiannis (2001) and Davies and Bouldin (1979). Yeh et al. (2014) developed a new cluster validity Index (CDV) that provides a quality measurement for the goodness of a clustering result for data and verify if clustering result is suitable.

Cluster validation can be characterized into two different groups, external clustering validation and internal clustering validation, which the main difference resides in whether or not external information is used for clustering validation (Halkidi & Vazirgiannis, 2002; Wang et al., 2009). An extensive comparative study of cluster validity indices can be found in Wu et al. (2009), Gurrutxaga et al. (2011) and Arbelaitz et al. (2013).

External validation methods require external information from the data to evaluate the extent to which the clustering structure discovered by a clustering algorithm matches some external structure, while interval validation methods evaluate the goodness of a clustering structure without needing external information. One example for external validation methods is entropy measure which evaluates the purity of clusters based on the given class labels. An example for internal validation measures is the Silhouette index which validates the clustering performance based on the pairwise difference of between and within cluster distances of all data points (Rendón et al., 2011; Rousseeuw, 1987). Silhouette plot was introduced by Rousseeuw (1987) in which the clusters are represented by a silhouette based on a proximity measure for the comparison of clusters tightness and separation showing which objects are well grouped within their cluster and which ones are not. The silhouette obtained for each cluster is plotted together in a single graph allowing the comparison and evaluation of the quality separation between clusters and an overview of the data structure. The average silhouette width provides an evaluation of clustering validity in a way to determine the appropriate number of clusters. Baarsch and Celebi (2012) performed an investigation of internal validity measured for k-means clustering approaching Silhouette Index, Calinski-Harabaz Index and Davies-Bouldin Index. Alok et al. (2014) developed and implemented an external cluster validity index based on Max-Min distance along data points and used a probabilistic approach to find the correct correspondence between the true and obtained clustering. To avoid errors in the iteration process there are certain criteria that can be used to estimate the optimum number of clusters before grouping the data. Clusters validity indexes can also be found in the works of Fujita et al. (2014), Kolesnikov et al. (2015), Yeh et al. (2014) and Zalik and Zalik (2011). Both external and internal validation measures can be applied not only to select the best algorithm for partition and to validate the number of clusters that best fit the data, they can also be used to previously estimate the optimal number of clusters before performing the partition into groups.

3.2. Methodology

In this work, an energy evaluation of an aromatics plant will be carry out. For that purpose, a detailed portrait of process units, energy consumptions and process variability is needed. One then proposes a methodology to extract and to partition operational data into clusters, thus identifying possible different operational scenarios. The step of the developed methodology is schematized in Figure 3.2.

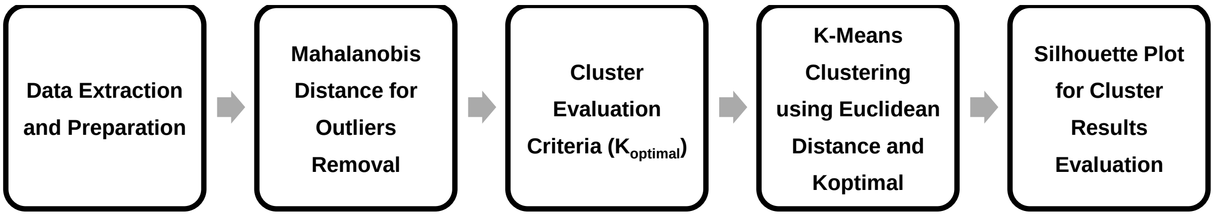


Figure 3.2: Steps for an accurate application of cluster analysis.

Data extracted from each process unit is pre-processed and cleaned to remove missing data and to eliminate possible outliers. From the resulting data, an optimal number of clusters that best fits each data set is found using certain cluster evaluation criteria. The attention of the problem proceeds of finding groups or clusters in the operational data of Pre-Distillation and of Arosolvan Units. K-means clustering algorithm is applied to analyse what patterns emerge taking into account the pre-determined optimal number of clusters (K_{optimal}) and using Euclidean Distance. The aim is to organize the data set into groups in such a way that operational measures within a group are more similar to each other than they are to operational measures belonging to a different group. In other words, the objective is to find out if there is a critical periods of energy consumption (different features in the data that would allow to distinguish groups) within the process unit in analysis. At the end, the quality of resulting clusters are analysed through Silhouette plot to evaluate how well-separated they are. The identified clusters correspond to different operational scenarios for further energy evaluation studies.

Step 1: Data Preparation and Cleaning

Pre-Distillation and Arosolvan Units of the aromatics plant were here analysed based on Process Flow Diagram (PFD) and Process and Instrumentation Diagram (PID). The collected operational data were provided by Galp Energia database for the period 2014 and 2015 in daily average and integrated as a data matrix in one single Excel document where columns represent variables and rows represent operational measures (observations). From the PFD and PID, many variables are measured, being chosen the ones having direct influence on heat exchanger networks: temperatures and flowrates.

Having gather all the variables and the information in one document, data cleaning was performed using Excel&VBA Macros. Missing values were found in the data due to equipment malfunction or because equipment shut down or failures in recording data. Thus, missing values were ignored and removed from the data, including some variables. Incoherent data, such as empty cells, zero or too low flow rates, zero and incoherent temperatures, etc., have also been eliminated from the database.

Step 2: Outliers Detection and Removal using Mahalanobis Distance

Regarding what had been said previously about types of methods to detect and eliminate possible outliers, a distance-based method was chosen for that purpose as it can provide more detailed and accurate results for these size datasets. Mahalanobis distance were applied using Software IBM SPSS Statistics to detect and remove outliers in terms of proximity from the datasets obtained for Pre-Distillation and Arosolvan Units.

Mahalanobis Distance scales the distance values by local cluster variances along the directions of correlation as in Equation 3.1. Considering normal distribution, Mahalanobis distance provides a standard test for outliers using mean and covariance matrix as estimators which are very sensitive to the presence of outliers (Aggarwal, 2013; Hair et al., 2010; Maesschalck et al., 2000).

$$\boldsymbol{MD^2} = (\boldsymbol{x} - \boldsymbol{\mu})\boldsymbol{C^{-1}}(\boldsymbol{x} - \boldsymbol{\mu})^{\boldsymbol{T}} \qquad \textbf{Equation 3.1}$$

Where:
MD^2 – squared Mahalanobis Distance;
x – Vector data;
μ - vector of mean values of independent variables;
C^{-1} – inverse covariance matrix of independent variables;
T – Indicates vector should be transposed.

As mentioned before, Mahalanobis Distance theory assumes that the data follow a normal multivariate distribution of p-dimensions, following a chi-square distribution with a number of degrees of freedom equal to the number of variables involved in the analysis. The distance from Mahalanobis takes into account the covariance matrix of the data of the p-dimensional matrix. Observations considered as outliers values are those with high Mahalanobis Distance values. Determining Mahalanobis Distance, this is interpreted by analysing the significance of the data ($p < 0.001$) and the corresponding normal chi-square distribution. Cases where observations are reported below 0.001 are considered outliers. This is a good methodology for detecting true outliers without the possibility of confusing them with the extreme values of the database.

Step 3: Estimation of the Optimal Number of Clusters

The determination of the optimal number of clusters ($K_{optimal}$) is an advantage when K-means clustering algorithm is applied, overcoming the drawback of a required interactive process to determine the best number of clusters that best fit each data set. $K_{optimal}$ was pre-determined using two internal cluster validity indexes to attain well-separated clusters with high accuracy and stability. These two clusters used were Davies-Bouldin criterion (Davies & Bouldin, 1979) and Silhouette Value Index Criterion (Rousseeuw, 1987) which were available in MATLAB Statistical Toolbox. These criteria were applied for the two data sets (Pre-Distillation and Arosolvan Units) to estimate the optimal number of clusters to be used in K-means clustering algorithm. The detailed description of both cluster evaluation criteria found in MATLAB Statistics Toolbox is presented here.

- **Davies-Bouldin Criterion (DBC)**

Davies-Bouldin criterion (DBC) evaluates the distance between the data within each cluster and between clusters (Davies & Bouldin, 1979). More precisely, DBC measures the ratio of within-cluster distance (average distance between each point in a cluster and its centroid) and between-cluster distance (average distance between each point in a given cluster and the centroid of other cluster), using Euclidean Distance. The DBC is defined as in Equation 3.2 in which D_{ij} is the within-to-between cluster distance ratio for the i^{th} and j^{th} clusters.

$$\boldsymbol{DBC = \frac{1}{k}\sum_{i=1}^{k} max_{j\neq i}\{D_{ij}\}}$$ **Equation 3.2**

D_{ij} can be specified as in Equation 3.3 in which $\bar{d}_i$ is the average distance between each point in the i^{th} cluster and the centroid of the i^{th} cluster, $\bar{d}_j$ is the average distance between each point in the i^{th} cluster and the centroid of the j^{th} cluster and $\bar{d}_{ij}$ is the Euclidean Distance between the centroids of the i^{th} and j^{th} cluster.

$$\mathbf{D_{ij} = \frac{(\bar{d}_i + \bar{d}_j)}{d_{ij}}}$$ **Equation 3.3**

The maximum value of D_{ij} represents the worst-case within-to-between clusters ratio for cluster i. For each process unit, the results are translated through a graph representation of the solutions provided by this criterion. The minimum value obtained in the graph corresponds to the optimal number of clusters for the data set which means that the optimal clustering solution ($K_{optimal}$) corresponds to the smallest DBC index value. This value results from the maximization of the distance of the points of a cluster in relation to other clusters. The application of this criterion requires the joint use of the K-means clustering algorithm to perform the grouping of the data.

- **Silhouette Value Index Criterion (SVC)**

Silhouette Value Index Criterion (SVC) evaluates how much a point is similar in relation to other points (within the same cluster) when compared to points in other clusters. More precisely, SVC measures the distance between points within the same cluster in relation to the distance between points in different clusters, computed using the square Euclidean Distance. The Silhouette Value for each point is a measure of how similar the points are in its own cluster, when compared to points in other clusters. It is specified through the Equation 3.4 in which S_i represents the value for the i^{th} point.

$$\mathbf{S_i = \frac{(b_i - a_i)}{\boldsymbol{max}(a_i, b_i)}}$$ **Equation 3.4**

In Equation 3.4, a_i is the average distance from the i^{th} point to other points in the same cluster as i, and b_i is the minimum average distance from the i^{th} point to points in a different cluster, minimized over clusters. For each process unit, the results are translated into a plot where the maximum value corresponds to the best definition of clusters.

Step 4: Finding Clusters using K-means Clustering Algorithm

The basic algorithm for k-means clustering is a six-step procedure starting by selecting the number of clusters, and then the method allocates the observation to its closest group using a distance measure, such as Euclidean distance, between the observation and the cluster centroid. Next, all the other observations are compared to each of the previous observations already allocated and placed in the group with highest similarity. The centroid point of each group is then recalculated using the assigned observations. The grouping process continues by determining the distance from all observations to the new group centres. If an observation is closer to the centre of another group, it is moved to other group which is closest to. The centres of its old and new groups are now recalculated. The process of comparing and moving observations where appropriate is repeated until there is no further need to move any observations and until there is no change in centroid point of each cluster.

K-means clustering algorithm, as explained before, is a technique that optimizes some criterion in order to partition the observations into specified or predetermined number of clusters. The MATLAB Statistics Toolbox has a function that implements the k-means clustering algorithm. The goal of this algorithm is to partition the data into *k* groups, which were pre-determined using the two criteria above, by minimizing the within-group sum-of-squares in relation to group means. The procedure implemented in this work is:

1) Specify the number of clusters *k* which is equal to the optimal number of clusters (k_{otimal}) estimated using the cluster evaluation criteria;
2) Define the Distance Measure to be applied which is square Euclidean distance by default;
3) Determine cluster centroids for each variable;
4) Calculate the distance between each observation and each cluster centroid;
5) Assign every observation to the closest cluster;
6) Calculate the centroid (i.e., the d-dimensional mean) of every cluster using the observations that were just grouped there.

MATLAB Statistical Toolbox provides a ***kmeans*** function that partitions data into *k* clusters, and returns the index (***idx*** function) of the cluster to which it has assigned each observation. K-means clustering operates on actual observations (rather than the larger set of dissimilarity measures), and creates a single level of clusters. ***Kmeans*** function finds a partition in which objects within each cluster are as close to each other as possible, and as far from objects in other clusters as possible. Different distance measures can be applied, depending on the kind of data that is being clustered. In this work, square Euclidean distance is the one to be used (***sqeuclidean*** function) which is also provided by MATLAB Statistical Toolbox.

Each cluster in the partition is defined by its member objects and by its centroid (mean) which is the point to which the sum of distances from all objects in that cluster is minimized. The ***kmeans*** function computes cluster centroids differently for each distance measure, to minimize the within-group sum-of-squares.

To evaluate how well-separated the resulting clusters are, a silhouette plot using the cluster indices output from ***kmeans*** is constructed for former cluster validation. The silhouette plot displays a measure of how close each point in one cluster is to points in the neighboring clusters. This measure ranges from +1, indicating points that are very distant from neighboring clusters, through 0, indicating points that are not distinctly in one cluster or another, to -1, indicating points that are probably assigned to the wrong cluster. The ***silhouette*** plot returns these values in its first output. Positive and high silhouette values mean well separated clusters, while negative silhouette values mean that points are not well assigned to none of the clusters.

3.3. Results and Discussion

Pre-distillation and Arosolvan units were the process units of the aromatics plant being evaluated in this work. The data extracted in daily average for the analysis correspond to the period 2014 – 2015 which were extracted and provided by Galp energia. Two independent data matrixes were built after data extracted (with temperatures and flowrates) from the instrumentational and control system with the following *nxp* dimensions, being n the number of observations and p the number of variables: 842x55 for Pre-Distillation Unit and 842x90 for Arosolvan Unit. After data pre-processing and treatment, removing missing data and incoherent values, the *nxp* dimensions of the two data matrixes were reduced to 740x55 for Pre-Distillation Unit and 689x86 for Arosolvan Unit. Note that, in the case of Arosolvan Unit, a reduction occurred in the number of variables in the data matrix, which means that these variables didn't had enough data to be considered in the dataset and thus, were eliminated due to missing and/or incoherent data. In addition, with Mahalanobis Distance, it was possible to identify and remove outliers within the two data matrices. The resultant final matrices obtained after data cleaning and outliers' removal have the following *nxp* dimensions: 706x55 for Pre-Distillation Unit and 620x86 for Arosolvan Unit. These were the two data sets used as input for cluster analysis.

For each process unit data matrix, the optimal number of clusters (K_{otimal}) were evaluated using Davis-Bouldin criterion (DBC) and Silhouette Value criterion (SVC) available in MATLAB Statistics Toolbox. For each process unit, the results were obtained through a graph representation of the solutions provided by each criterion.

- **Solutions obtained through Davies-Bouldin Criterion (DBC)**

For each process unit, the solutions obtained through the application of DBC criterion are shown in a graph representation in Figures 3.3 and 3.4 provided by this criterion.

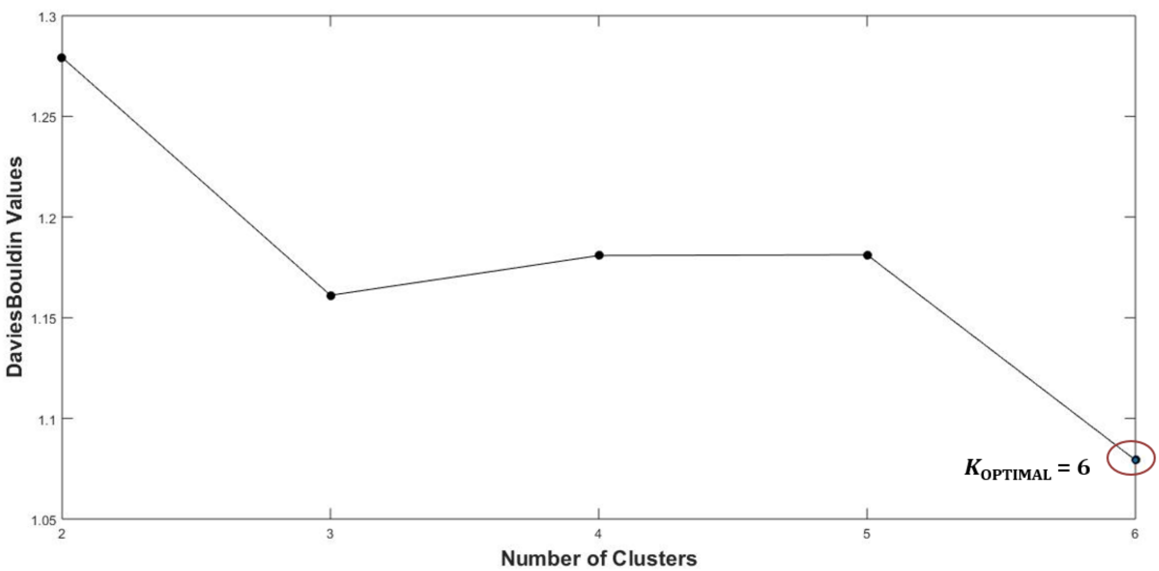


Figure 3.3: Graph representation of Davis-Bouldin Criterion solutions for Pre-Distillation Unit's data set.

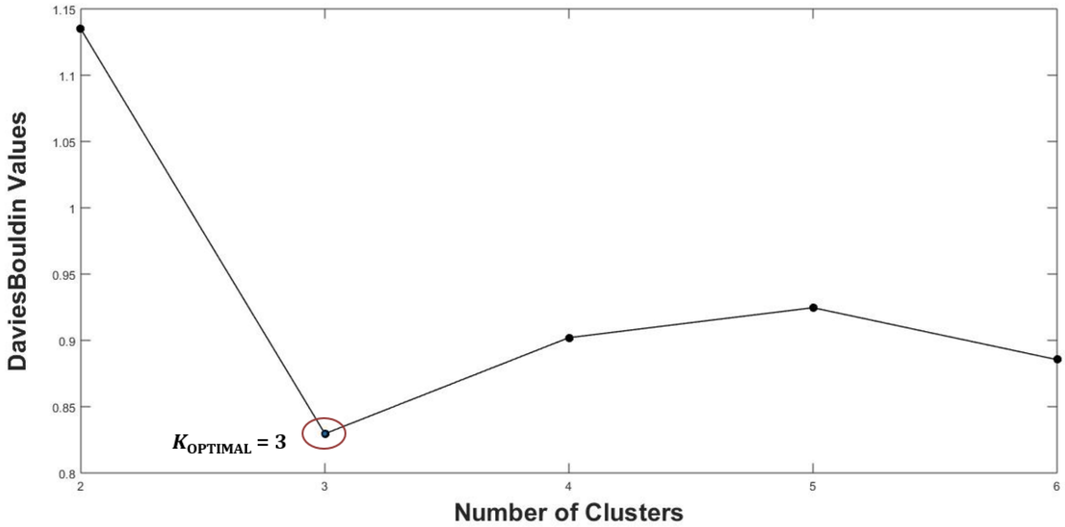


Figure 3.4: Graph representation of Davis-Bouldin Criterion solutions for Arosolvan Unit's data set.

Davies-Bouldin Criterion was evaluated considering a list of number of clusters to evaluate, which in this case was specified to test from 1 to 6 clusters for both process units. However, an inherited method was incorporated to evaluate additional numbers of clusters to guarantee that the optimal number of clusters was achieved. In this case, the number of clusters was evaluated to 10 clusters for both process units. For example, in the case of Pre-Distillation Unit, the optimal number of clusters obtained was 6 clusters. The inherited method guaranteed that this is the optimal number of clusters for Pre-Distillation Unit, not including the additional considering clusters (7 to 10) in the graph representation of the criterion. The same observation can be considered here for Arosolvan Unit.

The plots in Figure 3.3 and 3.4 show that $K_{optimal}$ value correspond to the lowest DBC value which is equal to 6 clusters for Pre-Distillation Unit and equal to 3 clusters for Arosolvan Unit, respectively, suggesting that these are the optimal number of clusters for each process unit.

- **Solutions obtained through Silhouette Value Index Criterion (SVC)**

Through the application of SVC criterion, the solutions obtained for each process unit are shown in a graph representation in Figures 3.5 and 3.6 provided by this criterion. The SVC criterion was evaluated considering a list of number of clusters to analyse, which in this case was specified to test from 1 to 8 clusters for both process units.

The plots in Figure 3.5 and 3.6 show that the highest SVC value occurs at 6 clusters for Pre-Distillation Unit and at 3 clusters for Arosolvan Unit, respectively, suggesting that these are the optimal number of clusters for each process unit. In both cases, the graph representation of the SVC criterion shown that the optimal number of clusters is reached for both process units and no additional number of clusters evaluation was required.

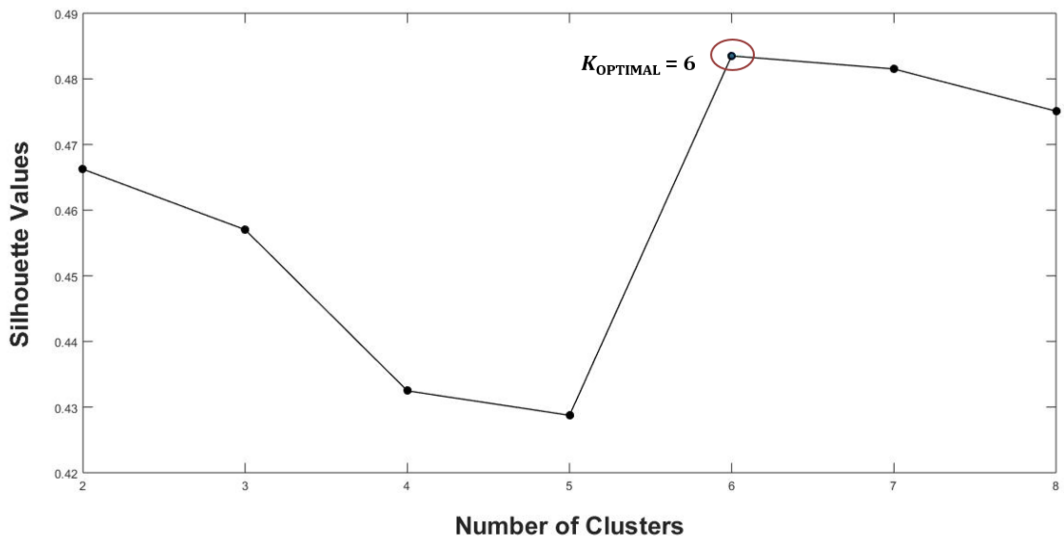


Figure 3.5: Graph representation of Silhouette Value Criterion solutions for Pre-Distillation Unit's data set.

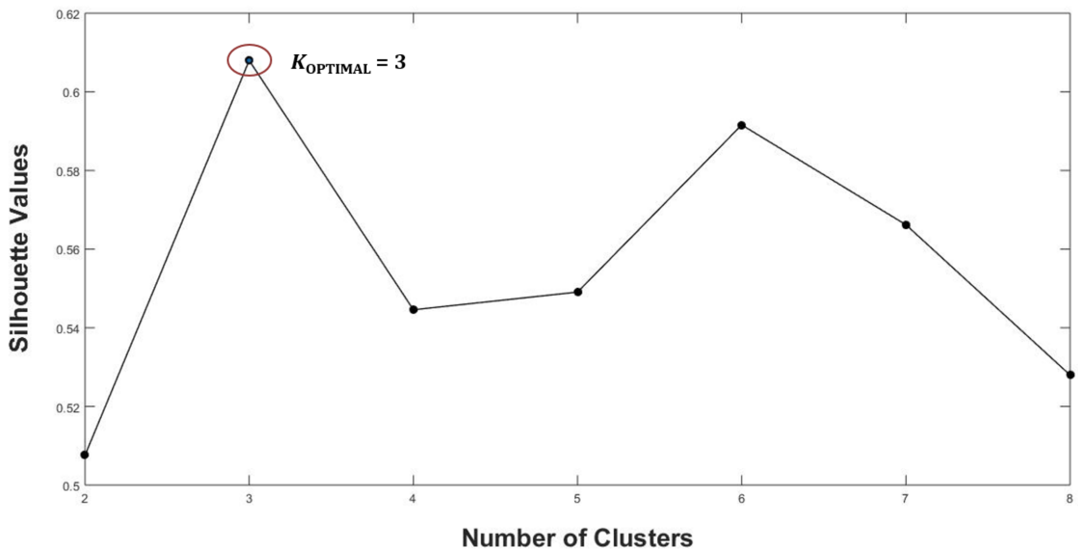


Figure 3.6: Graph representation of Silhouette Value Criterion solutions for Arosolvan Unit's data set.

The overall results obtained for $K_{optimal}$ for each process unit are summarized in Table 3.2.

Table 3.2: Results for K_{otimal} obtained through cluster evaluation criteria for each process unit.

Cluster Evaluation Criterium	$K_{optimal}$	
	DBC	SVC
Pre-distillation Unit	6	6
Arosolvan Unit	3	3

Both cluster evaluation criteria lead to the same results for the two process units (Table 3.2). It was obtained a K_{otimal} of 6 for Pre-Distillation Unit and a K_{otimal} of 3 for Arosolvan Unit. Consequently, k-means clustering algorithm was then applied considering the respective K_{otimal} for each process unit. The results of the partition were further validated through the visualization of the Silhouette plots, shown in Figure 3.7. From the observation of each plot, it is possible to verify that all clusters present high average silhouette values, which indicates a good distribution of data between clusters. Only few points are not well assigned to any of the clusters (negative silhouette values), possibly because these points may in fact be outliers not removed using Mahalanobis distance or extreme values. The interpretation and analysis of Mahalanobis Distance was done considering a significance value of 0.1 % used in literature, which for a probabilistic test of significance may be considered too low and thus, it may justify the negative values in the Silhouette plots as possible remaining outliers. Higher values for the probabilistic test of significance, such for example 1 % or maximum 5 %, could be used to assess whether these negative values continue to appear in the Silhouette plots.

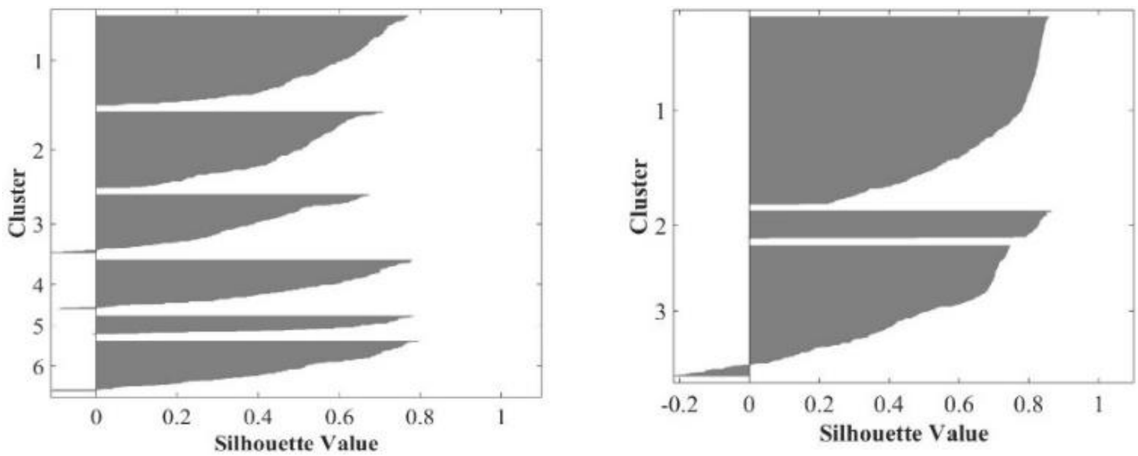


Figure 3.7: Silhouette plot for Pre-distillation Unit (left) and for Arosolvan Unit (right), after applying k-means clustering algorithm considering the respective value of $K_{optimal}$.

The identified clusters are representative of different operational scenarios for each process unit to which Pinch Analysis will be applied with the main purpose in finding energy targets (minimum utilities consumption) and in determining potential energy savings for each process unit. The results obtained for each operational scenario will be then compared to the results obtained for the global scenario (overall mean values) to verify if there is any critical scenario in terms of energy consumption.

3.4 Conclusions

In this work, data extraction for further energy performance analysis of Pre-Distillation and Arosolvan Units of the Aromatics Plant of Matosinhos Refinery was carried out. The procedure for data extraction relied on Process Flow Diagram (PFD), Process and Instrumentation Diagram (PID) and Heat Exchanger datasheets of each process unit. The data for the analysis was extracted in daily average from the instrumentation and control system of the respective process unit corresponding to the period 2014 – 2015. A data matrix in one single Excel document was built for each process unit, where columns represent variables and rows represent operational measures (observations). The variables measured are the ones with direct influence on heat exchanger networks: temperatures and flowrates.

A pre-treatment of the extracted data was performed for filtering and cleaning data, to exclude missing values and some variables, and to eliminate incoherent data. Outliers were also detected and removed from the data matrix applying Mahalanobis Distance which have mean and covariance matrix as robust estimators, being very sensitive to the presence of outliers. Finally, two data matrixes (with temperatures and flowrates) were obtained with the following *nxp* dimensions: 706x55 for Pre-Distillation Unit and 620x86 for Arosolvan Unit.

Cluster analysis was then performed to each data matrix using k-means clustering algorithm to define representative operational scenarios for the two main process units. Prior to the partition of the data into different clusters, the optimal number of clusters was estimated using two cluster evaluation criteria, Davis-Bouldin criterion (DBC) and Silhouette Value Index criterion (SVC). These criteria were able to identified 6 operational scenarios for Pre-Distillation Unit and 3 operational scenarios for Arosolvan Unit. The application of the different cluster evaluation criteria simplified the procedure to achieve the optimal number of clusters when using k-means clustering algorithm, overcoming the drawback of the interactive process to define the number of clusters that best suits the data.

The data partition resulting from k-means clustering algorithm considering the estimated optimal number of clusters were validated through Silhouette plots which indicated a good distribution of the data between clusters (high silhouette values) with only few points not well assigned to any of the clusters (negative silhouette values). The negative silhouette values could be possible outliers or extreme values. Higher values for the probabilistic test of significance used to interpret and analyze Mahalanobis Distance could be used to assess whether these negative values continue to appear in the Silhouette plots. The identified clusters are representative of different operational scenarios for each process unit.

It is concluded that cluster analysis showed potential to describe process operational data in terms of representative operational scenarios to be used as input for subsequent energy performance analysis. Pinch Analysis is then performed for each operational scenario thus finding energy targets (minimum utilities consumption) and potential energy savings for each process unit.

Chapter 4: Process Heat Integration and Retrofit Design using Heuristic Rules to Improve Energy Efficiency of Process Units

Abstract

The energy performance evaluation of Pre-Distillation and Arosolvan Units was performed using Pinch analysis considering different operational scenarios given by cluster analysis. For both process units, no significant differences were found between those scenarios in terms of energy savings and one global scenario was considered for further HEN improvement evaluation. In absolute terms, results showed substantial potential energy savings in Pre-distillation unit (34 %), much higher than those in Arosolvan unit (8.3 %). Cross-pinch exchanger elimination method and Pinch Design method were the retrofit methods considered in this work to find at least one possible solution for fixed energy targets. For Pre-Distillation unit, the best solution found correspond to a HEN with 14 heat exchangers with a total heat transfer area of 8467 m^2 for fixed energy targets. The required capital cost is 3.7 M€ with a payback period of 2.57 years. For Arosolvan unit, it was found a network with minimum energy requirements with 26 units and a total heat transfer area of 16,975 m^2. The required capital cost is 4.5 M€.

Key words: Aromatics Plant, Pinch Analysis, Retrofit Methods, Economic Analysis

4.1. Introduction

For every industry, the goal is to produce high quantity and quality products at lowest costs which are further integrated into a market. As seen in Figure 4.1, a process requires raw materials, energy and fresh water to produce the final products, while releasing heat, emissions and wastes to the environment (Gundersen, 2013; Relvas *et al.*, 2002). With the rapid industrial progress and economic growth, a negative side-effect came along to society and environment. Issues as energy, water saving, global warming and greenhouse gas emission (GGE) became one of the main focus of Business Sustainability and a political challenge for companies to review the way they consume fossil fuels, since this results in emissions of carbon dioxide and other pollutants (NO_x, H_2S, SO_x), and the way they manage waste water and disposal residues which cause environmental negative impacts and climatic changes (Klemeš *et al.*, 2011; Labuschagne *et al.*, 2005).

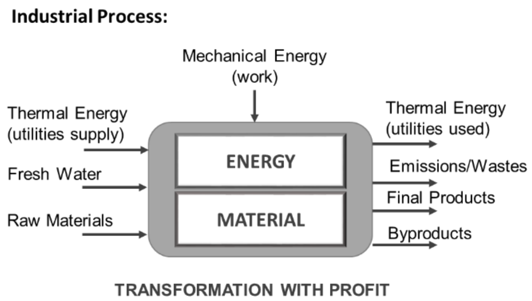


Figure 4.1: Industrial process representation (Gundersen, 2013).

The competitiveness between companies encouraged them to find the best available techniques (BAT) and methodologies to address these issues. One of the most powerful tools available is Process Integration (PI), which is a group of methodologies that when applied reduce consumption of resources in operating processes (raw-materials and energy usage) or harmful emissions (waste water and residue disposal) to the environment (Friedler, 2010; Klemeš *et al.*, 2011; Relvas *et al.*, 2002).

The International Energy Agency (IEA) defines PI as "*systematic and general methods for designing integrated production systems ranging from individual processes to total sites and with special emphasis on the efficient use of energy and reducing environmental effects*". This concept is very close to another system oriented technology: Process Synthesis. These two methodologies are integrated in Process System Engineering which by definition is Systems Engineering principles applied to processes. Figure 4.2 shows the relation between the three concepts (Gundersen, 2000; Klemeš *et al.*, 2011).

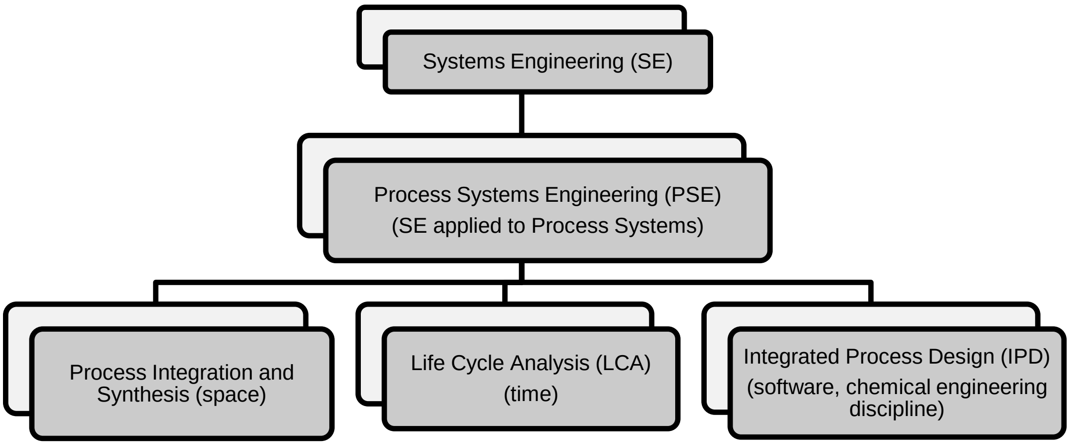


Figure 4.2: Process Integration among similar Terms (Gundersen, 2000).

Process Integration and Synthesis are approaches applied in space, which means they considered the whole plant, the entire site and sometimes the whole region. When the term PI is being used in this work, it refers to a certain industrial tasks and to methods to address those tasks to maximize savings (Gundersen, 2000). Examples of PI in industries:

- Heat Integration or Heat Recovery Pinch is applied for example in cooling and condensation integrated with heating and evaporation, identification of near-optimal level of heat recovery, design the heat exchanger network with minimum energy requirements, etc.;
- Power Integration is applied in co-generation;
- Chemical integration is applied to recover and reuse byproducts as raw materials in other plants, to recycle streams, reduce fresh water intake, reduce effluent emissions, etc.;
- Equipment Integration or Process Intensification is applied to incorporate multiple phenomena (reaction, separation, heat transfer) in the same equipment (Gundersen, 2000).

In the early stages of Process Integration, there was an overlapping of concepts of Process Integration and Energy Integration as the latter was largely associated with the concept of Pinch Analysis or Heat Recovery Pinch that gave birth to the first studies in the area of heat recovery. Pinch Analysis is associated to heat recovery by identifying the Pinch Point. The concept of Pinch Point and its identification has a significant importance as it is the first stage of a Process Integration study, because its identification provides information about the whole process and allows the analysis of potential solutions for integration. The continuous development of this field expanded the application to others. In the works of Smith *et al.* (2010), Dunn and El-Halwagi (2003) and Friedler (2010) is presented a state of the art regarding process integration techniques. The different methodologies have the same main objectives (targets) to guarantee an optimal performance of the process.

The main performance targets are the minimum energy requirements and cost, minimum equipment cost, minimum total capital cost, higher operability performance (high flexibility, controllability, switch ability to start up and shut-down or to new operations conditions) and finally, lower environmental negative impacts (emissions reduction and waste minimization). These methodologies can be applied to optimize heat exchanger networks, separation systems (distillation and evaporation), reactor systems, heat and power systems, steam and gas turbines and heat pumps, utility systems (steam systems, furnaces, refrigeration cycles), individual operating units or entire processes, total site (whole plant), or even considering regions. In addition, these methodologies can consider different types of industrial processes (continuous, batch and semi-batch processes), projects (new design, retrofit or debottlenecking), and thermodynamics (exergy in distillation and refrigeration). Conference on Process Integration, Modelling and Optimization for Energy Saving and Pollution Reduction (PRES) was introduced in 1998 where several works regarding these fields are presented and discussed. Some of the papers and developed works presented in this conference can be found in the review papers of Klemes and Stehlik (2003) and Klemes and Stehlık (2006). Past and recent developments in Process Heat Integration techniques can also be found in the works of Kumana and Al-Qahtani (2004), Morar and Agachi (2010), Klemes *et al.* (2013), Seferlis *et al.* (2015) and Liu *et al.* (2016).

Process Integration have been developed through other methodologies such as thermodynamics, heuristics and optimization. These methodologies can be applied alone or together considering a hierarchical analysis as shown in Figure 4.3. A study based on Pinch Analysis and Energy Performance Analysis are associated to thermodynamics field, while Hierarchical Analysis and Knowledge based systems are a result of the application of qualitative knowledge. The Optimization field involve the application of different mathematical programming tools. Recent developments in the application of thermodynamic methodologies, mathematical tools or both can be found in the paper reviews of Smith *et al.* (2010), Klemes and Kravanja (2013) and Sreepathi and Rangaiah (2014).

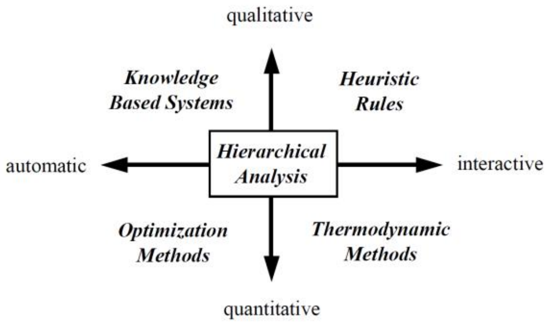


Figure 4.3: Hierarchical Analysis of a Process Integration methods (Gundersen, 2000, 2013).

Pinch Analysis has been largely applied in many industrial processes showing a great potential and simplicity in its application. However, it also presents some limitations that motivates to combine other techniques such as:

- Rigor of Pinch Analysis is sometimes replaced by Heuristic Rules to determine the number of units and the total minimum transfer area;
- Some graphical tools cannot handle forbidden matches between streams and simple rules for appropriate placement;
- Pinch Design method is a sequential procedure, starting with targets estimation, then develops and optimizes the design to achieve those targets. However, it only considers one match, one loop and one path at a time. It can´t handle multiple trades-off;
- Pinch Analysis provides a correct integration but, in some cases of network design, less costly and less complex designs can be found when ignoring Pinch Point;
- The procedure is time consuming but normally results in viable projects (Gundersen, 2013).

These limitations or restrictions must be identified prior to project design development. As Pinch Analysis can`t handle those restrictions, the alternative is to combine it with other technique such as mathematical programming to facilitate the achievement of the final solution.

4.2. Pinch Technology for Heat Recovery and Hierarchy of Process Synthesis

The sequential procedure of Process synthesis is schematized through the Onion Diagram in Figure 4.4. For each process unit (processes 1, 2 and 3), the analysis can be decomposed into layers (stages), starting with reaction units (first layer in the center of the onion diagram) where feeds, products, recycle concentrations and flowrates are targeted, which are needed for the following task. Follows the analysis of separation processes where heat and material balances are performed to set energy targets prior to heat exchanger network (HEN) evaluation and design represented by the third layer. This stage ensures that the energy targets are achieved during HEN design (Klemeš *et al.*, 2011; Linnhoff, 1998). The design of the reactors is dictated by the yield and conversion considerations and that of the separator by the need to flash off as much unreacted feed as possible. If the operating conditions of these units are accepted, then the design problem that remains is to get the optimum economic performance out of the system of heat exchangers, heaters and coolers (Kemp, 2007). The minimum energy requirements of the processes (heating and cooling demands) are provided by the central utility system and site heat and power systems (CHP) (Klemeš *et al.*, 2011; Linnhoff, 1998).

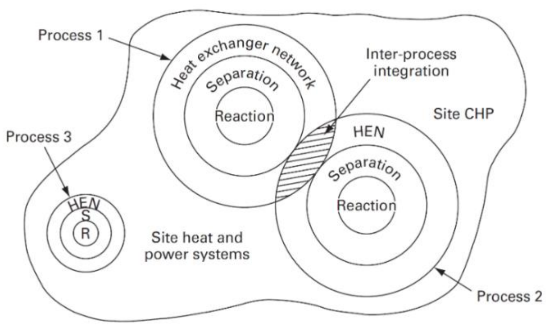


Figure 4.4: Onion Diagram which represents the hierarchy of process design (Kemp, 2007).

Process Synthesis can also be applied in an interactive process optimization problem. The main framework of process synthesis can be described as the following four steps:

1) Data Extraction – identification of the process integration problem (heat recovery maximization, fresh water intake minimization, wastes minimization, supply chains, etc.) and then collect the relevant data related to the problem.
2) Process Performance Targeting – determination of minimum energy requirements (heating and cooling demands to be satisfied by external utilities), minimum number of heat exchanger units, minimum heat transfer area, etc.
3) Process Modifications - setting energy targets allows to identify appropriate changes in the core process conditions which may include changes in operating conditions, changes in processes, removing units, adding new units, etc.
4) Network Design - the relevant process network for reusing or recovering the resources is obtained at the end of the application of the methodology. The design may consider various algorithms and sub-phases, such for example Pinch Design Algorithm which involves an initial construction of a HEN structure featuring the maximum energy recovery or minimum energy requirements (MER). A further step involves the evaluation of the trades-off between the energy costs for utilities and the investment costs for heat exchangers and piping (Klemeš, 2013).

Pinch Technology can also be extended to the site level considering the integration of more than two process units (in Figure4.4, it considers inter-process heat integration of processes 1 and 2) wherein appropriate loads on the various steam mains are identified through inter-process integration to minimize the site wide energy consumption. The overall methodology and analysis from the basic heat and material balance to the total site utility system allows to identify appropriate changes in the core process conditions that may have an impact on energy savings and capital costs. The thermodynamic bounds on heat exchange are used to estimate the utility needs and heat exchange area for a given heat recovery problem. The results are the lower bound on the utility demands and the lower bound on the required heat transfer area which are known as targets to achieve in practice and minimize the total cost of the HEN being designed (Kemp, 2007; Klemeš *et al.*, 2011; Linnhoff, 1998)

4.3. Setting Process Performance Targets

Pinch Analysis allows to estimate performance targets prior to heat exchanger network (HEN) design stage which are: minimum energy consumption (energy targets), minimum number of units, minimum total heat transfer area and minimum total annual cost. The previous estimation of these targets provides guidelines for HEN design and allows the comparison of any design with the "best possible" design.

4.3.1. Energy Targets

Energy targeting is the estimation of minimum external utilities consumptions (or total duty) that must be supplied and released from the process by the HEN. In addition, it sets the minimum temperature for energy supply and maximum temperature for release and often allows the determination of the optimum use of the available utilities if more than one external (hot and cold) utility is available. The available tools, which can be found in the books of Klemeš (2013), Kemp (2007) and Linnhoff (1998), are described next.

- **Hot and Cold Composite Curves**

Composite Curves are a temperature - enthalpy diagram used to evaluate heat recovery between multiple process streams (Linnhoff *et al.*, 1979). It is constructed by dividing the temperature axis into temperature intervals based on the supply and target temperatures of the process streams, and adding the respective enthalpy contributions (hot streams) and requirements (cold streams). These enthalpies are drawn against the corresponding temperatures resulting in two different curves, one representing the heating available from hot streams and a second one representing the cooling available from cold streams. In other words, this graphical tool in Figure 4.5 integrates all hot process streams into one hot composite curve (HCC) and all cold process streams into one cold composite curve (CCC).

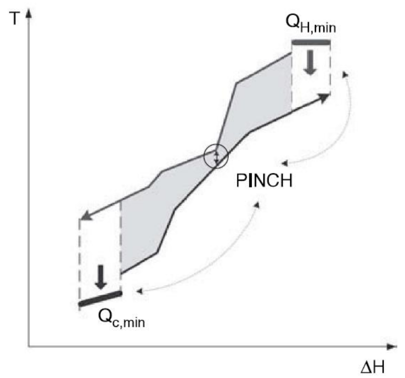


Figure 4.5: Example of hot and cold composite curve authorized by Klemeš *et al.* (2014).

The two composite curves are positioned relative to each other in such a way that HCC is always above the CCC. An overlapping region between the two curves is created representing the heat that can be recovered within the process. This region establishes a minimum temperature difference (ΔT_{MIN}) available between hot and cold streams located at pinch point that allows a feasible heat transfer between them. If the CCC is moved horizontally towards HCC until a point of the curve touches the HCC, ΔT_{MIN} becomes zero, which means that no heat transfer can take place as maximum heat recovery is achieved and the area required for that heat transfer is infinite. On the other hand, if the CCC is moved away from HCC, the gap region between the curves increases with ΔT_{MIN} and the potential of heat recovery decreases (lower heat transfer area requirements). Therefore, it is necessary to provide a ΔT_{MIN} value for a feasible heat transfer. This is a very important parameter because it is the point that gives the thermal level require to reuse streams properly. (Heggs, 1989; Klemeš *et al.*, 2011; Klemeš *et al.*, 2014).

On top of composite curves there is a gap where hot streams aren't available to supply heat to cold streams, being necessary to add a minimum external hot utility load ($Q_{HU,MIN}$) to satisfy this deficit amount of heat. Analogous, at the bottom of the composite curves, there is a gap where no cold streams are available to remove heat from hot streams being necessary to add a minimum external cold utility load ($Q_{CU,MIN}$) to remove the surplus amount of heat. The minimum external utilities required depend on ΔT_{MIN}

value: an increase in its value means higher minimum external utilities required for the process, decreasing the maximum heat that can possibly be recovered (Heggs, 1989; Klemeš *et al.*, 2014).

- **Problem Table Algorithm (PTA) and Heat Cascade**

Another tool to determine energy targets is Problem Table Algorithm (PTA) with Heat Cascade. PTA is an empiric procedure that uses shifted temperatures determined based on ΔT_{MIN} parameter to ensure that within any temperature interval, hot streams and cold streams are ΔT_{MIN} apart. Hot streams are set ½ ΔT_{MIN} below hot stream temperatures and cold streams are ½ ΔT_{MIN} above cold stream temperatures. In PTA, the enthalpy balance intervals are done for hot and cold streams together to allow the maximum possible heat recovery within each temperature interval (ensured by ΔT_{MIN}). This way, a full heat interchange within any interval temperature is possible and each interval has either a net surplus or net deficit of heat, avoiding the mistake of having both. Knowing the streams that run in each temperature interval, energy balances can be calculated. Therefore, it is possible to develop a feasible heat network assuming all heat surplus is removed through a cold utility and all the heat deficit is compensated by a hot utility. However, to avoid rejecting or accepting heat at inadequate temperatures, Heat Cascade is introduced together with PTA procedure.

Heat Cascade is a schematic representation of the cumulative heat passing through at a given temperature shifted interval. It uses enthalpy values where the hot streams are sources of heat and the cold streams are sinks of heat, both with the respective modified temperature intervals. The minimum temperature difference established is specified into the Heat Cascade. The hot streams supply heat to the temperature intervals according to their cooling requirements and the cold streams extract heat from the temperature intervals according to their heating requirements. The energy balances are established for each temperature interval. It starts with a zero-external heat input at the highest temperature, work down the column in the table, adding on the net heat change as a heat residual in each temperature interval from the highest to the lowest temperatures. This heat cascade contains negative heat flows (surplus) which is thermodynamically infeasible – Infeasible Heat Cascade – representing the bottleneck of the process (i.e. heat recovery pinch).Thus, the minimum net heat flow (the largest negative value or zero) in the cascade is considered and an equal amount of external hot utility is added to satisfy the deficit of the heat network. The minimum heat needed to make these residuals non-negative correspond to the minimum external heating requirement ($Q_{HU,MIN}$). Consequently, this amount of external hot utility is added to the first interval in the cascade, increasing all the net heat flows by this amount where the minimum value identified earlier becomes zero (pinch point). The heat removed in the final interval from the bottom of the heat cascade corresponds to the minimum external cold utility ($Q_{CU,MIN}$). This procedure guarantees a Feasible Heat Cascade and the maximum possible heat recovery (Klemeš *et al.*, 2014).

- **Grand Composite Curve (GCC)**

Grand composite curve (GCC) represented in Figure 4.6 is another temperature-enthalpy diagram resulting from heat cascade that represents the net heat flow (after adding external hot and cold utilities required) against the shifted interval temperatures. GCC represents the difference between the heat available from hot streams and the heat required by the cold streams relative to the pinch point at certain shifted temperature. The values of net heat flow at the top of GCC corresponds to the heat supplied to the cascade ($Q_{HU,MIN}$) and the values of net heat flow at the bottom of GCC corresponds to the heat that is removed from the heat cascade ($Q_{CU,MIN}$). The pinch point is located where net heat flow is zero (GCC touches vertical axis). It is a useful tool to verify if the pinch point occurs in the middle of the temperature range or at one end (called threshold problem) and identify other regions of low net heat flow or even double or multiple pinches. GCC may contain triangle regions, or pockets, of heat recovery achieved through heat transfer between hot and cold streams within the process, which means that there is some process integration already implemented in the process.

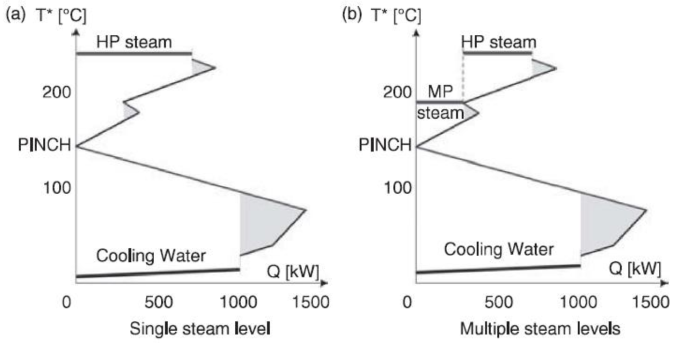


Figure 4.6: Grand composite curve to target single and multiple utilities with authorization of Klemeš *et al.* (2014).

Besides giving the energy targets of the overall process, GCC is a useful tool to give information about at what temperatures are needed the external utilities. Another way to optimize the energy consumption is to supply the heat at lower temperatures. This is the advantage of GCC towards previous tools. The energy required for the process can be supplied by different utility levels (such as high/medium/low pressure steam, refrigeration levels, hot oil circuit, furnaces flue gas, etc.). The main objective is to maximize the use of cheaper utility levels and minimize the use of expensive utility levels. Low pressure steam (LP steam) is cheaper than high pressure steam (HP steam) and cooling water is cheaper than refrigeration. Although the composite curves are useful to determine the overall energy targets, do not determine how much energy is needed to be supplied by different utility levels while GCC offers a clear visual representation of the selected utilities and the associated enthalpy change (Kemp, 2007; Klemeš *et al.*, 2014).

4.3.2. Minimum Number of Units or Heat Exchangers (N_{MIN})

After determining energy targets, the next step of heat integration is to estimate the minimum number of heat exchanger units (N_{MIN}) required, including heaters and coolers, prior to HEN design, which depends on the total number of process and utility streams (N) involved in heat transfer process according to Euler`s General Network Theorem (Equation 4.1), L is the number of independent loops and S is the number of separate components (subnetworks) (Ahmad *et al.*, 1990; Linnhoff and Ahmad, 1990).

$$N_{\mathbf{MIN}} = \mathbf{N} + \mathbf{L} - \mathbf{S} \qquad \textbf{Equation 4.1}$$

As the objective is to target the minimum number of heat exchangers ahead of network design, network features such as loops and number of subnetworks are not known. Thus, the parameter L is considered equal to zero to remove loops and the parameter S equal to 1 since the presence of subnetworks reduces the number of units. The Equation 4.1 can then be simplified into Equation 4.2.

$$\mathbf{U_{MIN} = N - 1}$$ **Equation 4.2**

In order to achieve energy targets, separate subnetworks must be designed above and below pinch point to debottleneck the process. Thus, Equation 4.2 must be applied separately to each subnetwork as there is no heat exchangers transferring heat across the pinch point in order to target the number of units compatible to energy targets. The total minimum number of heat exchangers for the network respecting energy targets is then given by Equation 4.3 (Klemeš *et al.*, 2014).

$$\mathbf{N_{min,MER} = (N-1)_{above\ Pinch} + (N-1)_{bellow\ Pinch}}$$ **Equation 4.3**

4.3.3. Minimum Heat Transfer Area (A_{MIN})

Composite curves used to determine energy targets for a given value of ΔT_{MIN} can also be used to determine minimum heat transfer area (A_{MIN}) required through Equation 4.4 to achieve energy targets. This procedure for area targeting assumes that heat is "vertically" exchanged between hot and cold composite curves across the whole enthalpy range. This assumption is equivalent to consider countercurrent area within the overall network and allows to achieve a minimum total surface area (Kemp, 2007; Linnhoff and Ahmad, 1990).

$$\mathbf{A_{MIN} = \sum_i \left[\frac{1}{\Delta T_{LM}} \sum_j \frac{\Delta H_j}{h_j}\right]}$$ **Equation 4.4**

where:
i: denotes i^{th} enthalpy interval
j: j^{th} stream
ΔT_{LM}: log mean temperature difference in interval
ΔH_j: enthalpy change of j^{th} stream
h_j: heat transfer coefficient of j^{th} stream

When the overall heat exchange is counter-current, minimum total area is achieved if global heat transfer coefficient is constant. The model was then extended by Linnhoff and Ahmad (1990) to allow different values for global heat transfer coefficient, which means different individual heat transfer coefficients (h-values). Vertical heat transfer based on composite curves are still valid when h-values are different. There are three effects in heat transfer when dealing with different h-values: resistance to heat flow due to lower h-values leads to higher heat transfer area, differences between coefficients may lead to lower overall area when temperature differences are higher for streams with lower h-values and isolation of low h-values by matching streams with low h-value with each other (Ahmad *et al.*, 1990; Linnhoff and Ahmad, 1990).

4.4. Heat Exchanger Network Retrofit Design using Heuristic Rules

Pinch analysis is performed when the main objective is to develop a new process or plant (grassroots design) or to improve the performance of an existing process or plant (retrofit design). The motivations for retrofit design projects could be the permanent change in feed or product specifications, an increase in demand which may be insufficient to build a new plant but high enough to raise the capacity of an existing one, improved safety, reduce operating costs, or accommodating new environmental specifications aimed at reducing emissions. The advantage of retrofit design against grassroots design is that, when debottlenecking a process or a plant, the existing equipment and piping must be used effectively, avoiding unnecessary investment even if it does not perform at its optimum. The profitability of a retrofit design must be maximized by maximizing the cost-saving on utilities minus the annualized capital cost. When the objective of the retrofit is to increase the energy savings of a heat exchanger network, the analysis should be undertaken concerning the minimization of utilities consumption of the existing units, focusing on either replacing or modifying the exchangers consuming excess of energy or removing or adding exchangers in parallel or series with the existing ones. Either way, the piping system must be also reviewed in order to accommodate the changes in the network which requires a certain investment (Klemeš *et al.*, 2011).

With the information provided by energy targets, and after identifying the limitations imposed by the operating conditions of process streams, the HEN of the existing plant can be synthesized to achieve the minimum energy requirements. Grid diagram is an efficient graphical representation tool for designing heat exchanger networks, which illustrates the counter-current flow of heat exchangers that helps to visualize and implement the decomposition of the network based on pinch point(s) location(s) as well as to study cross-pinch heat transfer. All the streams and matches are drawn relative to pinch temperatures. It helps to identify if a significant temperature location and if a stream starts above or below pinch point.

The application of pinch principles guarantees that no heater is used below pinch point as well as no cooler is used above pinch point, if only one pinch point exists, which will ensure that no heat is transferred across the pinch point and that the network will achieve energy targets. Grid Diagram is used to determine the minimum number of units that respects energy targets. It is important to notice that targeting for units takes place after targeting minimum utilities consumption, thus the types and amounts of different utilities needed are known and fixed prior to design.

The principles of pinch analysis are still the focus of the procedure for designing the retrofitted network. Above the pinch, the design must start at the pinch finding matches with cold streams on the same side that fulfil the first condition. In situations where is considered constant heat capacity flowrate (MCp) for all streams, the pinch point is always determined by the entry of a stream, either hot or cold. So heat capacity flowrate of hot streams must equal or be lower than cold streams and the number of hot streams must be equal or lower than the number of cold streams, as summed in Table 4.1. However, for retrofit cases, sometimes these rules are not sufficient (Kemp, 2007; Klemeš, 2013; Linnhoff, 1998)

Table 4.1: Stream matching rules above the pinch (Klemeš, 2013).

Stream Matching Rules	Above the Pinch	Below the Pinch
Heat Capacity Flowrate (MCp)	$MCp_{hotstreams} \leq MCp_{coldstreams}$	$MCp_{hotstreams} \geq MCp_{coldstreams}$
Number of streams	$N_{hotstream} \leq N_{coldstreams}$	$N_{hotstream} \geq N_{coldstreams}$

In retrofit cases, an evaluation of the existing plant is required to verify whether it is possible to make improvements, to reduce energy and to increase profitability. The first step in retrofit design is to decide which retrofit method is most suitable for the project. Two known retrofit methods considered in this work are: Pinch Design method with maximum re-use of existing exchangers and Cross-Pinch Exchanger Elimination Method (Kemp, 2007; Klemeš, 2013; Linnhoff, 1998).

4.4.1. Pinch Design Method with maximum re-use of existing exchangers

The Pinch Design Method, which was developed to design heat exchanger networks for new plants, have been extended for cases of maximum heat recovery of existing plants to achieve higher energy efficiency. Martin and Mato (2007) and Pereira *et al.* (2016) provided free educational software applications for heat exchanger design network based on Pinch Design Method.

The procedure for grassroots cases suggests starting the network design from the pinch point location and then to place heat exchanger matches (process-to-process) while moving away from the pinch point. Some considerations are here applied when placing those matches in order to obtain a network that respects minimum utilities usage, besides pinch golden rules and stream matching rules, such as no exchanger may have a temperature difference smaller than ΔT_{MIN}, all hot streams above the pinch must be matched up with cold streams and hot and cold streams entering the pinch must be given priority when matches are made above and below the pinch, respectively. In addition, when these design rules are not sufficient, it is necessary to split the streams so that heat exchange matches can be properly placed using also heuristic rules to decide how to divide the heat capacity flowrate between the branches. The procedure for retrofit cases is similar to the one described for grassroots design. The difference between procedures is that for retrofit cases it is considered the maximum re-used and reallocation of the existing heat exchangers (Kemp, 2007; Klemeš, 2013; Linnhoff, 1998).

4.4.2. Cross-Pinch Exchangers Elimination Method

This procedure starts with the existing heat exchanger network and change it towards a minimum energy requirement design. This approach also considers the current ΔT_{MIN} and the calculated energy targets and pinch temperature. The grid diagram is then constructed for the existing HEN, including exchangers, heaters and coolers, to identify which ones are the pinch violators. Then, it is possible to identify ways to add new matches to correct these inefficient zones using heuristic rules. The well-allocated heat exchangers are kept in the same place with the same stream matches and heat loads. The procedure is used to eliminate cross-pinch exchangers and starts to place heat exchangers matches (process-to-process) with the remaining process streams from the pinch point location while moving away from the pinch point. In this procedure, an additional heat transfer area is required for the new process-to-process stream matches or process-to-utility matches. These series of retrofit projects are ranked and the best ones can be chosen according to practical and economic criteria (Linnhoff, 1998). Li and Chang (2010) proposed an improved pinch-based retrofit procedure to reduce utility consumption of an existing heat exchanger network at minimum capital investment. The new procedure has cross-pinch method as first step to remove heat exchanger that is violating pinch point, and its heat loads on each hot and cold streams are both divided into two according to the pinch temperatures. Then, at both sides of the pinch point, streams are matched starting near pinch temperatures and then developed by moving away from the pinch sequentially according to temperature. The industrial heat exchangers are always almost over-designed by 15-30 % and the same heat exchange can be adopted to realize a new match between the same process streams if the heat load is closed to the original design level. This is also valid for Pinch Design Method when re-using existing heat exchangers.

4.5. Trades-off between Energy and Capital Costs for Retrofit Design

An energy efficient heat exchanger network design results in a trade-off between operating costs and investment costs. This is a complex situation and more complex for retrofit design cases where a capital investment has already been made.

The trade-off between energy and investment cost is dependent on the parameter ΔT_{MIN} value considered for the process. The lower ΔT_{MIN}, the higher is heat recovery and the lower is energy costs. But lower temperature driving forces means that higher heat transfer areas are needed and thus, capital costs are higher. On the contrary, higher ΔT_{MIN} increases energy costs due to lower heat recovery within the process but the capital costs decrease due to lower heat transfer area needed. Therefore, choosing the lowest ΔT_{MIN} seems to give maximum energy reduction but larger and costly heat exchangers. The surface area (A) required for heat transfer in a heat exchanger can be determined using Equation 4.5.

$$\mathbf{A = \frac{Q}{U\Delta T_{LM}}} \qquad \textbf{Equation 4.5}$$

The log mean temperature difference (ΔT_{LM}) parameter is determined by the inlet and outlet temperatures of process streams and depends on the configuration type of the streams. If heat exchanger operates in countercurrent, where hot streams enters at T_{h1} and leaves at T_{h2} and cold stream enters at T_{c1} and exits at T_{c2}, so that T_{c1} and T_{h2} are the "cold end" and T_{h1} and T_{c2} are the "hot end" of the exchanger, then ΔT_{LM} is given by Equation 4.6.

$$\mathbf{\Delta T_{LM} = \frac{\Delta T_h - \Delta T_c}{\ln\left(\frac{\Delta T_h}{\Delta T_c}\right)} = \frac{(T_{h1} - T_{c2}) - (T_{h2} + T_{c1})}{\ln\left(\frac{T_{h1} - T_{c2}}{T_{h2} - T_{c1}}\right)}} \qquad \textbf{Equation 4.6}$$

If hot streams temperature variation (ΔT_h) is equal to cold streams temperature variation (ΔT_c), then ΔT_{LM} cannot be defined and a simple difference in temperatures (ΔT) is used instead of Equation 4.6. It is possible to comprehend that heat exchanger surface area is inversely proportional to temperature difference. Thus, low values of ΔT_{min} lead to large and costly exchangers, as capital cost is closely related to heat transfer surface area. Even if one end of a heat exchanger has a high temperature difference, ΔT_{LM} is significantly influenced by the smaller temperature approach. A low ΔT_{MIN} value gives a low ΔT_{LM}.

Assuming that energy cost is only directly influenced by minimum utilities consumption and that heat exchanger cost is proportional to surface area, it is possible to estimate the trade-off between energy and capital costs.

Previous studies concluded that some processes have similar composite curves and therefore similar ΔT_{MIN} values. Linnhoff (1998) performed several studies resuming experience ΔT_{MIN} values. For petrochemical industries, as it is the case of typical aromatics plants, ΔT_{MIN} reference value is 10– 20 ºC. Although this assumption provides practical targets for retrofit modifications, it may result in non-optimal solutions which may promote losses of potential opportunities (Kemp, 2007; Klemeš, 2013; Linnhoff, 1998).

4.6. Literature Review

Other authors have been contributing for the development of process integration methodologies based on Pinch Technology. Nordman and Bernstsson (2001) presented two pinch technology based methods, being one of them a new composite curves developed for use in a targeting and options scanning stage in retrofitting. These curves were developed with the aim to overcome the disadvantages given by GCC in some retrofit situations. The temperatures in the GCC are not estimated correctly in existing systems having a heat demand that is large in relation to what could be achieved by enhanced heat recovery. Also, GCC does not give any information about the existing HEN in relation to the changes required in order to approach theoretical energy targets. These curves can therefore be used as an assessment of possible heat system improvements. This graphical tool provided a good representation of the existing HEN, including heaters and utility levels, from which relative investment cost for energy saving can be set.

The major problems found in literature deal with continuous composite curves. However, there are some cases, for example when a phase change of a process stream occurs, that is common to find discontinuities in composite curves and where no process stream exists within particular temperature range. Lakshmanan and Fraga (2002) addressed this problem by finding lower bounds on the optimal value of ΔT_{MIN} which reduces the range over which targeting needs to be carried out. Also, Lakshmanan and Fraga (2002) demonstrated that applying PTA directly is not possible to locate that lower bound and thus, it finds pinch points locations in which pinch design rules cannot be applied.

PTA is normally used to determine the energy targets and pinch point location prior to composite curves construction. Salama (2005) developed numerical techniques such as Simple Problem Table Algorithm (SPTA) to determine the optimal horizontal shift between composite curves and the limits on the ΔT_{MIN} prior to energy targets, pinch point location and GCC construction. Traditional PTA is composed by a lumping stage followed by a cascading stage. SPTA only deals with cascading stage in which energy is cascaded from the cold side to the hot side (reverse of traditional PTA) over an ordered set of stream and target temperatures of the input data. This numerical technique showed potential when determining energy targets and cogeneration and can eliminate PTA in Pinch Design Method. The bounds on ΔT_{MIN} allow to determine true design pinches making the design method easier to be applied.

Later, Salama (2006) developed another numerical technique to determine the optimal heat energy targets in heat pinch analysis based on a geometrical approach that consists in using the horizontal shift between cold composite curve and the stationary hot composite curve to determine the critical lower bound on ΔT_{MIN}. Salama (2009) developed an enthalpy flow rate technique that allows the construction of a new enthalpy-temperature diagram called complement grand composite curve (CGCC). This new curve aims to determine the differential temperature distribution between the composite curves as a function of the enthalpy flow rate variable. The temperature differential information is needed for heat exchange area estimation and in multiple utility targeting.

Castier (2007) extended utility targeting procedure based on new rules to determine minimum utilities required and to guarantee that utilities will be utilized at conditions with the least departure from the pinch temperature, increasing network's thermodynamic efficiency and reducing utilities cost. This new procedure is based on a direct extension of the problem table analysis without the need of GCC. Composite curves and GCC are approximations because heat capacities do depend on temperatures and thus, enthalpies are not a linear function. Moreover, as mixtures may change phase, their composition also change, modifying the latent heat of the phase transition. With rigorous calculated thermodynamic properties, the closest approach between hot and cold composite curves may occur between temperature intervals or inside them. Castier (2012) developed a rigorous multiple utility targeting algorithm to overcome those drawbacks found using thermodynamic tools contributing to a higher energy efficiency by providing design guidelines to avoid using utilities at unnecessary temperatures.

Bandyopadhyay and Sahu (2010) presented a simple modification on the traditional PTA algorithm to target the minimum utility requirements in a HEN. The Modified PTA procedure lies in determining the net heat capacity flowrate in each temperature interval without identifying individual hot or cold streams considering an algebraic sum of the heat flows corresponding to any particular interval. Energy targeting procedure and GCC are achieved in the same way as in traditional PTA. This modification allows to extend the application of PTA in cases of heat-integrated water allocation networks.

Although Pinch Analysis provides excellent tools to estimate energy targets and to provide design guidelines, it lacks in selecting the right data and in interpreting local inefficiencies in an existing HEN. Those issues were addressed by Savulescu *et al.* (2013) who developed an alternate visualization tool of composite curves – Steam Mapping - to facilitate and increase the receptivity of its practice in industrial companies. This visualization technique illustrates the actual energy distribution of a targeted plant revealing the allocation of energy sources and sinks within the whole plant. It also helps to identify possible bottlenecks in the existing HEN based on temperature levels and heat loads to find fast and effective retrofit solutions.

Yong *et al.* (2015) introduced the Shifted Retrofit Thermodynamic Grid Diagram (SRTGD) to identify favorable retrofit solutions as it allows an easier visualization of HEN arrangements and key parameters such as heat capacity flowrates, temperatures and temperature differences. This new procedure accounts simultaneously thermodynamic insights, stream capacities and topology factors. Also, it can incorporate pinch analysis to identify process pinches and network pinches.

The second pinch technology based method developed by Nordman and Bernstsson (2001) was a matrix method for identifying cost efficient ways of improving a HEN in retrofit projects enabling to consider all important parameters that affect HEN retrofit cost. The goal is to find an optimal cost by minimizing the use of heat exchanger area in the network. This can be done by introducing new heat exchangers and/or by using existing ones more efficiently. Moreover, the choice made depends on economic factors such as electricity price, price of heat and total investment space, and technical factors such as controllability and flexibility.

In existing heat exchanger networks, it is found some disturbances and variabilities in operating conditions such as inlet/outlet temperatures and mass flowrates. Tellez *et al.* (2006) developed the methodology "Fuzzy Design Reliability Theory" that takes into account the ability, flexibility and resiliency to meet the design requirements at different operating conditions. The main advantage of this methodology is the consideration of the engineer in order to determine the expected variations in process that may occur. These variations will be taken in consideration, mainly the occurrence of disturbances that must be rejected by the process. Thus, this new methodology determines the HEN resiliency of the process to tolerate and to recover from disturbances and process behavior variability.

Pinch Analysis-based techniques have found applications in several cases for the countercurrent exchanger networks. Sun and Luo (2011) presented two procedures, one for co-current heat exchanger and other for multipass heat exchangers, taking into account the thermodynamic insights of Pinch Technology. For the co-current flow, composite curves and PTA are modified and compared to the ones obtained with countercurrent flow. In composite curves for co-current flow, the modified hot streams are drawn by reversing the original hot composite curve derived from the traditional pinch analysis. Multipass heat exchangers involve part countercurrent and part co-current flow and are mostly derived from FT (correction factor for fouling) design method. Composite curves for multipass heat exchangers are constructed by properly combining the temperature intervals based on the previous analysis of the HEN with co-current exchangers only, assuming that cold streams are on the shell side and hot streams are on the tubes side.

Grid Diagram Table was introduced by Abbood *et al.* (2012) as a general and alternative tool of composite curves, PTA and grid diagram to determine energy targets, pinch point location as well as for HEN retrofit. Grid Diagram Table combines numerical and visualization advantages of the key geometric observations that link composite curves to the fundamentals of pinch points and heat capacity flowrates and energy balances to determine energy targets. This tool allows to represent stream interval temperature scale and to be used as tool to visualize pinch point violations which are useful for a rapid and effective HEN retrofit.

Gandalla (2015) developed a new graphical tool that allows to describe an existing heat exchanger network including details of exchanger matches plotting hot streams temperatures versus cold streams temperatures, heaters and coolers. It also helps to identify inefficient zones within the network using pinch analysis principles determining this way the potential of energy savings.

Bakar *et al.* (2016) presented a systematic technique to select the optimal ΔT_{MIN} using a trade-off plot for designing a flexible and operable heat exchanger network. Although it does not consider global optimization, it takes into account the insights of process design (energy targets), control (flexibility and operability) and cost performance in early stage of HEN design.

In the last few years, bridge analysis concept has been applied in HEN retrofit situations which offers an energy transfer diagram (ETD) tool to illustrate the variation of flowrate of cascaded heat with temperature and an energy transfer curve (ETC) representing the flowrate of cascaded heat in each heat exchanger involving process-to-process and process-to-utility matches. Bonhivers *et al.* (2016) combined pinch analysis with bridge analysis to reduce minimum energy requirements by decreasing the flowrate of cascaded heat in the entire temperature range between hot and cold utilities for the removal of cross-pinch transfers.

Other innovative techniques and application fields can be found in Table 4.2 and 4.3.

Table 4.2: Other Examples of Pinch Analysis reasearch, innovation and application fields (part I).

Authors	Research and Innovation	Application field and Achievements
Özkan and Dinçer (2001)	Pinch Design Method with an improved Problem Table Algorithm (IPAT) that allows to determine heat loads in each temperature interval without using shifted temperatures and to determined pinch points and energy targets.	Crude Petroleum Unit of TÜPRAS Petroleum Refinery: 22 % in energy savings with an investment cost of 3.58 million euros for 7393 m^2 added and a payback period of 1.69 years.
Matijaseviae and Otmaeiae (2002)	Traditional Pinch Analysis Application	Nitric Acid Plant of Kutina Petrochemical Industry (Croatia): threshold case study in which only cold utilities are needed reducing 3.8 MW of utilities consumption with 357,120 $/year in operating costs and 43,185 $/year in annualized capital costs for 10 years. The payback time resulted in 15 months.
Bengtsson *et al.* (2002)	Advanced Pinch Curves at real temperatures instead shifted temperatures to estimate energy targets, and Matrix Method to minimize heat exchanger area of HEN retrofit (Nordman and Bernstsson, 2001). Cost-optimal solution are chosen based on physical distance between streams, types of heat exchangers, heat transfer coefficients, annual pressure-drop cots, annual maintenance costs, and fouling.	Pulp and Paper Mill of Skoghall Mill (Swedish): advanced pinch curves estimated a maximum heat recovery of 8 MW, being able to recover only 5 MW with matrix method using the heat recovered in other parts of the process.
Yoon *et al.* (2007)	Data extraction from the process (temperatures, heat duty, heat capacity of each process stream and available utility data); Grid Diagram of current heat exchanger network for retrofit analysis; HEN improvement and investment cost evaluation considering different exchanger materials using capital cost estimation method of Guthrie (2007) considering a module factor for a more accurate equipment cost.	Ethylbenzene Process of LG chemicals in Yeosu, Korea: the retrofit case saves energy cost by $0.61 million/year (5.6% of the total energy cost savings) and necessary capital investment is $0.17 million.
Kralj (2009)	Graphical Heat Integration Estimation Technique: Analysis of Process Efficiency using Grand Composite Curve to estimate energy targets using fraction of maximum possible heat integration method (0 to 1, being 1 maximum energy efficiency); Modifying the process to achieve energy targets.	Formaldehyde production process: maximum heat recovery of 3.5 MW with a fraction of maximum possible heat integration 0f 0.86. There is a 5 % increase in production.
Piacentino (2011)	Heat Loads Plot was used to evaluate heat integration potential of process streams; Exergy Destruction Factor to evaluate the inefficiency of temperature profiles for each heat exchanger; Driving Force Plot was used to evaluate HEN improvements; A spider-type diagram was introduced to identify a hierarchy order between retrofit topologies solutions and the most promising relaxation paths for each network topology.	Aromatics Plant: Retrofit of existing HEN networks based on existing and innovative techniques to perform a diagnosis to achieve Minimum Energy Requirements.

Table 4.3: Other Examples of Pinch Analysis reasearch, innovation and application fields (part II).

Dagde and Piagbo (2012) and Piagbo and Dagde (2013)	The automatic heat exchanger retrofit function of Aspen Energy Analyzer was used for retrofitting, minimizing streams segmentation and the number of heat exchangers in the network. Possible retrofit solutions were evaluated by modifying utility exchangers, re-sequencing heat exchangers, re-piping heat exchangers and adding heat exchangers and new area. Finally, cross pinch exchangers were identified and eliminated and retrofit solutions were compared.	Industrial Plant of Crude Distillation Unit (CDU) of a functional refinery in Port Harcourt, Nigeria. Retrofit solutions were found by modifying utility exchangers and re-sequencing heat exchangers which were able to achieve lower operational costs by 0.21% with minimum area modification costs by 5 %. No more economical viable solutions were found with, re-piping heat exchangers and adding heat exchangers and new area. However, eliminating cross pinch exchangers showed huge energy and costs savings (16.6%), being the most promising of the retrofit designs, although investment costs would need to be considered.
Rikhtegar and Sadighi (2013)	Pinch technology-based study of heating and cooling of material streams in a large-scale olefins plant identifies major opportunities for energy savings.	Olefin Plant of South Iran at Bandar Iman with a 411,000 tons/year of ethylene production capacity. Composite curves obtained with KBC SuperTarget Software shown a potential of energy savings of 194.8 GJ/hr.
Milosevic *et al.* (2013)	The authors show an overview of Pinch Technology as an indispensable tool in optimising process units with respect to energy efficiency. Pinch Principles are shown as useful tool to improve the performance of existing process units and not just pertain to new designs and large retrofit projects.	Industrial pre-heat train of an atmospheric crude oil distillation unit (CDU). The potential of energy savings showed to be 22.7 MW, being 65 % of the efficiency gap closed by adding area with a payback period of 1.5 years and the remaining 35 % efficiency gap closed by Path Pinch Method.
Dogãn (2013)	Heat Integration projects were developed to delivery significant savings which required detailed simulation and case-specific heat integration analysis.	Industrial pre-heat train of an atmospheric crude oil distillation unit (CDU). Industrial hydrocracker and hydrodesulphurisation units (HDS).
Oluleye *et al.* (2015)	A raking criterion was introduced for evaluating opportunities that utilize recovered energy from the available waste heat in process sites. Associated with each opportunity found, it takes into account the potential to reduce green-house gas emissions and the economic factors (cost and benefits).	A Petroleum Refinery was used as a case study. Results showed that there is potential in waste heat to increase efficiency in the use of fuel by 16 % and reduce emissions by 11 % when only economic on-site utilization opportunities are explored.
Kamel *et al.* (2017)	Temperature driving force (TDP) new graphical representation is used as an analysis method to retrofit heat exchanger networks to boost energy efficiency and generate cost-effective opportunities.	An existing modern refinery in Egypt is retrofitted by structural and non-structural modifications using TDP curves. Results showed a potential of energy savings of 10.5 % with minor structural modifications, achieving some 60 % of that potential with Pinch Analysis. This new technique provides valuable contribution owing to its rigorousness, pinch-based characteristics, systematic procedure application, and easy interpretation. However, it's both difficult and time consuming, mainly for industrial practices.

4.7. Economic Analysis of Heat Exchanger Network Retrofit

The economic evaluation of heat exchanger retrofit projects requires the estimation of capital costs, in addition to operating costs, associated with the construction of the network. The capital cost must take into consideration, not only the costs of new heat exchangers, but also the costs associated of re-using the existing heat exchangers. A number of other parameters must be taken into consideration such as physical distance between streams, types of heat exchangers, space requirements, auxiliary equipment, heat transfer coefficients, annual pressure-drops costs and annual maintenance costs and fouling (Ahmad *et al.*, 1990; Nordman and Bernstsson, 2001).

There are several methods that can be found in literature. A good review of those methods can be found in the books of Coker (2007) and Turton *et al.* (2018). The estimating procedure of the total full capital cost of the retrofitted heat exchanger network used in this work is the Bare Module Cost for Equipment by Turton *et al.* (2018) which considers only the cost of new exchangers, including installation. The Bare Module Equipment Cost takes into account direct and indirect projects expenses associated with the installation of the equipment. Direct costs are related to the equipment costs, materials required for installation and the labour required to install equipment and material. Indirect costs include logistics, construction and contractor engineering expenses. A more detail description of these expenses are presented in Annex VI.

This module costing technique is the most common and most applied in engineering projects for a preliminary cost estimation. It relates total costs since the purchased cost of the equipment that is evaluated for some based conditions. In this work, the conditions specified for the base case are: 1) equipment is fabricated using carbon steel (CS) which is the most common construction material; and 2) equipment operates at near ambient temperature. For different base case conditions, multiplying factors must be used according to equipment type, specific system pressure and specific materials of construction.

The Bare Module Equipment Cost (C_{BM}) considering direct and indirect project expenses for each equipment can be determined through Equation 4.7 in which are included the purchased cost for base case conditions (C_p^0) and bare module cost factor (F_{BM}) that corresponds to the multiplication factor to account the items that address direct and indirect project expenses plus the specific materials of construction and operating pressure.

$$\boldsymbol{C_{BM} = C_p^0 F_{BM}} \qquad \textbf{Equation 4.7}$$

The C_{BM} is estimated considering the purchased costs for the equipment at base conditions that must be available with the corresponding bare module factor and factors account for different operating pressures and materials of construction which depend on the equipment type. The bare module cost for shell-and-tube heat exchangers is given in Equation 4.8 in which the values of constants B_1 and B_2 can be obtained in Annex VI for heat exchangers.

$$\boldsymbol{C_{BM} = C_p^0 (B_1 + B_2 F_p F_M)} \qquad \textbf{Equation 4.8}$$

The purchased equipment costs (C_p^0) of new equipment and pressure factor (F_p) from Equation 4.8 above is obtained through the next Equations 4.9 and 4.10, respectively.

$$log_{10}C_p^0 = K_1 + K_2 log_{10}(A) + K_3[log_{10}(A)]^2 \quad \text{Equation 4.9}$$

$$F_p = C_1 + C_2 log_{10}P + C_3(log_{10}P)^2 \quad \text{Equation 4.10}$$

From Equation 4.9, parameter A is the size of the equipment in terms of heat transfer area and constants K_1, K_2 and K_3 can be obtained using equipment cost data in Table VI.2 in Annex VI for heat exchangers. From Equation 4.10, parameter P is the operating pressure of the equipment and the values for the constants C_1, C_2 and C_3 can be estimated using pressure factors for process equipment data in Table VI.3 in Annex VII for heat exchangers. However, in this work, the bare module cost for ambient pressure and carbon steel construction for the type of equipment material (material factor, FM) and the bare module factor for the equipment at these conditions are determined considering F_M and F_p equal to 1 as indicated in Turton et al. (2018).

The information required for an equipment module estimation is based on data provided along the years which means that it is recommended to use inflation factors to report the costs to the current year of cost estimation. Therefore, it is considered cost indices to adjust for the effects of inflation on equipment costs and the Chemical Engineering Plant Cost Index of the year 2001 (CEPCI = 394) was assumed for all inflation adjustments. Using the values provided by Turton *et al.* (2018), CEPCI was updated using interpolation for the year 2018 (CEPCI = 591.3).

Payback period (PBP) is here used as an economic decision criterion together with total investment cost to evaluate months of investment. It is an estimation of the time required to recover total capital investment in the retrofitted project (Turton *et al.*, 2018).

4.8. Methodology

A process-level heat integration using Pinch Analysis is performed to evaluate energy efficiency of Pre-Distillation and Arosolvan Units by determining the maximum heat recovery that is possible to achieve within each process unit. A general methodology applied for this evaluation can be followed through the scheme in Figure 4.7.

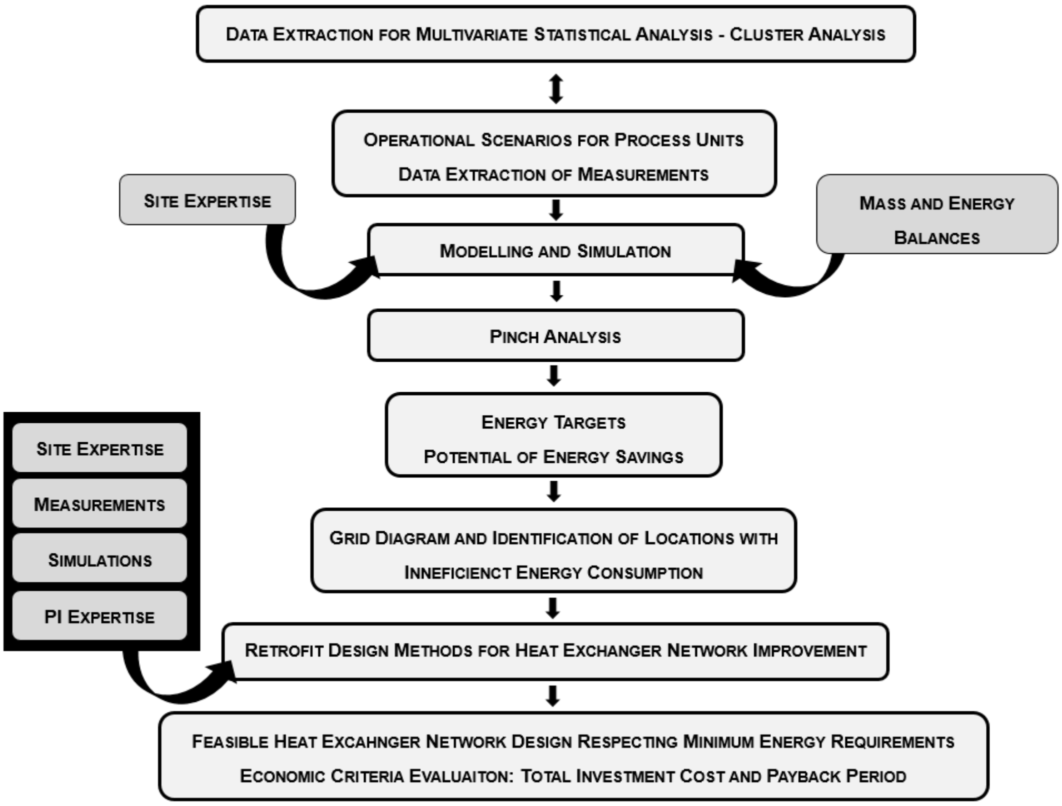


Figure 4.7: Schematization of the methodology applied to evaluate the potential of energy savings.

Cluster analysis discriminated different operational scenarios for Pre-Distillation Unit and for Arosolvan Unit to be used here for an energy performance analysis. Thermal data of each cluster was gathered for this purpose. Also, it was considered a global scenario defined by the overall mean values to verify if there is a significant difference in energy consumption and in the potential of energy savings between the different operational scenarios and global scenario.

Prior to any analysis, thermal data (temperatures and flowrates of process streams and utilities) were extracted from the different clusters, and mass and energy balances for each operational scenario were verified.

The potential of energy savings is determined based on the difference between actual utilities consumption within process unit obtained through operational scenarios and minimum utilities requirements (energy targets) to run the same process obtained using tools of Pinch analysis. The current heat exchanger network of the individual process units is represented using grid diagram to easily identify inefficient zones of energy consumption and, based on the scope of energy savings, apply retrofit methods to find possible network improvement solutions that allow to achieve a network with maximum heat recovery.

Step 1: Determination of Actual Utilities Consumption for Individual Process Units

Total actual utilities consumption are determined for each operational scenario (clusters) and for global scenario of individual process units. The actual utilities consumption translate the type and loads of hot and cold utilities that are being currently consumed by the process unit.

Some considerations described in Annex III were implemented while extracting thermal data. Mass and energy balances are performed to each process stream using software Aspen Plus 8.0 and simulation model HEATX in order to predict the heat available from hot process streams and heat required of cold process streams. For each stream are predicted its physical properties (heat capacity (cp) and latent heat (λ)) considering the operational data of the installed heat exchanger. These physical properties are determined from the composition established for each process stream based on the data provided by the Laboratory of Matosinhos Refinery, which for confidential reasons will not be here provided. The same defined composition was used for the different operational scenarios and global scenarios.

The operating conditions used (stream flow rates and supply and target temperatures) are the ones obtained for each operational scenarios and global scenario. Operating pressures of the different heat exchangers in the process units' network were considered constant and equal to the design data given in the equipment datasheets, Process Flowsheet Diagrams (PFD) and Process and Instrumentation Diagrams (P&ID).

Step 2: Estimation of Energy Targets

Energy targets were estimated using hot and cold composite curves of Pinch Analysis which were constructed through Aspen Energy Analyzer considering heat loads and supply and target temperatures of process streams for all the considered operational scenarios and global scenario.

Through heat exchangers design data, several values to attribute to ΔT_{MIN} were found and used to evaluate energy targets possible to be achieved. Though, there are typical values for ΔT_{MIN} that can be established according to the type of industry. As the aromatics plant is an intermediate plant between refinery and chemical and petrochemical industries, the latter is considered. For chemical and petrochemical industries, the typical values for ΔT_{MIN} are between 10 - 20 ºC, according to the typical values for various types of processes presented in Linnhoff (1998). However, as a rule of thumb, rating values below 10 ºC should be avoided. Therefore, energy targets were estimated for several minimum temperature difference values in the range between 10 – 20 ºC for both process units, as it is in the range considered for chemical and petrochemical industries.

Step 3: Evaluation of Potential of Energy Savings and Operating Costs (OPEX)

Energy targets thus estimated are compared to actual utilities consumptions between operational scenarios and between operational scenarios and global scenario for each process unit. Potential energy savings traduce in percentage the excess of heat that could be recovered within each process unit through process-level heat integration. The potential of energy savings were obtained for each operational scenario and for global scenario of each individual process unit with the goal of identifying different (and possibly critical) energy consumption scenarios for the subsequent energy optimization studies.

Step 4: Heat Exchanger Network representation using Grid Diagram

In Aspen Energy Analyzer, a grid diagram is used to represent the actual heat exchanger network of each individual process unit as it is a graphical visualization tool that allows a clear representation of streams and heat exchangers, a clear identification of streams temperatures and a clear visible pinch point locations and its implications. Actual heat exchangers areas of the current heat exchanger network were determined for the operating conditions of the process units, considering the standard value given by Aspen Energy Analyzer for an individual heat transfer coefficient of 720 kJ/(m^2.hr.ºC) for all process streams.

Moreover, heat transfer operations are shown which allows to easily identify the inefficient zones of energy consumption within the network, namely those where heat is being transferred across pinch point(s). These inefficient zones are to be eliminated in the following step using retrofit design methods based on heuristic rules of Pinch Analysis to achieve fixed energy targets.

Step 5: Heat Exchanger Network Retrofit Methods based on Heuristics rules

An evaluation of possible modifications in the current heat exchanger network of each process unit is performed to achieve energy targets and to increase energy efficiency through the application of retrofit methods based on heuristic rules (Pinch principles). The aim is to explore and find various options for network improvement considering fixed energy targets without getting into specific details of flow-sheet changes. This translates in finding retrofit design solutions for network improvement using grid diagram constructed through Aspen Energy Analyzer and considering the obtained performance targets (energy targets, minimum number of units and minimum heat transfer area) during the analysis for specific modifications of the heat exchanger network using pinch analysis principles and retrofit methods. In a retrofit project, the installation of new equipment, the additional heat exchanger surface area and/or the re-allocation of existing heat exchangers is expected.

For the process units of the aromatics plant, two retrofit methods are used to develop and analyse possible retrofit projects which are: A) Cross-Pinch Exchanger Elimination Method that makes incremental changes to the existing network to eliminate inefficient zones of energy consumption; and B) Pinch Design Method with maximum re-use of existing exchangers by deleting the existing network of the grid diagram and re-designed it considering re-use of existing exchangers in place of new ones between the same streams or the reallocation to new functions (duties).

A) Cross-Pinch Exchanger Elimination Method

As mentioned before, from the grid diagram it is possible to identify the heat exchangers that are violating the pinch point(s), which means that these heat exchangers are transferring heat across the pinch and, thus are considered inefficient zones of energy transfer within the network.

The identified cross-pinch exchangers are removed from the network. Cross-pinch heat loads are then divided into parts according to the corresponding pinch temperatures. For this purpose, incremental heat transfer area is required to the existing network. The unmatched split loads of each process stream is combined with other process streams and/or utilities according to the side of the pinch point (above or below pinch point). The remaining process streams are combined according to pinch principles: feasibility temperatures at pinch point(s) and match placements should start at the pinch and then developed by moving away from the pinch sequentially according to temperature. Above pinch points, total heat loads of hot process streams should be assigned to cold process streams and, bellow pinch point, total heat loads required by cold process streams should be supplied by hot process streams. The new matches can be assigned to the existing heat exchangers that were primarily eliminated, if possible, to maximize the re-use of the available heat transfer area and at the same time minimize the additional area required to achieve maximum heat recovery with minimum investment cost. In addition, in the application of this retrofit method, it is considered that well-allocated heat exchangers are left out of the retrofit study, as well as its duties and operating conditions are left unchanged.

B) Pinch Design Method with maximum re-use of existing exchangers

The traditional Pinch Design method is manly applied for grassroots designs. However, this method can be adapted for retrofit cases by considering the existing heat exchangers of the current network and make best use of the available heat transfer area during retrofit study. Briefly, Pinch Design Method (PDM) for retrofit cases consists in deleting the existing network of the grid diagram, including possible branches, and re-design it by following the heuristic rules applied in traditional PDM. At the end, the new matches can be assigned to the available heat exchangers. This way, the method allows to maximize the re-use of the available heat transfer area for new matches between the same streams and or different streams and simultaneously minimize additional area required to achieve maximum heat recovery with minimum investment cost.

In both retrofit design methods, the pinch design principles are here considered: the network design starts from the pinch point, where it is the most restricted part of the design due to temperature differences approaching ΔT_{MIN}, and then start to place heat exchanger matches while moving away from the pinch point having in consideration that no exchanger may have a temperature difference at hot and cold ends smaller than ΔT_{MIN}, no process-to-process heat transfer may occur across pinch and no inappropriate use of utilities is allowed (hot utilities are consumed above pinch point and cold utilities are consumed below pinch point).

To reduce process energy requirement, changes in the heat and material balance could be considered, such as changing the parameters of operating conditions (for example, operating pressures and flow ratios of a distillation column, pump-around flowrates, etc.). However, in the retrofit projects of the process units, changes in operating units and operating conditions is not possible and solutions are found based on fixed energy targets.

Step 6: Evaluation of Investment cost using Capital Equipment-Cost Program (CAPCOST)

After the implementation of the retrofit methods to achieve a HEN with minimum energy requirements, heat exchangers areas were estimated considering an individual heat transfer coefficient of 720 kJ/(m^2.hr.ºC) for all process streams, which is the standard value given by Aspen Energy Analyzer Software tool, including in its tutorial.

It is then possible to rank the retrofit projects and choose the best ones according to economic criteria. Capital cost and payback period are estimated for the required network modifications to achieve energy targets using Bare Module Cost for Equipment at base conditions having in consideration the maximum re-use of the existing heat exchangers. In both Pre-Distillation and Arosolvan Units, all heat exchangers can be re-used and reallocated for different stream matches, including reboilers (as all are thermo-syphon type). The only heat exchangers that will not be re-used are the air coolers as air cooling utility will stop being consumed and only cooling water will be considered as cold utility in both process units.

The industrial heat exchangers are almost always over-designed by 15-30 %, which was also assumed in both process units, when reallocating existing heat exchangers. Thus, the same heat exchanger can be adopted for a new match. In addition, heat exchangers that are kept in the same position with the same function don't have any cost associated. Heat exchangers being reallocated to new stream matches and heat loads have an installation cost associated which corresponds to 20 % of a new equipment cost determined through Bare Module Equipment Cost. For new exchangers, total Bare Module Equipment Cost is considered.

The Chemical Engineering Plant Cost Index of the year 2001 (CEPCI = 394) was assumed for all inflation adjustments. Using the values provided by Turton *et al.* (2018), CEPCI was updated using interpolation for the year 2018 (CEPCI = 591.3) to update the investment cost.

4.9. Results and Discussion

Pre-Distillation and Arosolvan Units have operated with high energy consumption along the years. Hence, it is essential to analyse the processes performance behaviour in terms of its actual energy consumption and to evaluate opportunities to minimize operational costs without compromising the processes itself, the respective operating conditions, its product quality and availability. Improvements in the heat exchanger network within each process unit are here considered through the application of retrofit methods using heuristic rules in case heat recovery opportunities are found. Therefore, it is crucial to review the current situation of each process unit and define a proper case study.

4.9.1. Thermal Stream and Utility Data Extraction

For each process unit, thermal data was extracted from the defined global scenario (overall mean values) and from the different operational scenarios (clusters) to be used for a process energy performance analysis. The procedure for process data extraction is described in Annex III.

For analysing a heat exchanger network, process and utility streams involved in each heat exchanger were identified and the heat loads were determined using the extracted thermal data (flowrates and supply and target temperatures). The material and energy balances were applied if and when required based on considered flowsheet of process units.

The enthalpy of individual process streams, as well as its physical properties, of the installed heat exchangers were predicted using the simulation model HEATX of Aspen Plus 8.0. The simulation model HEATX also required the definition of streams components and compositions which were defined based on the data supplied by the laboratory of Matosinhos Refinery. This information is not provided due to company's confidentiality. Actual utilities data, which are given in Tables 4.4 and 4.5, were supplied by the company and were used to determine the actual utilities consumptions for both process units, respectively, through Aspen Plus simulations. In both process units are being consumed medium pressure steam (MP steam), cooling water (CW) and air cooling.

Table 4.4: Actual Utilities data used for Pre-Distillation Unit.

Utilities	Temperatures	F (tons/hr)	Q (MW)	Q_{TOTAL} (MW)
MP Steam (14.5 barg)	200 -199 ºC	6.5	5.47	23
Cooling Water	20 – 30 ºC	73.9	0.858	
Air Cooling	20 – 70 ºC	1,203	16.7	

Table 4.5: Actual Utilities data used for Arosolvan Unit.

Utilities	Temperatures	F (tons/hr)	Q (MW)	Q_{TOTAL} (MW)
MP Steam (14.5 barg)	215 -175 ºC	10.8	17.5	45
	195 – 175 ºC	22.6	8.5	
Cooling Water (CW)	10 – 20 ºC	56.6	0.657	
Air Cooling	20 – 70 ºC	2,887	18.36	

In Pre-Distillation Unit, it is consumed MP steam as external hot utility at saturated conditions with a temperature of 200 ºC at 14.5 barg. As for external cold utilities, cooling water and air cooling are being consumed in the range between 20 ºC - 30 ºC and 20 ºC to 70 ºC, respectively. Arosolvan Unit consumes MP Steam at 215 ºC and at 195 ºC at 15.0 bar which means that is consumed in both superheated and saturated states (temperature saturation is 200 ºC at 15.0 bar). As for cold utilities, it is consumed CW and Air Cooling in the range between 20 ºC - 40 ºC and 20 ºC - 70 ºC, respectively.

The results obtained for operating conditions found with global scenario and considering the actual utility data above are presented in Annex III for Pre-Distillation and Arosolvan Units.

As an additional note, it was only considered the installed heat exchangers that operate continuously in both process units. Heat exchangers that only operate periodically to establish some temperature balances are left out of the analysis, as well as drum condensers. For example, in Pre-Distillation Units, the following heat exchangers E0110, E0117, E120, E0106, E0113 and E0116 identified in Figure 2.4 are not considered in the analysis. The heat exchangers considered are shown in Annex I for Pre-Distillation Unit and in Annex II for Arosolvan Unit.

Process- Level Pinch Analysis is performed to both process units. Tools provided by Pinch Analysis are used to quantify energy targets and to evaluate the influence of the potential of energy savings in the operating costs (or energy costs) of each process unit.

4.9.2. Energy Targets and Potential of Energy Savings

Pinch Analysis is then performed for each operational scenario thus finding energy targets (minimum utilities consumptions) and potential of energy savings (maximum heat recovery) for each process unit. Energy targets are determined from hot and cold composite curves (HCC and CCC, respectively) through Aspen Energy Analyzer considering heat loads and supply and target temperatures of process streams for each operational scenario and global scenario.

One purpose of this study was to evaluate the influence of the energy targets in the operating costs by only considering medium pressure steam as hot utility and cooling water as cold utility, which means that air coolers would be eliminated from the current heat exchanger networks and replaced by new coolers in both process units. The same operating conditions for the utilities used in Pre-Distillation Unit are equally considered here. In Arosolvan Unit, due to the demands of the operating conditions, new conditions for the utilities were established. The updated Utility Data are shown in Tables 4.6.

Table 4.6: New Utilities data conditions considered for Pre-Distillation and Arosolvan Units.

Utilities	Pre-Distillation Unit	Arosolvan Unit
MP Steam (14.5 barg)	200 -199 ºC	200 -199 ºC
Cooling Water	20 – 30 ºC	10 – 20 ºC

For this purpose, it is considered as external utilities MP Steam at saturated temperature of 200 ºC with an operating pressure of 14.5 barg for both process units and cooling water at 20 ºC for Pre-Distillation Unit and at 10 ºC for Arosolvan Unit. That inlet temperature of 10 ºC is possible to be supplied due to the chiller of cooling tower in operation within utility system.

Process-Level Pinch Analysis is then performed to estimate energy targets for all operational scenarios using composite curves for a ΔT_{MIN} value of 10 ºC. This parameter value was estimated using heat exchangers design data. Composite curves built considering global scenario for both process units are presented in Figure 4.8. From Figure 4.8, it can be concluded that ΔT_{MIN} determines the relative location of hot and cold streams, being an important variable for setting the amount of heat recovery.

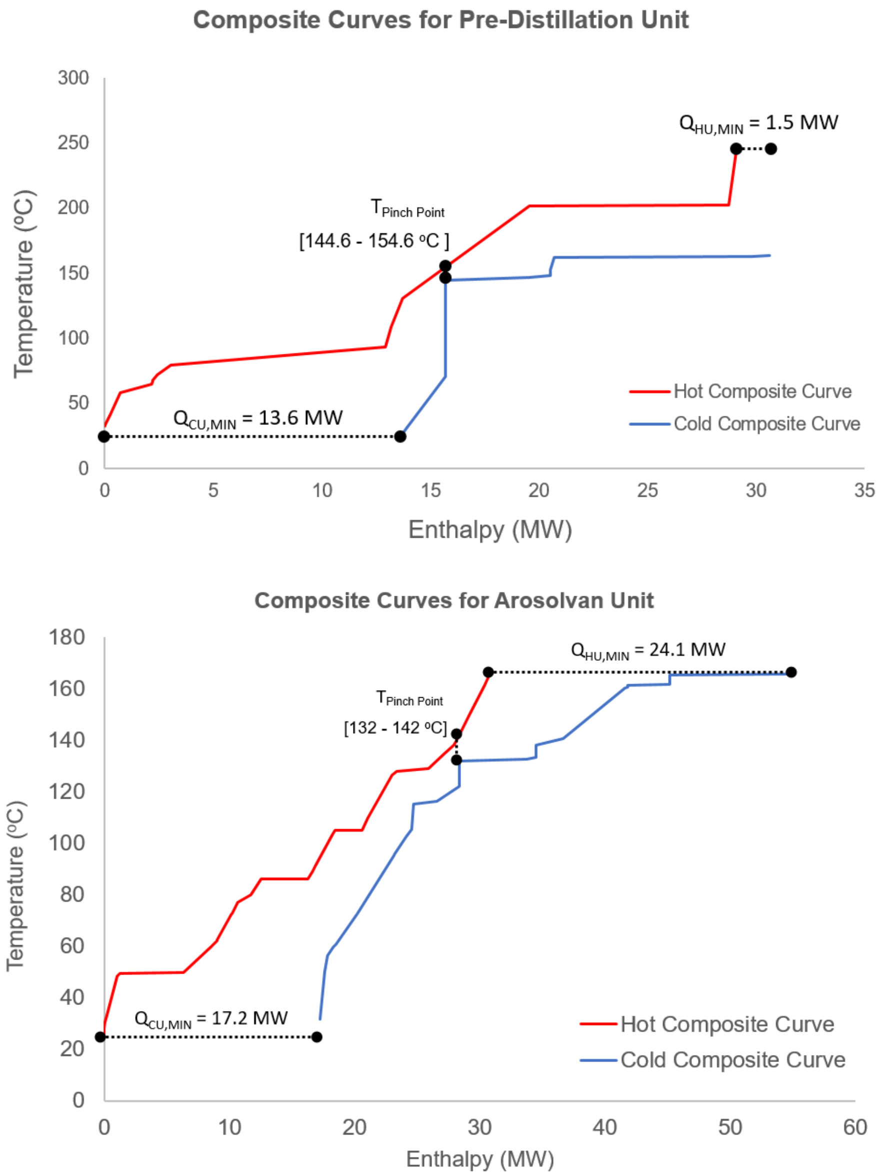


Figure 4.8: Composite Curves for Pre-Distillation Unit and for Arosolvan Unit for a ΔT_{MIN} of 10 ºC.

Through heat exchangers design data, several values to attribute to ΔT_{MIN} were found and used to evaluate the maximum heat recovery that it is possible to be achieved. The ΔT_{MIN} values were also attributed taking into account the typical values for a chemical and petrochemical plant (10 - 20 ºC), being values bellow 10 ºC avoided. The results obtained for energy targets varying with ΔT_{MIN} values are presented in Annex IV for both Pre-Distillation and Arosolvan Units. From these results, it was verified that an increase in ΔT_{MIN} value leads to lower energy savings. Pre-Distillation Unit shows potential in energy savings from 26.8 % to 34 % decreasing ΔT_{MIN} value. Arosolvan Unit shows potential in energy savings from 1.8 % to 8.3 % decreasing ΔT_{MIN} value. No heat recovery opportunities were found for ΔT_{MIN} values higher than 15 ºC in the case of Arosolvan Unit.

Energy targets were then obtained for both process units and for all operational scenarios through composite curves for a ΔT_{MIN} value of 10 ºC in which minimum hot and cold utilities consumptions ($Q_{HU,MIN}$ and $Q_{CU,MIN}$, respectively) are shown. Energy targets thus calculated were compared to actual utilities consumptions, estimated through Aspen Plus simulations of the installed heat exchangers during thermal data extracted procedure. Potential energy savings traduces in percentage the excess of heat that could be recovered within each process unit through process heat integration. Total actual utilities consumptions, total minimum values ($Q_{HU,MIN}$ + $Q_{CU,MIN}$) and the difference between them are presented in Tables 4.7 and 4.8, for each distinct operational scenario and for global scenario.

Table 4.7: Energy targets for Pre-Distillation unit.

Operational Scenarios	Total Actual Utilities Consumption (MW)	Total Minimum Utilities Consumption (MW)	Potential Energy Savings (%)
Global	23.0	15.1	34.0
1	23.9	14.4	40.0
2	21.9	15.0	31.5
3	23.4	15.7	32.8
4	20.8	14.4	30.5
5	27.2	18.4	32.5
6	26.2	16.8	35.8

Table 4.8: Energy targets for Arosolvan unit.

Operational Scenarios	Total Actual Utilities Consumption (MW)	Total Minimum Utilities Consumption (MW)	Potential Energy Savings (%)
Global	45.0	41.3	8.3
1	46.8	44.5	4.8
2	46.2	40.1	13.1
3	42.3	38.2	9.6

In both process units, total actual utilities consumptions for the different operational scenarios are close to each other and close to the ones for the global scenario. The same observation is valid when comparing total minimum utilities consumption. Thus, in both process units, identified scenarios are not in fact that much different in terms of utilities consumption and hence global scenario is considered for further analysis.

Regarding potential of energy savings, Pre-Distillation Unit has a minimum hot and cold utilities consumptions of 1.5 MW and 13.6 MW, approximately, as it is possible to see in composite curves (Fig. 4.8). Thus, comparing total minimum utilities consumption (15.1 MW) with actual utilities consumption (23 MW), it is possible a total maximum heat recovery of 7.9 MW which corresponds to a 34.0 % for Pre-Distillation Unit. As for Arosolvan Unit, it is required a minimum hot and cold utilities consumption of 24.1 MW and 17.2 MW, approximately (Fig. 4.8), achieving an 8.3 % of potential of energy savings.

Thus, comparing total minimum utilities consumption (41.3 MW) with actual utilities consumption (45 MW), it is possible a maximum heat recovery of 3.7 MW for Arosolvan Unit. These results show that there is potential to achieve more energy efficient processes, that potential being higher for Pre-Distillation Unit than for Arosolvan Unit.

4.9.3. Savings in Operating Costs

Operating costs were evaluated considering global scenario for each process unit. The actual operating costs affected by each type of external utility being currently consumed in Pre-Distillation and Arosolvan Units are shown in Table 4.9.

Table 4.9: Actual Operating Costs of Pre-Distillation and Arosolvan Units.

Operating Costs (KEUR/year)	Pre-Distillation Unit	Arosolvan Unit
MP Steam	2,079	9,885
CW	41.2	31.54
Air Cooling	163.7	418.1
Total Operating Cost	2,284.2	10,335

Results show that Pre-Distillation Unit has a hot utility cost of 2.01 MEUR/year and a cold utility cost of 0.20 MEUR/year, being the total operating costs of 2.28 MEUR/year. As for Arosolvan Unit, hot utility consumption has an annual cost of 9.89 MEUR/year and cold utility consumption has an annual cost of 0.32 MEUR/year, being the total operating costs of 10.3 MEUR/year. These results show that between cold utilities, air cooling is the cold utility that contributes for a higher operating costs as its costs depends on the electricity provided to the drivers of the air coolers and not on the amount of heat being transferred in the air cooler. As none of the process units have air coolers that allow to vary heat transfer velocities in the drivers, the operating costs regarding air cooling will not change significantly and it will only depend on the electricity provided to the motors. In addition, as there is no certainty regarding the costs values used to estimate the utility cost for air cooling, this utility is excluded for the purposed study.

Therefore, the aim here is to evaluate operating costs savings by eliminating the consumption of air cooling as cold utility in both process units, consuming only cooling water, even in cases of process streams as top product of distillation towers. In Table 4.10 are presented the results of actual operating costs and operating costs for fixed energy targets.

Table 4.10: Operating Costs Savings considering energy targets for Pre-Distillation and Arosolvan Units.

Process Unit	Actual Operating Costs (MEUR/year)	Target Operating Costs (MEUR/years)	Operating Costs Savings (MEUR/year)
Pre-Distillation	2.28	1.23	1.05
Arosolvan Unit	10.3	9.99	0.31

Results show that Pre-Distillation Unit has a total target operating cost of 1.23 MEUR/year, achieving an operating costs savings of 1.05 MEUR/year (corresponding to a reduction in 45 %). Arosolvan Unit has a total target operating cost of 9.99 MEUR/year, achieving an operating costs savings of 0.31 MEUR/year (corresponding to a reduction in 3.4 %).

4.9.4. Pre-Distillation Unit: Retrofit Solutions for a HEN with Minimum Energy Requirements

Maximum heat recovery within Pre-Distillation Unit were quantified through the estimation of energy targets. Inefficient zones of energy consumptions within the current HEN are here identified using grid diagram and possible modifications are analysed through the application of retrofit methods using heuristic rules to eliminate these inefficient zones and thus, to achieve minimum energy requirements.

Grid diagram representing the current HEN of Pre-Distillation Unit was constructed in Aspen Energy Analyzer and considering the operational data presented in Annex V. The grid diagram is shown in Figure 4.9.

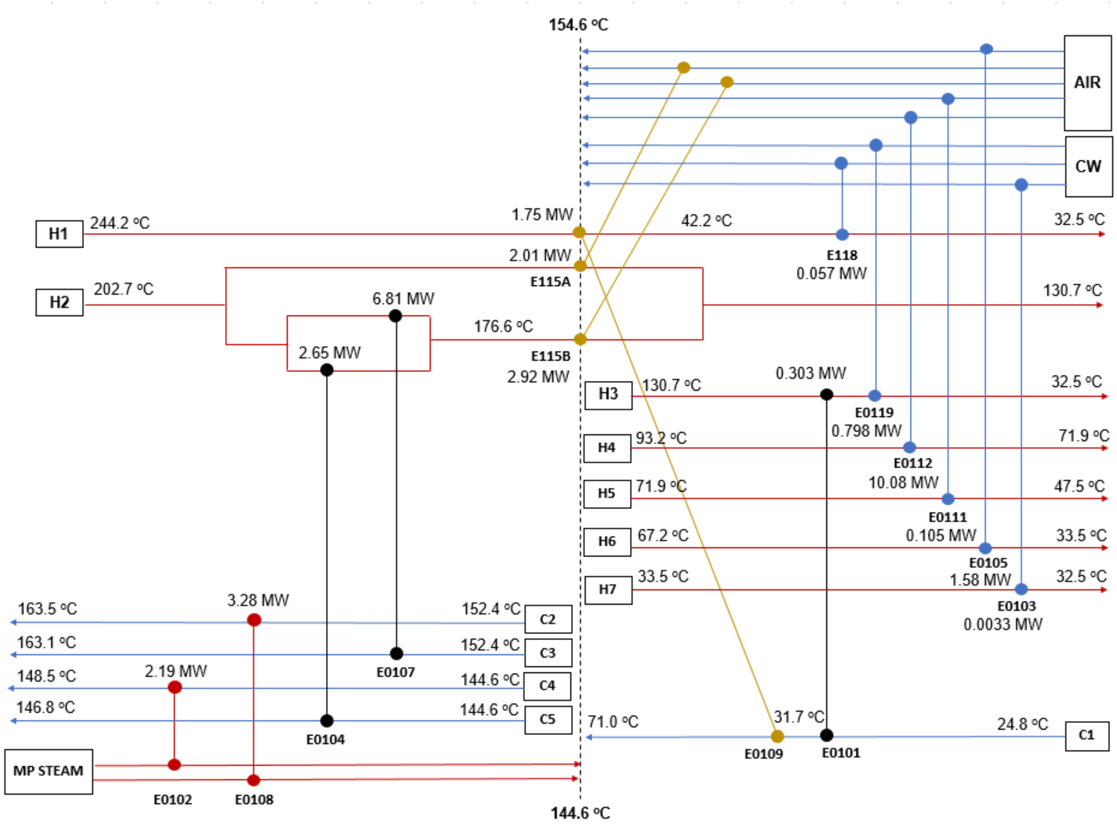


Figure 4.9: Actual Heat Exchanger Network of Pre-Distillation Unit.

The pinch hot and cold temperatures, as determined from the composite curves (Fig. 4.8), are also shown on the grid diagram (Fig. 4.9) which for Pre-Distillation Unit is 144.6 – 145.6 ºC. The pinch point location is represented as a vertical line cutting the network into two regions: one subnetwork above the pinch (heat sinks) shown on the left and one subnetwork below the pinch (heat sources) shown on the right. The hot process streams in red are represented on the top of the figure while cold process streams in blue are represented bellow the figure. The highest temperatures of process streams are represented on the left side and the lowest temperatures on the right side. Thus, hot process streams run from the left side to the right side while cold process streams run from the left side to the right side.

The heat exchangers transferring heat between process-to-process streams and process-to-utility streams are represented by a vertical line joining circles on the two matched streams. Process-to-process heat exchangers are identified in black, heaters are differentiated as red and coolers as blue. The cold utilities (CW and Air) are above the hot process streams bellow pinch point and the hot utilities (MP steam) are below the cold process streams above pinch point.

In addition, it is possible to identify 7 hot process streams and 5 cold process streams. In total, there are 14 heat exchangers (4 process-to-process heat exchangers, 4 reboilers, 3 coolers and 5 air coolers) with a total heat transfer surface area of 8941 m^2 which was determined considering heat transfer in counter-current. Results can be found in Annex III. The heat exchangers areas were determined considering a constant and by default value of 720 kJ/(m^2.hr.ºC) provided by Aspen Energy Analyzer for the individual heat transfer coefficient for all process and utility streams, as the aim is to obtain purely indicative values for total heat transfer area and for the associated investment cost.

As mentioned before, grid diagram is a helpful visualization tool to identify zones of inefficient heat integration, namely those where heat is being transferred across the pinch point. Currently, there are 3 heat exchangers marked in yellow transferring heat across pinch point which are E0109 (process-to-process heat exchanger) and E0115A/B (two air coolers). These are the inefficient zones to be eliminated using retrofit methods.

Through Aspen Energy Analyzer, it is also possible to estimate the minimum number of units and the total minimum heat transfer area required to achieve fixed energy targets. For this case, and for the considerations mentioned above, it was estimated a minimum number of units of 14 heat exchangers with a total minimum area required of 7010 m^2. Although the current HEN of Pre-Distillation Unit achieves minimum number of units targeted, the actual total heat transfer area is much higher than the minimum required exceeding by 1931 m^2. Thus, the next step is to apply the retrofit methods, cross-pinch elimination method and pinch design method, to eliminate the inefficient zones of energy consumption quantifying the total heat transfer area required for fixed energy targets and also assuming a constant and by default value of 720 kJ/(m^2.hr.ºC) for the individual heat transfer coefficient for all process and utility streams given by Aspen Energy Analyzer Software tool tutorial.

Cross-Pinch Exchangers Elimination Method and Pinch Design Method, both with maximum re-use of existing heat exchangers, are applied to obtain retrofit design solutions for the current HEN of Pre-Distillation Unit. The retrofit design solutions are evaluated based on some economic criteria, such as total investment cost and payback period. Indeed, it is possible to obtain independent solutions involving structural and non-structural modifications to the network that can be ranked according to the investment required and just choose the best one that respects fixed energy and operating costs targets.

For the implementation of both methods, a few rules must be followed: a) no exchanger may have a temperature difference lower than the specified ΔT_{MIN} for each process unit (10 ºC); b) no heat transfer may occur across the pinch as energy targets are fixed and the aim is to find a retrofit solution with maximum heat recovery; and c) no inappropriate use of utilities is allowed which means that hot utilities and cold utilities are only consumed above and below pinch point, respectively.

Total investment cost is estimated using bare module equipment cost which is a procedure applied to estimate the cost of new equipment. The data required for this procedure is presented in Annex VI which corresponds for CEPCI of 394 for the year 2001. This value was assumed for all inflation adjustments to update the investment cost for the year 2018 (CEPCI = 591.3). Thus, some considerations are also here considered to estimate a proper investment cost for the re-use of the existing equipment such as: i) new equipment cost are determined following the traditional procedure of the bare module equipment cost; ii) well-allocated heat exchangers or heat exchangers with the same streams match and heat duties do not have a cost associated (zero cost); and iii) the re-use and reallocation of the existing and available heat exchangers to new stream matches and/or heat duties have only an installation cost associated corresponding to 20 % of a new equipment cost (a percentage estimated through bare module equipment cost procedure data). Moreover, heat exchangers are designed above the required capacity (maximum over 15-30%) which means that even for higher loads that might exist, the existing heat exchanger might be re-used in the network.

Results obtained with Cross-Pinch Exchanger Elimination Method

From the application of cross-pinch elimination method using Aspen Energy Analyzer and applying pinch principles and heuristic rules, one of many possible heat exchanger network retrofit solutions was obtained which is shown in Figure 4.10. This retrofit solution was obtained by considering firstly the hot process streams with higher duties transferring heat across the pinch and dividing its heat loads to be transferred with cold process streams. Secondly, minimum temperature differences at the hot and cold ends of the counter-current heat exchangers have to respect ΔT_{MIN} of 10 ºC, which means that matches placement should start at the pinch and then moved away from the pinch sequentially according to process streams temperatures. At last, remaining process streams are matched with the respective type of utility depending if it is above or below the pinch point.

Above pinch point, it was necessary a total of 8 heat exchangers to achieve minimum hot utility requirements (1.5 MW) with a total estimated heat transfer area of 5648 m^2. From these heat exchangers, two reboilers (E0104 and E107) are well-allocated in the network with a total heat transfer area of 2377 m^2. Also, the reboiler E0102 (480 m^2) can be re-used and reallocated in the place of NU- 5 to perform a new duty. Thus, a total heat transfer area of 2857 m^2 is re-used above pinch point. The remaining 5 heat exchangers have a total additional heat transfer area of 2791 m^2 that is required to add to the network. A total capital cost of 1,944 k€ is required for network modifications above pinch.

To achieve minimum cold utility requirements (13.6 MW) bellow pinch point, it was also necessary 8 heat exchangers with a total heat transfer area of 2820 m^2. As heat exchanger E0101 (33.2 m^2) was well-allocated and the two coolers E0103 (5 m^2) and E0119 (222 m^2) could be reused in the network for the same stream matches, a total of 260 m^2 heat transfer area is re-used without any cost associated. Only 5 additional units with 2560 m^2 were required to fulfil that purpose. A total capital cost of 1,774 k€ is needed for network modifications below pinch.

The resultant network retrofit solution required a total of 16 number of units corresponding to a total heat transfer area of 8468 m^2, which 3117 m^2 corresponds to a total re-used heat transfer area of existing equipment (6 heat exchangers) and 5351 m^2 corresponds to a total additional heat transfer area requirements (10 heat exchangers). A total investment cost of 3,718 k€ is required for the retrofit project using cross-pinch exchanger elimination method with a payback period of 3.5 years. As it is possible to verify, the solution found exceeds minimum number of units target by 2 exchangers (exceeding 6.7% of the initial target) and exceeds about 1457 m^2 of minimum total heat transfer area target (exceeding 20.5% of the initial target). Therefore, other better solutions can be found possibly with other retrofit methods, as with the application of pinch design method re-using existing heat exchangers.

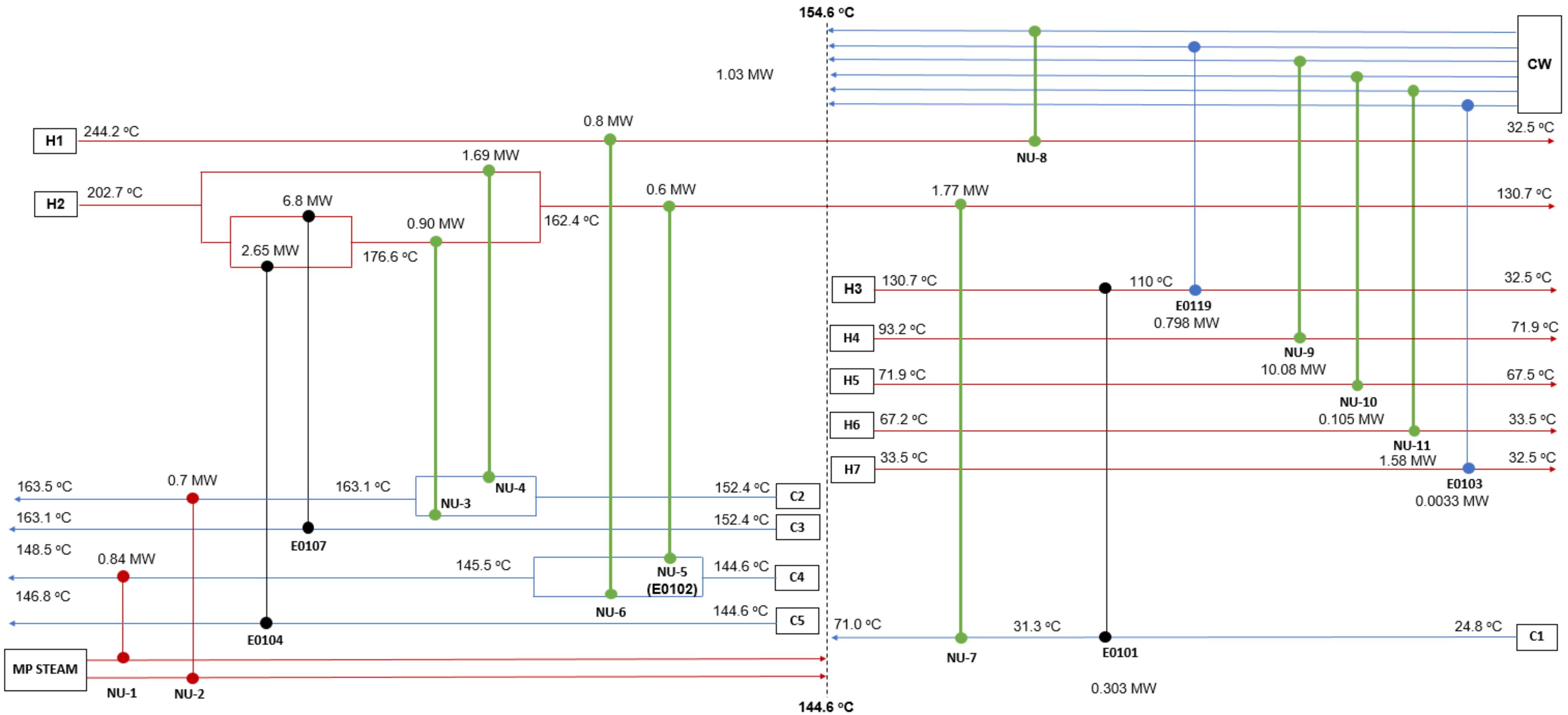


Figure 4.10: Grid diagram of retrofit network solution for Pre-Distillation Unit resultant from cross-pinch exchanger elimination method using heuristic rules.

Results obtained with Pinch Design Method for Retrofit Design

For this retrofit study, it is considered basically a new heat exchanger network with the main difference that existing heat exchangers can be re-used and re-allocated to perform the same or new duties. New heat exchangers might also be required. Also stream branches are eliminated from the grid diagram. The network retrofit solution obtained with this method is represented in the grid diagram shown in Figure 4.11. This retrofit solution was obtained using the heuristic rules starting with hot process streams with higher heat capacity flowrates and/or heat loads to be transferred with cold process streams. Secondly, minimum temperature differences at the hot and cold ends of the counter-current heat exchangers have to respect ΔT_{MIN} of 10 ºC, which means that matches placement should start at the pinch and then moved away from the pinch sequentially according to process streams temperatures. At last, remaining process streams are matched with the respective type of utility depending if it is above or below the pinch point.

Above pinch point, it was necessary 6 heat exchangers to achieve minimum hot utility requirements (1.5 MW) with a total heat transfer area of 4543 m^2. However, some of the existing heat exchangers can be re-used and re-allocated for new duties to minimize total additional heat transfer area. For the net heat source, 4 heat exchangers can be re-used (E0102, E0104, E0107 and E0108) as all of them are shell and tube reboilers (thermosiphon type) which means they can be re-allocated for new duties: E0102 and E0104 are used in parallel to serve the new duty of HEATX-4, E0107 is reused to serve the new duty of HEATX-3, and E0108 is reused to serve the new duty of HEATX-5. The resultant total re-used of the 4 heat exchangers is 3996 m^2, approximately, with only an installation cost associated. Therefore, the required additional area to achieve fixed hot utility target is 547 m^2 with a total capital cost of 0.967 k€ for network modifications above pinch. The results can be found in Annex VII.

For fixed cold utility target (13.6 MW) bellow pinch point, it was required 8 heat exchangers with a total heat transfer area of 2920 m^2, approximately. The existing heat exchangers that can be re-used to minimize additional heat transfer area are E0103, E0109 and E0118 which are shell and tube type heat exchangers. Re-using these exchangers, it is possible to re-use a total heat transfer area of 528 m^2. For the net sink source, 5 additional heat exchangers are required with a total additional area of 2392 m^2 with a total capital cost of 1,734 k€ for network modifications above pinch.

To sum up, the resultant network retrofit solution required a total 14 number of units corresponding to a total heat transfer area of 7463 m^2, which 4524 m^2 corresponds to a total re-used heat transfer area of existing equipment (7 heat exchangers) and 2940 m^2 corresponds to a total additional heat transfer area requirements (7 heat exchangers). As it is possible to verify, the solution respects total minimum number of units target (14 heat exchangers) but exceeds about 453 m^2 of minimum total heat transfer area target (exceeding 6.5 % of the initial target) with a total capital cost of 2,702 k€ for network retrofit project with a payback period of 2.57years. The results obtained with correcting cross-pinch method and pinch design method for retrofit cases are summarized in Table 4.11.

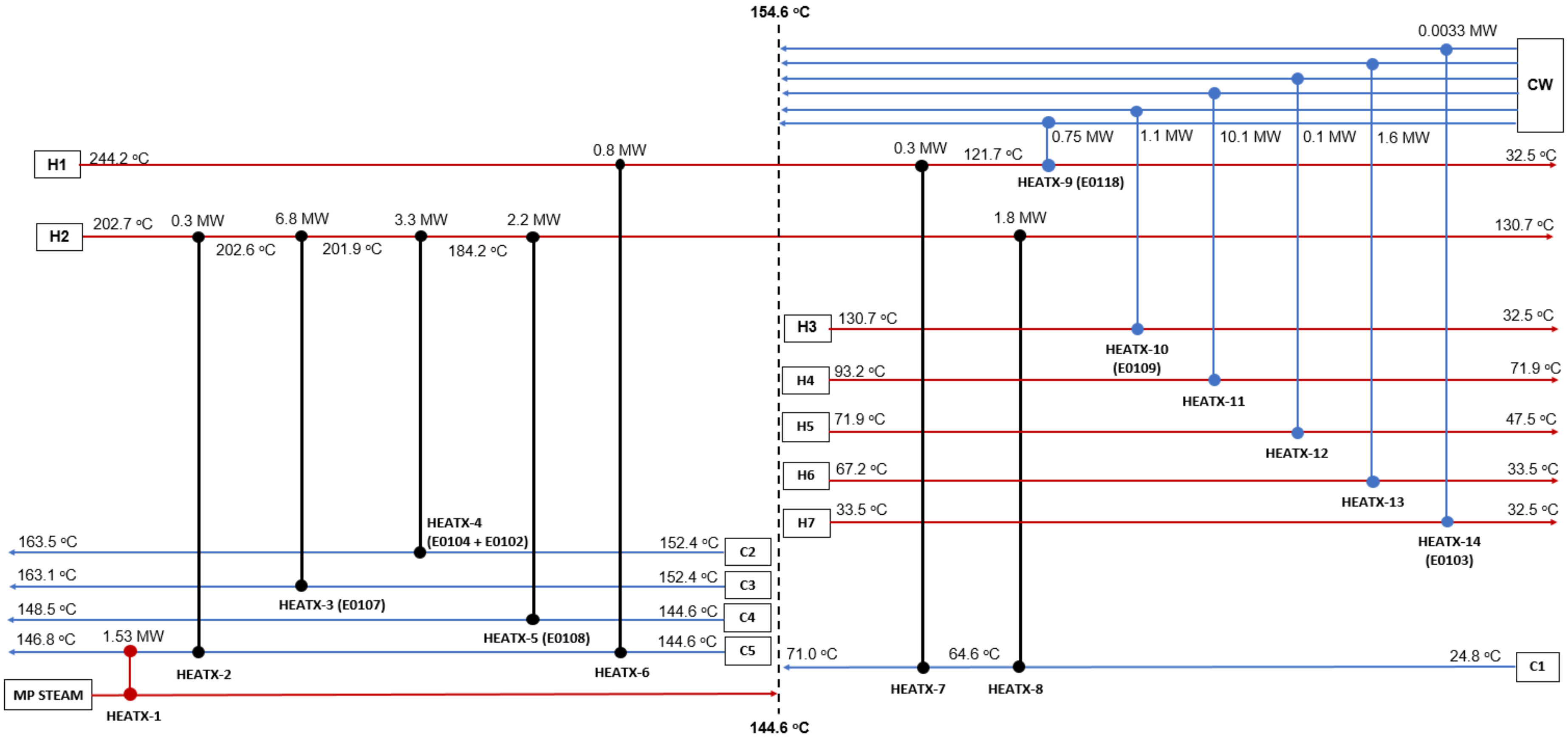


Figure 4.11: Heat Exchanger Network retrofit solution using Pinch Design Method for Retrofit Design applying heuristic rules for Pre-Distillation Unit.

Table 4.11: Overall results obtained with cross-pinch exchanger elimination method and pinch design method for retrofit cases.

Retrofit Method	Cross-Pinch Exchangers Elimination Method	Pinch Design Method
Retrofit Solution No	Solution 1	Solution 2
Total No Units	16	14
Total Re-used Area (m^2)	3,117	4,524
Total Additional Area (m^2)	5,351	2,940
Total Area (m^2)	8,467	7,463
Total Capital Cost (k€)	3,768	2,702
Payback Period	3.54	2.57

From Table 4.11, despite the possibility in re-using existing exchangers, it is possible to verify that for the fixed energy targets and operating costs, a better solution is found using Pinch Design Method for retrofit design (Solution 2) as it requires less units and less heat transfer area than cross-pinch heat exchanger elimination method (Solution 1). In addition, with cross-pinch elimination method, it is obtained higher investment cost and payback period than the pinch design method for retrofit cases. This occurs because in cross-pinch heat exchanger elimination method, an incremental in heat transfer area is required with lower possibilities in re-using existing heat exchangers and a higher number of new equipment is required. On the other hand, some heat exchangers remain unaltered and only the incremental heat transfer area is accounted. With Pinch Design method, there is a higher possibility in re-using the maximum existing heat exchangers of the current network (except for the air coolers that are replaced for new coolers) and the mainly factor in the capital cost is the reallocation and installation of those equipment which is equivalent to 20 % of the cost of new equipment. For this reason, pinch design method for retrofit design offers a better retrofit solution for fixed energy targets as it offers lower investment cost.

4.9.5. Arosolvan Unit: Retrofit Solutions for a HEN with Minimum Energy Requirements

Process operating data of Arosolvan Unit for the construction of grid diagram is presented in Annex V. Grid diagram shown in Figure 4.12 represents the current heat exchanger network of Arosolvan Unit. The pinch hot and cold temperatures, as determined from the composite curves (Fig. 4.9), are also shown on the grid diagram which for Arosolvan Unit are 132.0 – 142.0 ºC. The heat exchangers transferring heat between process-to-process streams and process-to-utility streams are represented using the same analogy as in grid diagram of Pre-Distillation unit.

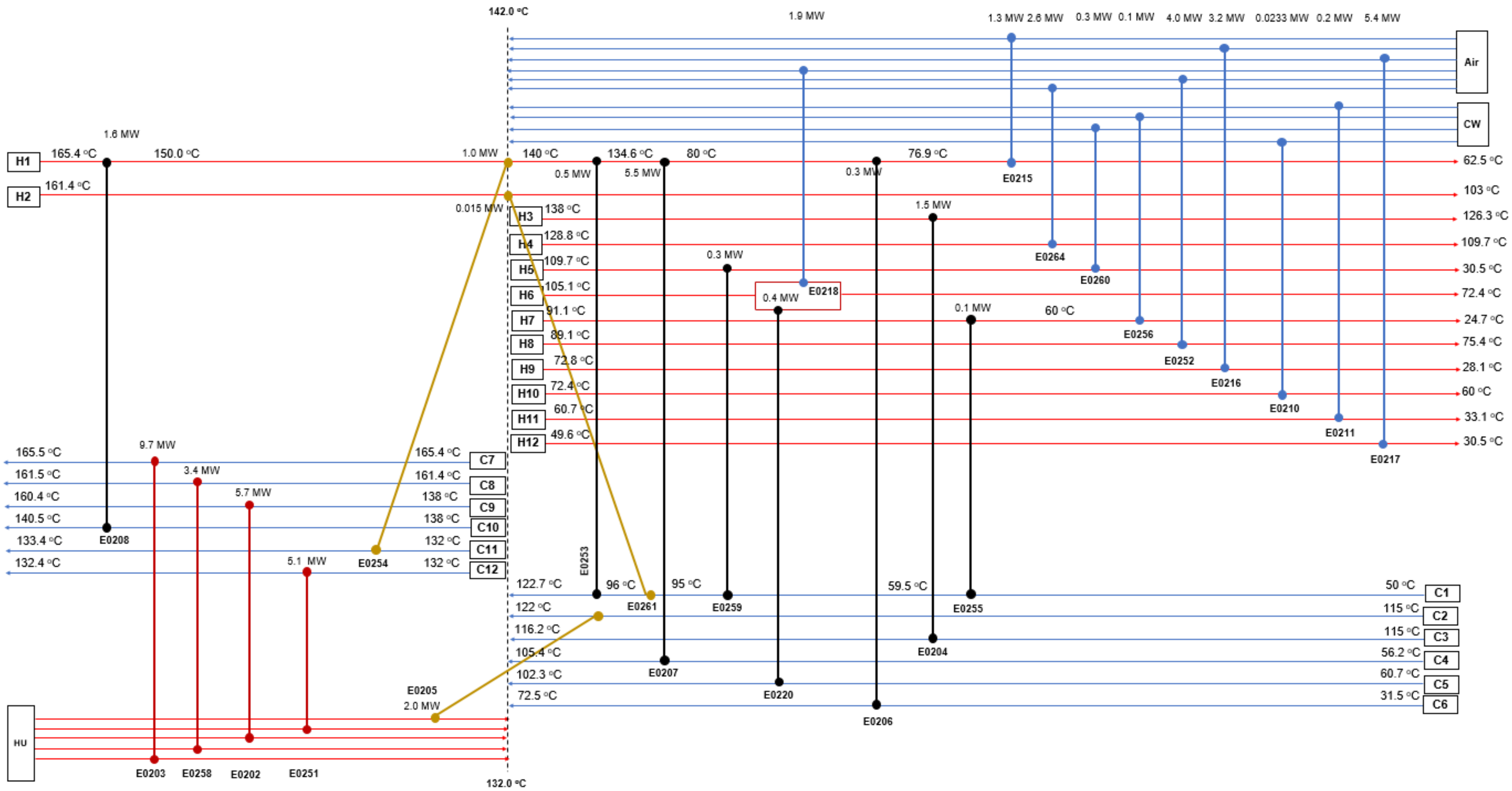


Figure 4.12: Grid Diagram representing the actual Heat Exchanger Network of Arosolvan Unit.

The process unit is composed by 12 hot process streams and 12 cold process streams. In total, there are 25 installed heat exchangers (8 process-to-process heat exchangers, 7 reboilers, 4 coolers and 6 air coolers) with a total heat transfer surface area of 26,270 m^2 which was determined considering heat transfer in counter-current. Results can be found in Annex III. The heat exchangers areas were also determined considering a constant and by default value of 720 kJ/(m^2.hr.ºC) for the individual heat transfer coefficient for all process and utility streams to obtain purely indicative values for total heat transfer area and for the associated investment cost.

Through Aspen Energy Analyzer, for the mentioned utility data conditions required, it is targeted the minimum number of units (N_{MIN}) and the total minimum heat transfer area (A_{MIN}) required to achieve fixed energy targets (24 MW of heating and 17 MW of cooling). For this case, and for the considerations mentioned above, it was estimated an N_{MIN} of 26 with an A_{MIN} required of 15,187 m^2 for counter current.

Currently, there are 3 heat exchangers marked in yellow transferring heat across pinch point which are E0254 and E0261 (process-to-process heat exchangers) and E0205 (process-to-utility heat exchanger). These are the inefficient zones to be eliminated from the network by applying the two retrofit methods.

Cross-Pinch Heat Exchangers Elimination Method for Arosolvan Unit

Cross-pinch exchangers elimination method is first applied which requires making incremental changes to the existing network to achieve fixed energy targets. Exchanger E0208 above pinch point and exchangers E0204, E0206, E0207, E0220, E0253 and E0255 bellow pinch point are considered well-allocated and thus excluded from the retrofit problem. The remained streams, which includes the ones transferring heat with hot and cold utilities, were considered to make best use of heat transfer between process-to-process streams.

From the application of cross-pinch exchanger elimination method using Aspen Energy Analyzer, and using the same principles and heuristic rules, no viable solution was found without violating the hot and cold ends of process-to-process stream matches. Some of the remained streams to be matched do not respect the minimum temperature differences at the hot and cold ends of the counter-current heat exchangers, requiring ΔT_{MIN} lower than 10 ºC to obtain possible solutions.

Pinch Design Method for retrofit of Arosolvan Unit

Pinch Design Method is applied in which the existing heat exchangers can be re-used and re-allocated to perform the same or new duties. New heat exchangers might also be required. The same procedure applied for Pre-Distillation Unit is also considered for the retrofit of Arosolvan Unit. The network retrofit solution obtained with this method is represented in grid diagram shown in Figure 4.13.

Above pinch point, it was necessary 8 heat exchangers to achieve minimum hot utility requirements (24 MW) with an approximated total heat transfer area of 7240 m^2. However, some of the existing heat exchangers can be re-used and re-allocated for new duties to minimize total additional heat transfer area. For the net heat source, 6 heat exchangers can be re-used (E0203/HEATX-1, E0258/HEATX-2), E0202/HEATX-3, E0251/HEATX-5 and E0208/HEATX-6) as all of them have closed heat transfer areas. The results can be found in Annex VIII. Total re-used heat transfer area is 6586 m^2, approximately. On the other hand, it is required 2 new heat exchangers (HEATX-4, HEATX-7 and HEATX-8) resulting in an additional area of 654 m^2. These modifications require an investment cost of 0.132 k€.

For fixed cold utility target (17.2 MW) bellow pinch point, it was required 18 heat exchangers with a total heat transfer area of 9735 m^2, approximately. The existing heat exchangers that can be re-used to minimize additional heat transfer area are: E0204 and E0205 (HEATX-12), E0256 (HEATX-14), E0255 (HEATX-15), E0214 and E0260 (HEATX-17), E0206 (HEATX-19), E0204 (HEATX-23), E0261 (HEATX- 24) and E0207 (HEATX-26). Re-using these exchangers, it is possible to a total re-used heat transfer area of 4703 m^2. For the net sink source, 11 additional heat exchangers are required with a total additional area of 5032 m^2. These modifications require an investment cost of 4,404 k€.

The resultant network retrofit solution required a total 26 heat exchangers corresponding to a total heat transfer area of 16,975 m^2 of which 11,288 m^2 corresponds to a total re-used heat transfer area of existing equipment (13 heat exchangers) and 5687 m^2 corresponds to a total additional heat transfer area requirements (15 heat exchangers). It is needed a total capital cost of 4,537 k€. As it is possible to verify, the solution respects total minimum number of units target (26 heat exchangers) for fixed energy targets but exceeds about 1788 m^2 of minimum total heat transfer area target (exceeding 8.4 % of the initial target) due to the re-use of the existing exchangers. It is possible to verify that for the fixed energy targets and operating costs, it is found a viable solution using Pinch Design Method for retrofit design. As the operational cost savings obtained for this process units are too low, the payback period is not here used as economic criterion for decision making as the investment costs are enough as based decision, in this case.

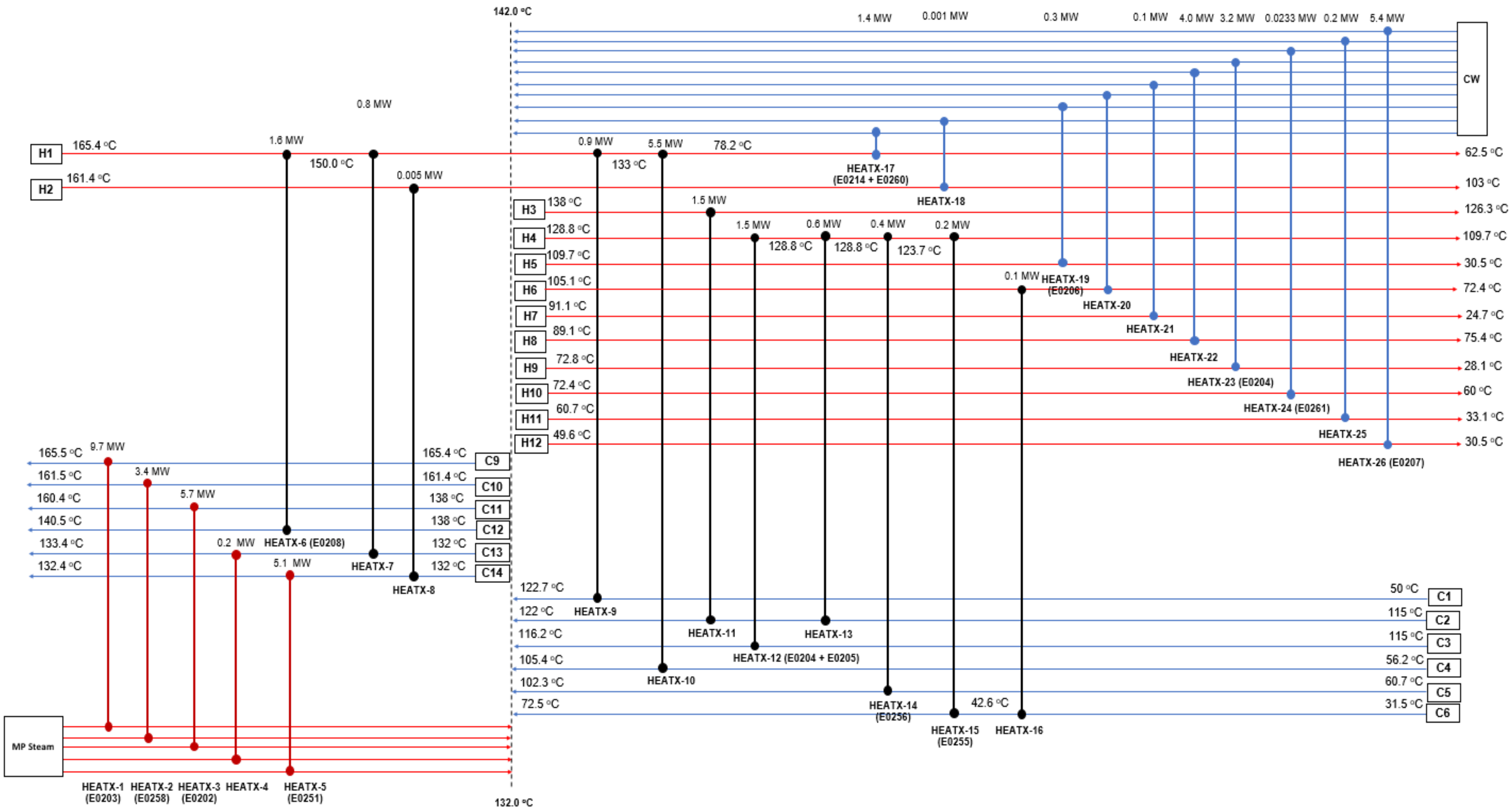


Figure 4.13: Heat Exchanger Network retrofit solution using Pinch Design Method applying heuristic rules for Arosolvan Unit.

4.10. Conclusions

The potential of energy savings for Pre-Distillation and Arosolvan Units were evaluated considering different operational scenarios (clusters) and global scenario (overall mean values). These potentials were compared between all scenarios showing no significant difference in terms of potential of energy savings. Therefore, it is possible a potential of energy savings of 34 % (7.9 MW) for Pre-Distillation Unit and of 8.3 % (3.7 MW) for Arosolvan Unit. The operating costs savings correspond to 1.05 M€ for Pre-Distillation and 0.31 M€ for Arosolvan Units, respectively.

Energy targets were then estimated for global scenario and for a ΔT_{MIN} of 10 ºC for both process units. A minimum hot and cold utilities consumption of 1.5 MW and 13.6 MW, respectively, was estimated for Pre-Distillation Unit. For Arosolvan Unit, it was estimated a minimum hot and cold utilities consumption of 24 MW and 17.2 MW. The current heat exchanger network of each process unit was represented in a grid diagram to identify the inefficient zones of energy consumptions within the network, namely those transferring heat across pinch point. In both process units, it was found three heat exchangers violating the pinch point. To eliminate these inefficient zones, two retrofit methods using heuristic rules were applied in a way to achieve networks with minimum energy requirements: cross-pinch exchanger elimination method and pinch design method. The retrofit design solutions were ranked according to total investment cost and payback period.

In the case of Pre-Distillation Unit, the best retrofit design solution for fixed energy targets was found applying pinch design method. To achieve minimum energy requirements, it is necessary 14 heat exchangers with a total heat transfer area of 7463 m^2. From these total heat transfer area, 4524 m^2 correspond to total re-used area of the existing heat exchangers (total of 6 heat exchangers re-used) and 2940 m^2 correspond to a total additional heat transfer area required for new 8 heat exchangers. A total investment cost of 2,702 k€ is required 2.57 years.

In the case of Arosolvan Units, only one solution was found using pinch design method as with cross-pinch exchanger elimination method no solution was found without violating the ΔT_{MIN} of 10 ºC at hot and cold ends of the heat exchangers. Using pinch design method, it was found one possible solution requiring 26 heat exchangers with a total heat transfer area of 16,975 m^2. From these area, 11,288 m^2 correspond to total re-used area of the existing heat exchangers (total of 15 heat exchangers re-used) and 5687 m^2 correspond to a total of additional heat transfer area required for new 11 heat exchangers. The structural and non-structural modifications of the current network to achieve minimum energy requirements requires a total capital cost of 4,537 k€ which is a higher investment to proceed to any modification of Arosolvan Unit and thus, it is suggested to continue to operate as the actual situation

So far, the best retrofit solution found for Pre-Distillation unit corresponds to the one obtained with the implementation of pinch design method due to the fact that, although higher modifications in the network are required, the possibility in re-using the maximum of the existing equipment is higher than in cross-pinch exchanger elimination method. In this method, although part of the structure of the network is fixed, the possibility in re-using existing exchangers is lower and a higher investment cost in new equipment is required due to the incremental heat transfer area needed to eliminate the inefficient zones of energy consumption. Nevertheless, optimization studies using mathematical programming models are further applied to obtain optimal solutions for fixed energy targets which will be compared to the ones obtained using Pinch Analysis and heuristic rules.

Chapter 5: Aromatics Plant Site Wide Energy Performance Analysis

Abstract

Total Site Heat Integration is a methodology used to identify heat recovery opportunities across multiple process units or industrial plants linked through a central utility system that works as an intermediate energy carrier between them. Here, a direct and indirect heat integration analysis is performed to identify heat transfer opportunities for the whole site through the integration Pre-Distillation and Arosolvan Units. Heat recovery opportunities are evaluated using a single grand composite curve comprising both process units as a single unit (direct heat integration) and total site profiles to evaluate heat recovery opportunities using intermediate utilities (indirect heat integration), giving both the overall heating and cooling demands for the whole site. The evaluation was performed for minimum temperature differences of 10 ºC and 15 ºC. Inter-process heat recovery showed higher potential in heat recovery through direct heat integration than intra-process heat recovery (within each individual process units) for both minimum temperature differences. Total site profiles revealed a heat transfer stage between 130 ºC and 144.6 ºC for a minimum temperature differences of 15 ºC, where process heat sources can generate utilities to be supplied to process heat sinks, corresponding to 680 kW. The methodology proposed here was able to easily identify the amount of heat that is possible to be exchanged between the two analysed process units of the aromatics plant.

Key words: Aromatics Plant, Pinch Analysis, Total Site Analysis, Energy Targets.

5.1. Introduction

Heat recovery opportunities can be identified within each individual process or/and between processes. Process-level pinch analysis allows to understand important factors, balancing the increase high value products with rational energy consumption and the most cost promising process modifications prior to (re)design. For a better energy consumption evaluation, this methodology has been expanded from a single process to large plants. As individual process units might operate independently and occupy different subsections of the site, the overall site may not be fully analysed. Therefore, total site improvement, as a simultaneous approach to consider individual process units issues alongside site wide utility planning and energy in all forms, provides an overview of the potential of energy reduction and associated emissions for the whole site (Klemeš *et al.*, 2014; Linnhoff, 1998).

Total Site concept using Pinch Technology as background was introduced by Dhole and Linnhoff (1992). Industries like refinery and petrochemicals integrate several individual process units as part of large plants, which are interlinked with one another to exchange raw materials, intermediate products, side products and energy carriers (utilities). Total Site Heat integration (TSHI) identifies additional inter-process heat recovery opportunities across different individual processes via central utility system (Klemes *et al.*, 1997; Linnhoff, 1998).

TSHI translates the complex interactions between utility systems for individual plants, the incorporation of utilities into networks for individual plants, and the incorporation of heat and power systems. The steam supply from a source plants and the steam demand of sink plants are balanced by the production of steam and generation of power in the utility system (Bagajewicz and Rodera, 2000). Indirect heat integration with intermediate fluids or through a central utility system, although it offers higher process flexibility and control, it lacks in achieving maximum energy recovery opportunities. This occurs because the use of intermediate fluids to transfer heat from one process to the other reduces the interval of effective heat transfer between pinches by an addition of different minimum approach temperatures. Thus, the energy savings potential is lower when compared to direct integration. Also, the number of heat exchangers can be higher than in direct integration, which leads to higher costs. In direct heat integration, different processes are combined and treated as a single process and provides the maximum energy savings with the maximum possible heat transfer across different processes. Processes with different pinch locations offer potential for energy recovery through site level integration. However, direct integration may involve complex networking with multiple streams, crossing the individual battery limits and demanding more equipment to overcome this problem which increases cost. Also, direct integration may involve topological disadvantages and chemical as well as safety hazards due to direct integration of far away streams. Comparing to indirect integration, direct integration offers less operational flexibility and controllability of the overall plant. The trade-off is between the capital cost of extra heat exchangers and the operating cost associated with equipment and utility usage (Bandyopadhyay *et al.*, 2010; Hui and Ahmad, 1994; Klemeš *et al.*, 2014).

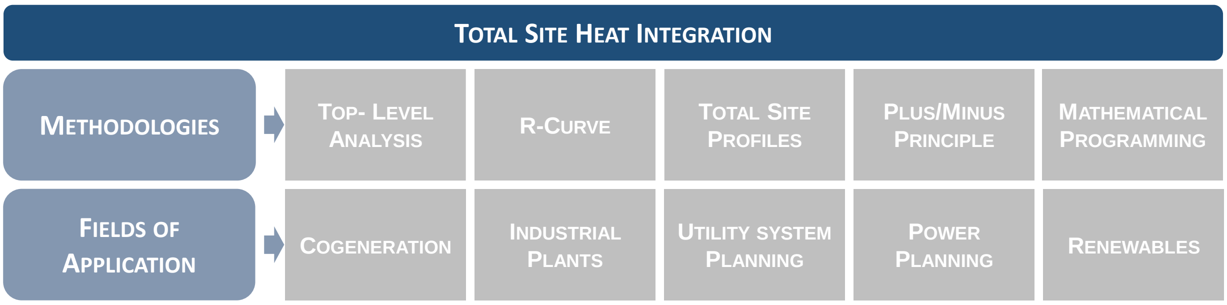


Figure 5.1: Total Site Integration main applications.

Figure 5.1 describes the main application fields and methodologies developed along the recent years for a total site improvement. Total Site Targeting method allows waste heat from processes to be used as a source of heat in other processes. Waste heat sources are converted to steam and passed to processes that are in heat deficit through the steam system. It targets the amounts of steam used and generated by the combined individual processes, the amount of heat recovery that can be achieved through the steam system, the amount of steam that has to be supplied by steam generators, and the potential co-generation that can be produced by distributing the stream through the Total Site system (Klemes *et al.*, 1997). Total Site Analysis procedure evaluates how much of steam levels are required to supply to a site, to maximize power generation, to evaluate the requirements of additional systems (such cogeneration systems combining heat and power) or heat exchangers between process streams of separated processes to identify opportunities to recover heat by raising steam from process streams bellow the pinch point and used as an intermediate utility in other processes, to evaluate the benefits of a heat recovery project that saves steam when considering the loss in power generation, and to evaluate the optimal temperatures of utility levels considering the whole site (Linnhoff, 1998).

A site-wide heat recovery is performed to identify heat sources and heat sinks on the site, which stem from the individual site processes through the construction of grand composite curves (GCC), a Pinch Analysis tool to evaluate heat integration opportunities. These curves are the base of total site profiles giving the heat sources and heat sinks required for the whole site. The energy required for the process can be supplied by different utility levels (such as high/medium/low pressure steam, refrigeration levels, hot oil circuit, furnaces flue gas, etc.). The main objective is to maximize the use of cheaper utility levels and minimize the use of expensive utility levels. Low pressure steam (LP steam) is cheaper than high pressure steam (HP steam) and cooling water is cheaper than refrigeration. Although the composite curves are useful to determine the overall energy targets, do not determine how much energy is needed to be supplied by different utility levels while GCC offers a clear visual representation of the selected utilities and the associated enthalpy change (Klemeš *et al.*, 2014; Klemeš, 2013; Linnhoff, 1998).

Sophisticated methods were developed for total site analysis, such as Total Site Analysis™ of Skelland and Petella (1993), Advent™ of AspenTech and SuperTarget™ of Linnhoff-March. Lygeros *et al.* (1996) developed a total site integrator software for a total site integration and design of the utility system. Wolff *et al.* (1998) developed a site modelling procedure called SitEModelling™ to be used by companies to conduct energy optimization studies of all essential plants and whole sites using pinch technology, process simulation, process synthesis and to determine projects economic benefits.

Despite the availability of process integration tools enabling the targeting of utility systems to achieve the site-wide minimum energy requirements, there are additional barriers when heat integration is extended to a total site which some are indicated in Table 5.1.

Table 5.1: Advantages and disadvantages of Total Site Heat Integration.

	Total Site Heat Integration	Reference
Advantages	▪ Great benefit to share the large investment for the utility system between more individual processes integrated in the overall site; ▪ Offers exchanging utilities and enabling Heat Integration between separate processes, via intermediate energy carriers. ▪ Common utility system allows processes to exchange utilities: the high-temperature cooling demand of a process may be used for utility (e.g. steam) generation instead of serving the demand with utility cooling; ▪ Lower temperature cooling demands in other processes can sometimes be served by the process-generated utility instead of applying boiler steam, utility hot oil or furnace flue gas.	Klemeš *et al.* (2014)
Disadvantages	▪ Plant interdependence; ▪ Variations in the heating and cooling demand as well as unexpected or planned process unit shutdowns can affect the surrounding processes when these are integrated; ▪ Layout influences piping costs which is proportional to the distance between the plants. Heat exchanger location has important implications on the cost. ▪ The type of fluid influence stream matching and selection of suitable utilities in order to maintain an effective heat transfer coefficient; ▪ Issues that may limit or forbid certain stream matches increase cold and hot utilities above the minimum requirements; ▪ The limits on environment emission affect the technology and equipment selection which influences cost.	Chew *et al.* (2013b) Bungener *et al.* (2015)

A complete review of the challenges and potentials of modelling tools for TSHI and utility system optimization and of further research developments and software packages to face the new challenges imposed by the need to account for the process sustainability can be found in Varbanov *et al.* (2017a) and Varbanov *et al.* (2017b). Total Site to integrate industrial complexes of different companies has also been attempted. Retrofit of an entire cluster consisting of several processing plants is a complex task, which requires large investments and a great deal of collaboration between different companies. For future improvements, the potential to significantly increase energy efficicency is through energy collaboration between different chemical clusters (Eriksson *et al.*, 2015; Hackl *et al.*, 2011; Hackl and Harvey, 2015). Some literature examples applied to site wide industrial plants and utility and cogeneration systems are presented next.

5.1.1. Site Wide Heat Recovery using Total Site Analysis

Dhole and Linnhoff (1992) introduced total site concept to a cogeneration process within a utility system to target for fuel, co-generation, emissions and cooling ahead of design. Energy targets are set using temperature-enthalpy site profiles derived from individual processes GCC known as total site profile or site source-sink profiles (SSSP). The monotonic parts of GCC called pockets indicate the level of intra-process heat recovery within a process which may be removed when deriving SSSP to account inter-process heat recovery. Site-wide targets are based on a given number of steam levels and pressures followed by an analysis of various site related proposals prior to design with reference to site expansion, process and utilities modifications.

Klemes *et al.* (1997) following the work of Dhole and Linnhoff (1992) expanded pinch analysis application of single processes to site-wide application through the development of a valuable and viable industrial procedure for targeting and planning energy costs and emissions reduction at factory site level. The methodology was applied to one acrylic polymer manufacturing plant, three refineries and one tissue paper mill. With the new procedure, it was possible to set targets for improvement and expansion opportunities in individual process units, as well as in an overall production sites, improving sites infrastructure too. The application of total site analysis to large industrial complexes produced 30 % energy savings and 10 % capital costs, overall. Matsuda *et al.* (2009) developed a long-term energy saving plan resulting from the application of R-curve analysis and Site Source-Sink Profiles (SSSP) analysis to an heavy chemical industrial complex (31 processes such as petrochemical, refinery, power company, etc.) of Kashima in Japan with the aim to reduce energy consumption. Although the complex was already working with high efficiency, it was found room for energy savings through sharing energy among the various process industries by implementing the central gas turbine combined utility centre, and the proposed modifications to the steam headers. Later, Matsuda *et al.* (2012) used total site profiles to target energy savings of a large scale steel plant reducing an amount of 21 MW of cooling demands. Also, there was evaluated the possbility of implementing a combined system of two power generation systems (6.2 MW and 12.3 MW) and a heat utilization system for the removal of CO_2.

So far, to set total site targets, traditional total site approach assumed that the whole site operates with the same minimum allowed temperature difference. The assumption of a single global ΔT_{MIN} for all the processes may lead to an inaccurate estimation of the overall total site heat recovery targets. Fodor *et al.* (2010) extended traditional total site analysis by introducing individual ΔT_{MIN} for the different processes to provide a more realistic evaluation of the capital-energy trade-offs since the complete intra and inter-process heat recovery potential would be revealed. The extended approach revealed high potential for improvement achieving 37 % of LP steam recovery and reducing by 14 % that HP steam demand and 39 % cooling demand. Later, Fodor *et al.* (2012) presented a further improvement by considering a ΔT_{MIN} for each individual process dealing with stream specific ΔT_{MIN} inside each process by setting different ΔT contribution (ΔT_{cont}) and also using different ΔT_{cont} between the process streams and the utility systems, which allows for more explicit estimation of the energy and heat exchanger area targets. Nemet *et al.* (2012) evaluated the capital cost for the generation and use of site utilities (e.g. steam, hot water, cooling water), which enables the evaluation of the trade-off between heat recovery and capital cost targets for total sites, thus allowing to set optimal ΔT_{min} values for the various processes.

Nemet *et al.* (2012) implemented plus/minus principle to deal with the addition of new processes or units in the already existing total site and also achieving maximum heat recovery. The inclusion of new units and processes were done and evaluated at two levels. One way is to consider adding an operating unit to the current utility system and the total site profiles remain the same. Other way is to change total site including more processes and total site profiles change. The level of these changes in the site are evaluated using Plus/Minus principle to allow the most beneficial integration of new units. Chew *et al.* (2013a) and Chew *et al.* (2015b) also showed the advantages of Plus/Minus Principle to target process modifications at the selected sections to improve total site heat recovery. Liew *et al.* (2014b) developed a total site retrofit framework involving a petrochemical plant as case study to achieve significant energy savings when considering direct and indirect heat recovery retrofit options. Plus/Minus principle was further applied to evaluate the correct locations of heat surpluses and deficits and lead to appropriate total site retrofit solutions.

Boldyryev *et al.* (2013) upgraded total site methodology by selecting the optimal temperature levels for intermediate utilities to acccount the trade-off between capital and heat recovery. Total Site Source-Sink Porfiles are used to target minimum heat transfer area by proposing different intermediate utilities for each enthalpy interval defined between Site Source Profile and Site Sink Profile. Total minimum heat transfer area for the presented case study on Total Site was reduced by 32 % in comparission with the traditional methodology showing potential in reducting capital cost for heat exchangers network design on Total Site level. Boldyryev *et al.* (2014) presented further improvement to decrease even more capital costs for Total Site heat recovery by using different utility levels. Selecting appropriate temperate of intermediate utilities implies a reduction in heat transfer area up to 49 %.

Chew *et al.* (2015a) evaluated the incorporation of the principles keep hot stream hot (KHSH) and keep cold stream cold (KCSC) to evaluate the changes of total site profiles in order to maximize temperature driving forces and the hot stream supply and/or target temperatures, and to minimize the cold stream supply and/or cold supply and target temperatures. These principles on single processes showed that it is possible to reduce energy targets and/or capital costs by increasing the temperature driving forces. More detailed can be found in Kemp (2007) and Klemeš *et al.* (2011).

Song *et al.* (2017) introduced a new graphical tool to overcome some drawbacks of the implementation of GCC, which may generate intricate HENs, and of waste heat source/sink in the existing heat exchanger network (HENs), which may miss some possible heat recovery potential. This new procedure involves the application of Interplant Shifted Grand Composite Curve (ISCC) to determine the maximum feasible heat recovery potential via indirect interplant heat integration and the minimum flowrate of a single-circuit intermediate medium used. With the case study presented, the new tool graph showed potential to increase 43 % of energy savings and much easier and simpler to be applied than the other two methods.

Tarighaleslami *et al.* (2017) used an improved target algorithm to unify TSHI that estimates improved TSHI targets for sites that require utilities. There is a difference between this new procedure and the traditional procedure. While the new procedure sums process level utility targets to form the basis of total site utility targets, the conventional method uses total site profiles based on the excess process heat deficits/surpluses to set total site targets. The improved total site target algorithm and the traditional methodology was applied in three industrial case studies, representing a wide variety of processing industries, and showing that higher energy savings can be achieved with the new procedure.

5.1.2. Total Site Analysis of Utility Systems, Cogeneration Systems and Power Planning

Total Site concept was firstly applied by Dhole and Linnhoff (1992) to a cogeneration process within a utility system. The concept was further extended to improve utility systems and power planning and later, to renewable energy systems. The central utility system consumes fuel, generates power and supplies heat, power and steam at different pressures through several steam mains, providing the energy required to run the different individual processes. Total Site Targeting methodology is applied using different tools to synthesise the entire total site system, which includes process utility and heat exchanger network design integrated with site utility system.

Dhole and Linnhoff (1992) applied total site concept together with an exergy analysis making use of Carnot Factor to produce targets to aim fuel savings, identifying the trade-off between fuel and power generation and optimising utility level temperatures for minimum total cost. The results showed more benefits in modifying than expanding the process by including a new turbine to compensate MP steam production. The disadvantage of this procedure, although it establishes a link between the heat exchanger network and utility system by using exergy analysis, it lacks in establishing the proper energy-capital trade-off, special for heat exchanger networks.

Later, Hui and Ahmad (1994) made further improvements to optimize energy and capital cost for heat recovery among processes through process exergy analysis. The optimization of the utility levels is achieved by reducing the exergy loss of the heat exchanger networks, using exergy grand composite curves (EGCC), which will directly benefit the power generation in the utility system. Exergy losses is reduced by changing utility loads and levels which also reduces the total exergetic cost of utilities. The cost of utilities directly affects the design of process systems considered for total site analysis. The developed methodology allowed to take into account the effect on the utility system when an energy-capital trade-off in a heat exchanger network is determined. Processes exergy analysis for steam costing allows to use the resulting steam as an interface between the utility plant and the processes. With this cost interface, the subsequent design of the utility system and heat exchanger network of the different processes can be treated as two separated tasks.

A shaftwork targeting methodology based on thermodynamic insights on cogeneration was developed by Sorin and Hammache (2005) with the aim to overcome the drawbacks of the methodology developed by Rassi (1994). The methodology applies a Site Utility Grand Composite Curve (SUGCC) which are obtained from the source and sink site composite curves. This graphical tool allows to express the indirect heat recovery through steam mains. It is a thermal profile that represents each steam main by its saturation temperature and steam generation and usage loads. Shaftwork production is targeted using SUGCC by analysing the defined areas obtained of heat loads and temperatures and to multiply the areas by a proportionality constant conversion factor obtained through a steam turbine simulation. However, the methodology showed some drawbacks. The power is not linear to the saturation temperature differences between inlet and outlet pressures, and the very high pressure steam and cooling targets cannot be accurately visualized on the SUGCC. The modified Site Utility Grand Composite Curve (SUGCC) of Sorin and Hammache (2005) allow to determine potential for cogeneration, fuel and cooling requirement. The modified SUGCC allows to visualize VHP consumption, thus fuel consumption, shaftwork production and cooling targets. With modified SUGCC it is possible to target shaftwork production as in this procedure the power is a non-linear function of the input and output of temperatures but rather a linear function of the difference in Carnot factors between the heat source and heat sink for the given inlet temperature of the heat source. This way, the drawbacks of the methodology proposed by Rassi (1994) were overcome. As for examples of industrial implementation, Manesh *et al.* (2013) and Pirmohamadi *et al.* (2019) applied SUGGC to evaluate the potential of cogeneration system efficiency within site utility system of a total site refinery plants.

Bandyopadhyay *et al.* (2010) developed a similar procedure proposed by Dhole and Linnhoff (1992) in which a site grand composite curve is generated to incorporate the assisted heat transfer of a total site and to estimate cogeneration potential of an overall site. The term SGCC should not be confused with the site utility grand composite curve (SUGCC). Site utility grand composite curve (SUGCC) is essentially the GCC of the site level utility interactions. Site grand composite curve (SGCC) is the GCC at the site level prior to the consideration of the utility levels. It is essentially the grand composite curve of the site source and sink profiles after incorporating assisted heat transfer (the pockets of GCC are taken into account). Assisted heat transfer is considered to achieve maximum indirect heat integration between processes in which heat transfer outside the region between process pinch points of individual grand composite curves plays an important role to estimate the cogeneration potential. Assisted heat transfer taking into account pockets of grand composite curves was also considered. The segments of GCC were shifted and the regions intersecting regions of different segments are to be eliminated as these regions do not have sufficient drive force for inter-process heat integration. This way, additional energy saving opportunities are found across processes. With SGCC, site level energy targets, including multiple level utility targeting, can be estimated.

Gorsek *et al.* (2006) presented a pratical industrial application composed of two processes, a cogeneration system and two main steam distribution levels with the illustration of the combination of computer simulation, energy integration and cost estimation to perform an effective process analysis. Supertarget computer programming was used to calculate heat cascades and energy targets. A process-level pinch analysis and a total site integration considering cogeneration within utility systems is performed. To evaluate the individual processes, an Extended Grand Composite Curve (EGCC) is used which is composed of a GCC that is extended with utility composite curves (UCCs). While the GCC represents indirect heat exchange (energy flows from hot utilities through the heat exchanger network to cold utilities), UCCs graphically reproduce direct heat exchange between energy sources and energy sinks. With this interpretation, energy availability analysis of the whole process is possible. A modified Site Source-Sink Profile was then used to give detailed insight into the site utility system configuration, heating and cooling demands and cogeneration design, thus enabling a design of an ideal interface between the site processes and the site utility system. Modified SSSP were used to compare the heat delivered by the exhaust steam from a turbine against the heating requirements of the process to be integrated. Profile matching was used to explore the relationship between the heat flow available in a steam turbine exhaust and the process heat flow acceptance requirements. Such analysis estimated realistic targets for central site combustion, total electric power and emissions.

Another tool developed for cogeneration system heat integration is R-curve that provides guidelines for cogeneration efficiency for a given site power-to-ratio demand of a utility system. Ghaebi *et al.* (2012) applied R-curve tool to a large industrial CHP site, which generate heat and power simultaneously. Targets of total site cooling demand were also set based on total annual cost of total trigeneration (combined cooling, heating and power). The research shown a possibility to use extra LP steam of a total site to supply heating demand of an absorption chiller system. It was suggested to integrate it within the utility system of the total cogeneration site to decrease or eliminate LP steam waste. Karimkashi and Amidpour (2012) extended R-curve concept by introducing two new curves to analyse total site of an industrial system. This graphical tool deals only with simple utility systems, and doesn't takes into account multiple steam distribution levels and complex steam turbine configuration. Also, it assumes constant isentropic efficiencies for steam turbines, which leads to non-realistic results. To overcome these drawbacks, "R-ratio vs. Total Annual Cost (TAC) curve" and "R-ratio vs. Emissions (EM) curve" were included to determine total annual cost of total site utility system to demonstrate the emissions impact.

Ren *et al.* (2018) developed a software to estimate the potential of cogeneration of a total site utility system of a refinery plant. The simulator is used to calculate the temperatures of steam mains, steam flowrates and shaft power rates. Shaft power generation by steam turbines in expansion zones were also simulated. This approach was compared to other procedures in the literature and some advantages were found as the new method needs neither establishing iterative calculation, nor programming procedure, and it requires fewer parameters. In addition, the calculation of the steam turbine capital cost and environmental footprints are considered in the targeting procedure to provide decision makers with a more complete picture of the designed sites. This should allow them to efficiently screen and compare the major design options on the basis of both economic and environmental performance.

Another methodology developed for TSHI considering utility systems was Top- Level Analysis which evaluates heat and power needs of a site using existing utility consumption of plants rather than energy targets. Top-level Analysis is another procedure to obtain total site profiles. As explained before, total site profiles can be derived based on GCC of individual processes considered in the whole site. Although it is a valid procedure, it assumes that all potential heat recovery projects can be implemented, which is not necessarily true, especially for combined heat and power systems. Thus, Top-Level Analysis shows more advantages, especially in retrofit situations, as it considers utility requirements for the individual processes which will be higher and more realistic. Also, data can be extracted more easily and accepts heat integration arrangements that are already in place in the individual processes (Kemp, 2007). Makwana *et al.* (1998) applied top-level analysis to an industrial complex that expedites the energy retrofit and operations management. The two-step procedure translates its performance and establishes the potential of improvement and economic directions in terms of specific energy saving target. The economic directions help to identify promising heat exchanger networks modifications with minimum capital cost. Site efficiency and its limits are identified by creating a power generation efficiency curve.

On the opposite, Bungener *et al.* (2015) carried out a multi-period total site analysis on a petrochemical site of Stenunngsund, Sweeden. Total Site Profiles (TSP) and Total Site Composites (TSC) were constructed to target site-wide heat integration opportunities for the utility system. Possible modifications on system were identified to maximize heat recovery. A new graphical approach based on TSP and TSC was developed to design new utility systems using an intermediate fluid. The work showed benefits in replacing the entire hot utility consumption by a recovered process heat using an improved utility system. A multi-period total site sensitivity analysis was also performed to identify the impact of units' shutdowns on the improved utility system. However, shutdowns of some units would challenge the feasibility of the proposed site integration.

Liew *et al.* (2012) presented four main contributions for Total Site Heat Integration through the extension of Problem Table Algorithm (PTA) to total site analysis, through the introduction of Total Site Sensitivity Table (TSST) to analyse a site's overall sensitivity to plant maintenance, and to explore the effects of plant shutdown or production changes on heat distribution and utility generation systems over a Total Site. Multiple utility levels can be determined in both the PTA and TS-PTA, and the Total Site Utility Distribution (TSUD) table to design Total Site utility distribution network. The application of TSST allows to identify possible measures that can be taken into account during the design and operational stages to ensure other site utility supplies are not disrupted. Liew *et al.* (2013) improved TSST to be used as a systematic tool to characterise the effects of a plant maintenance shutdown, to determine the operational changes needed for the utility production and to plan mitigation actions. This tool can be used to determine the optimum size of a utility generation system, to design the backup generators and piping needed in the system and to assess the external utilities that might need to be bought and stored. Liew *et al.* (2014a) developed a numerical heat cascade algorithm for heat integration across total site processes considering different layout problems to achieve minimum multiple utility targets. The algorithm also evaluates the effects of pressure drops and heat losses in different locations of utility system. This enhanced methodology improves the accuracy of the existing total site targeting methodology by considering the effects of plant layout in a total site system.

5.2 Methodology

A site wide energy performance analysis is carried out to evaluate inter-process heat recovery which means the maximum heat recovery that is possible to be achieved when considering Pre-Distillation and Arosolvan Units as a whole site. For this purpose, two procedures are here considered: direct heat integration and indirect heat integration. Both procedures have Pinch Analysis as its background. A schematic representation of a site wide energy performance analysis procedure is shown in Figure 5.2.

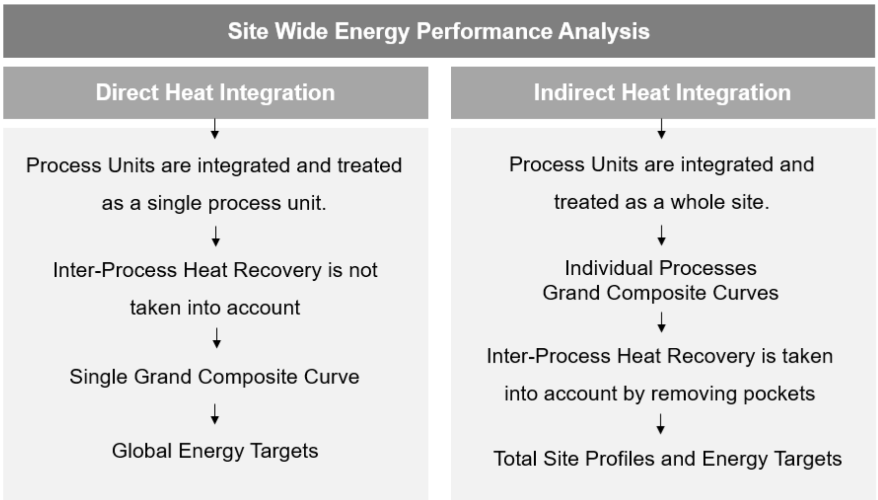


Figure 5.2: Strategy used for Total Site Improvement.

Direct heat integration considers that both process units operate as a single unit and a single grand composite curve is built comprising both process units to evaluate energy targets. For an indirect heat integration analysis, a total site analysis is performed to estimate the maximum heat recovery that is possible to be achieved using intermediate fluids provided by the central utility system. Follows next a more detailed description of both procedures.

- **Direct Heat Integration using a Single Grand Composite Curve**

In direct heat integration, Pre-Distillation and Arosolvan Units are integrated and treated as a single unit to estimate the maximum energy savings with the maximum possible heat transfer between process streams across the two process units. Processes with different pinch locations offer potential for energy recovery through site level integration. For this purpose, a single grand composite curve is constructed using Aspen Energy Analyzer considering two ΔT_{MIN} values: 10 ºC and 15 ºC. Global energy targets are obtained through the single grand composite curves and compared to the total energy targets achieved through intra-process heat integration (energy targets obtained for individual process units). In addition, global energy targets are compared to the total actual utilities consumptions that are being consumed by both process units to estimate the amount of heat recovery that it is possible to be achieved. Therefore, an accurate comparison between inter and intra-process heat recovery is carried out to evaluate which of the two options is the most advantageous for further energy optimization studies.

- **Indirect Heat Integration using Total Site Analysis**

Total Site Analysis follows an analogous procedure of Pinch Analysis, starting with the selection of the data to be extracted and considered in total site heat integration and improvement. Energy targets are then set for the minimum practical energy needs to run each process unit, and an evaluation in terms of inter and intra-process heat recovery is performed to analyse which of the two options is the most advantageous for further energy optimization studies.

Step 1: Minimum Temperature Difference (ΔT_{min}) Parameter Specification

The specification of a ΔT_{MIN} for heat exchange between the process streams of each individual process unit to be considered in the analysis is required. For this study, two different ΔT_{MIN} values (10 ºC and 15 ºC) are considered to evaluate energy targets.

Step 2: Process-Level Pinch Analysis

For an adequate total site evaluation, data extraction is performed using individual processes grand composite curves which are obtained using Aspen Energy Analyzer and considering the specified ΔT_{MIN} value. In this case, the same ΔT_{MIN} was considered for both process units. These curves are an enthalpy-temperature diagram which gives pinch point location, the overall minimum heating and cooling demands (energy targets) of each individual process unit and it lays open the interface between process and utilities for the given process unit. As the number of processes units to be integrated is small, and only two, the data extraction from GCC can be used to identify the potential of heat recovery.

The procedure for targeting intra-process heat recovery considers several energy integration aspects: i) heat recovery among the streams inside the process; ii) the profile above pinch point location represent a net heat sink, whereas the profile below the process pinch represents a net heat source; iii) minimum external hot and cold utilities consumption; iv) targets for multiple utility levels.

Step 3: Data Extraction of the heat sources and heat sinks

Total Site Profiles (TSP) or Site source-sink profiles (SSSP) are built using data extracted from GCC of each process unit. There are two options to obtain total site profiles: a) take all heat sources and sinks from the processes, regardless of the opportunities for intra-process heat recovery; or b) take only the net heat sources and net heat sinks from the individual processes, accounting for intra-process heat recovery. The choice here is rather the intra-process heat recovery (or the pockets in grand composite curves) is taken into consideration and not extracted as data for total site analysis. If pockets are to be extracted from the process, then the heat source of the pocket (a hot stream segment) will need to be able to generate a hot utility (usually steam) and the cold sink will have to be heated by an external hot utility (again steam) provided by central utility system. Here, option b) is used. Parts of the grand composite curve are left out of the analysis. The monotonic parts, or the also called "pockets" of the curve, are isolated by sealing off with vertical lines. Thus, the remaining parts left are the net heat source and sink elements to be satisfied by the central utility system.

Step 4: Shift the extracted segments to the temperature scale

Source and sink elements of the resulting grand composite curve after step 3 are shifted in its temperatures. Source element temperatures are reduced by ½ ΔT_{MIN} and sink element temperatures are increased by ½ ΔT_{MIN}. This step is analogous to process-level pinch analysis to obtain the grand composite curves. Site composite curves are double shifted to give a total ΔT shift of ΔT_{MIN}. If different values of ΔT_{MIN} apply to different processes, then each set of process data is given its individual shift in ΔT_{MIN} before the streams are combined in the construction of the site composite curves. This shifting in temperatures reverts the temperature scale back from shifted to real temperatures, as to obtain grand composite curves, real temperatures are shifted using the inverse process. This way, it occurs a feasible heat exchange at the selected value of the minimum approach temperature in the heat exchangers into the curve.

Step 5: Creating Total Site Profiles

The construction of total sites from the modified grand composite curves simply involves the generation of "composite curves" from the shifted source and sink elements. From grand composite curve of each process, the residual heat sources and heat sinks are identified, moving from the single process level to a total site analysis. The site heat source profile is then constructed by combining the heat source data from Pre-Distillation and Arosolvan Units into a single profile, which is analogous to the hot composite curve for a single process. The site heat sink profile is formed by combining the heat sink data from both process units, being analogous to that of cold composite curves. The composite curve for net heat source elements are called "Site Source Profile" and the composite curve for net heat sink elements are called "Site Sink Profiles". Total site profiles are in real temperatures. These are used together to set targets for total site improvements, giving a perspective of surplus heat and heat deficit for all the processes on the site.

The maximum limit of the heat recovery is reached when the two site profiles touch and cannot be shifted further (limit factor for further integration). Total Site Pinch point divides the problem into net heat sink and net heat source. The remaining site sink profile heat demand is met by the supply of steam from a central boiler. Excess heat is removed by cooling water or produces very low pressure steam.

Step 6: Potential of Energy Savings Evaluation

The energy targets obtained through inter-process heat integration and energy targets obtained through total site analysis are compared to each other and to the total actual utilities consumption comprising both process units. This comparison will allow the designer to decide which of the two options between inter and intra-process heat recovery is more advantageous for the aromatics plant for further specific network retrofit designs.

5.4. Results and Discussion

For the aromatics plant in study, a site-wide energy performance analysis is carried out to evaluate the potential of heat recovery when considering direct and indirect heat integration between Pre-Distillation and Arosolvan Units.

Direct heat integration was evaluated by considering both process units as a whole which means it is considered that they operate as a single unit. In this way, a single grand composite curve was constructed to evaluate the heat recovery opportunities through the direct use of the process streams of both units. The GCC comprising both process units is presented in Figure 5.3 for a ΔT_{MIN} of 10 ºC.

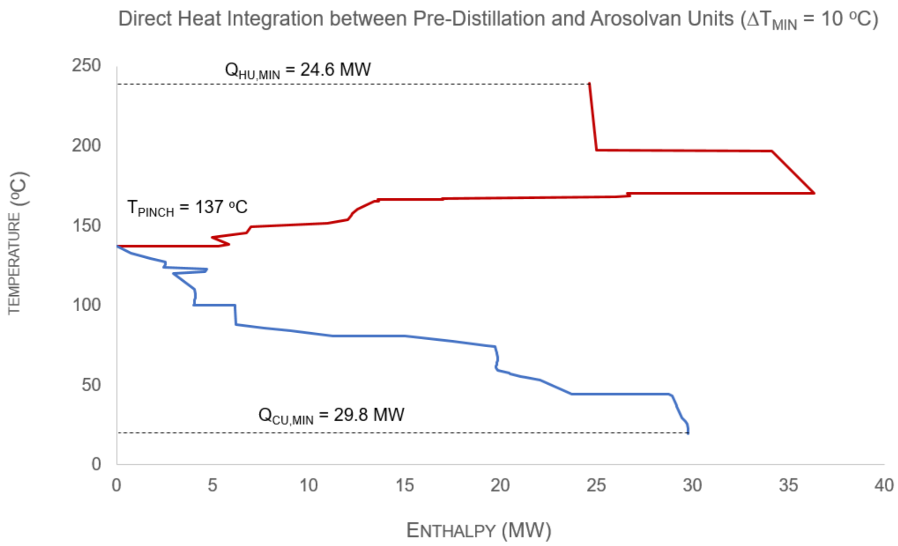


Figure 5.3: Direct heat integration between Pre-Distillation Unit and Arosolvan Unit considering a ΔT_{MIN} of 10 ºC.

When direct heat integration is considered, the resultant total minimum utilities consumption of the integration between the two process units must be equal or lower than the sum of the total minimum utilities consumption obtained for each individual process units determined by its individual composite curves (Figure 4.10). If the total minimum utilities consumption resulting from the integration between the two units is lower than the total energy targets obtained for each process unit, than a higher heat recovery is possible when considering direct heat integration. The overall energy targets considering intra and inter-process heat recovery is presented in Table 5.2 for a ΔT_{MIN} of 10 ºC.

Table 5.2: Comparison between results obtained with intra-process heat recovery and inter-process heat recovery through direct heat integration of both process units for a ΔT_{MIN} of 10 ºC.

Energy Targets	**Intra-Process Heat Recovery**		**Inter-Process Heat Recovery**
	Pre-Distillation Unit	Arosolvan Unit	
Hot Utility (MW)	1.5	24.1	24.6
Cold Utility (MW)	13.6	17.2	29.8
Total Consumption (MW)	15.1	41.3	54.4

In previous chapter, it was determined the total actual utilities being consumed within each process unit. In Pre-Distillation Unit, it is being consumed a total of 23 MW of utilities, while in Arosolvan Unit, a total of 45 MW. In overall, it is being consumed a total of 68 MW in utilities to satisfy both process units.

For a ΔT_{MIN} of 10 ºC, the resultant total energy targets through intra-process heat recovery are 15.1 MW for Pre-Distillation Unit and 41.3 MW for Arosolvan Unit, giving a total minimum energy consumption of 56.4 MW. When both process units are integrated as a single unit, the resultant total energy targets through inter-process heat recovery considering direct heat integration is 54.4 MW, indicating that it is possible to recover 2 MW more through the maximization of heat exchange between process streams of both units. Comparing these results to the total actual utilities being consumed in both process units (68 MW), it is verified that there is higher heat recovery opportunities when considering direct inter-process heat recovery (13.6 MW) than with intra-process heat recovery (11.6 MW).

This evaluation was also performed considering a ΔT_{MIN} of 15 ºC, as it was previously verified that there is still heat recovery opportunities for higher ΔT_{MIN} than 10 ºC in both process units. The GCC integrating both process units is presented in Figure 5.4. The overall energy targets considering intra and inter-process heat recovery is presented in Table 5.3.

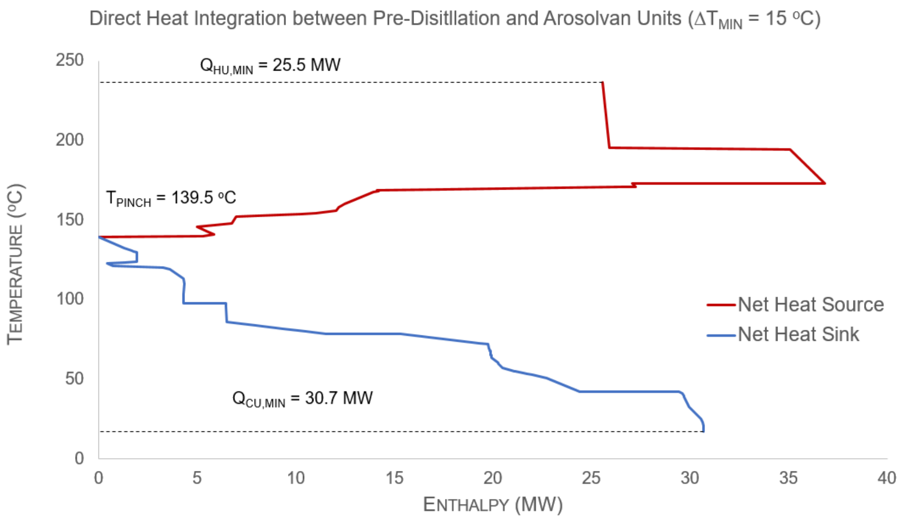


Figure 5.4: Direct heat integration between Pre-Distillation Unit and Arosolvan Unit considering a ΔT_{MIN} of 15 ºC.

Table 5.3: Comparison between results obtained with intra-process heat recovery and inter-process heat recovery through direct heat integration of both process units for a ΔT_{MIN} of 15 ºC.

Energy Targets	**Intra-Process Heat Recovery**		**Inter-Process Direct Heat Recovery**
	Pre-Distillation Unit	Arosolvan Unit	
Hot Utility (MW)	1.94	25.6	25.5
Cold Utility (MW)	14.0	18.6	30.7
Total Consumption (MW)	16.0	44.2	56.2

For a ΔT_{MIN} of 15 ºC, the resultant total energy targets through intra-process heat recovery are 16.0 MW for Pre-Distillation Unit and 44.2 MW for Arosolvan Unit, approximately, giving a total minimum energy consumption of 60.2 MW. As a single unit, the resultant total energy targets through inter-process heat recovery considering direct heat integration is 56.2 MW, indicating that it is possible to recover 4 MW more of energy consumption, approximately. Comparing these results to the total actual utilities being consumed in both process units (68 MW), it is verified that there is higher heat recovery opportunities when considering direct inter-process heat recovery (11.8 MW) than with intra-process heat recovery (7.8 MW).

From the results presented for the two attributed values of ΔT_{MIN}, it is verified that for lower ΔT_{MIN} value leads to a higher energy targets when considering both intra and inter-process heat recovery. However, higher opportunities of heat recovery are found when considering inter-process heat recovery than when considering intra-process heat recovery for both ΔT_{MIN} values. Moreover, higher heat recovery opportunities are found for a ΔT_{MIN} of 10 ºC than for a ΔT_{MIN} of 15 ºC when considering direct inter-process heat recovery. This occurs because intra-process heat integration is not taken into account when direct heat integration is being analysed and therefore, the opportunities found through inter-process heat recovery are higher as there are more process streams available from one process unit to exchange heat with process streams of the other process unit.

However, when inter-process heat recovery is being considered there is the disadvantage of having the need to overcome the drawbacks of the battery limits of each process unit and the distance between the process streams involved to achieve maximum energy recovery. Therefore, more equipment and piping is required to overcome this problem which increases total cost and thus, the energy savings obtained for both cases scenarios do not justify further HENs modifications studies.

Indirect heat integration using an intermediate fluid to exchange heat between Pre-Distillation and Arosolvan Units was also carried out to find inter-process heat recovery opportunities. Total Site Analysis was used for this purpose to identify heat recovery opportunities through intermediate utilities. Thus, Total Site Profiles were built using data extracted from GCC of each individual process unit. For a ΔT_{MIN} of 10 ºC, individual process grand composite curves were obtained using Aspen Energy Analyzer which are shown in Figures 5.5 and 5.6.

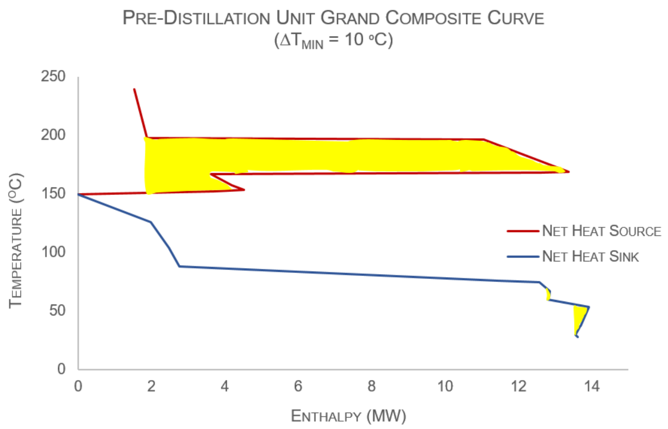


Figure 5.5: Pre-Distillation unit grand composite curve for a ΔT_{MIN} of 10 ºC.

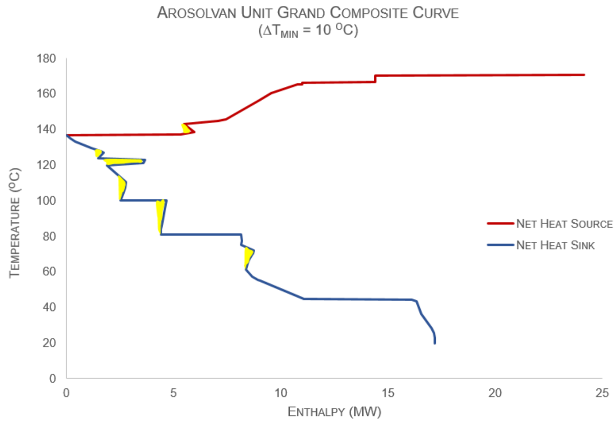


Figure 5.6: Arosolvan unit grand composite curve for a ΔT_{MIN} of 10 ºC.

Intra-process heat recovery was also analysed to evaluate heat recovery opportunities within the process unit by identifying the existing pockets in each GCC. In GCC of Pre-Distillation unit (Figure 5.5), with pinch point located at shifted temperature of 149.6 ºC, one pocket was identified in net heat source above pinch point and two pockets in net heat sink below pinch point. In GCC of Arosolvan unit (Figure 5.6), with pinch point located at shifted temperature of 137 ºC, it was identified one pocket in net heat source above pinch point and five pockets in net heat sink below pinch point.

In each process GCC, the pockets were identified and removed using linear interpolation. The remained segments of each net heat source and net heat sink were extracted to build site source profile and site sink profile. Plotting site source-sink profiles together, it results in a total site profile presented in Figure 5.7.

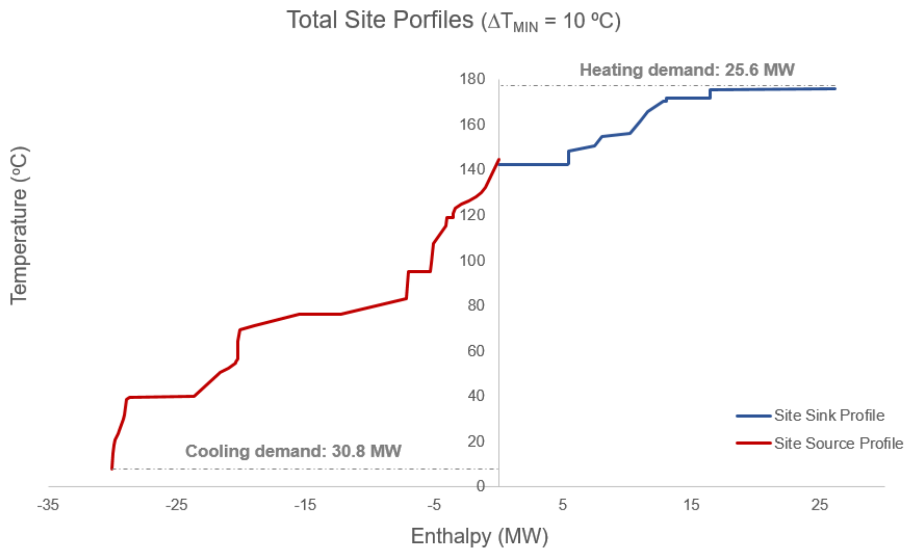


Figure 5.7: Total Site Profiles integrating U100 and U200 considering a ΔT_{MIN} of 10 ºC.

From total site profiles in Figure 5.7, it is shown a total amount of heating demand equal to 30 MW and a cooling demand of 26 MW, approximately. It is also verified that for a ΔT_{MIN} of 10 ºC there is no heat recovery opportunities considering the integration between both process units, as no heat transfer stage was created between heat sources and heat sinks. As in the profiles, the points are coincident which means that there is no temperature interval to establish a heat transfer stage. Thus, no heat can be transferred from heat sources to heat sinks through a generated utility or through an intermediate utility.

Total site profiles were also obtained considering a ΔT_{MIN} of 15 ºC to evaluate possible inter-process heat recovery opportunities. Individual Grand Composite Curves are presented in Figures 5.8 and 5.9.

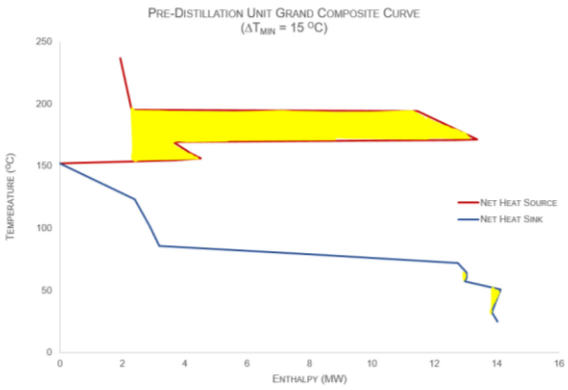


Figure 5.8: Pre-Distillation unit grand composite curve built for a ΔT_{MIN} of 15 ºC.

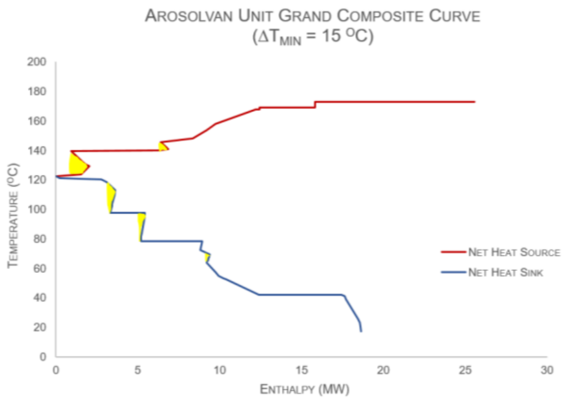


Figure 5.9: Arosolvan unit grand composite curve built for a ΔT_{MIN} of 15 ºC.

In GCC of Pre-Distillation unit (Figure 5.8), with pinch point located at shifted temperature of 152 ºC, the number of pockets that represent heat recovery opportunities within the process unit are the same above and below the pinch point as the ones found for ΔT_{MIN} of 10 ºC. In GCC of Arosolvan unit (Figure 5.9), with pinch point located at shifted temperature of 122 ºC, two pockets were now found in net heat source above the pinch and three pockets were found in net heat sink below pinch point. In both process units, heating and cooling demand increased with ΔT_{MIN}, which means that, besides decreasing the potential of energy savings as discussed before, heat recovery opportunities within the process are less than the ones gained with a ΔT_{MIN} of 10 ºC.

After excluding the segments that give shape to the pockets, the remained segments of each net heat source and net heat sink was extracted to build site source profile and site sink profile. Plotting site source-sink profiles together, it results in a total site profile presented in Figure 5.10.

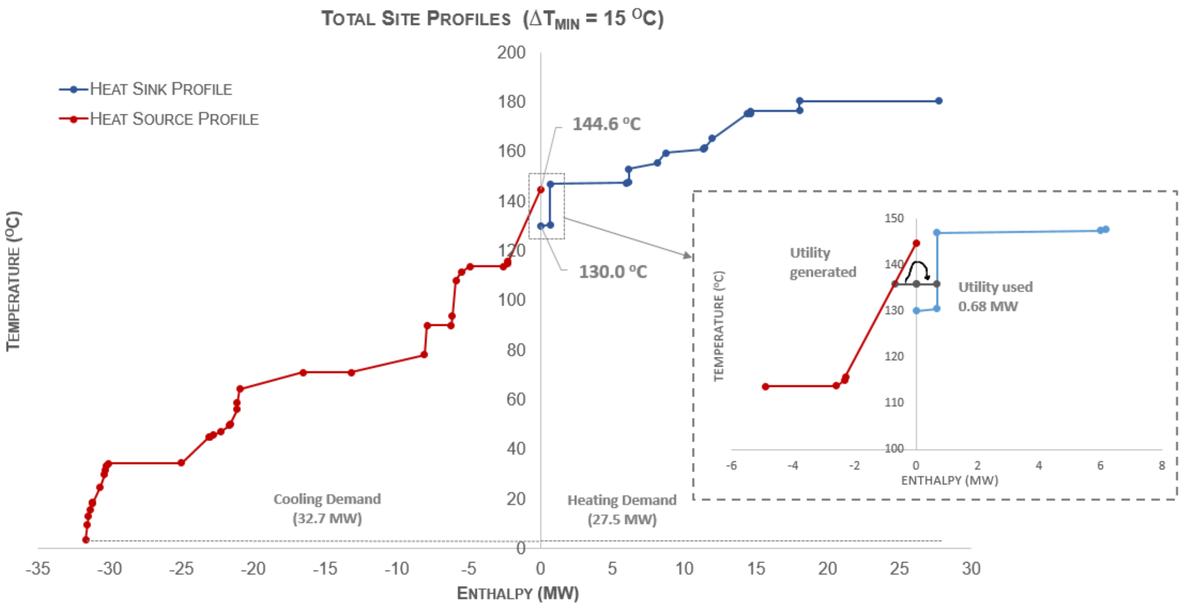


Figure 5.10: Total Site Profiles integrating U100 and U200 considering a ΔT_{MIN} of 15 ºC.

From total site profiles for ΔT_{MIN} of 15 ºC in Figure 5.10, it verifies that it was created a small heat transfer stage between 130 and 144.6 ºC where heat sources can transfer heat to heat sinks through a generated utility or an intermediate utility from the central utility system. The heat that can be transferred corresponds to a small value of 680 kW. Yet, the amount of heat available is unworthy in relation to the capital cost of the generating equipment.

Moreover, the segment of heat sinks integrating the heat transfer stage is vertical which means that there is a reboiler that can be heated through the intermediate utility by changing operating conditions. However, changes in operating conditions are not a hypothesis in this study. Nevertheless, an evaluation of utilities site composite curves would be required to determine which utility from the central utility system has the operating temperature between the heat transfer stage temperature intervals to perform such task.

5.5. Conclusions

An evaluation of heat recovery opportunities was performed considering direct and indirect heat integration between Pre-Distillation and Arosolvan Units of Matosinhos Refinery's Aromatics Plant.

Direct heat integration was first analysed by considering both process units as one single unit to evaluate the potential of energy savings. The analysis involved the construction of a single grand composite curve comprising both process units using Aspen Energy Analyzer to identify opportunities of energy savings without taking into account intra-process heat recovery. The analysis was performed considering ΔT_{MIN} of 10 ºC and 15 ºC obtaining better results in terms of energy savings for lower ΔT_{MIN} when considering direct inter-process heat recovery due to the fact that intra-process heat recovery is not taken into account. This means that the higher ΔT_{MIN} value, the lower are the opportunities in heat recovery. Therefore, for a ΔT_{MIN} of 10 ºC, a total minimum utilities consumption of 56.4 MW was obtained considering intra-process heat recovery, while a total minimum utilities consumption of 54.4 MW was achieved with inter-process heat recovery, approximately. Comparing these results to the ones obtained for the total actual utilities consumption (68 MW), higher energy savings are obtained considering inter-process heat recovery (13.6 MW) than with intra-process heat recovery (11.6 MW).

Indirect heat integration using intermediate fluids was also performed. The analysis involved the evaluation of heat recovery opportunities after intra-process heat recovery takes place (pockets of grand composite curves are excluded from the analysis) and with the point of view of process heat sources and heat sinks that can be met by heat recovery through a generated intermediate utility, thereby minimising the amount of steam that has to be supplied by central utility system.

After maximizing heat recovery within individual process units, total site profiles comprising heating demands required (Site Source Profile) and cooling demands needed (Site Sink Profile) by both process units were obtained considering two different ΔT_{MIN} values. A ΔT_{MIN} of 10 ºC was considered for both process units to build individual grand composite curves. From total site profiles, it concludes that no heat transfer stage was created between heat sources and heat sinks and thus, there is no available heat to be transferred from heat sources to heat sinks through a generated utility. For a ΔT_{MIN} of 15 ºC for both process units, the heating and cooling demands for the whole site were 32.6 MW and 27.5 MW, respectively. The resulting total site profiles shown a heat transfer stage between 130 and 144.6 ºC where heat sources can transfer heat to heat sinks through a generated utility. However, the amount of heat that can be transferred corresponds to a small value of 680 kW, being unworthy when compared to capital costs of required equipment to achieve these target. Yet, the segment of heat sinks integrating the heat transfer stage is vertical indicating that there is a reboiler that can be heated through the intermediate utility by changing operating conditions. However, changes in operating conditions are not a hypothesis in this study.

To conclude, the results found in both direct and indirect heat integration do not justify being considered in further analysis due to the equipment and piping costs required to overcome the drawbacks of the battery limits of each process unit and the distance between the process streams involved to achieve maximum energy recovery.

Chapter 6: Optimization and Synthesis of Heat Exchanger Networks for Retrofit Design Solutions

Abstract

A new hybrid methodology, combining pinch analysis and mathematical programming tools, is here proposed for the retrofit of heat exchanger networks with minimum investment cost, and respecting minimum energy requirements. These are first estimated through the construction of composite curves provided by pinch analysis. A grid diagram is then used to represent the current network and to locate inefficient zones of heat integration. These are then redesigned using mathematical programming tools, and in particular the sequential optimization approach, where the minimum number of heat exchangers is first determined and, in a second stage, the minimum cost network synthesized. The final solution is then constructed on the top of this optimal solution, trying to maximize the reuse of already existing exchangers. This hybrid methodology is applied to the Pre-Distillation and Arosolvan Units of Matosinhos Refinery's Aromatics Plant and results compared with those obtained through pinch analysis and heuristic retrofit rules. In both cases, heuristic rules result in retrofit solutions with lower estimated investment cost, the difference being small in the case of the Pre-Distillation Unit. The hybrid methodology using mathematical programming was expected to produce better solutions and in fact, in most cases, it generates networks with a lower total transfer area, including new and reused heat exchangers. However, these solutions may be suboptimal in terms of new investment needed, since the procedure used to reallocate existing units still needs to be improved (namely incorporating reallocation decisions in the optimization formulations).

Key words: aromatics plants, retrofit of HEN, pinch analysis, optimal process synthesis.

6.1. Introduction to Process Optimization

Optimization of industrial processes aims to provide information on how to perform certain sustainability tasks as optimization problems and what tools are available for solving these problems. When attempting to improve the process and its economic performance at some level, for example reducing resource demands and environmental impacts, process modelling can facilitate some decisions in terms of process design and operation policies to follow. When building a model using mathematical formulation some characteristics of the process must be considered from process phenomena and unit operations to technological constrains and company rules.

Sustainability tasks as optimization problems can be related to new system designs, to the synthesis of a new processing network, and to the retrofit design and operational improvements in heat exchange, reactor, and separation networks. In the case of existing processes or industrial plants, these optimization tasks can include maximizing heat recovery, maximizing process efficiency, minimizing water use and wastewater discharged. The optimization problem consists of a performance criterion defined by an objective function to be maximized or minimized, and thus, to find the best available option according to process characteristics, some of which are fixed with respect to the choice to be made (parameters) and others are allowed to vary (variables). However, some of these variables are dependent variables according to process specifications and internal relationships. The remaining variables are decision variables that are to be manipulated by the optimization tool. The objective function must be formulated as a function of the decision and/or dependent variables.

The continuous and discrete domains and constraints of the model define a feasible region for the optimization problem that contains the solutions from which to choose according to the designed criteria and the decision variables involved. Common process criteria are to minimize the process operating cost, to minimize total annualized cost (including capital costs), to minimize consumption of a certain resources or product or to maximize profit. Decision variables can be continuous type or integer type. Continuous variables are assigned to model properties (flow rates, component concentrations and temperatures, for example) that vary within the feasible region. Integer variables are assigned to model the status of operating devices as well as the selection/exclusion of options for operating units in synthesis problems. Also, the model can include different types of constraints. Mass and energy balances, for example, are equality constrains, while limitations for flowrates, temperatures, pressures, components concentrations, etc., are defined through inequality constraints.

The mathematical formulations that are used to solve these optimization tasks are usually mixed integer nonlinear programming (MINLP) problems. These are often disintegrated into mixed integer linear programming (MILP) problems and nonlinear programming (NLP) problems. The modelling and optimization platform General Algebraic Modelling (GAMS) available in GAMS Development Corporation (2018) is coupled with the state-of-art solvers (e.g. CPLEX for MILP problems, CONOPT for NLP problems and BARON for MINLP problems), and is the tool used in this work. The algorithms for continuous optimization are in most of the solvers classical algorithm based on derivatives. Regarding the integer part, the two main methods are cutting planes method and branch and bound. Cutting planes method consists in adding constraints to force integrality and various algorithms have been developed on this basis. Branch and bound method consists of a decomposition strategy in which the binary variables are gradually relaxed to the corresponding continuous domain [0;1] and the binary solution delimited according to the results of these relaxed problems (Kemp, 2007; Williams, 2013).

Process synthesis and process design tasks at industrial scale tend to involve a significant number of operating units. One of the main fields of application is HEN synthesis. Targeting is an important tool which delimits the underlying design or operation task to which the optimization is being applied. With estimated targets, it is possible to define upper bounds on the network performance and/or lower bound on investment cost. For HEN synthesis, maximum energy recovery targets can be first established, and HENs with reasonable cost thereafter synthesized. It should be however noted that the solution thus obtained is seldom the global minimum for the total annualized cost, which is the sum of annual operating costs and annualized investment costs.

In HEN synthesis, a good practice is to perform targeting for a heat recovery problem. Targeting provides the information on the network potential performance in terms of energy consumption. Pinch analysis can be used aside to estimate the best possible performance of the network by using simple models even before using rigorous design procedures, saving valuable time. The estimated targets can be used primarily to determine which operations and units should be included or left out of the design study. This approach can simplify network design if the number of operations is large and the targets can be used as guidelines in the network synthesis. Generally, the main objective is to either achieve the targets exactly or to approach them closely with the final design. If the targeting model is too idealized, then the produced estimates will serve as loose performance or cost bounds, not as tight bounds. If the targeting model is exact or if at least captures all key factors at the corresponding design stage, then targeting procedure also provides convenient partitioning of the original design space. This makes it easier to decompose the problem and simplify the remaining actions. A good example is the division of HEN in the two regions above and below the pinch in Heat Integration based on pinch point location (Biegler *et al.*, 1999; Floudas, 1995; Kemp, 2007).

6.2. Heat Exchanger Network Synthesis using Mathematical Programming Tools

Heat exchanger network synthesis has been approached using Pinch Analysis and Mathematical Programming Methods. In chapter 4, it was demonstrated the various layers of process integration and design through the onion diagram of Linnhoff (1998) and Pinch Technology based approaches were described and considered in this work to design HENs. Here, Mathematical Programming tools are addressed for HEN synthesis. Mathematical Programming tools have been progressing since the 1980s and in the first contributions the focus was on reducing energy consumption, thus having the concept of heat recovery pinch as central. Then, the aim became the reduction of total cost including energy and investment in transfer area, and also aspects as flexibility and operability of the designed network (Gundersen and Naess, 1988; Kemp, 2007).

Many research papers focus more on systematic and general methods to address HENs synthesis problems in a way to extend theoretical approaches to realistic approaches for their application to real industrial problems, where complexity of the network is often higher and specific technical details may be critical. For instance, a rigorous description of phase change or the variation of transport properties with temperature may be critical aspects in practical applications, and they are often overlooked in the research literature. Other factors still not fully addressed in the literature are complex flow configurations and materials of construction of the heat exchangers (Gundersen and Naess, 1988; Sieniutycz and Jesowski, 2009).

Grossman *et al.* (2000), Furman and Sahinidis (2002) and Morar and Agachi (2010) presented review papers of HENs synthesis for new plants. For existing plants, Gundersen and Naess (1988) provided an evaluation of existing HEN retrofit methods until 1988, and considering the industry perspective. Jezowski (1994) continued the evaluation work until 1993, followed by Sreepathi and Rangaiah (2014). Such methods can provide optimal designs of new plants with optimal level of energy consumption, and improve heat recovery of existing plants through retrofit designs of their HENs.

Different retrofit approaches have been proposed by either increasing heat transfer area, reassigning existing exchangers and/or using heat transfer enhancements able to increase heat transfer coefficients. Mathematical programming methods involve formulation of a mathematical model which represents a set of alternative retrofit designs in which the optimization algorithm searches for the optimal network satisfying energy/cost requirements (Smith *et al.*, 2010; Sreepathi and Rangaiah, 2014). Sequential methodology and Simultaneous methodology are the two main mathematical optimization techniques described here for HEN synthesis. Furman and Shahinidis (2001) discussed in their paper the computational complexity of this methodologies providing new insights to structural properties of HEN synthesis problem.

6.2.1. Sequential Methodology

In this section, a state of the art of a sequential, rigorous and automatic mathematical programming approach is described for HENs synthesis problems. Heat recovery network is the major component affecting the overall performance of process system. Thus, the task is to exchange the available heat of all process streams in order to reduce utilities consumption. When multiple utilities are considered, the cost of utilities is usually the dominant factor to synthesize HEN for which the utility cost is at a minimum.

The first studies decomposed the problem into sequential tasks: 1st minimum utility consumption or cost target; 2nd Minimum number of matches target for the obtained utility target; and 3rd Network derivation for minimum investment cost respecting minimum utility consumption and minimum number of matches. The methodology is schematized in Figure 6.1. This decomposition approach considers total cost based on utility and investment costs, minimizing the components of utility, units and investment costs. It assumes that energy cost is the dominant factor and that minimum number of units solutions needs to meet minimum energy requirements and minimum investment solution.

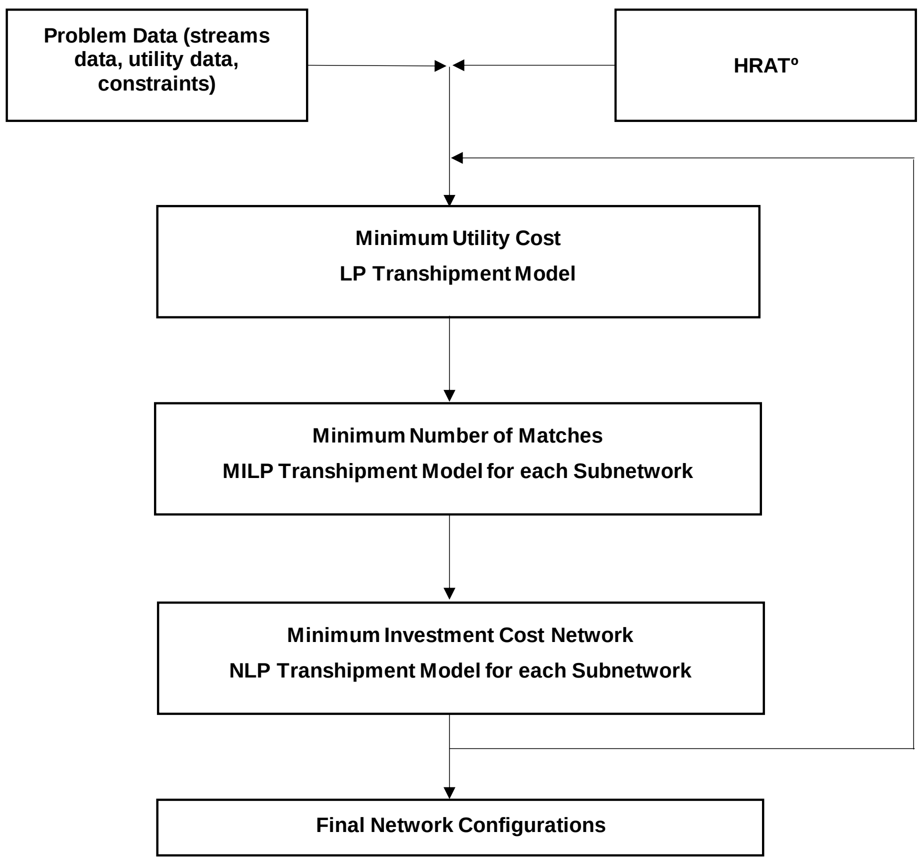


Figure 6.1: Methodology decomposition steps for HEN synthesis (Floudas, 1995).

Describing Figure 6.2, for a given Heat Recovery Approach Temperature (HRAT), LP model is used to target minimum hot and cold utilities consumption and/or cost target providing also the location of the pinch point(s) if it occurs dividing the network into subnetworks. Next, a MILP model is applied for each subnetwork to determine the minimum number of matches between process-to-process streams and process-to-utility streams and its respective heat loads. NLP model is then applied considering the optimal solution obtained through LP and MILP models to formulate a superstructure whose solution provides the minimum investment cost network configuration (Floudas, 1995).

To determine minimum number of matches, Cerda and Westbergerg (1983) developed a transportation model that was further extended to a transhipment model by Papoulias and Grossman (1983). The transhipment model searches the optimum network for transporting a commodity (a product) from sources (where it is produced) to intermediate nodes (warehouses where it is stocked) and then to destinations (markets). Using the same analogy for HEN, as shown in Figure 6.2, heat is the commodity transferred from hot process streams and hot utilities (sources of heat) to cold process streams and cold utilities (destinations) via temperature intervals (warehouses) for a feasible heat transfer. Temperature intervals are determined through the partitioning of temperature range defined by hot and cold process streams and intermediate utilities (if they exist). The nodes on the left represent the sources while the nodes on the right represent the destinations. The intermediate warehouses are the temperature intervals partitioned from temperature range. The arrows represent the heat flows from sources to warehouses, from the warehouses to destinations and from one warehouse to the one immediately bellow. Also, in the top temperature interval the only heat entering are from the hottest utility and the hot process streams while in the bottom temperature interval the only heat exiting are from the coldest utility and cold process streams (Biegler *et al.*, 1999; Floudas, 1995).

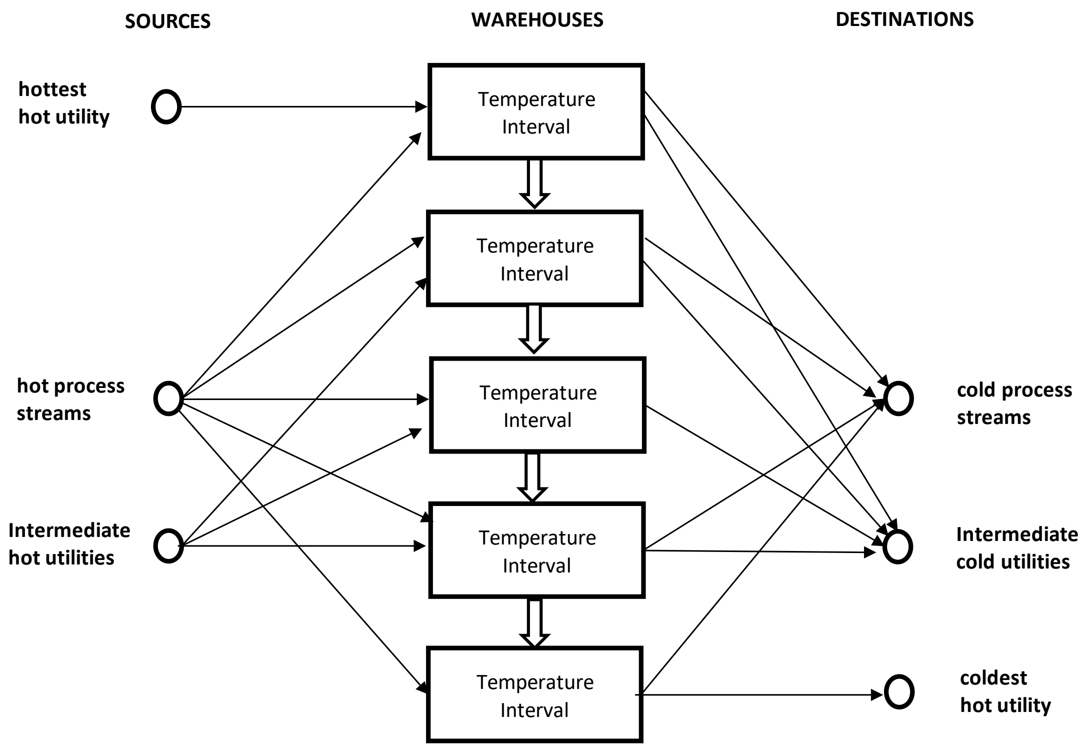


Figure 6.2: Analogy between transhipment model and heat exchanger network (Floudas, 1995).

Papoulias and Grossmann (1983) presented in their paper a number of transhipment models for the systematic synthesis of heat recovery networks. The LP model versions were set to predict minimum utilities consumption or cost with and without restricted matches. The MILP model version were set to develop networks that involve minimum number of heat exchanger units with possible splitting and mixing streams, and where preferences can be assigned to the matches by attributing weights to specify different levels of priority. The advantage of this model is that it can account changes in process synthesis that enhance heat integration and can lead to improved heat recovery networks.

Floudas *et al.* (1986) worked further in a model where heat loads distribution (HLD) is transformed into a network, which means a given quantity of heat is transferred between a hot and a cold stream, that satisfies the fewest number of units given by MILP model solution and the maximum energy recovery given by LP model solution. This network is generated based on a C-F superstructure, name given for the superstructure developed by Floudas *et al.* (1986), as shown in Figure 6.3, and optimized through a non-linear program (NLP) model.

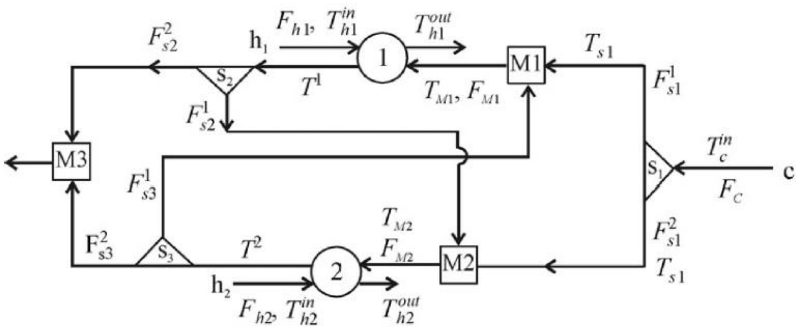


Figure 6.3: C-F superstructure exemplification for a given cold process stream (Kemp, 2007).

The C-F superstructure is a representation of all alternative networks structures, and each subnetwork determined by pinch point(s) location(s) are solved using a nonlinear programming (NLP) model. The key elements of this superstructure rely on mixers at the inlets of all heat exchangers, splitters at the outlets of all heat exchangers, a mixer at each output stream and a splitter at each input stream. Each mixer at the inlet of each exchanger is connected to the input splitter and to the splitters of the other exchangers. Each splitter at the outlet of each exchanger is connected to the output mixer and to the mixers of the other heat exchangers. These superstructure also considers all possible configurations: parallel structure, series structure, parallel-series structure, series-parallel structure and bypass structure. The exchanger minimum approach temperature (EMAT) can or not be relaxed for each match, and if the parameter is relaxed, the EMAT parameter is treated instead as a variable lower than specified lower bound. NLP model solution gives the near-optimal network configuration with minimum investment cost based considered for the modifications set up in MILP model (Floudas, 1995; Floudas *et al.*, 1986; Kemp, 2007).

Ciric and Floudas (1989) proposed a systematic two stage approach for the optimal redesign of HENs whilst the first stage involves a MILP formulation to determine the number of matches and the cost associated with each potential match of streams, including possible options for modifications. Thus, it is possible to obtain information about exchangers that could be reassigned or newly installed, and whether there is a need to increase or decrease the area of the existing exchangers. The second stage involves the formulation of a NLP model to determine the retrofitted network that minimizes the total modification cost. In the same work, Ciric and Floudas (1989) proposed a MINLP model as an alternative to solve the same problem by treating the previous two stages simultaneously and investigated issues related to attaining the best retrofit solution. Ciric and Floudas (1990) proposed a MINLP formulation without considering network decomposition that selects process stream matches and match-exchangers assignments on the base of actual area requirements, as opposed to estimates of area and/or piping costs, while simultaneously optimized the C-F superstructure.

In the work of Gundersen and Grossmann (1990) is presented different approaches of the transhipment model that allows the relaxation of exchange minimum approach temperature (EMAT) at the extremes of the exchangers to evaluate the network complexity in terms of splitting, mixing and by pass streams. However, the trade-off between minimum number of units and total area requirements are not taken into account. The authors choose to keep the decomposition of the problem proposed by Floudas *et al.* (1986) and add heuristic rules to the selection of matches in MILP model (transhipment model). One version of the transhipment model used by the authors was the Vertical MILP Transhipment model in which heat is transferred vertically from the hot to the cold composite curve resulting in a spaghetti design in a network with a very large number of splitters, mixers and heat exchangers. This means that a further loop-breaking procedure is necessary and it cannot guarantee the optimal design. A transhipment model combining temperature intervals and enthalpy intervals was developed allowing matches according to temperature intervals based on EMAT while the heat loads distribution is determined from enthalpy intervals based on HRAT to achieve lower total area requirements and associated total cost. Gundersen *et al.* (1996) applied the same methodology to overcome the limitations of sequential methodology, for example not considering area when selecting matches, and it is an alternative to simultaneous methodology using MINLP model which shows problems with non-convexities and local optima.

Papalexandri and Pistikopoulos (1998) proposed a decomposition-based approach for process optimization and simultaneous heat integration applied to an Industrial Process. The authors approached the industrial problem as a sequential approach in which addressed simultaneously with heat integration within one optimization problem exploiting interactions between process structure, operating conditions and energy recovery. Limitations of the methodology were overcome as the representation of heat integration alternatives including stream mixing, splitting multiple matches, detailed thermodynamic properties, hot-hot and cold-cold heat exchange matches.

In sequential methodology, LP model allows to maximize heat recovery or minimize utilities consumption cost. Moreover, the approach although considers multiple utilities and restricted matches, it does not considered multiple pinches if they occur. Jezowski *et al.* (2000) developed a MILP model which allows the determination and identification of simultaneous pinches if they do exist at conditions of minimum cost of multiple utilities for heat capacity flow-rates varying within ranges. Later, Jezowski *et al.* (2001), maintaining the goal of minimizing number of units and heat loads of utilities, developed a MILP model to eliminate exchangers by breaking loops across pinches thus reducing the number of matches to a global optimum. The approach showed to be useful in retrofitting cases such for example to make some units free for other services or to create path heater-cooler and, hence, increase heat recovery within the network.

Pettersson (2005) applied sequential approach based on LP and MILP models to generate networks for industrial size heat exchanger networks synthesis problems with the difference that instead of decomposing the design task into different sequential targets, the problem is decomposed into subproblems with the same target but with varying degree of relaxation. Thus, utility and investment costs are considered at one extent in each stage. Moreover, at each stage, some of the potential matches can be excluded in further stages which reduces the size of the design problem and permitting a more detailed model at the next stage. Anantharaman *et al.* (2010) used a sequential and interactive framework with the main aim of finding near optimal heat exchanger networks for industrial size problems. The industrial problem is decomposed in subsequent subtasks involving the minimum energy consumption targeting (LP relaxation model), minimum number of units targeting (vertical MILP model) finding sets of matches and its respective heat loads, and network generation and optimization (NLP model). The minimum number of units' problem was reformulated to reduce the gap using physical insights and heuristic rules. The sequential framework showed that model solution times depend mainly on the number of binary variables and on specific model characteristics. The results showed that the model solution time is too long for a sequential framework and improvements are required to solve large industrial problems.

EL-Temtamy and Gabr (2012) upgraded sequential methodology to handle flexible heat exchanger networks for multiperiod process. The approach adapts to changes in streams' supply and target temperatures and heat capacity flowrates using multiperiod transhipment models. Multiperiod LP and MILP models are applied to target utility requirements and the heat exchanger configuration that respects minimum number of units, providing different solutions corresponding to different interactive runs, while remaining flexible to ensure maximum energy recovery at each period of operation. This approach showed higher potential for flexible HENS than single step approaches for overall cost optimization as they are only optimal for short time and are not energy efficient. Miranda *et al.* (2017) also applied sequential approach to handle multiperiod heat exchanger networks synthesis by adding to C-F superstructure new by-pass streams and an improvement in NLP model.

The work of Bagajewicz *et al.* (2013) demonstrated the application of two different HEN retrofit methods to a large industrial complex of a crude unit: Pinch Design Method (thermodynamic method) and Heat Integration Transportation Model (HIT) described through mathematical formulation models. The results showed better solutions using mathematical programming method and the authors pointed out the difficulties in achieving a better economic viable solution using Pinch Technology. However, the mathematical programming method are less popular in industrial practice due to the difficulty in setting up models due to the higher complexity of the problem.

Cheng *et al.* (2014) extended sequential methodology to a total site chemical plant comprising three industrial plants. For maximum energy recovery, Cheng *et al.* (2014) developed a systematic design procedure to take into account whole site savings costs appropriately allowing to maximize the financial benefit of each plant at each stage of the optimization subtasks. The subtasks are similar to the traditional sequential methodology starting to determine the lowest acceptable utility costs and the proper heat flows between every pair of plants and also their fair trade prices (LP model). Then, minimum number of matches and corresponding heat duties are determined (MILP model), following the optimization of the network configuration (NLP model). The superstructure and the model constraints can be built in the same way as in the traditional sequential methodology but using an alternative objective function in which it is adopted the maximization of individual total annualized cost savings simultaneously.

Kim and Bagajewicz (2016) extended the sequential methodology and C-F superstructure developed by Floudas *et al.* (1986) for the case of grassroots design which required reformulations to account several stream matches between two streams, activates splitting control and allows for mixing temperature control. Also, the authors added a new lifting partitioning algorithm to solve the problem globally. The new approach allowed to obtain network structures that single step models, such simultaneous methodology, cannot provide.

6.2.2. Simultaneous Methodology

A simultaneous methodology was developed in early 1990s by Yee and Grossmann (1990) as an alternative to sequential methodology to deal with HEN synthesis as a single-task problem in which all decisions on utiliy consumption or cost, number of matches, and network configuration are treated simultaneously via optimization using MINLP model. This methodology consists of a general superstructure, as shown in Figure 6.4, based upon the problem data and the assumptions of a stage-wise representation.

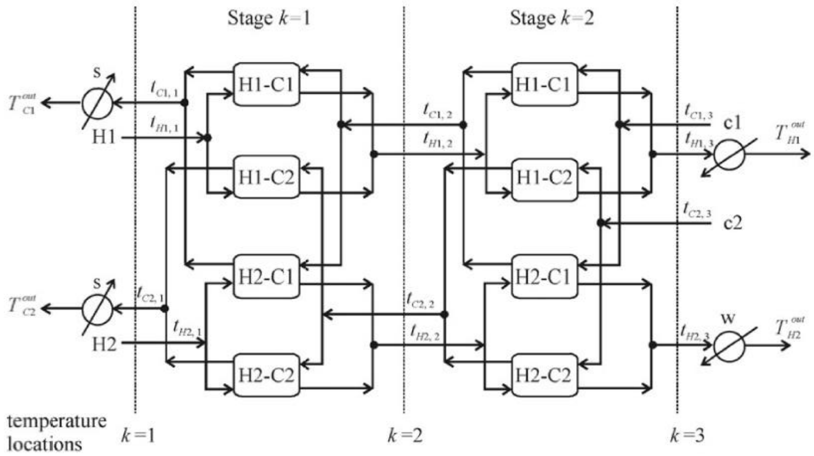


Figure 6.4: Representation of Y-G superstructure for HEN synthesis (Kemp, 2007).

Given a set of two hot process streams (H1 and H2) and two cold process streams (C1 and C2), the Y-G superstructure (Figure 6.4), name given for the stage-wise superstruture developed by Yee and Grossmann (1990), consists of a number of stages determined by the maximum number between the existing number of hot process streams and cold process streams involved in the optimization problem. In this case, as there is two hot process streams and two cold process streams, the maximum number of stages is equal to 2 (Stage k = 1 and Stage k = 2). In each stage, different possibilities for stream matching and sequencing can take place with a restriction imposed by isothermal mixing assumption at the nodes between each stage. Each stream is split into a number of streams equal to the number of potential matches which are directed to the exchangers representing each potential match. The outlets of each exchanger features the same temperature and are mixed at a mixing point where the temperature of the considered stream at the next stage is defined. The outlet temperature of each stream and at each stage are treated as unknown variables. Moreover, heaters are placed at the highest temperature region (left side of temperature location k = 1) of the cold process stream and coolers are placed at the lowest temperature region of the hot process stream (right side of temperature location k = 3).

The isothermal mixing assumption at each node between each stage implies that a process stream is split at each stage into a number of streams that are equal to the possible matches (parallel configuration) and the outlets temperatures of all matches are the same and equal to the unknown temperature of the considered stream from this stage. Energy balances to be considered are the overall energy balance for each stream within each stage and the overall energy balance of each process stream. For an isothermal mixing, energy balances around each heat exchanger and around mixing points (nodes) are not necessary due to considering parallel configuration at each stage for each stream, and by determining the optimal temperatures of each stage, it is possible to determine the flow rates at each split stream (Floudas, 1995; Kemp, 2007).

In the works of Zamora and Grossmann (1997) and Zamora and Grossmann (1998), simultaneous methodology of Yee and Grossmann (1990) is used along with its noncovex MINLP SYNHEAT model introduced by the logarithmic mean temperature difference (LMTD). The authors presented a rigorous optimization method for the synthesis of HEN under the simplifying assumption of no stream splitting. A new class of approximating planes that bound the LMTD from above, and a convex MINLP model that is linearly constrained, predicts lower bounds for the minimum total annual cost of the network. This model is embedded within branch and bound algorithm that performs a spatial search in the domain of the networks temperatures. The solutions provided a set of promising networks configurations that are globally optimized to search for the global optimum network configuration and operating conditions. Later, Zamora and Grossmann (1998) proposed an approach that relies on the use of two new different sets of underestimators for the heat transfer area to overcome the nonconvexities of MINLP model and treat it as convex MINLP model that predicts tighter lower bounds to the global optimum.

Yee and Grossmann (1988) developed also another methodology for the retrofit problem that also simultaneously optimizes the stream matches and network configuration. The difference in simultaneous methodology of Yee and Grossmann (1988) is that the structural modifications result in a superstructure where energy recovery, heat loads, minimum approach temperature (EMAT) and stream matches are not fixed.

Sorsak and Kravanja (2002) upgraded the stage-wise superstructure of Yee and Grossmann (1990) by taking into account different types of heat exchangers in the simultaneous methodology model. The authors performed an initialization of the problem to reduce the time efficiency necessary to solve MINLP model. The initialization for the first MINLP interaction was done using NLP subproblems to cover all feasible matches and exchanger types in the superstructure. Moreover, Björk and Westerlund (2002) extended the stage-wise superstructure model in a way to consider non-isothermal mixing. By removing the assumption of isothermal mixing from the initial model, it is possible to find better solutions for network configurations for the case of constant heat-capacity flowrates and heat transfer coefficients. Konukman *et al.* (2002), maintaining the assumption of isothermal mixing in the stage-wise superstructure model, the synthesis of maximum energy recovery in HEN structures considers a certain operational flexibility is accomplished through a single-stage, non-interactive, superstructure-based, simultaneous MILP formulation to satisfy a given structural-flexibility target. In the works of Frausto-Hernández *et al.* (2002) and Frausto-Hernández *et al.* (2003), the simultaneous MINLP model was extended to assume the effect of allowable pressure drop instead of constant film heat transfer coefficients. Ravagnani and Caballero (2007) proposed a two-step approach for HEN synthesis and detailed design of heat exchangers. The first step involves a similar model based on stage-wise superstructure representation considering stream splitting and constant heat transfer coefficients. In further step, the heat exchangers are detailed designed and the streams heat transfer coefficient recalculated. This way, the results obtained for different values of heat transfer coefficient can be compared along with global cost.

Isafiade and Fraser (2008) proposed an interval-based MINLP superstructure model in which the intervals are defined by the supply and target temperatures of hot and cold streams, including utilities. The model can simultaneously trade-off energy, heat transfer area and number of units while generating a near optimal network superstructure. In the model are considered matches constraints, streams with different heat transfer coefficients and multiple utilities. In further work, Isafiade and Fraser (2010) extended the interval-based MINLP superstructure model to handle multi-period operations in which supply temperature, target temperature and flowrates of streams can vary over a specified range. Na *et al.* (2015) modified stage wise superstructure to incorporate utility substages to consider multiple utilities.

Ponce-Ortega *et al.* (2008) proposed a modification in the simultaneous methodology stage-wise superstructure model by introducing isothermal streams with appropriate constraints that allow the handling of streams with phase change and streams that also involve sensible heat effects. Also, within the formulation, the assumption of isothermal mixing between stages is kept in the model and an approximation of the logarithmic mean temperature difference for streams with phase change and sensible heat changes inside the exchanger was used. The model is based on an MINLP formulation and provides the network with minimum total annual cost, which includes capital cost of the exchangers and the utility costs. In further work, Ponce-Ortega *et al.* (2010) extended the developed approach to incorporate utilities at each stage. Hasan *et al.* (2010) propose an approach to overcome the assumption of constant heat capacity flowrates and isothermal streams in simultaneous methodology by including process streams phase change with an "equivalent" sensible heat change with a fictitious heat capacity that gives the heat duty for the underlying phase change over 1 K. Many multicomponent process streams suffer phase change within a range of temperatures and assuming that they are isothermal which can be inaccurate and lead to inferior networks. A MINLP model and a solution algorithm to incorporate non-isothermal phase change in heat exchanger networks synthesis was proposed by approximating the nonlinear temperature-enthalpy diagram via empirical cubic correlations and including also a procedure to ensure minimum temperature approach at all points in the exchanger.

Results showed significant cost reductions, even when applied to industrial problems, when compared with existing processes. To overcome the limitation of simultaneous methodology to provide better networks configurations, Huang *et al.* (2012) used the modified stage-wise superstructure of Hasan *et al.* (2010) to handle HEN synthesis with non-isothermal mixing. In the model, the authors included improved temperature bounds and logical constraints to obtain better solutions. Liang *et al.* (2013) also approach stage-wise superstructure of Yee and Grossmann (1990) to a synthesis model with non-isothermal mixing by including nonlinear heat mixing balances at each exchanger and mixers and using heuristics as an initialization strategy to obtain feasible solutions.

So far, multiperiod heat exchanger networks synthesis have been approached with sequential approach. Recent works of Zhang *et al.* (2015), Short *et al.* (2016), Isafiade and Short (2016) and Pavão *et al.* (2018) extended simultaneous methodology for multi-period heat exchanger network synthesis by applying multi-period MINLP model.

6.2.3. Comparison between Heat Exchanger Design Synthesis Strategies

In this chapter, two approaches are presented and discussed for heat exchanger design synthesis: sequential methodology and simultaneous methodology. A comparison review between these two methodologies can be found in the paper of Vidyashankar and Narasimhan (2010).

The sequential methodology is a decomposed-based approach that handles HEN synthesis in subsequent and separated subtasks which results are dependent on the previous subtasks. The application of this methodology in retrofit design studies showed good quality networks with respect to total annualized cost. On the other hand, this approach cannot simultaneously optimize different costs associated with HEN design and the trade-offs between energy and capital cost are not taken into account appropriately. This disadvantage comes from the fact that an HRAT value is initially selected and the partitioning into subnetworks affect the number of units and areas of the units in the HEN configuration which may lead to suboptimal networks. The selection of matches' tasks using MILP model may provide multiple feasible combinations of matches' tasks that may be evaluated and give different total investment costs in further optimization subtask. Another complexity that arises is in the optimization of C-F superstructure configuration networks using NLP model which may provide several local solutions. The evaluation of different solutions to determine optimal network required an interactive process due to the specification of HRAT value that is initially required.

At industrial perspectives, some large industrially sized problems may require longer computational time due to a higher number of process streams and variables. In addition, NLP model behaves as a non-convex curve, which may cause some difficulties in finding a global optimum. The advantages of this methodology is allowing a much greater involvement of the designer. In addition, in contrast to the pinch technique, the dual-temperature approach method allows a finite heat flow across the pinch point by choosing an exchange minimum temperature approach (EMAT) in heat exchangers. EMAT is relaxed when its value is lower than temperature intervals approach temperature (TIAT) used in temperature partitioning into temperature intervals and lower than HRAT which is used to target the maximum energy recovery (MER). The relaxation of strict-pinch case (heat cannot be transferred across pinch point) into a pseudo-pinch case (heat can be transferred across pinch point) increases the chance of getting HENs that are more practical with better operability features, fewer stream splits and a lower number of units (Floudas, 1995; Galli and Cerda, 1998; Gundersen and Grossmann, 1990).

Simultaneous methodology simplifies HEN superstructure in a number of stages determined by the number of hot and cold process streams involved. When the number of stages becomes large, for example in industrial large sized problems, multiple potential matches are considered and the model becomes more complex even with the benefit of having linear constraints. In addition, as opposite of C-F superstructure, the stage-wise superstructure of Yee and Grossmann (1990) does not considered all the structural configuration alternatives due to isothermal mixing assumption. In cases in which HEN configurations have splits present, this assumption may lead to an overestimation of the area cost and hence the investment cost. If splits are present, the resulting HEN structure may feature more heat exchangers than needed. Also, the assumption of isothermal mixing neglects from consideration the structures in which a split stream goes through two or more exchangers in series. In addition, in stage-wise superstructures there is a limitation that the process stream does not exchange heat with many other process streams. It requires as input the maximum number of times that two streams can exchange heat (Floudas, 1995).

6.2.4. Hybrid Methodology

In this work, two approaches of HEN synthesis have been described, one using thermodynamic insights and another based on mathematical programming. However, some researches support the idea of rather than using either one of these approaches, there has been a trend to make best use of the combination of both approaches called hybrid methodology. A paper review incorporating hybrid methods is presented by Sreepathi and Rangaiah (2014).

Hybrid methods combines thermodynamic-heuristics methods with mathematical programming methods, making the best use of the strengths of both methodologies such as allowing user interaction and can be applied to large problems. In order to solve industrial problems, the user interaction may have an important role to play. Although the industrial practice is using primarily pinch analysis concepts, the complexity of the decisions involved, the large number of options to be considered and the require automation and speed in decision making justify the need for new retrofit technologies such as mathematical models. Retrofit problems include changes for the reduction of utilities consumption, appropriate structural modifications, number and type of units to be purchased, changes in the installed heat transfer area, repipping of streams and reassignment of matches. These decisions can be addressed using hybrid methodologies (Briones and Kokossis, 1996).

Briones and Kokossis (1996) presented in their paper the application of a hybrid methodology combining mathematical programming and pinch analysis methods. The authors considered applying the decomposition scheme to address the retrofit HENs problem as a multi-task that includes targets for structural modifications and heat transfer area changes, development and optimization of the retrofitted network and the analysis of its complexity against economic penalties and trade-offs. The results showed that the decomposition enables viable designs to be processed for final optimization. The methodology allows interactions with engineer/designer at different stages of the decision making process and explores different scenarios for the retrofit problem.

Asante and Zhu (1996) and Asante and Zhu (1997) developed a new procedure that consists of a two stages approach for retrofit HEN design of a Crude Unit, consisting of a modification selection stage and an optimisation stage. The first stage is a diagnosis stage that allows user interactions to identify and select minimum number of topology modifications to be made to the original HEN. These topology modifications must enable a desire heat recovery target to be achieved. The HEN topology resulting from these modifications is optimized to produce the final retrofit design. The procedure is automated and allows user interaction, making the best use of both methodologies. The methodology showed potential to offer an efficient, systematic and automatic methodology for the retrofit design. However, as contrary of MINLP simultaneous methodology, this procedure does not guarantee a retrofit network with minimum cost. In spite of this, it ensures that the final retrofit costs remain close to minimum.

More recent works of hybrid methodology combining Pinch Analysis and Mathematical Programming tools can be found. Corredor (2012) applied hybrid methodology to an industrial natural gas processing plant to obtain the best design on energetic use by optimizing heat exchanger surface area, utilities consumption and economic costs. Angsutorn *et al.* (2014) applied Pinch Analysis and MINLP stage-wise model with relaxation technique for HEN synthesis. Pinch Analysis identified the optimal pinch point and HRAT value to avoid large heat exchanger areas and which decomposes the problem into the two regions above and below pinch point. Then, the mathematical programming technique with relaxation is applied to reduce the number of heat exchangers and generate the final HEN design. The hybrid methodology showed lower computational time effort due to HEN synthesis with two smaller size parts defined by pinch point location.

6.3. Methodology

A hybrid methodology combining Pinch Analysis and a sequential methodology is used in this work for heat exchanger network (HEN) synthesis of Pre-Distillation and Arosolvan Units to develop optimal retrofit design solutions. For each process unit, HEN synthesis is handled in subsequent inter-dependent tasks that are sequentially optimized via separable mathematical programming models. A general schematic representation of the methodology applied is shown in Figure 6.5.

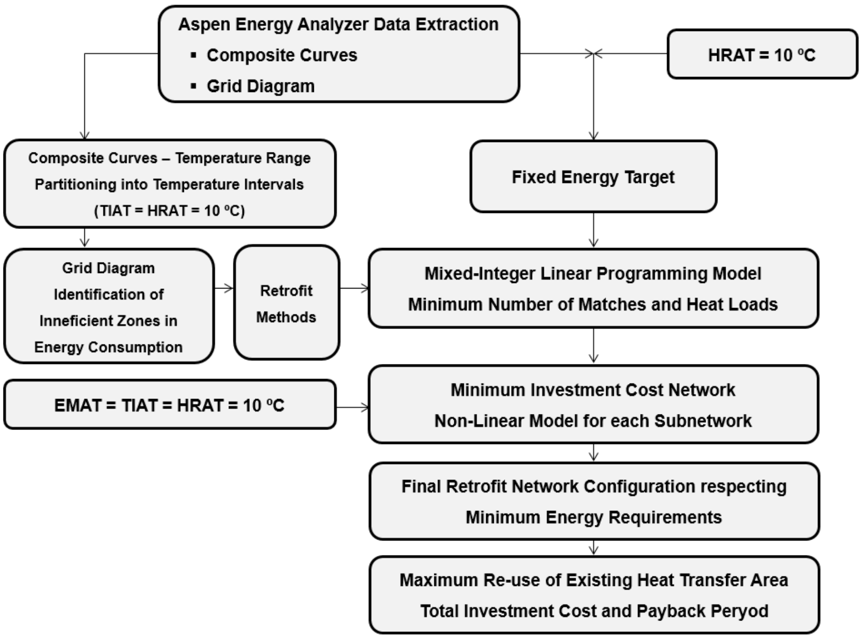


Figure 6.5: Hybrid methodology for heat exchanger network synthesis of Pre-Distillation and Arosolvan Units.

For a heat recovery approach temperature (HRAT) of 10 ºC, the constructed composite curves and the respective energy targets and pinch point location previously estimated are here considered for both Pre-Distillation and Arosolvan Units. The grid diagram used to represent the current heat exchanger network of each process unit was also here considered based on which the inefficient zones of energy consumption were identified, namely those where heat is transferred across pinch point. These inefficient zones will be redesigned in the second phase of this methodology using sequential optimization models considering two retrofit methods: cross-pinch exchanger elimination method and pinch design method.

Sequential methodology decomposes the problem into two and inter-dependent tasks: i) determination of the minimum number of units (matches) and its respective heat loads for fixed energy targets using mixed-integer linear programming model (MILP model); and ii) derivation of a C-F superstructure network above and below pinch point and determination of the optimal network configuration for minimum investment cost using non-linear programming model (NLP model) for a given fixed energy targets and minimum number of units. The superstructure considers all possible configurations from which the optimization method searches for the optimal network configuration satisfying the given constraints. This sequential approach assumes that the energy cost is the dominant factor and that the minimum number of units solutions needs to meet the energy targets and the minimum investment cost.

The total investment cost associated to the optimal overall network configuration is determined considering Bare Module Equipment Cost method. This method is traditionally applied to estimate the cost of new equipment. In this case, and in both retrofit methods, it is considered the maximum re-use of the existing heat exchangers, minimizing the requirements of additional heat transfer area. Therefore, an adjustment is required in the total investment cost after the reallocation of the existing heat exchangers, if and when required.

- **Retrofit Problem Definition**

From grid diagram representing the current heat exchanger network of each process unit, data was extracted obtaining a set of hot process streams (H_i) to be cooled and a set of cold process streams (C_j) to be heated. For each process stream, it is defined the supplied/inlet temperature (T_{INLET}) and its target/outlet temperature (T_{OUTLET}) associated with a specific heat capacity flowrate (MCp). Also, it is considered for both process units the consumption of only one type of hot utility (HU) and one type of cold utility (CU), of which conditions are the same as used in Pinch Analysis.

The data extracted procedure from the grid diagram depends on the retrofit method to be used. In this work, the same retrofit methods are considered: cross-pinch exchanger elimination method and pinch design method for retrofit design. For each procedure, it is considered the following:

A) As described in previous chapter, the aim of applying cross-pinch exchanger elimination method is to eliminate the heat exchangers that are transferring heat across pinch point. From the grid diagram of the current heat exchanger network, these inefficient zones of energy consumption are identified and process data from these zones are extracted (inlet and outlet temperatures and heat loads). Using these data, a second heat exchanger network is developed to be redesigned using optimization tools. Well-allocated units, considered efficient zones in energy consumption of the initial network, are left out of the optimization study. Process streams data from matches involving process-to-utility streams are also considered to make best use of heat transfer between process-to-process streams;

B) In Pinch Design Method for retrofit design, the overall network is redesigned as if a new network, which means that all heat exchangers are removed from the network as well as streams splits and mixers.

Based on stream matches solution, all possible superstructure configurations are drawn for the network with flowrates and temperatures of all process streams, including stream splits and phase change phenomena occurring in some process streams. When phase change occur, their enthalpy are modelled as piecewise linear functions of temperature with different slopes below bubble points, between bubble and dew-points, and above dew points. The procedure is further described.

In both retrofit methods, it is considered the maximum re-use and reallocation of the existing heat exchangers after obtaining the optimal overall network configuration. The heat transfer areas were determined considering counter-current heat exchange and a constant and by default values of individual heat transfer coefficients provided by Aspen Energy Analyzer (720 kJ/((m^2.hr.ºC)) for all process and utility streams for the estimation of heat exchanger areas. As stated before, heat transfer areas and associated costs are purely indicative values. The optimal network configuration is the one that respects minimum investment cost required for minimum heat transfer area for fixed energy targets and minimum number of units.

- **Definition of Temperature Intervals through Composite Curves**

A composite curve is considered for each retrofit design method, and its respective process data, considering an HRAT equal to 10 ºC. From composite curves are defined the temperature intervals to be considered in MILP model for the determination of minimum number of units (N_{MIN}) and its respective heat loads.

In HEN synthesis, there are three temperature approaches that are used as parameters at different stages that restrict and simplify the problem when they are fixed. These parameters are:

- Heat Recovery Approach Temperature (HRAT) to quantify energy targets;
- Temperature Interval Approach Temperature (TIAT) to partition the temperature range into temperature intervals and to control the residual flows out of the temperature intervals;
- Exchange Minimum Approach Temperature (EMAT) to specify the minimum temperature difference between two streams exchanging heat within an exchanger.

The three parameters are related through Equation 6.1. In general, HRAT is allowed to vary while TIAT may be set equal to HRAT (strict pinch case). In this study, strict pinch case is considered as no heat is allowed to be transferred across pinch point. It is also considered an EMAT value of 10 ºC.

$$\mathbf{HRAT \geq TIAT \geq EMAT} \quad \textbf{Equation 6.1}$$

Temperature intervals (k) are defined through the partitioning of temperature ranges of hot and cold process streams within the composite curves considering a TIAT of 10 ºC to control the residual heat flows from one interval to the next. It is also assumed that there is only one hot utility and one cold utility being supplied at the top and at the bottom of the temperature range, respectively. In cases where a phase change occurs during the temperature variation of a process stream, the temperature partitioning is modified and the heat loads of the three segments of phase change are considered within its respective temperature intervals. The process stream is then treated the same way as one phase process stream. Problem table analysis and heat cascade are performed to determine the heat loads in each defined temperature intervals for each retrofitted method. Its results are used as input to MILP transhipment model for the determination of the minimum number of units for the fixed energy targets.

- **Minimum number of units (N_{MIN})**

The subnetworks of the HEN delimited by pinch point location, one above the pinch and one below the pinch, are treated independently. A MILP transhipment model is applied to determine the minimum number of matches between process-to-process streams and process-to-utility streams along with its respective heat loads.

As described in the book of Floudas (1995), the MILP model is based on problem table analysis and heat cascade. The variables involved in the model are a mixed set of continuous and binary variables. Therefore, the model corresponds to a mixed integer linear programming (MILP) problem. The problem is solved in General Algebraic Modelling System (GAMS) using CPLEX algorithm and it searches for global optimal solution. The solution provides the minimum number of matches and their correspondent heat loads for each subnetwork. To write MILP transhipment model, it is needed to define the main indices and sets as follows:

$TI = \{ k \mid 1, 2, .., k \},$
$HP_k = \{ i \mid hot\ process\ stream\ i\ is\ present\ in\ interval\ k \},$
$CP_k = \{ j \mid hot\ process\ stream\ j\ is\ present\ in\ interval\ k \},$
$HU_k = \{ i \mid hot\ utility\ i\ is\ present\ in\ interval\ k \},$
$CU_k = \{ j \mid cold\ utility\ i\ is\ present\ in\ interval\ k \},$
$i : hot\ process\ stream\ and\ hot\ utility,$
$j : cold\ process\ stream\ and\ cold\ utility,$
$k : temperature\ interval.$

The input data or parameters to represent the heat loads of temperature intervals:

$Q_{ik}^{H} : heat\ load\ of\ hot\ process\ stream\ i\ entering\ temperature\ interval\ k,$
$Q_{jk}^{C} : heat\ load\ of\ hot\ process\ stream\ j\ entering\ temperature\ interval\ k.$

Then, the variables to represent the potential heat flows are introduced:

$QS_{ik} : heat\ load\ of\ hot\ utility\ i\ entering\ temperature\ interval\ k,$
$QW_{jk} : heat\ load\ of\ cold\ utility\ j\ entering\ temperature\ interval\ k,$
$R_k : heat\ residual\ load\ out\ of\ temperature\ interval\ k,$

Q_{ik}^{H} and Q_{jk}^{C} are parameters since they are specified from the data through problem table analysis and heat cascade and temperature partitioning procedure. The heat loads of hot process stream *i* in temperature interval k are traduced through Equation 6.2 where F_i is the flowrate of hot stream *i*, Cp_{ik} is the heat capacity of hot process stream *i* in interval *k* and ΔT_{ik} is the temperature change of hot stream *i* in interval *k*. The heat loads for cold process streams *j* in temperature interval *k* is traduced through Equation 6.3 where F_j is the flowrate of hot stream *j*, Cp_{jk} is the heat capacity of hot process stream *j* in interval *k* and ΔT_{jk} is the temperature change of hot stream *j* in interval *k*.

$$\boldsymbol{Q_{ik}^{H} = F_i (Cp)_{ik} \Delta T_{ik}} \qquad \textbf{Equation 6.2}$$

$$\boldsymbol{Q_{ik}^{C} = F_j (Cp)_{jk} \Delta T_{jk}} \qquad \textbf{Equation 6.3}$$

The representation of each temperature interval k is in Figure 6.6 where are indicated the associated variables (hot and cold utility heat loads, heat residuals) and the parameters (hot and cold process streams heat loads).

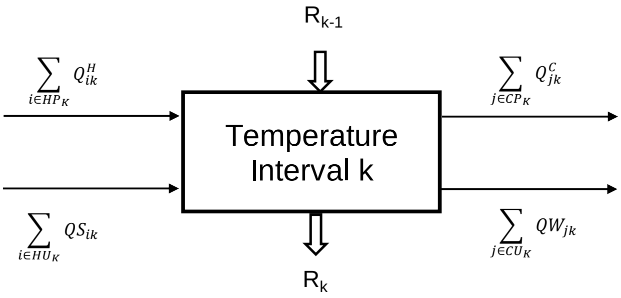


Figure 6.6: Heat loads of k temperature interval (Floudas, 1995).

In Figure 6.6, heat enters in temperature interval k from hot streams and utilities whose temperature range includes part of or the whole temperature interval and from the previous temperature interval (k- 1) that is at a higher temperature via heat residual (R_{k-1}). As this heat residual is in excess, it can be used in the respective interval. On the other hand, the heat loads exiting temperature interval k are used by cold streams and utilities whose temperature range includes part of the whole temperature interval and directed to the next temperature interval that is at a lower temperature interval via the heat residual R_k which is in excess and cannot be used in the k interval. Also, at the top and bottom temperature interval (k = 1 and k = K, respectively) there is no heat residual entering or exiting ($R_k = R_K = 0$). All the variables defining heat loads are positive as indicated by the constraint in Equation 6.4.

$$\left.\begin{array}{r} \boldsymbol{R_k \geq 0} \\ \boldsymbol{QS_{ik} \geq 0} \\ \boldsymbol{QW_{jk} \geq 0} \end{array}\right\} \boldsymbol{k \in TI}$$ **Equation 6.4**

The overall energy balance around temperature interval *k* are traduced through Equation 6.5 which is a linear equality constraint.

$$\boldsymbol{R_k - R_{k-1} + \sum_{j \in CU_k} QW_{jk} - \sum_{i \in HU_k} QS_{ik} = \sum_{j \in HP_k} Q_{ik}^H - \sum_{i \in CP_k} Q_{ik}^C}$$ **Equation 6.5**

The main objective of MILP model is to determine the heat exchange between all pairs of streams excluding utilities considering each match, amount of heat load of each match and amount of heat residual of each hot process stream/utility. The existence of each match is modelled via the introduction of a binary variable (y_{ij}) such as indicated in Equation 6.6. In this, it is excluded the matches (ij) that include hot and cold utilities.

$$\boldsymbol{y_{ij} = \begin{cases} 1, \ if\ match\ (ij) takes\ place,\ i \in HP\ U\ HU,\ j \in CP\ U\ CU \\ 0,\ otherwise \end{cases}}$$ **Equation 6.6**

The amount of heat load for each match (*ij*) is modelled through the introduction of continuous variables (Q_{ij}) which is the heat exchanged in a match (*ij*) at interval k. The variable Q_{ijk} is the heat load of match (*ij*) over all intervals of the subnetwork under consideration. Through Equation 6.7 is determined the heat loads for each match (*ij*).

$$\boldsymbol{Q_{ij} = \sum_k Q_{ijk}} \qquad \textbf{Equation 6.7}$$

The heat residual of each hot process stream/utility exiting each temperature interval k is modelled by Equation 6.8 which introduces the continuous variables R_{ik} which is the residual heat of hot process stream/utility *i* out of temperature interval k and R_k is the total residual heat exiting interval k.

$$\boldsymbol{R_k = \sum_i R_{ik}} \qquad \textbf{Equation 6.8}$$

The MILP transhipment model can be represented as indicated in Figure 6.7 in which a hot process stream H1 and a hot utility S1 can potentially exchange heat with a cold process stream C1. Thus, there is a potential of two matches: (H1, C1) and (S1, C1).

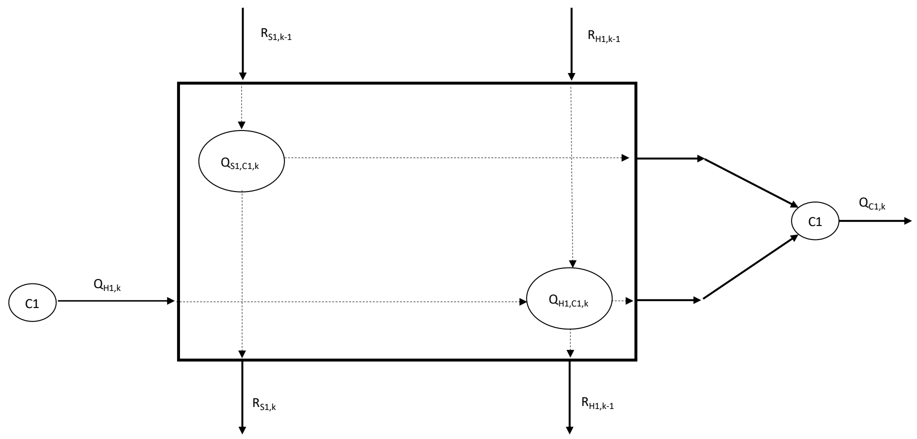


Figure 6.7: Graphical representation of a temperature interval *k* for a MILP transhipment model (Floudas, 1995).

In Figure 6.7, the variables $Q_{S1,C1,k}$ is a variable even if it is known the amount of hot utility S1 that enters at the upper temperature interval. Also, the residuals $R_{S1,k-1}$ and $R_{S1,k}$ are unknown and hence are variables. Known fixed quantities are $Q_{H1,k}^{H}$ and $Q_{C1,k}^{C}$ which represent the heat available from hot stream H1 and the heat needed by stream C1 at interval k, respectively. The residuals $R_{H1,k-1}$, $R_{H1,k}$ and $Q_{H1,C1,k}$ are variables. After introducing the binary and continuous variables to target the minimum number of matches, the MILP model considers the following:

i. Energy balances for each hot process stream and at each temperature interval k,
ii. Energy balances for each hot utility and at each temperature interval k,
iii. Energy balances for each cold process stream and at each temperature interval k,
iv. Energy balance for each cold utility and at each temperature interval k,
v. Definitions of total residual flows at each interval,

vi. Definitions of heat loads of each match,
vii. Relations between heat loads Q_{ij} and binary variables y_{ij},
viii. Nonnegativity constraints on continuous variables,
ix. Zero top and bottom residual constraints,
x. Integrality conditions on y_{ij}.

The objective function is a linear sum of all y_{ij} variables and minimizes the number of matches between process-to-process streams and process-to-utility streams. The mathematical model to target minimum number of matches can be formulated as follows:

$$\min \sum_{i \in HPUHU} \sum_{J \in CPUCU} y_{ij}$$

$$s.t.$$

$$R_{i,k} - R_{i,k-1} + \sum_{j \in CP_k UCU_k} Q_{ijk} = Q_{ik}^{H}, \qquad i \in HP_k, k \in TI$$

$$R_{i,k} - R_{i,k-1} + \sum_{j \in CP_k} Q_{ijk} = Q_{ik}^{H}, \qquad i \in HU_k\,, k \in TI$$

$$\sum_{i \in HP_k UHU_k} Q_{ijk} = Q_{jk}^{C}, \qquad j \in CP_k\,, k \in TI$$

$$\sum_{i \in HP_k} Q_{ijk} = \ Q_{jk}^{C}, \qquad j \in CU_k, k \in TI$$

$$R_k - \sum_{i \in HP_k UHU_k} R_{ik} = 0, \qquad k \in TI$$

$$Q_{ij} = \sum_{k \in TI} Q_{ijk}$$

$$L_{ij} y_{ij} \leq Q_{ij} \leq u_{ij} y_{ij}$$

$$Q_{ijk} \ \geq 0, k \in TI;\ R_{ik} = 0, k \in TI$$

$$R_0 = R_1 = 0$$

$$y_{ij} \ \in \{0, 1\}$$

In the model are excluded the possible matches between hot and cold utilities by not including y_{ij} variables for that purpose in the objective function as well as in constraints. The energy balances are linear constraints in residuals and heat loads. The relationship between continuous variables and binary variables are linear since L_{ij} and U_{ij} are parameters that correspond to lower and upper bounds, respectively, on the heat exchange of each match (*ij*). These constraints guarantee that if a match does not exist, then its heat load should be zero. Otherwise, if the match takes place, then its heat load should be between its lower bound and the upper bound (maximum heat that can be transfer between a hot and cold stream). Therefore:

$$if\ y_{ij} = 1, then\ L_{ij} \leq Q_{ij} \leq U_{ij}$$

$$if\ y_{ij} = 0, then\ 0 \leq Q_{ij} \leq 0\ and\ hence\ Q_{ij} = 0$$

Lower and upper bounds values can be properly defined to reduce the computational effort of solving the model. The tighter the bounds, the less effort is required even though the same solution can be obtained for arbitrarily large lower and upper bounds ranges. To determine the upper (U_{ij}) and lower (L_{ij}) bounds on the heat loads for each potential match in each considered subnetwork, it is important to considered the following cases: no matches restrictions, required matches, forbidden matches, preferred matches, and restricted heat loads on matches. In this case, no restrictions are imposed on matches and thus, the upper bound U_{ij} of potential match (ij) is given by the minimum of the heat loads of streams i and j as in Equation 6.9. The lower bound L_{ij} is used primarily to avoid small heat exchangers and in this case with no restrictions it is considered L = 0.

$$\boldsymbol{U_{ij} = min}\{\textstyle\sum_{k\in TI} \boldsymbol{Q^{H}_{ik}}, \sum_{k\in TI} \boldsymbol{Q^{C}_{jk}}\} \qquad \textbf{Equation 6.9}$$

In addition, the MILP model can provide several global solutions with the same objective function and it is very straightforward to generate all such solutions for further examination by incorporating appropriate integer cuts.

- **Development of Subnetworks superstructure to determine optimal configuration**

The third step is to formulate a C-F superstructure based on the optimal solution obtained through MILP model in which is considered all possible configurations for the retrofitted network. These include the alternatives of: i) parallel structure, ii) series structure, iii) parallel-series, iv) series-parallel, and v) by-pass. The key elements of these superstructures is they embed heat exchanger units, mixers at inlets of each exchanger, splitters at the outlets of each exchanger, a mixer at each output stream, and a splitter at each input stream. The advantage of these superstructures is in considering individual stream superstructures which can be derived independently. The variables of the interconnecting streams to be considered are also indicated (heat capacities, flowrates, and temperatures).

A NLP model is used for this purpose to determine the optimal subnetwork configuration solution. When dealing with process stream with phase change, their enthalpy are modelled as piecewise linear functions of temperature with different slopes below the bubble-points, between bubble and dew points, and above dew points. Binary variables are needed to describe these enthalpy functions and thus NLP model becomes a MINLP model. All models are solved using GAMS coupled with BARON solver. The overall network configuration corresponds to a minimum investment cost network.

In this step, some considerations are taken into account such as: fixed and variable target temperatures, different types of streams involved (gas, phase change and liquid), counter-current heat exchangers, carbon steel as material of construction, constant operating pressure ratings and constant and by default values of individual process streams heat transfer coefficients (720 kJ/((m^2.hr.ºC)).

To determine the minimum investment cost structure out of many alternatives supplied by the HEN superstructure, it is defined the following variables and constrains:

i) Variables:

- Flow rates heat capacities of each stream;
- Temperatures of each stream;
- Areas of the heat exchangers;

ii) Constraints:

- Mass balances for the splitters;
- Mass balances for the mixers;
- Energy balances for the mixers and exchangers;
- Feasibility constraints for heat exchange, and
- Nonnegativity constraints.

The objective function of the model is the minimization of the investment cost of the heat exchangers that are postulated in the superstructure. The objective function is written in function of bare module equipment cost (CBM) which takes into account the considerations described above to define the problem. The objective function used for the subnetworks above and below pinch point can be represented through Equations 6.10.

$$\boldsymbol{CBM = \sum Cp^{0}_{(i,j)} \times FBM} \qquad \textbf{Equation 6.10}$$

The mentioned constrains are not of the same nature. Mass balances for splitters and mixers, feasibility constrains for heat exchangers and no negativity constrains are all linear constraints. The energy balances for mixers and exchangers are nonlinear constrains, since they have bilinear products of unknown flow rates of the interconnecting streams times their unknown respective temperatures. The objective function is also nonlinear function of the driving temperature forces expressed in logarithmic temperature difference (LMTD) form. Here, it is considered the Patterson (1994) approximation given in Equation 6.11 for the determination of LMTD in the heat exchanger project equation. Hence, the mathematical model is a nonlinear programming NLP problem.

$$\mathbf{LMTD} = \frac{2}{3}\left(\left(\Delta\mathbf{T^{H}_{IN}} - \Delta\mathbf{T^{C}_{OUT}}\right) \times \left(\Delta\mathbf{T^{H}_{OUT}} - \Delta\mathbf{T^{C}_{IN}}\right)\right)^{1/2} + \frac{1}{3}\left(\frac{(\Delta\mathbf{T^{H}_{IN}}-\Delta\mathbf{T^{C}_{OUT}})\times(\Delta\mathbf{T^{H}_{OUT}}-\Delta\mathbf{T^{C}_{IN}})}{2}\right) \qquad \textbf{Equation 6.11}$$

The optimal solution of NLP problem will give information on all temperatures and flow rates of the streams in the superstructure, as well as heat transfer areas of new heat exchangers and respective total investment cost, determining automatically the optimal configuration of the network.

The same adjustments in total investment costs considered in Chapter 4 are also here performed when applying Bare Module Equipment Cost method. The total investment cost through this method is determined considering the purchase of new equipment. As in both retrofit method is considered the maximum re-use and reallocation of the existing heat exchangers of the current heat exchanger network. Therefore, some adjustments were considered to determine the total heat transfer area requirements resultant from the re-use of existing heat exchangers instead of the new ones obtained through the model. In other words, the attribution of the heat transfer area of the existing heat exchangers is only performed after obtaining the optimal configuration network. Consequently, it is also required an adjustment of the respective investment cost involved in reallocating these equipment.

The same considerations to estimate a proper investment cost for the re-use of the existing equipment are: i) new equipment cost are determined following the traditional procedure of the bare module equipment cost; ii) well-allocated heat exchangers or heat exchangers with the same streams match and heat duties do not have a cost associated (zero cost); and iii) the re-use and reallocation of the existing and available heat exchangers to new stream matches and/or heat duties have only an installation cost associated corresponding to 20 % of a new equipment cost (a percentage estimated through bare module equipment cost procedure data). Moreover, heat exchangers are designed above the required capacity (maximum over 15-30%) which means that even for higher loads that might exist, the existing heat exchanger might be re-used in the network.

The Chemical Engineering Plant Cost Index of the year 2001 (CEPCI = 394) was assumed for all inflation adjustments. Using the values provided by Turton *et al.* (2018), CEPCI was updated using interpolation for the year 2018 (CEPCI = 591.3) to update the investment cost.

It is then possible to rank the retrofit projects and choose the best ones according to economic criteria. Capital cost and payback period are estimated for the required network modifications to achieve energy targets using Bare Module Cost for Equipment at base conditions having in consideration the maximum re-use of the existing heat exchangers. In both Pre-Distillation and Arosolvan Units, all heat exchangers can be re-used and reallocated for different stream matches, including reboilers (as all are thermo-syphon type). The only heat exchangers that will not be re-used are the air coolers as air cooling utility will stop being consumed and only cooling water will be considered in both process units.

- **Procedure to model phase change behaviour of a process stream**

The enthalpy variation of a process stream at a given temperature (E(T)) is a type of nonlinear function that can be represented by integer variables. The enthalpy variation curve is a piecewise linear curve as represented in Figure 6.8 in which: T_{REF} is the reference temperature at which enthalpy is determined; T_{BP} is the boiling point temperature (saturated liquid); T_{DP} is the dew point temperature (saturated vapour); and T_{UP} is the maximum (upper bound) temperature of a process stream.

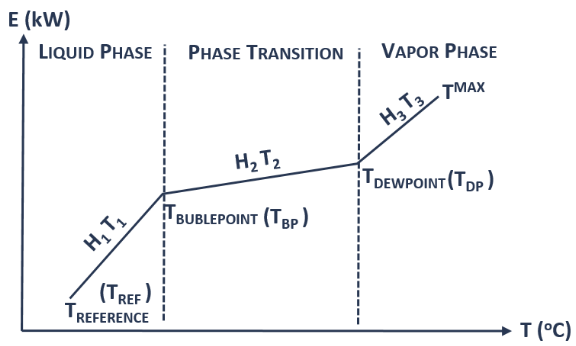


Figure 6.8: Representation of enthalpy variation curve of a process stream .

To model the enthalpy curve, it is expressed any value of E(T) as the sum of three variables as represented through Equation 6.12 in which H_1 is the enthalpy of liquid phase, H_2 is the enthalpy of phase change and H_3 is the enthalpy of gas phase. Thus, the enthalpy for each of these variables is linear.

$$\boldsymbol{E(T) = H_1 + H_2 + H_3} \qquad \textbf{Equation 6.12}$$

Where,

$$0 \le \delta_1 \le T_{BP} \quad \text{and} \quad \delta_1 = T_1 - T_{REF}$$
$$0 \le \delta_2 \le T_{DP} \quad \text{and} \quad \delta_2 = T_2 - T_{BP}$$
$$\boldsymbol{0 \le \delta_3 \le T_{UB}} \quad \text{and} \quad \boldsymbol{\delta_3 = T_3 - T_{DP}} \qquad \textbf{Equation 6.13}$$

The variables have been defined so that:

- δ_1 correspond to the amount of which temperature variable T_1 exceeds reference temperature (T_{REF}) but is less or equal to bubble point temperature (T_{BP}).
- δ_2 correspond to the amount of which temperature variable T_2 exceeds bubble point temperature (T_{BP}) but is less or equal to dew point temperature (T_{DP});
- δ_3 correspond to the amount of which temperature variable T_3 exceeds dew temperature (T_{DP}) but is less or equal to maximum temperature of the process stream (T_{UB}).

And the total enthalpy variation is given by:

$$\boldsymbol{H_1 = cp^L(T_1 - T_{REF})} \qquad \textbf{Equation 6.14}$$

$$\boldsymbol{H_2 = cp^{FICT}(T_2 - T_{BP})} \qquad \textbf{Equation 6.15}$$

$$\boldsymbol{H_3 = cp^G(T_3 - T_{DP})} \qquad \textbf{Equation 6.16}$$

If this interpretation is to be valid, it is also required that $T_1 = T_{BP}$ whenever $\delta_2 > 0$ and that $T_2 = T_{DP}$ whenever $T_3 > 0$. However, these restrictions on the variables are just constraints conditions and can be modelled by introducing the following two binary variables:

$$W_1 = \begin{cases} 1\ if\ T1\ is\ at\ is\ upper\ bound\ (T_1 = T_{BP}) \\ 0\ otherwise\ (T_1 < T_{BP}) \end{cases}$$

$$W_2 = \begin{cases} 1\ if\ T2\ is\ at\ is\ upper\ bound\ (T_2 = T_{DP}) \\ 0\ otherwise\ (T_2 < T_{DP}) \end{cases}$$

Then, the mentioned constraints can be replaced by:

$(T_{BP} - T_{REF})W_1 \le T_1 - T_{REF} \le (T_{BP} - T_{REF})$	$\delta 1 = T_1 - T_{REF}$	$T_1 \le T_{BP}$
$(T_{DP} - T_{BP})W_2 \le T_2 - T_{BP} \le (T_{DP} - T_{BP})W_1$	$\delta 2 = T_2 - T_{BP}$	$T_{BP} < T_2 < T_{DP}$
$0 \le T_{UP} - T_{DP} \le (T_{UP} - T_{DP})W_2$	$\delta 3 = T_3 - T_{DP}$	$T_{UP} \ge T_3 \ge T_{DP}$

These constraints ensure that the proper conditional constraints hold. Note that:

- $W_1 = 0$ and $W_2 = 0$ to maintain the feasibility for the constraint imposed upon δ_2 and reduces to:
  $T_1 - T_{REF} \leq T_{BP} - T_{REF}$ $\delta 2 = 0$ and $\delta 3 = 0$

- $W_1 = 1$ and $W_2 = 0$ then reduces to:
  $T_1 = T_{BP}$ and $T_2 - T_{REF} \leq T_{DP} - T_{BP}$ and $\delta 3 = 0$

- $W_1 = 1$ and $W_2 = 1$ then reduces to:
  $T_1 = T_{BP}$ and $T_2 = T_{DP}$ and $T_{UP} \geq T_3 \geq T_{DP}$

- $W_1 = 0$ and $W_2 = 1$ is not feasible and it doesn`t happen.

Hence, we observe that there are three feasible combinations for the values of W1 and W2. To calculate the final temperature value:

$$T - T_{REF} = (T_1 - T_{REF}) + (T_2 - T_{BP}) + (T_3 - T_{DP}) \qquad \textbf{Equation 6.17}$$

6.4. Results and Discussion

In previous chapter, for both Pre-Distillation and Arosolvan units, Pinch Analysis was applied to estimate energy targets through construction of composite curves using Aspen Energy Analyzer. Grid diagrams were constructed to represent the current HEN through which were easily identified the inefficient zones of energy consumption within each process unit. Here, and considering the different retrofit methods, the inefficient zones identified are eliminated using optimization tools to obtain retrofit solutions that respect fixed energy targets and minimum number of units with minimum investment cost as possible. The results are then compared to the ones obtained with retrofit methods based on heuristic rules. The results obtained for Pre-Distillation and Arosolvan Units are discussed next.

Pre-Distillation Unit

Energy targets, pinch point location and the grid diagram representing the current heat exchanger network (Chapter 4) of Pre-Distillation Unit are here considered. The inefficient zones of energy consumption within the network were already identified and correspond to the heat exchangers operating across the pinch point: E0109 and E01115 A/B. HEN synthesis problem is decomposed into sequential steps applied to both subnetworks divided by pinch point location, above and below pinch point, as the aim is to achieve an optimal HEN with maximum heat recovery and therefore, no heat is allowed to be transferred across pinch point (strict-pinch case).

The two retrofit methods are applied using sequential methodology that involve subsequent mathematical programming models with the aim to eliminate these inefficient zones. Two retrofit approaches are considered in the application of this methodology: cross-pinch exchanger elimination method and pinch design method.

Retrofit Design Solutions using Cross-Pinch Exchanger Elimination Method

In cross-pinch elimination method, it is considered a second heat exchanger network built with only the data extracted of the process streams involved in the inefficient zones of the current HEN. Also, process streams involved in process-to-utility matches were considered to make best use of the heat transfer between process streams and to replace air coolers with coolers. Well-allocated process-to-process heat exchangers and the respective streams or part of the streams involved were left out of the optimization study. For the new set of hot process streams and cold process streams, and considering the respective heat loads and operating conditions of the installed heat exchangers, it was constructed a new composite curve as shown in Figure 6.9. The new composite curves show that energy targets and pinch point location remained equal to the ones estimated for the initial network.

The partition of temperature range procedure using the new composite curves was applied to determine the temperature intervals for a TIAT of 10 ºC. Each kink point of the hot composite curve was considered to determine the respective temperature in the cold composite curve. The same analogy is applied for the cold composite curve. Therefore, for the subnetwork above pinch point were determined 5 temperature intervals while for the subnetwork below pinch point were determined 7 temperature intervals.

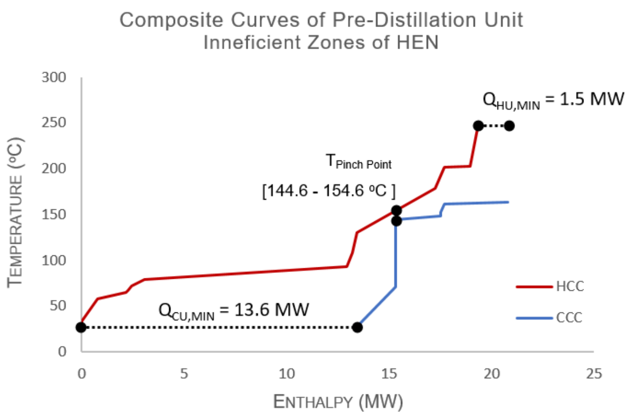


Figure 6.9: Composite curves considering process streams data of the inefficient zones of HEN network of Pre-Distillation Unit.

The temperature intervals are set in descending order for a problem table analysis and heat cascade dealing with process streams with phase change. The results were used as input for MILP model to determine the optimal solution for the minimum number of heat exchangers (N_{MIN}). In addition, it was also determined the upper bounds of heat loads that can be transferred from a hot stream to a cold stream which correspond to the minimum between the heat available by hot stream and the heat needed by cold stream. The results obtained for the upper bounds are presented in Annex IX. MILP model was then solved for each subnetwork using GAMS with CPLEX algorithm. Integer cuts were also included in the model to obtain different possible solutions. The solutions found for the subnetworks above and below pinch point are shown in Tables 6.1 and 6.2, respectively.

Table 6.1: Possible solutions for minimum number of units determined through MILP model for the remaining network above pinch point of Pre-Distillation Unit.

$Q_{MATCHES}$	Solution No 1		Solution No 2		Solution No 3	
(KW)	C4	C2	C4	C2	C4	C2
MP Steam	-	1486.4	-	1486.4	-	1486.4
H1	764.8	-	66.6	698.2	299.0	465.8
H21	520.3	1245.8	670.7	1095.4	986.1	780.0
H22	905.0	547.8	1452.8	-	905.0	547.8

Table 6.2: Possible solutions for minimum number of units determined through MILP model for the remaining network below the pinch point of Pre-Distillation Unit.

$Q_{MATCHES}$	Solution No 1		Solution No 2		Solution No 3		Solution No 4		Solution No 5	
(KW)	C1	CW	C1	CW	C1	CW	C1	CW	C1	CW
H1	-	1042.2	-	1042.2	-	1042	-	1042.2	-	1042.2
H21	246.5	-	173.8	72.8	246.5	-	246.5	-	246.5	-
H22	1471.2	-	1471.2	-	1398.5	72.8	1471.2		1471.2	-
H3	-	798	-	798	-	798	-	798	-	798
H4	-	10084	-	10084	-	10084	-	10084	-	10084
H5	32.2	72.8	105	-	105	-	-	105	28.9	76.1
H6	-	1578.7	-	1578.7	-	1578.7	32.2	1546.478	-	1578.7
H7	-	3.3	-	3.3	-	3.3	-	3.3	3.3	-

MILP model searches for global solution for the minimum number of units (N_{min}) giving its respective stream matches and heat loads. For the subnetwork above pinch point (Table 6.1), there was no more than three different solutions found, which means that there is no more possible solutions for the matches than the ones presented. Solution number 3 has one more unit than solutions number 1 and 2 and thus, it is decided to exclude this solution from the analysis. Solution no 1 was chosen for the retrofit study. The results of MILP model showed that it is required a minimum number of 6 units above the pinch to achieve 1.5 MW of MP steam.

From solutions found for the subnetwork below pinch point (Table 6.2), there was 5 different solutions found in terms of heat loads distribution between matches for the same minimum number of units. The first solution was chosen for the retrofit study. The results of MILP model showed that it is required a minimum number of 9 units below the pinch to achieve 13.6 MW of cooling water.

The next step is to derive a streams C-F superstructure for each subnetwork considering the matches obtained with MILP model that includes all alternative network configuration structures, such as parallel structure, series structure, parallel-series, series-parallel, and by pass. The superstructures derived for the subnetworks above and below pinch point considering minimum number of units obtained with MILP model are shown in Annex IX. The superstructure above pinch point for hot process streams and for cold process streams are exemplified here through Figure 6.10 and 6.11.

These alternative configurations are integrated in each stream superstructure as it incorporates one input, one output, a number of heat exchangers equal to the matches in which the stream is involved, and all possible connections from input to the units, between each pair of units, and from the units to the output. Taking for example stream H21, this input stream has a splitter (S1) that features of a number of outlet streams equal to the number of heat exchangers (2) that are associated with this stream given by MILP model solution. The H21 outlet stream has a mixer (M3) that features of a number of inlet streams equal to the number of heat exchangers (2) that are associated with this stream. All heat exchangers connected to stream H21 have a mixer at its inlet (M1 and M2) and a splitter at is outlet (S2 and S3). The mixers at the inlet of each heat exchanger are connected to the input splitter and the splitters of the other heat exchangers: M1 is connected to S1 and S3 and M2 is connected to S1 and S2. The splitters at the outlet of each exchanger are connected to the output mixers and the mixers of the other heat exchangers: S2 is connected to M2 and M3 and S3 is connected to M1 and M3.

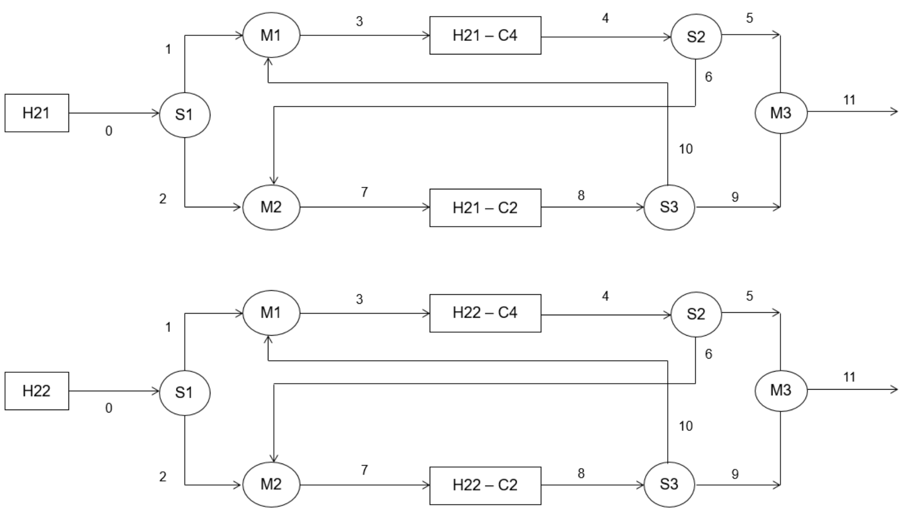
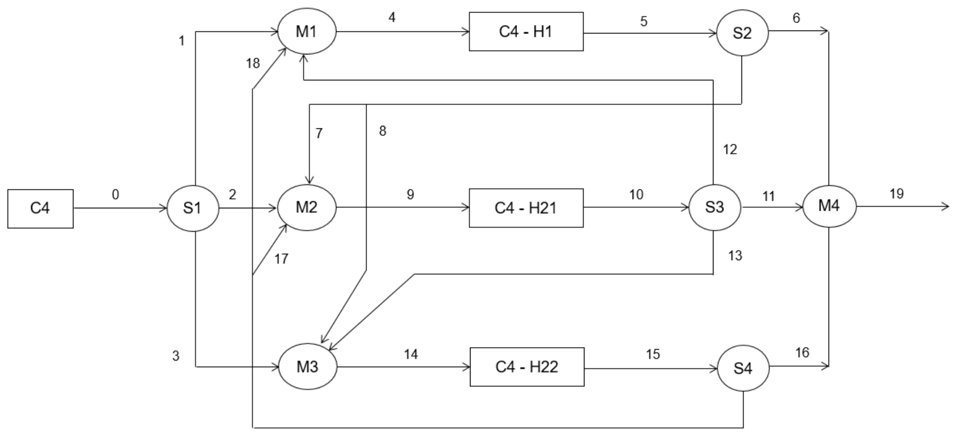


Figure 6.10: Streams superstructure for HEN subnetwork above pinch point for hot process streams considering inefficient zones of energy consumption network for Pre-Distillation Unit.



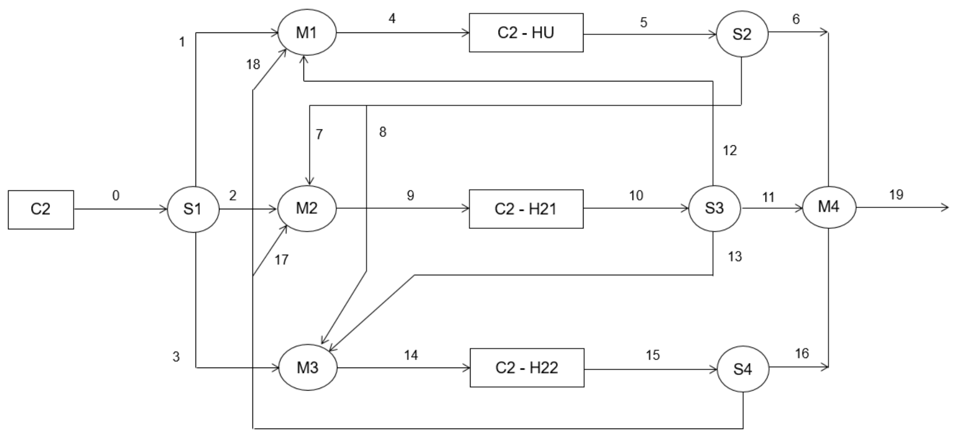


Figure 6.11: Streams superstructure for HEN subnetwork above pinch point for cold process streams considering inefficient zones of energy consumption network for Pre-Distillation Unit

As it is possible to observe from Figure 6.11, the superstructure derived for the subnetwork below pinch point is more complex than the one derived for the subnetwork above pinch point as it involves more interconnections between heat exchangers, mixers and splitters.

To obtain the optimal configuration of the subnetwork above pinch point, considering all stream superstructures, a MINLP model is solved as there are process streams with phase change involved in the subnetwork. For the subnetwork below pinch point a NLP model is solved, as there is no process stream with phase change involved. In both models are included mass balances at each splitter and mixer and energy balances at each mixer and heat exchanger. Mixers are here considered as non-isothermal mixers. Hot and cold ends of the heat exchangers much be equal or higher than the specified ΔT_{MIN} (10 ºC). Both models were solved using GAMS with BARON algorithm which searches for global optimal solution. Then, the stream superstructures are combined into one optimal overall network structure which is shown in Figure 6.12 through a grid diagram.

The optimal configuration solutions obtained for the individual streams superstructures above and below pinch points are shown in Annex IX. The optimal network configuration obtained for streams structures above pinch point for hot and cold process streams are presented in Figure 6.13.

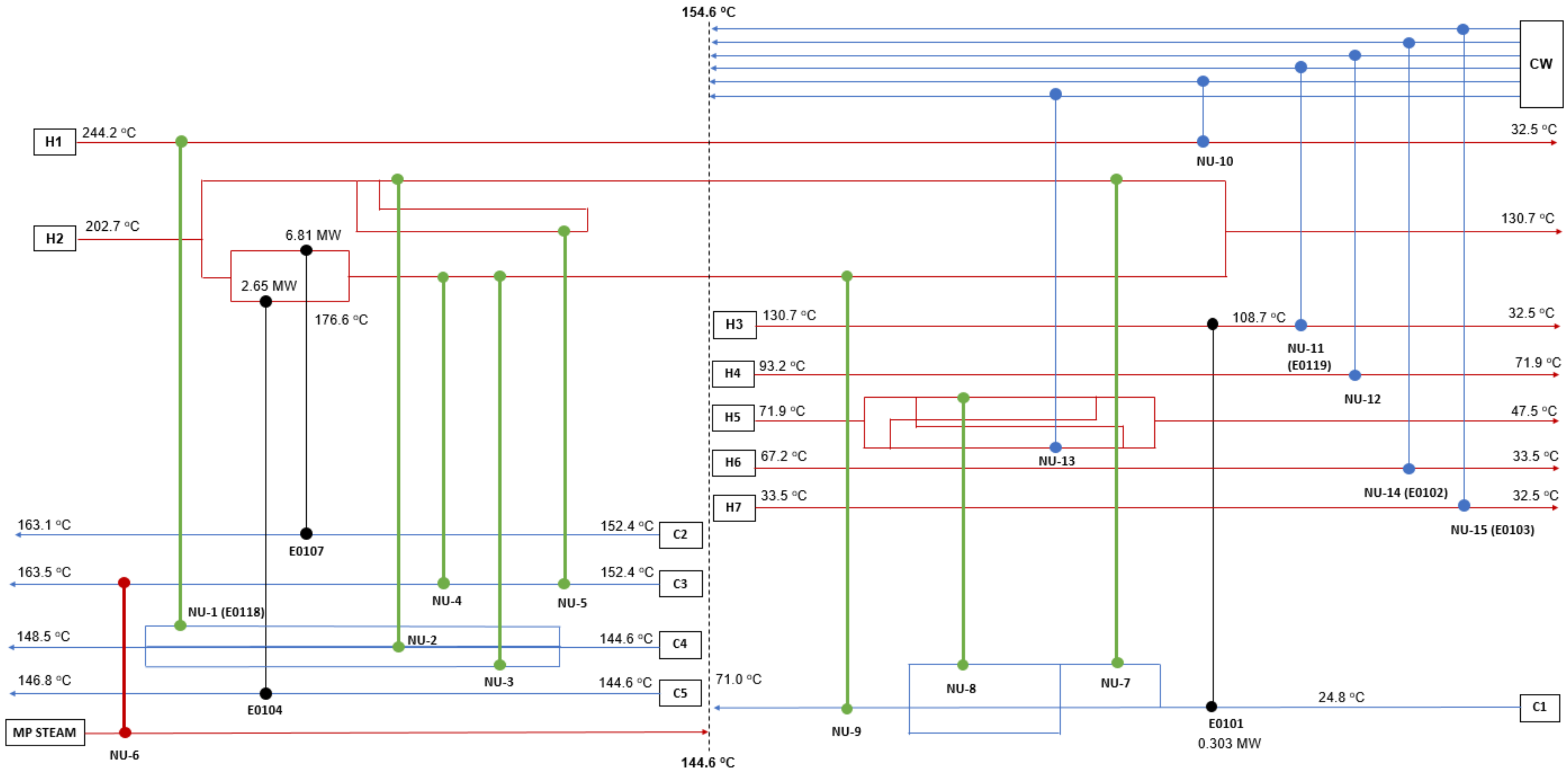
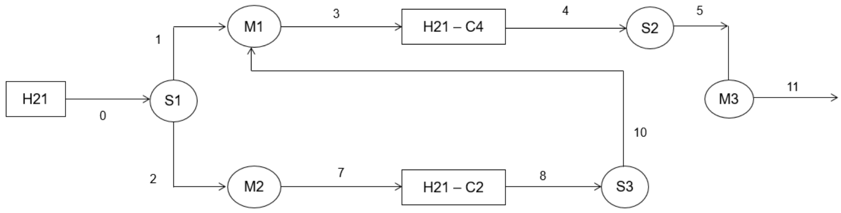
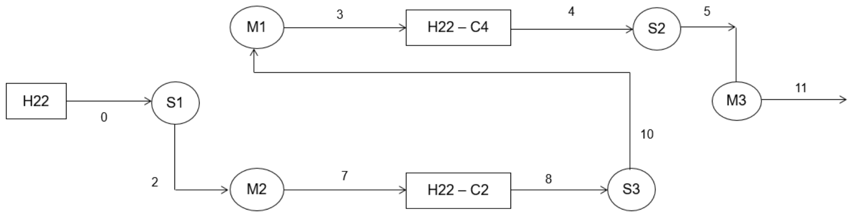


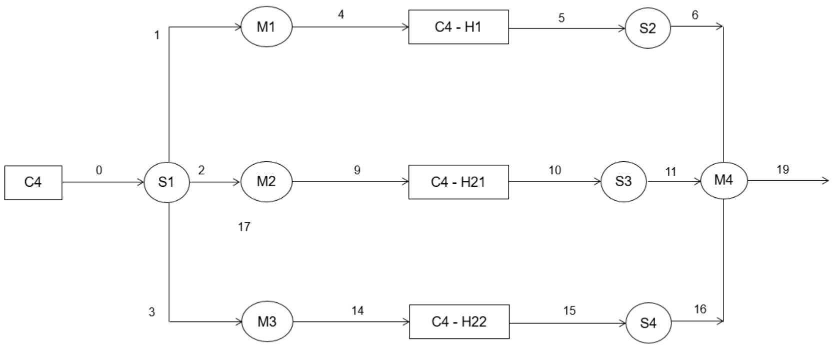
Figure 6.12: Optimal network retrofit solution obtained using hybrid methodology and considering cross-pinch exchanger elimination method for Pre-Distillation unit.



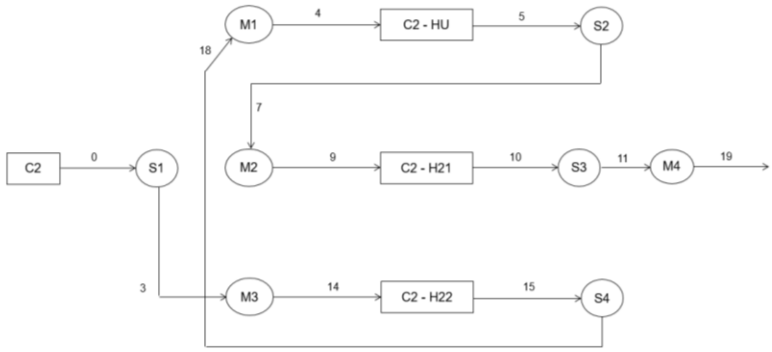
C8 CUT (H21)		
Stream	F (TON/HR)	T (°C)
0	15.438	202.7
1	0.419	202.7
2	15.019	202.7
3	15.438	201.686
4	15.438	154.6
5	15.438	154.6
7	15.019	202.7
8	15.019	201.66
10	15.019	201.66
11	15.438	154.6



C8 CUT (H22)		
Stream	F (TON/HR)	T (°C)
0	94.835	178.2
2	94.835	178.2
3	94.835	169.301
4	94.835	154.6
5	94.835	154.6
7	94.835	178.2
8	94.835	169.301
10	94.835	169.301
11	94.835	154.6



C6/C7R1 (C4)		
Stream	MCP (MJ/HR)	T (°C)
0	2021.539	144.6
1	705.965	144.6
2	480.234	144.6
3	835.34	144.6
4	705.965	144.6
5	705.965	148.5
6	705.965	148.5
9	480.234	144.6
10	480.234	148.5
11	480.234	148.5
14	835.34	144.6
15	835.34	148.5
16	835.34	148.5
19	2021.539	148.5



C8/C9R2 (C2)		
Stream	MCP (MJ/HR)	T (°C)
0	1063.784	152.4
3	1063.784	152.4
4	1063.784	154.254
5	1063.784	159.284
7	1063.784	159.284
9	1063.784	159.284
10	1063.784	163.5
11	1063.784	163.5
14	1063.784	152.4
15	1063.784	154.254
18	1063.784	154.254
19	1063.784	163.5

Figure 6.13: Results for streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network.

For the subnetwork above pinch point, the MINLP model coupled with BARON gives an optimal solution in short period of time. It was obtained a total heat transfer area of 7285 m^2 for the 8 required heat exchangers to achieve fixed hot utility target of 1.5 MW. The heat transfer area re-used and required, as well as a detailed discrimination of the investment cost considering bare module equipment cost method, are presented in Annex IX. In this case, two heat exchangers were considered well-allocated in the initial network (E0104 and E0107) with a total heat transfer area of 2377 m^2 and thus, no investment cost is associated. The heat exchanger E0119 with a heat transfer area of 222 m^2 can be re-used in the place of new unit NU-1. Therefore, it is possible a total re-used heat transfer area of 2599 m^2. A total additional heat transfer area for the 5 new heat exchangers of 1739 m^2 is required (NU- 2 to NU-6). This retrofit project has a bare module cost of 1,198 k€, considering new and re-used equipment.

For the subnetwork below pinch point, a NLP model coupled with BARON as algorithm gives an optimal solution in short period of time. The optimal configuration for streams interconnection superstructure of this subnetwork is presented in Annex IX. It was obtained a total heat transfer area of 2947 m^2 for the 10 required heat exchangers to achieve fixed hot utility target of 13.6 MW. The heat transfer area re-used and required, as well as a detailed discrimination of the investment cost considering bare module equipment cost method, are presented in Annex IX. In this case, one heat exchanger were considered well-allocated in the initial network (E0101) with a total heat transfer area of 33 m^2 and thus, no investment cost is associated. The heat exchangers E0119 (301.2 m^2) can be re-used in the place of NU-11, E0102 (480 m^2) can be re-used in the place of NU-14 and E0103 (4.7 m^2) can be re-used in the place of NU-15. Therefore, a total re-used heat transfer area of 824 m^2. A total additional heat transfer area for the 6 new heat exchangers of 2124 m^2 is required (NU- 2 to NU-6).This retrofit project it would have a total investment cost of 1,541k€, considering new and re-used equipment.

The resultant network retrofit solution required a total 18 number of units, including well allocated heat exchangers, corresponding to a total heat transfer area of 7285 m^2, which 3423 m^2 corresponds to a total re-used heat transfer area of existing equipment (7 heat exchangers) and 3863 m^2 corresponds to a total additional heat transfer area requirements (11 heat exchangers). A total investment cost of 2,740 k€ is required for the retrofit project using cross-pinch exchanger elimination method with a payback period of 2.61years.

Results obtained with Pinch Design Method for Retrofit Design

Pinch design method for retrofit design is now applied. The same approach used in the retrofit using heuristic rules are here considered: all heat exchangers, branches, splitters and mixers are eliminated from the current heat exchanger network. Therefore, there is no need to construct new composite curves and the same initial composite curve is here used for the partitioning of temperature ranges into temperature intervals. For the subnetwork above pinch point were determined 6 temperature intervals and for the subnetwork below pinch point were determined 7 temperature intervals.

The optimal solution for the minimum number of heat exchangers (N_{MIN}) was determined with MILP model using the results obtained with problem table analysis and heat cascade as input. In addition, the upper bounds for the heat loads that can be transferred between streams are presented in Annex X for the subnetworks above and below pinch point. Solutions were found for each subnetwork using GAMS with CPLEX as algorithm. Integer cuts were also included in the model to obtain different possible solutions. The solutions found for the subnetworks above and below pinch point are shown in Tables 6.3 and 6.4, respectively.

Table 6.3: Possible solutions for minimum number of units determined through MILP model for the remaining network, above and below the pinch point.

Solution	Q_{MATCH} (kW)		C6C7R1	C6C7R2	C8C9R1	C8C9R2
			C4	C5	C3	C2
1	STEAM	HU	1425	0	0	109
	C9CUT	H1	765	0	0	0
	C8CUT	H2	0	2650	6815	3171
2	STEAM	HU	1425	0	109	0
	C9CUT	H1	765	0	0	0
	C8CUT	H2	0	2650	6706	3280
3	STEAM	HU	1534	0	0	0
	C9CUT	H1	656	0	0	109
	C8CUT	H2	0	2650	6815	3171

Table 6.4: Possible solutions for minimum number of units determined through MILP model for the remaining network, above and below the pinch point.

Solution	Solution 1		Solution 2		Solution 3		Solution 4		Solution 5	
Q_{MATCH} (kW)	REFORMATE (C1)	CW	REFORMATE (C1)	CW	REFORMATE (C1)	CW	REFORMATE (C1)	CW	REFORMATE (C1)	CW
C9CUT (H1)	0	1042	0	1042	0	1042	0	1042	0	1042
C8CUT1 (H2)	1768	0	1768	0	1768	0	1768	0	1768	0
C8CUT2 (H3)	0	1101	180	921	0	1101	0	1101	0	1101
BTCUT1 (H4)	180	9904	0	10084	285	9799	0	10084	0	10084
BTCUT2 (H5)	105	0	105	0	0	105	0	105	105	0
C5CUT1 (H6)	0	1579	0	1579	0	1579	285	1294	180	1399
C5CUT2 (H7)	0	3.3	0	3.3	0	3.3	0	3.3	0	3.3

From the five solutions shown in Table 6.3, it was verified that no more than three possible different solutions were found. Solution number 3 has one more unit than solutions number 1 and 2 and thus, it is excluded from the analysis. Between solutions 1 and 2, the first solution was considered for the retrofit study. The results of MILP model showed that it is required a minimum number of 6 units above the pinch to achieve 1.5 MW of MP steam.

From the five solutions shown in Table 6.4, there was 5 different solutions found in terms of heat loads distribution between matches for the same minimum number of units. The first solution was considered for the retrofit study. The results of MILP model showed that it is required a minimum number of 8 units below the pinch to achieve 13.6 MW of cooling water.

The next step is to determine a configuration that respects the solutions obtained in the previous sequential steps for each subnetwork. Based on these information, it is possible to postulate all stream superstructure which is shown in Annex X for the subnetwork above and below pinch point. The streams superstructures show the same complexity as the ones obtained in cross pinch exchanger elimination method. In the superstructures are also indicated the variables of the interconnecting streams to be considered (heat capacities, flowrates and temperatures). To obtain the optimal configuration of each subnetwork, a MINLP model is solved as there are process streams with phase change involved in the network above pinch point and a NLP model below pinch point. Both models were solved using GAMS with BARON algorithm which searches for global optimal solution.

The optimal configuration of the overall network structure is shown in Figure 6.14 through a grid diagram. The optimal configuration for streams interconnection superstructure of this subnetwork above and below the pinch point are presented in Annex X, as well as its respective detail discrimination of heat transfer area obtained for each unit and the bare module equipment cost.

For the subnetwork above pinch point, a MINLP model using BARON as algorithm was solved giving an optimal solution in a short period of time. It was obtained a total heat transfer area of 4678 m^2 for the 6 required heat exchangers to achieve fixed hot utility target of 1.5 MW. In this case, two heat exchangers can be re-used (E0107 and E0108 in the place of HEATX-3 and HEATX-4, respectively) with a total heat transfer area of 3020 m^2 and thus, only an installation cost of their reallocation is accounted in the investment cost. A total additional heat transfer area for the 4 new heat exchangers of 1658 m^2 is required (HEATX-1, HEATX-2, HEATX-5 and HEATX- 6). This retrofit project above pinch point has a minimum bare module equipment cost of 1,441 k€, considering new and modified equipment and installation cost.

For the subnetwork below pinch point, a MINLP model using BARON as algorithm was solved giving an optimal solution in a short period of time. It was obtained a total heat transfer area of 3078 m^2 for the 8 heat exchangers required to achieve fixed cold utility target of 13.6 MW. In this case, it was possible to re-use 4 existing heat exchangers, being those E0118 (222 m^2) in place of HEATX-7, E0101 (33.2 m^2) in place of HEATX-8, E0109 (361.2 m^2) in place of HEATX-11 and E0103 (4.7 m^2) in place of HEATX- 14. For these heat exchangers, only the installation cost associated to its reallocation are taken into account in the investment cost. A total re-used heat transfer area of 561 m^2 is possible. A total additional heat transfer area for the 6 new heat exchangers of 2517 m^2 is required. This retrofit project it would have a minimum bare module cost of 1,811 k€, considering new and modified equipment and installation cost.

The resultant network retrofit solution required a total of 14 heat exchangers corresponding to a total heat transfer area of 7756 m^2, which 3581 m^2 corresponds to a total re-used heat transfer area of existing equipment (6 heat exchangers) and 4175 m^2 corresponds to the total additional heat transfer area requirements (8 heat exchangers) for the overall optimal network configuration. A total investment cost of 3,252 k€ is required for the retrofit project using pinch design method with a payback period of 3.10 years.

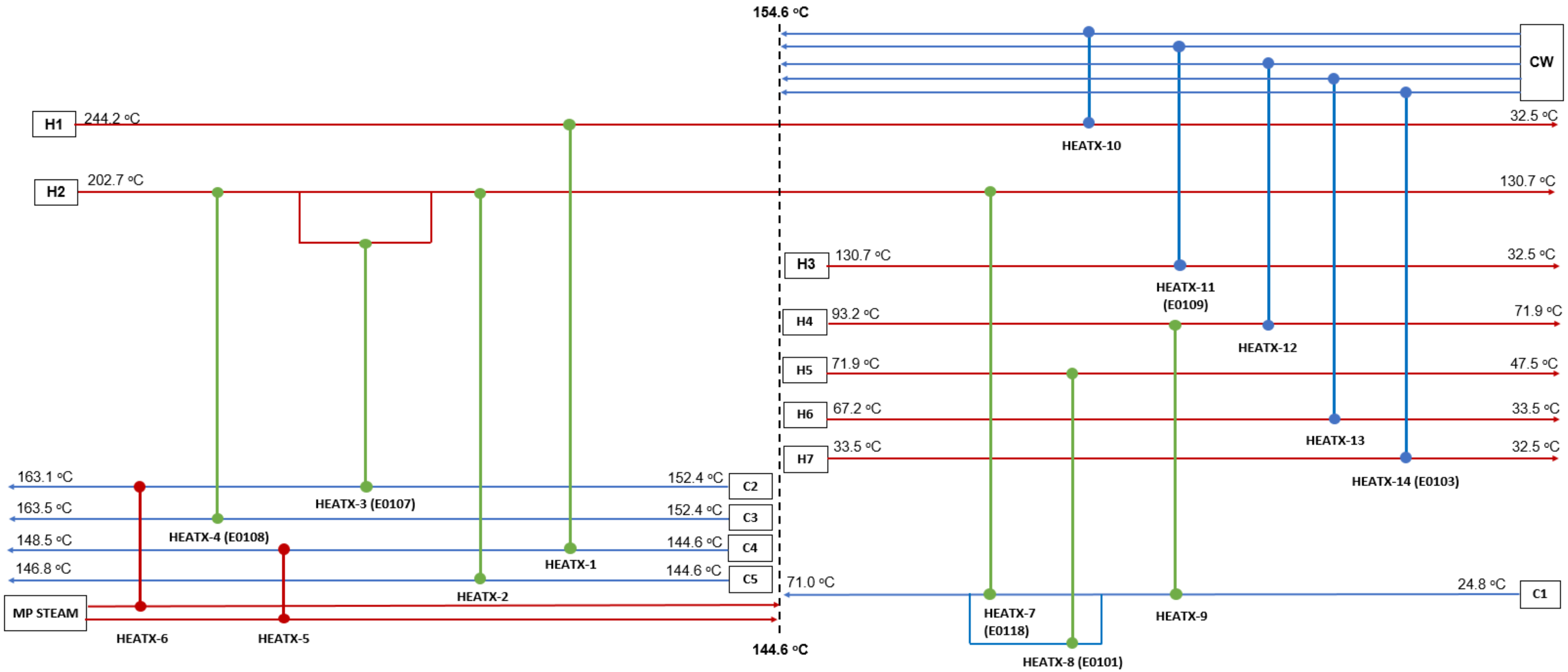


Figure 6.14: Optimal retrofit solution obtained using hybrid methodology and considering Pinch Design Method for Pre-Distillation unit.

The results using the retrofit methods applying hybrid methodology are now compared with the ones obtained with retrofit methods using heuristic rules in previous Chapter 4. The results are summarized in the next Table 6.5.

Table 6.5: Comparison of retrofit design solutions obtained with cross-pinch exchanger retrofit method using heuristic rules and hybrid methodology for Pre-Distillation Unit.

Retrofit Design Solutions	Heuristic Rules		Hybrid Methodology	
	Cross-Pinch Exchangers Elimination Method	Pinch Design Method	Cross-Pinch Exchangers Elimination Method	Pinch Design Method
Solution No	1	2	3	4
Total No Units	16	14	18	14
Total re-used Area (m^2)	3117	4524	3423	3581
Total Additional Area (m^2)	5351	2940	3863	4175
Total Area (m^2)	8468	7464	7286	7756
Total Capital Cost (KEUR)	3,718	2,702	2,740	3,252
Payback Period (years)	3.54	2.57	2.61	3.10

Comparing the results obtained with hybrid methodology presented in Table 6.5, it is possible to conclude that the best retrofit solution is the one obtained with cross-pinch exchanger elimination method which offers lower capital cost and payback period. With this method it is possible to achieve fixed energy targets (15.1 MW) with lower total heat transfer area requirements. Also, although it is re-used lower heat transfer area (3423 m^2) of the existing equipment, it requires lower additional heat transfer area (4432 m^2) when compared to the ones obtained with pinch design method. Pinch design method, although it is achieved targeted minimum number of units estimated through Pinch Analysis, it offers higher heat transfer area requirements. Despite there is available higher re-used heat transfer area of existing units (3581 m^2) than the one available in cross-pinch exchanger elimination method, it is required higher additional heat transfer area for new equipment which implies higher investment costs.

Comparing now the results obtained with hybrid methodology to the ones obtained with retrofit methods using heuristic rules, it is verified that pinch design method based on heuristic rules gives better solution not only in terms of minimum number of units but also it demands lower additional heat transfer area than any other retrofit solutions obtained. Also, the solution 2 obtained with this method allows higher re-use of the existing equipment and only it is associated the reallocation and installation cost. For these reasons, the total investment cost is lower. However, it is to be noted that a closer solution no 3 to solution no 2 in terms of total investment cost and payback period is obtained with cross-pinch exchanger elimination method using hybrid methodology maybe due to the different types of configurations that are considered in the C-F superstructure that are not possible to considered using thermodynamic-heuristic rules. Nevertheless, it was expected better solutions with hybrid methodology, the assumption of other types of configurations in the network superstructures may lead to different heat transfer area requirements than the already existing ones and thus, the possibility in re-using the existing heat exchangers is reduced. Another possible reason is in the fact that the optimal solution obtained using hybrid methodology is lost as the existing heat transfer area requirements are reallocated after obtaining the optimal network. An additional procedure should be incorporated in the model to attribute the existing areas to the new matches using binary variables.

Arosolvan Unit

Energy targets, pinch point location and the grid diagram representing the current heat exchanger network of Arosolvan Unit are here considered. The inefficient zones of energy consumption within the network were already identified and correspond to the heat exchangers operating across the pinch point: E0254 and E0261 (process-to-process heat exchangers) and E0205 (process-to-utility heat exchanger). In this process unit, only cross-pinch exchanger elimination method is applied to eliminate these inefficient zones as no solution was found using heuristic rules. In addition, it is not of the company interest in considering in investing in a new network, but only in minimum modifications. Well-allocated heat exchangers and the respective streams or part of the streams involved were left out of the optimization study. These equipment remaining unaltered: E0208, E0253, E0207, E0259, E0220, E0206, E0204, and E0255. Therefore, the remaining streams data was used to draw a second heat exchanger network to synthesize and eliminate these inefficient zones using sequential methodology. The overall network is divided by pinch point location, above and below pinch point, as the aim is to achieve an optimal HEN with maximum heat recovery and therefore, no heat is allowed to be transferred across pinch point (strict-pinch case).

For the new set of hot and cold process streams, and considering the respective heat loads and operating conditions of the installed heat exchangers, it was constructed a new composite curve as shown in Figure 6.15. The new composite curves show that energy targets increased (24.9 MW of hot utility and 17.9 MW of cold utility) compared to the initial estimated energy targets, although lower than actual utilities consumption. Also, pinch point location changed being established new hot and cold pinch temperatures (118.8 – 128.8 ºC).

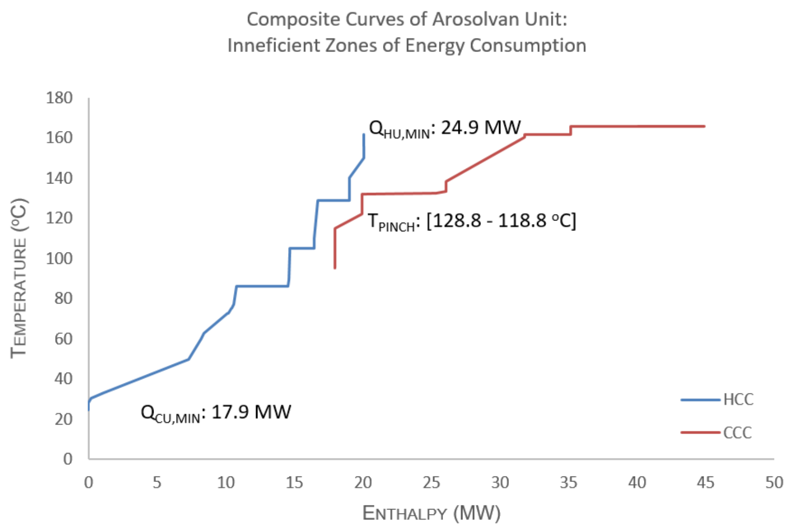


Figure 6.15: Composite curves considering process streams data of the inefficient zones of HEN network.

The partition of temperature range procedure was applied using the new composite curves determining 10 temperature intervals for the subnetwork above pinch point while for the subnetwork below pinch point were determined 8 temperature intervals.

Problem table analysis and heat cascade were performed considering phase change phenomena of process streams. The respective results were used as input for MILP model to determine the global optimal solution for the minimum number of heat exchangers (N_{MIN}). The results obtained for the upper bounds are presented in Annex XI. MILP model was then solved for each subnetwork using GAMS with CPLEX as algorithm. Integer cuts were also included in the model to obtain different possible solutions. The solutions found for the subnetworks above and below pinch point are shown in Tables 6.6 and 6.7, respectively.

For the subnetwork above pinch point, there was no more than 3 different solutions found, which means that there is no more possible solutions for the matches than the ones presented. Solution number 3 has one more unit than solutions number 1 and 2 and thus, it is excluded from the analysis. Between solutions 1 and 2, the first solution was considered for the retrofit study. The results of MILP model showed that it is required a minimum number of 8 units above the pinch to achieve 24.9 MW of MP steam.

For the subnetwork below pinch point, there was 4 different solutions found in terms of heat loads distribution between matches for the same minimum number of units. The first solution was considered for the retrofit study. The results of MILP model showed that it is required a minimum number of 9 units below the pinch to achieve 17.9 MW of cooling water.

Table 6.6: Possible solutions for minimum number of units determined through MILP model for the remaining network above pinch point.

Solution No	Q_{MATCH} (ij)	SOLVENT (NMP+MEG) R1	T0252 BTM R1	EXTRACT R2	T0251 BTM R1	T0251 BTM R2	SOLVENT GLICOL R2
1	MP Steam	9740	3390	5730	915.055	5080	0
	SOLVENT (NMP+MEG)	0	0	0	104.945	0	915.055
	C9CUT	0	0	0	0	0	8.373
2	STEAM	9740	3390	5730	1020	4975.055	0
	SOLVENT (NMP+MEG)	0	0	0	0	104.945	915.055
	C9CUT	0	0	0	0	0	8.373
3	STEAM	9740	3390	5625.055	1020	5080	0
	SOLVENT (NMP+MEG)	0	0	104.945	0	0	915.055
	C9CUT	0	0	0	0	0	8.373

Table 6.7: Possible solutions for minimum number of units determined through MILP model for the remaining network below the pinch point.

UB (kW)	Solution No 1			Solution No 2			Solution No 3			Solution No 4		
	AROMATICS EXTRACTED	SOLVENT GLICOL R2	CW	AROMATICS EXTRACTED	SOLVENT GLICOL R2	CW	AROMATICS EXTRACTED	SOLVENT GLICOL R2	CW	AROMATICS EXTRACTED	SOLVENT GLICOL R2	CW
SOLVENT (NMP+MEG)	0	0	1309	0	0	1309	0	0	1309	0	0	1309
C9 CUT	0	0	6.627	0	0.976	5.651	6.113	0	0.514	1.5	0	5.127
TOLUENE	15	1096.571	1460.429	15	1095.595	1461.405	8.887	1096.571	1466.542	13.5	1096.571	1461.929
TOLUENE DIST	0	0	304	0	0	304	0	0	304	0	0	304
PURE WATER	0	0	1903.007	0	0	1903.007	0	0	1903.007	0	0	1903.007
BENZENE	0	0	3983.9	0	0	3983.9	0	0	3983.9	0	0	3983.9
PURE BENZENE	0	0	94.4	0	0	94.4	0	0	94.4	0	0	94.4
EXTRACT RECYCLE PROD	0	0	3155	0	0	3155	0	0	3155	0	0	3155
PURE WATER DIST	0	0	23.3	0	0	23.3	0	0	23.3	0	0	23.3
LIGHT NON AROMATICS	0	0	236	0	0	236	0	0	236	0	0	236
AROMATICS SAT GLICOL	0	0	5434	0	0	5434	0	0	5434	0	0	5434

The next step is to derive a subnetwork superstructure considering the matches obtained with MILP model that includes all alternative network configuration structures. The superstructures derived for the subnetworks above and below pinch point are shown in Annex XI. To obtain the optimal configuration of each subnetwork, a MINLP model is solved as there are process streams with phase change involved in the network below pinch point and a NLP model above pinch point. Both models were solved using GAMS with BARON algorithm which searches for global optimal solution. The solution obtained for the individual streams superstructures are shown in Annex XI. Then, the stream superstructures are combined into one overall superstructure which has considered all configurations for each subnetwork. The optimal configuration of the overall HEN superstructure of the network is shown in Figure 6.16 through a grid diagram. The optimal configuration for streams interconnection superstructure of this subnetwork above and below the pinch point are presented in Annex XI, as well as its respective detail discrimination of heat transfer area obtained for each unit and the bare module equipment cost.

For the subnetwork above pinch point, an MINLP model using BARON as algorithm was solved giving an optimal solution in short period of time. It was obtained a total heat transfer area of 4622 m^2 for the 8 required heat exchangers to achieve fixed hot utility target of 24.9 MW. In this case, a total of 5 heat exchangers can be re-used: E0202 (1168 m^2) and E0254 (865.8 m^2) in place of NU-4, E0258 (891 m^2) in place of NU-6, E0211 (153.2 m^2) in place of NU-7 and E0251 (754.8 m^2) in place of NU-8. These corresponds to a maximum re-use of heat transfer area of 3833 m^2. A total additional heat transfer area for the 4 new heat exchangers of 789 m^2 is required (HEATX-1, HEATX-2, HEATX-5 and HEATX- 6). This retrofit project it would have a minimum bare module cost of 1.163 k€, considering new and modified equipment and installation cost.

For the subnetwork below pinch point, a MINLP model using BARON as algorithm was solved giving an optimal solution in a short period of time. It was obtained a total heat transfer area of 7033 m^2 for the 9 required heat exchangers to achieve fixed hot utility target of 17.9 MW. In this case, it was possible to re-use 3 existing heat exchangers, being those E0260 (162 m^2) in place of NU-11, E0261 (5.5 m^2) in place of NU-18 and E0256 (109 m^2) in place of NU-19. For these heat exchangers, only the installation cost associated to its reallocation are taken into account in the investment cost. A total re-used heat transfer area of 277 m^2 is possible. A total additional heat transfer area for the 6 new heat exchangers of 6755 m^2 is required. This retrofit project it would have a minimum bare module cost of 4,957 k€, considering new and modified equipment and installation cost.

The resultant network retrofit solution required a total of 28 heat exchangers corresponding to a total heat transfer area of 16,341 m^2, which 4110 m^2 corresponds to a total re-used heat transfer area of existing equipment (6 heat exchangers), 4687 m^2 corresponds to the total heat transfer area of the 8 well-allocated heat exchangers and 7544 m^2 corresponds to the total additional heat transfer area requirements (8 heat exchangers) for the overall optimal network configuration. A total investment cost of 6,120 k€ is required for the retrofit project using pinch design method, being a significantly higher investment considered by the company and thus, this retrofit solution is not considered a possible viable solution to be implementation. As the operational cost savings for this process units are too low, the payback period is not evaluated for this case and the investment costs show to be the only criterion required for decision making.

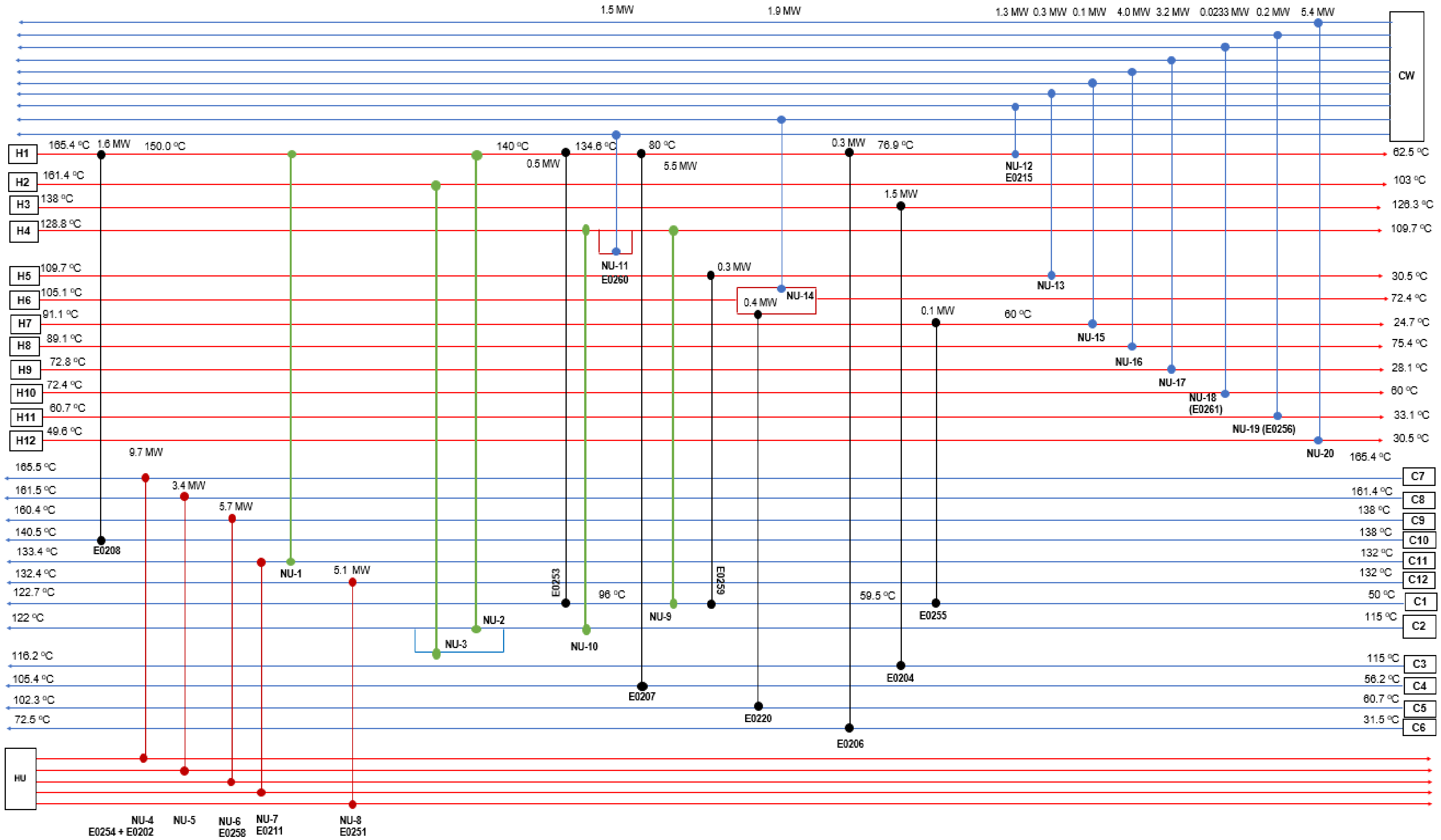


Figure 6.16: Optimal retrofit solution obtained using hybrid methodology and considering cross-pinch exchanger elimination method for Arosolvan unit.

The results obtained using hybrid methodology based on cross-pinch exchanger elimination method were compared to the previous results obtained with pinch design method using heuristic rules. The results are summed up in Table 6.8.

Table 6.8: Comparison of retrofit design solutions obtained with cross-pinch exchanger retrofit method using heuristic rules and hybrid methodology for Arosolvan Unit.

Retrofit Method	**Heuristic Rules**	**Hybrid Methodology**
	Pinch Design Method	Cross-Pinch Exchangers Elimination Method
Retrofit Solution No	Solution 1	Solution 2
Total No Units	26	28
Total Re-used Area (m^2)	11,288	8797
Total Additional Area (m^2)	5687	7544
Total Area (m^2)	16,975	16,341
Total Capital Cost (k€)	4,537	6,120

From the results shown in Table 6.8, it is possible to verify that pinch design method based on heuristic rules gives better solution not only in terms of minimum number of units but also demands lower additional heat transfer area when compared to the retrofit solution given by hybrid methodology. Also, the solution 1 obtained allows higher re-use of the existing exchangers and only is associated the reallocation and installation cost. For these reasons, the total investment cost is significantly lower than the one obtained with hybrid methodology. The same reasons discussed in the study cases of Pre-Distillation Unit are also applied here. Although it was expected better solutions with hybrid methodology, due to the application of optimization models, the assumption of other types of configurations in the network superstructures may lead to different heat transfer area requirements than the already existing ones and thus, the possibility in re-using the existing heat exchangers is reduced. In addition, the modification of pinch point location and the increase in energy targets when applied cross-pinch exchanger elimination method using hybrid methodology, lead to lower energy savings and thus, lower total heat transfer area requirements. These might also be the reason for the limitation of the re-use of the existing heat exchangers. Consequently, the optimal solution obtained using hybrid methodology is lost as the existing heat transfer area requirements are reallocated after obtaining the optimal network.

6.5. Conclusions

Pre-Distillation Unit and Arosolvan Unit of Matosinhos Refinery´s Aromatics Plant are here subjected to a heat integration and optimization study in order to maximize heat transfer efficiency and thus reduce operating costs. For this purpose, a hybrid methodology, combining pinch analysis and sequential methodology, is developed for the retrofit of heat exchanger networks respecting energy targets and minimum number of units for a minimum investment cost.

Retrofit design solutions were obtained considering two retrofit methods: cross-pinch exchanger elimination method and pinch design method. In the retrofit method, only process stream data of the inefficient zones of energy consumption were considered as input for sequential methodology and by process stream data involved initially in utility matches to make best use of heat transfer between process-to-process streams. For this case scenario, new composite curves were required to evaluate energy targets and the location of pinch point. The aim was to eliminate those inefficient zones without altering well-allocated heat exchangers which were left out of the optimization study. The second scenario corresponded to a redraw of the overall heat exchanger network using pinch design method as if it was a grassroots. In both retrofit methods, it was considered the maximum re-use of the existing heat exchangers and a readjustment in the total investment cost after obtaining the optimal configuration solution of the overall network.

For Pre-Distillation Unit, both methods were applied using heuristic rules and hybrid methodology. From the analysis of the four retrofit design solutions, the best solution found was the one achieved with pinch design method using heuristic rules. For this solution, an investment cost of 2,702k€ is required for a total re-used and additional heat transfer area of 7463 m^2 for a total of 14 heat exchangers and fixed energy targets (1.5 MW and 13.6 MW of hot and cold utility consumptions, respectively). Also, this solution allows higher re-used heat transfer area which reduces significantly the investment cost required as for this re-used area only installation cost is accounted. The second best solution found was Solution 3 obtained with cross-pinch exchanger elimination method with a total investment cost of 2,740k€ for a total re-used and additional heat transfer area of 7285 m^2 for a total of 15 heat exchangers for the same fixed energy targets. Cross pinch exchanger elimination method using hybrid methodology showed also promising results when compared to pinch design method using heuristic rules.

For Arosolvan Unit, no solution was found using cross-pinch exchanger elimination method using heuristic rules and for this reason, the same retrofit method was applied using hybrid methodology. However, considering only the process data of the inefficient zones of energy consumption led to an increase in energy targets and a modification in pinch point location. The optimal solution found required a total investment cost of 6,120 k€ for a total re-used and additional heat transfer area of 16,341 m^2 for a total of 28 heat exchangers and fixed energy targets (24.9 MW and 17.9 MW of hot and cold utility consumptions, respectively). However, this solution requires higher additional heat transfer area than the one obtained for the retrofit solution found with pinch design method using heuristic rules. The solution obtained with pinch design method using heuristic rules required lower number of units (26) with a total heat transfer area of 16,975 m^2 which requires a total investment cost of 4,537 k€. However, the investment costs obtained using both approaches are extremely high for the company expectations, which means that none of these solutions are considered viable for further analysis and implementation.

Better solutions were expected in both case studies with hybrid methodology, due to the application of optimization models. However, the assumption of other types of configurations in the network superstructures may lead to different heat transfer area requirements than the already existing ones and thus, the possibility in re-using the existing heat exchangers is reduced. Consequently, the optimal solution obtained using hybrid methodology is lost as the existing heat transfer area requirements are reallocated after obtaining the optimal network.

Chapter 7: Conclusions and Future Works

The present work entitled "Energy Optimization of Matosinhos Refinery's Aromatics Plant" is integrated in the Doctoral Program in Refining, Petrochemical and Chemical Engineering (EngIQ) which started in the academic year 2014-2015. This PhD project was developed in the Aromatics Plant of Galp energia Matosinhos Refinery, which is an energy intensive consumer plant because it handles several processes that require high energy demands, being necessary significant reformulations to reduce energy consumption and operating costs.

The Aromatics plant integrates two main process units that are here subjected to an energy performance analysis: Pre-Distillation Unit and Arosolvan Unit. Pre-Distillation Unit is the "front end" of the aromatics plant processing reformate into different fractions: light gasoline, a mixture of benzene and toluene, a mixture of xylene isomers and heavy aromatics for solvents production. The mixture of benzene and toluene is sent to Arosolvan unit in which benzene and toluene are separated into individual final products. The aim of this project is to implement strategies of energy integration and optimization in the two process units of the aromatics plant to improve its energy consumption at heat exchangers networks level.

For an energy performance evaluation, data was extracted from both process units in daily average from the instrumentation and control system of the respective process unit corresponding to the period 2014 – 2015. The variables measured are the ones with direct influence on heat exchanger networks: temperatures and flowrates. Data pre-processing and treatment was performed to remove missing and incoherent data. Outliers were also detected and removed using Mahalanobis Distance which have robust estimators for outliers detection. Two data matrixes were obtained with the following *nxp* dimensions: 706x55 for Pre-Distillation Unit and 620x86 for Arosolvan Unit.

For each data set, different operational scenarios were obtained using k-means clustering algorithm, a clustering analysis technique which partitions the data into different groups (clusters). Two cluster evaluation criteria were applied to determine the optimal number of clusters to be considered in the partitioning of the data set: Davis-Bouldin Criteria and Silhouette Value Criteria. These criteria were able to identify 6 clusters for Pre-Distillation Unit and 3 clusters for Arosolvan Unit. Silhouette plots were used to evaluate the quality of the different clusters which indicated well separated clusters and only few points not well assigned to any of the clusters. These clusters represent operational scenarios which were used as input for subsequent energy performance analysis of each process units.

To improve the efficiency of the processes units, two strategies were considered in this work. One strategy was Process Heat Integration using Pinch Technology and the other one was Optimization using a hybrid methodology combining Pinch Analysis and sequential methodology. Process-level Pinch Analysis was performed for each operational scenario and for a global scenario (overall mean values) of each process unit to estimate energy targets and the potential of energy savings. These potentials were compared concluding that there is no significant difference in terms of energy savings and utilities consumption and thus, the global scenario was considered for further energy integration and optimization studies. Therefore, it is possible a potential of energy savings of 34 % (7.9 MW) for Pre-Distillation Unit and a potential of energy savings of 8.3 % (3.7 MW) for Arosolvan Unit, considering a

ΔT_{MIN} of 10 ºC in both cases. The operating costs savings correspond to 1.05 M€ and 10.3 M€ for Pre-Distillation and Arosolvan Units, respectively.

A site wide energy performance analysis considering direct and indirect heat integration was also carried out. With direct heat integration, which considers that both process units are integrated as single unit, a total minimum utilities consumption of 56 MW was obtained considering intra-process heat recovery, while a total minimum utilities consumption of 54 MW was achieved with inter-process heat recovery, for a ΔT_{MIN} of 10 ºC. Total Site Analysis was the approach considered for an indirect heat integration evaluation which considers heat recovery using intermediate fluids. Total Site Profiles was the tool used to estimate energy targets for the whole site. A transfer heat stage was identified for a ΔT_{MIN} of 15 ºC in which only 680 kW can be transferred through a generated utility. The direct and indirect heat integration energy targets are considered unworthy and do not justify being used in further analysis nor for practical implementation due to equipment and piping costs required to overcome the drawbacks of the battery limits of each process unit and the distance between the process streams involved to achieve maximum energy recovery.

Retrofit design solutions were obtained for each process unit considering two retrofit methods: cross-pinch exchanger elimination method and pinch design method. The two methods were applied using heuristic rules and hybrid methodology. The best retrofit solution was selected based on total capital cost and payback period. For Pre-Distillation Unit, the best retrofit solution was found with pinch design method using heuristic rules. For this solution, an investment cost of 2,702 k€ is required, with a payback period of 2.57 years, for a total of 14 heat exchangers and a total heat transfer area of 7463 m^2 for fixed energy targets. However, a closer solution was found when considering cross-pinch exchanger elimination method using hybrid methodology being able to achieve an investment cost of 2,740 k€ with a payback period of 2.61. These results show that, it was possible to achieve an optimal solution with less HEN modifications to achieve minimum energy requirements. For Arosolvan Unit, the best retrofit solution found was also the one obtained with pinch design method using heuristic rules requiring 26 heat exchangers with a total heat transfer area of 16,975 m^2 which requires a total investment cost of 4,537 k€, which is considered a very high investment and a no viable solution for implementation.

Better solutions were expected in both case studies with hybrid methodology, due to the application of optimization models. However, the heat transfer area and its respective investment costs of the optimal network is determined considering the purchase of new equipment. For this reason, the optimal solution using hybrid methodology is lost as the existing heat transfer area is reallocated after obtaining the optimal network and thus, it is necessary to recalculate the investment cost required for the installation of these equipment. For future work, it would be interesting to integrate in the superstructure configuration model the attribution of the existing areas using binary variables to determine the actual minimum investment cost of the optimal network. In addition, the assumption of other types of configurations in the network superstructures may lead to different heat transfer area requirements than the already existing ones and thus, the possibility in re-using the existing heat exchangers is reduced.

In this work, the aim was to find heat exchanger network retrofit solutions for fixed energy targets and for this purpose a hybrid methodology integrating a sequential methodology was applied. In future works, a trade-off between operating costs and investments costs could be analysed by applying a different type of methodology, such as simultaneous methodology. Other considerations could be integrated in the referent study and in both referred methodologies, such as the use of more than one type of hot and cold utilities, different heat exchanger types and material, individual heat transfer coefficients specified for each process unit and utility, etc.

The energy integration and optimization of the Aromatics Plant was performed considering the already existing processes and strategies were implemented to obtained realistic solutions to achieve higher efficient processes without changing operating conditions nor considering the replace of the existing processes for new and more advance ones. For future work, new and more advanced technologies might be considered to improve process units or to evaluate an upgrade of the Aromatics Plant.

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Annexes

Annex I. Listing of Equipment of Heat Exchanger Network of Pre-Distillation Unit

The heat exchanger network of Pre-Distillation unit integrates several types of heat exchangers from shell and tube heat exchangers, coolers, heaters, reboilers, air coolers and drum condensers. The list and description of the installed heat exchangers are presented in Table I.1.

Table I.1: List of exchangers found in the heat exchanger network of Pre-distillation Unit.

Exchangers	ID	Description
Process-to-Process Heat Exchangers	E-0101	Reformate feed pre-heater
	E-0109	Reformate feed pre-heater
	E-0110	C8/C9+ cut cooler to cool clay towers feed (R0115 A/B)
Reboilers using hot utility	E-0102	Depentanizer tower reboiler (T0101)
	E-0108	Reboiler of BT cut tower (T0102)
Reboilers	E-0104	Depentanizer tower reboiler (T0101)
	E-0107	Reboiler of BT cut tower (T0102)
Cooling water	E-0103	$C5^-$ cut distillate cooler
	E-0117	Cooler to cool BT cut distillate from air cooler E-0111
	E-0118	$C9^+$ cut cooler before storage
	E-0119	C8 cut cooler before storage
	E-0120	$C8/C9^+$ cut cooler before storage
Drum Condensers	E-0106	Condenser for vapours residue of drum D0101
	E-0113	Condenser for vapours residue of drum D0102
	E-0116	Condenser for vapours residue of drum D0103
Air Coolers	E-0105	Air cooler to cool C5-cut from the top of depentanizer tower (T0101)
	E-0111	Air cooler to cool BT cut distillate from drum D0102
	E-0112	Air cooler to cool BT cut from the top of BT cut tower (T0102)
	E-0115 A	Air cooler to cool C8 cut from the top of $C8/C9^+$ tower (T0103)
	E-0115 B	Air cooler to cool $C8/C9^+$ cut from the top of $C8/C9^+$ cut tower (T0103)

Annex II. Listing of Equipment of Heat Exchanger Network of Arosolvan Unit

The heat exchanger network of Arosolvan unit integrates several types of heat exchangers from shell and tube heat exchangers, coolers, heaters, reboilers, air coolers and drum condensers. The list and description of the installed heat exchangers are presented in Table II.1.

Table II.1: List of exchangers considered in the heat exchanger network of Arosolvan unit.

Equipment	ID	Description
Heat Exchangers	E0206	Store BT is pre-heated
	E0207	Extract is pre-heated before being fed to extract recycle tower
	E0220	Water destillation tower condenser
	E0204	Reboiler of Water Distillation Tower (T0204)
	E0255	Aromatics Extracted are pre-heated before being fed to clay treatment tower and benzene from tower T0251 is cooled.
	E0260	Toluene distillate is cooled.
	E0259	Clay treatment feed is pre-heated.
Reboilers	E0202	Reboiler of tower T0202 heated by medium pressure steam
	E0205	Reboiler from water Distillation tower (T0204)
	E0251	Reboiler from Benzene tower (T0251)
	E0258	Reboiler from Toluene tower (T0252)
	E0208	Reboiler from tower T0202 heated by solvent from tower T0203
	E0254	Reboiler from Benzene tower (T0251)
	E0261	Bottom product from toluene tower (T0252) is cooled
Coolers	E0211 A/B	Non-aromatics from the top of tower T0205 are cooled
	E0210	Water wash cooler
	E0256	Pure benzene is cooled
	E0262	Bottom product from toluene tower (T0252) is cooled
Air Coolers	E0215	Solvent cooler
	E0216	Extract recycle stream obtained from top tower T0202 is cooled
	E0217	Aromatics separated from solvent in top tower T0203 is condensed
	E0218	Pure water from T0204 is cooed
	E0252	Extract recycle stream from tower T0252 is cooled
	E0264	Pure toluene from top tower T0252 is condensed

Annex III. Data Extraction from Process Flowsheet to Energy Consumption Analysis

The required data for an energy performance evaluation involves the identification of the main process streams, process stream heating and cooling information, heat exchangers involved and utilities type information. Data extraction is a very time consuming and critical activity, since the quality and realism of the retrofit solutions depend on the accuracy of the data.

In this work, two steps for data extraction were considered. First, data was extracted based on PFD and P&ID and Instrumental and Control System implemented in each process Unit. The data extracted contained only the variables with direct influence on heat exchanger transfer phenomena (temperatures and flowrates). These data sets were pre-processed and treated (removing missing data, incoherent data and possible outliers) for a multivariate statistical analysis through the application of a clustering technique to obtain different (and possibly critical) operational scenarios in terms of energy consumption. Secondly, data was extracted from each cluster to define the conditions in terms of temperatures and flowrates of the different operational scenarios. This second step is equivalent to the second data extraction procedure in this work for further accurate energy performance analysis.

Data Extraction from a process means collecting and processing Stream Data and Utility Data. Stream data integrates heating and cooling requirements of process streams, including evaporation and condensation of process streams (phase change), while Utility Data is in reference to heating and cooling requirements provided by utilities consumed within the process. Other types of data may also be collected if needed, such as economic data: cost of heat exchangers, operating costs (utilities consumption cost), heat exchangers costs, economic parameters, etc.

In retrofit cases, data is collected from process measurements which may require some data reconciliation. Missing operating data, which are not available and given by process instrumentation and control system, can be estimated using process simulations. In addition, it is possible to use the original specification sheets for the heat exchangers and use measurements from the plant. However, there are some situations in which measurements are missing and instruments may either not functioning or may give wrong data. In these cases, mass and energy balances are a very important task for data reconciliation. Some of these variables, which could not be extracted from instrumentation and control system of the process unit, were calculated from others performing energy and mass balances to the top and bottom of distillation columns and to heat exchangers.

Data Extraction from Process Unit Flowsheet for Energy Savings Evaluation

For an intra-process level Pinch Analysis, thermal data must be extracted from the operating process flowsheet, including the identification of process heating and cooling demands. In this step, heat and material balances are applied to determine the missing information of the process. The important information needed of process streams and utilities available to perform Pinch Analysis is:

- Supply/inlet (T_{inlet}) and target/outlet (T_{outlet}) temperatures of each stream;
- Mass flowrates (F);
- Average specific heat (Cp);
- Average heat capacity flowrate (MCp);

- Enthalpy of vaporization and condensation when occurs phase changes;
- Average heat transfer coefficient (h) of process streams;
- Global heat transfer coefficient (U) of a heat exchanger;
- External hot utility (HU) and cold utility (CU) costs;

For example, mass balance are required in the determination of the bottom and top product of the distillation columns, and energy balances are required to determine the heat exchanged between two streams or the heat required for a condensation or vaporization process. Heat is the energy that is transferred when there is a temperature difference occurring from the highest temperature to the lower temperature until thermal equilibrium is achieved (temperature difference is zero). Heat is associated to many industrial processes such as distillation units, evaporation units, heat exchangers networks, etc. Heat transfer rate (Q) measures the heat that is transferred through time and the heat flux ($\dot{Q}$) is the quantity of heat that is transfer along time and by heat transfer area (A) as in Equation III.1.

$$\mathbf{q} = \frac{\dot{\mathbf{q}}}{\mathbf{A}}$$ **Equation III.1**

A heat exchanger allows the heat transfer between two or more fluids at different temperatures. The design of a heat exchanger must have in consideration the heat transfer effects between the involved fluids and the pressure drop that fluids suffer crossing the heat exchanger. Heat exchangers are used in many industrial processes: distillation processes, refrigeration processes, heat recovery systems, etc. To design a heat transfer equipment or to analyze an existing one, it is necessary to establish a relation between the quantities of heat transferred with the inlet and outlet temperatures of the fluids, global coefficients of heat transfer and heat transfer surface area.

The energy balances to hot and cold fluids allows to obtain certain equations that establish the relation between the mentioned variables. In cases where heat is transfer in an isothermal system, which means heat transferred to the exterior of the system is not significant, is therefore not considered. Moreover, if kinetic and potential energy are not significant, if a phase change does not occur, and if the specific heat can be considered constant, then the energy balance to hot and cold fluids can be translated through the Equations III.2 and III.3, respectively. When a hot and a cold process streams transfer heat within the same heat exchanger, the heat supplied by the hot process stream (q_h) is equal to the heat required by the cold process stream (q_c).

Hot Fluid: $$\mathbf{q_h = m_h c_{p,h}(T_{q,in} - T_{q,out})}$$ **Equation III.2**

Cold Fluid: $$\mathbf{q_c = m_c c_{p,c}(T_{c,out} - T_{c,in})}$$ **Equation III.3**

In industrial plants, when condensation and evaporation operating units coexist within the overall process, some process streams suffer phase change. Thus, it is necessary to quantify the required enthalpy changes of process streams. From thermodynamics, a phase change corresponds to a total enthalpy flow (H) that a process stream undergoes when changing conditions. The enthalpy flow during a phase change (between bubble point and dew point of a process stream) can be determined through Equation III.4 where m is the mass flowrate (kg/hr) and λ is the specific enthalpy (kJ/kg) giving change in enthalpy flow the energy units (kJ/s = kW). The enthalpy flow varies according to temperature and heat capacity. For pure components, the process of a phase change occurs at saturation temperature. For mixtures, the process of a phase change is linear between dew point and bubble point of the mixture.

$$\mathbf{H} = \boldsymbol{md\lambda} \qquad \textbf{Equation III.4}$$

The overall energy balance for a process stream with phase change is given in Equation III.5.

$$\mathbf{Q} = \boldsymbol{m}\mathbf{cp}(\mathbf{T_{vapor}} - \mathbf{T_{DEWPOINT}}) + \boldsymbol{m\lambda} + \boldsymbol{m}\mathbf{cp}(\mathbf{T_{BUBLEPOINT}} - \mathbf{T_{Liquid}}) \qquad \textbf{Equation III.5}$$

In addition, enthalpy calculation of a process stream is in general a complicated function directly affected by stream pressure, temperature and composition. In Heat Integration, process streams are defined with fixed flowrates and compositions. In cases in which one of these conditions changes, a new process stream is considered. For example, a process stream as a top product of a distillation tower has the same composition as its distillate. However, in Heat Integration, these are considered two different process streams due to different flowrates. The influence of the pressure effect on enthalpy is here ignored to simplify the study. Another condition that was taken into account to simplify Pinch Analysis was the consideration of a constant heat capacity (cp) for process streams without phase change and a piece-wise linear relation with temperature and enthalpy variation for process streams with phase change (defined as segments in Aspen Energy Analyzer considering its dew and bubble points and its respective heat loads). In further energy optimization studies using mathematical programming model is developed to describe phase change behavior of a process stream.

Another important equation is heat exchanger project equation (Equation III.6) which establishes the relation between the thermal power, heat transfer surface area, global coefficient of heat transfer and the average of temperature differences between hot and cold fluids involved in heat transfer process more suitable for the heat exchanged in analysis. The parameter ΔT_{LM}, which is the average temperature difference between fluids, is determined based on the type of heat exchanger.

$$\mathbf{Q} = \mathbf{UA\Delta T_{LM}} \qquad \textbf{Equation III.6}$$

Data Extraction Principles

Some heuristic rules were developed for data extraction from a process flowsheet, which were introduced by Linnhoff (1998), that are considered here during the extraction of data within clusters:

a) All features of the given flowsheet or an existing design must not be considered to keep the degrees of freedom open in order not to overlook promising solutions for heat recovery systems;

b) Streams at different temperatures should not be mixed as it may eliminate potential heat recovery solutions. In this case, this condition may bring advantage and disadvantage for the analysis, depending on its level and the processes involved. For example, in heat exchanger networks, mixers of the same process streams with the same composition can act as a heat exchanger, thus saving capital cost. On the other hand, mixing streams with different composition is only an option if the streams are entering the same unit operation, such as a chemical reactor;

c) Utilities stream data shouldn't be included to establish minimum utility requirements. However, there are cases where it is not so easy to distinguish whether a stream is a process stream or acts as a utility;

d) There is a certain reluctance in the process industries to accept heat integration solutions from an operational point of view. Thus, do not accept the prejudice of colleagues against heat integration. However, it is a fact that most industrial processes are heavily integrated, and rather than focusing on maximum heat recovery, one should focus on correct or appropriate heat integration. In addition, it should be mentioned that when the economic potential of heat integration is established and well documented, it is often easier to get acceptance for such projects.

e) Distinguish between soft and hard stream data. It is important to differentiate that some stream data must be considered as hard specifications, while others can be adjusted if that improves or simplifies the heat recovery system. For example, an inlet temperature to a distillation column must often be regarded as a hard specification (not changed), while the target temperature of a process stream going to some sort of storage can be manipulated (example of soft process data). Specifying a low target temperature for a hot product stream going to storage than the minimum required will increase the need for external cooling if the target temperature is below the pinch temperature. Instead, this cooling could have been taken care of by nature itself through convective heat losses to the environment.

Data Extraction for Pre-Distillation Unit and Arosolvan Unit

For an energy efficiency evaluation of Pre-Distillation and Arosolvan Units, it was considered the data extracted and reconciled for the equipment listed in Annex I and II, respectively. Also, it was only considered the installed heat exchangers that operate continuously. Heat exchangers that only operate periodically to establish some temperature balances are left out of the analysis. For example, in the case of Pre-Distillation Unit, heat exchangers operating periodically (E0110, E0117 and E0120) and drum condensers (E0106, E0113 and E0116) were not considered in the analysis.

The resultant thermal data for the global scenario of Pre-Distillation Unit is here presented in the Tables III.1 to III.4. The resultant thermal data for the global scenario of Arosolvan Unit is here presented in the Tables III.5 to III.8.

Table III.1: Heat loads of the installed process-to-process heat exchangers of Pre-Distillation Unit.

ID	Heat Exchanger Type	TEMA	Stream	Stream type	F (kg/hr)	Cp (kJ/kgºC)	T_{inlet} (ºC)	T_{outlet} (ºC)	MCp (MW/ºC)	Q (MW)	Actual Area (m^2)
E0101	Exchanger	Double Pipe	C8's cut	Hot	19,465	2.55	130.7	108.7	0.0138	0.303	33.20
			Reformate	Cold	75,309	2.10	24.8	31.7	0.0439		
E0109	Shell&Tube	BES Horizontal (floating head)	$C9^+$ cut	Hot	11,634	2.68	244.2	42.2	0.00866	1.75	301.2
			Reformate	Cold	75,309	2.13	31.7	71.00	0.0445		

Table III.2: Heat loads of the installed reboilers of Pre-Distillation Unit.

ID	Heat Exchanger Type	TEMA	Stream	Stream type	F (kg/hr)	Cp (kJ/kgºC)	ʎ (kJ/kgºC)	T_{inlet} (ºC)	T_{outlet} (ºC)	MCp (MW/ºC)	Q (MW)	Actual Area (m^2)
E0102	Reboiler Thermosyphon	BEM Vertical (fixed tubes)	MP Steam	Hot	2,780	-	2832	215	215	-	2.19	474.9
			$C6/C7^+$ cut R1	Cold	-	-	-	144.6	148.5	0.562		
E0108	Reboiler Thermosyphon	BES Vertical (floating head)	MP Steam	Hot	3,723	-	2832	215	215	-	3.28	1139
			$C8/C9^+$ cut R2	Cold	-	-	-	152.4	163.5	0.295		
E0104	Reboiler Thermosyphon	BES Vertical (floating head)	C8's cut	Hot	26,579	1.87	-	202.7	202.6	0.010	0.00105	484.4
						311	1768	202.6	201.7	2.296	2.21	
						2.47	-	201.7	178.2	0.019	0.441	
			$C6/C7^+$ cut R2	Cold	-	-	-	144.6	146.8	1.205	2.65	
E0107	Reboiler Thermosyphon	BES Vertical (floating head)	C8's cut	Hot	68,257	1.87	410	202.7	202.6	0.027	0.0027	1930
						311	1768	202.6	201.7	5.89	5.66	
						2.47	51.8	201.7	178.2	0.0489	1.15	
			$C8/C9^+$ cut	Cold	-	-	-	152.4	163.1	0.637	6.81	

Table III.3: Heat loads of the installed coolers of Pre-Distillation Unit.

ID	Heat Exchanger Type	TEMA	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	Actual Area (m^2)
E0103	Cooler	BEM Horizontal (fixed tubes)	$C5^-$ cut distillate	Hot	4740	2.51	33.5	32.5	0.00330	0.0033	8.031
			Cooling water	Cold	284	4.18	20	30	0.00033		
E0118	Cooler	BEM Horizontal (fixed tubes)	$C9^+$ cut	Hot	11,634	1.82	42.2	32.5	0.00588	0.057	107.3
			Cooling water	Cold	4909	4.18	20	30	0.0057		
E0119	Cooler	BES Horizontal (floating head)	C8 cut	Hot	19,465	1.94	108.7	32.5	0.0105	0.798	257.6
			Cooling water	Cold	68727	4.18	20	30	0.0798		

Table III.4: Heat loads of the installed air coolers of Pre-Distillation Unit.

ID	Heat Exchanger Type	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	ʎ (kJ/kg°C)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	Actual Area (m^2)
E0105	Air cooler	$C5^-$ cut	Hot	13,985	1.85	-	67.2	64.6	0.00731	0.019	1250
					-	2033	64.6	58.1	0.202	1.31	
					1.30	-	58.1	33.5	0.0103	0.253	
		Air	Cold	113904	1	-	20	70	0.0316	1.58	
E0112	Air cooler	BT Cut	Hot	95,317	-	2055	93.2	79.3	0.691	9.61	2698
					2.41	-	79.3	71.9	0.0641	0.474	
		Air	Cold	726048	1	-	20	70	0.202	10.08	
E0111	Air cooler	BT Cut	Hot	35,854	2.38		71.9	67.5	0.0239	0.105	27.42
		Air	Cold	7560	1	-	20	70	0.00210	0.105	
E0115 B	Air cooler	C8's Cut	Hot	94,836	2.21	-	178.2	130.7	0.0615	2.92	271.3
		Air	Cold	210240	1		20	70	0.0584	2.92	
E0115 A	Air cooler	C8 cut	Hot	15,438	1.87	-	202.7	202.6	0.00607	0.000607	142.2
					-	1949	202.6	201.7	1.333	1.28	
					2.47	-	201.7	178.2	0.0311	0.732	
		Air	Cold	144908	1		20	70	0.0403	2.01	

Table III.5: Heat loads of the installed process-to-process heat exchangers of Arosolvan Unit.

ID	Heat Exchanger Type	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	MCp (kJ/kg)	Q (kJ/hr)
E0206	Shell&Tube	BT cut	Cold	11,283	2.14	31.5	72.5	0.00671	0.275	24146	990000
		Solvent (NMP,MEG)	Hot	148,979	2.14	80	76.90	0.0887		319355	
E0207	Shell&Tube	Extract	Cold	173091	2.32	56.2	105.4	0.111	5.48	400976	19728000
		Solvent (NMP,MEG)	Hot	148,979	2.41	135	80.0	0.0996		358691	
E0220	Shell&Tube	Water vapor	Hot	530	2330	105.1	105.06	8.263	0.3305	29745000	1189800
					4.33	105.06	72.4	0.00066	0.0215	2370	77400
		Solvente NMP + Water	Cold	12640	2.41	60.7	102.3	0.00846	0.352	30462	1267200
E0204	Shell&Tube	Extract Recycle	Hot	180683	2.47	138	126.3	0.124	1.45	446154	5220000
		Solvent Glicol + Water	Cold	-	-	115	116.2	1.208		4350000	
E0255	Shell&Tube	Pure Benzene	Hot	5225	2.01	91.1	60	0.00291	0.0906	10487	326160
		Aromatics Extracted	Cold	24480	1.40	50	59.5	0.00954		34333	
E0259	Shell&Tube	Tolueno Distillate	Hot	13482	2.02	109.7	75	0.00758	0.263	27285	946800
		Aromatics Extracted	Cold	24480	1.09	59.5	95	0.00741	0.263	26670	946800
E0253	Shell&Tube	Solvent (NMP,MEG)	Hot	148979	2.44	140	134.6	0.101	0.546	364000	1965600
		Aromatics Extracted	Cold	24480	3.01	96	122.7	0.0204		73618	

Table III.6: Heat loads of the installed reboilers of Arosolvan Unit.

ID	Heat Exchanger Type	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	λ (kJ/kg)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	MCp (kJ/kg)	Q (kJ/hr)
E0202	Reboiler	MP Steam	Hot	7394	-	2832	195	175	-	5.73	-	20628000
	Thermosyphon	Extract reflux	Cold	-	-	-	138.4	160.4	0.2605		937636	
E0203	Reboiler	MP Steam	Hot	12,584	-	2832	195	174	-	9.74	-	35064000
	Thermosyphon	Solvent (NMP + MEG) R1	Cold	-		-	165.4	165.5	97.4		3.51E+08	
E0205	Reboiler	MP Steam	Hot	2603	-	2832	195	175	-	2.02	-	7254000
	Thermosyphon	Solvent Glicol + Water	Cold	-	-	-	115	122.4	0.272		980270	
E0251	Reboiler	MP Steam	Hot	6453		2832	195	174	-	5.08	-	18288000
	Thermosyphon	T0251 BTM Liquid	Cold	-	-	-	132	132.4	12.7		45720000	
E0258	Reboiler	MP Steam	Hot	4309	-	2832	195	175	-	3.39	-	12204000
	Thermosyphon	T0252 BTM Liquid	Cold	-	-	-	161.4	161.5	33.9		1.22E+08	
E0208	Reboiler	Solvent (NMP,MEG)	Hot	148979	2.53	-	165.4	150	0.105	1.61	377065	5806800
	Thermosyphon	Extract WNA reflux 1	Cold	-	-	-	138	140.5	0.645		2322720	
E0254	Reboiler	T0251 BTM Liquid	Cold	-	-	-	132	133.4	0.731	1.02	2633143	3686400
	Thermosyphon	Solvent	Hot	148,979	2.47		150	140	0.102		368640	
E0261	Reboiler	C9 cut (T0252 BTM Liq)	Hot	-	-	-	161.4	103	0.000257	0.015	925	54000
	Thermosyphon	Aromatics Extracted	Cold	24480	2.21	-	95	96	0.015		54000	

Table III.7: Heat loads of the installed coolers of Arosolvan Unit.

ID	Heat Exchanger Type	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	MCp (kJ/kg)	Q (kJ/hr)
E0211 A/B	Shell&Tube	Light Non Aromatics	Hot	12971	2.37	60.7	33.1	0.00855	0.236	30783	849600
		Cooling Water	Cold	20325	4.18	20	30	0.0236		84960	
E0210	Shell&Tube	Pure Water Destillate	Hot	2615	4.33	72.4	65	0.00315	0.0233	11335	83880
		Cooling Water	Cold	2007	4.18	20	30	0.00233		8388	
E0256	Shell&Tube	Pure Benzene	Hot	5225	1.84	60	24.7	0.00267	0.0944	9627	339840
		Cooling Water	Cold	8130	4.18	20	30	0.00944		33984	
E0260	Shell&Tube	Toluene	Hot	13482	1.82	75	30.5	0.00681	0.303	24512	1090800
		Cooling Water	Cold	26096	4.18	20	30	0.0303		109080	

Table III.8: Heat loads of the installed air coolers of Arosolvan Unit.

ID	Heat Exchanger Type	Stream	Stream type	F (kg/hr)	Cp (kJ/kg°C)	λ (kJ/kg)	T_{inlet} (°C)	T_{outlet} (°C)	MCp (MW/°C)	Q (MW)	MCp (kJ/kg)	Q (kJ/hr)
E0215	Air Cooler	Solvent (NMP,MEG)	Hot	148979	2.19	-	76.9	62.54	0.0906	1.30	326156	4683600
		Air Cooling	Cold	93672	1	-	20	70	0.0260		93672	
E0216	Air Cooler	Extract recycle product	Hot	25356	1.61	-	72.8	62.2	0.0113	0.120	40755	432000
					-	388	62.2	48.5	0.1993	2.73	717372	9828000
					2.16	-	48.5	28.1	0.0152	0.31	54706	1116000
		Air Cooling	Cold	227520	1	-	20	70	-	3.16	-	11376000
E0217	Air Cooler	Aromatics, Glicol	Hot	46161	-	390	49.6	49.4	25	5.00	90000000	18000000
					1.79	-	49.4	30.5	0.0230	0.434	82667	1562400
		Air Cooling	Cold	1956240	1	-	20	30	-	5.43	-	19562400
E0218	Air Cooler	Water vapor	Hot	2864	-	2245.3	105.1	105.06	44.68	1.79	160830000	6433200
					4.46	-	105.06	72.4	0.00355	0.116	12786	417600
		Air Cooling	Cold	137016	1	-	20	70	-	1.90	-	6850800
E0252	Air Cooler	Benzene (top product)	Hot	34596	1.31	-	89.1	86	0.0125	0.0389	45174	140040
					-	389	86	85.98	187	3.74	673200000	13464000
					2.04	-	85.98	75.4	0.0196	0.207	70435	745200
		Air Cooling	Cold	286985	1		20	70	-	3.99	-	14349240
E0264	Air Cooler	Tolueno	Hot	23754	1.54	-	128.8	128.77	0	0	0	0
					-	349	128.77	128.77	23	2.30	36581	8290800
					2.16	-	128.77	109.7	0.014263	0.272	51348	979200
		Air Cooling	Cold	185400	1	-	20	70	-	2.58	-	9270000

Annex IV. Energy targets evaluation for different ΔT_{MIN} values

Through heat exchangers design data, several values to attribute to ΔT_{MIN} were found and used to evaluate energy targets possible to be achieved. Though, the typical values for ΔT_{MIN} for the type of industry were respected. For chemical and petrochemical industries the typical values for ΔT_{MIN} are between 10 - 20 ºC. Therefore, energy targets were estimated for several minimum temperature difference values in this range found using heat exchanger design data for both process units. The results are presented in Tables IV.1 and IV.2.

Table IV.1: Results for the variation of potential of energy savings with ΔT_{MIN} for Pre-Distillation Unit.

ΔT_{MIN} (°C)	Utilities	Actual Consumption (MW)	Total Real Consumption (MW)	Energy Targets (MW)	Total Minimum Consumption (MW)	Energy Savings (MW)	Total Energy Savings (MW)	Potential of Energy Savings (%)
10	Heating	5.12	22.9	1.525	15.1	3.60	7.8	34.0
	Cooling	17.8		13.62		4.2		
11	Heating	5.12	22.9	1.608	15.3	3.51	7.6	33.3
	Cooling	17.8		13.7		4.1		
15	Heating	5.12	22.9	1.939	16.0	3.18	7.0	30.4
	Cooling	17.8		14.03		3.8		
16	Heating	5.12	22.9	2.02	16.1	3.10	6.8	29.7
	Cooling	17.8		14.11		3.7		
20	Heating	5.12	22.9	2.352	16.8	2.77	6.1	26.8
	Cooling	17.8		14.44		3.4		

Table IV.2: Results for the variation of potential of energy savings with ΔT_{MIN} for Arosolvan Unit.

ΔT_{MIN} (°C)	Utilities	Actual Consumption (MW)	Total Real Consumption (MW)	Energy Targets (MW)	Total Minimum Consumption (MW)	Energy Savings (MW)	Total Energy Savings (MW)	Potential of Energy Savings (%)
10	Heating	26	45.0	24.1	41.2	1.90	3.8	8.4
	Cooling	19.0		17.1		1.9		
15	Heating	26	45.0	25.56	44.2	0.44	0.8	1.8
	Cooling	19.0		18.62		0.4		
17	Heating	26	45.0	26.01	45.1	0.0	0.0	0.0
	Cooling	19.0		19.07		0.0		
20	Heating	26	45.0	26.68	46.4	0.0	0.0	0.0
	Cooling	19.0		19.74		0.0		

Annex V. Readjust Data to Represent Current Heat Exchanger Network in Grid Diagram

Grid diagram is a graphical tool of Pinch Analysis useful to represent the current heat exchanger network. Aspen Energy Analyzer is used to construct grid diagrams for each process unit. Thus, it is required a readjustment of the data to specify it in the software, such as the process streams and its operating conditions: supply temperatures (T_{INLET}), target temperatures (T_{OUTLET}), heat loads (Q) and heat capacity flowrates (MCp), which is the product of the specific heat capacity of the process stream (Cp) and the mass flow rate of the process stream. The input data to be used in Aspen Energy Analyzer for hot and cold process streams of Pre-Distillation Unit are presented in Tables V.1 and V.2 and of Arosolvan Unit in Tables V.3 and V.4.

Table V.1: Input data of cold process streams of Pre-Distillation Unit for Aspen Energy Analyzer.

ID	Process Stream		F (kg/hr)	T_{inlet} (ºC)	T_{outlet} (ºC)	Q (MW)	MCp (MW/ºC)
C1	Reformate	↗	75309	24.8	31.7	0.303	0.0439
				31.7	71.0	1.75	0.0445
C2	C8C9 R1	↗	963077	152.4	163.1	6.81	0.6364
C3	C8C9 R2	↗	446968	152.4	163.5	3.28	0.295
C4	C6C7 R1	↗	863905	144.6	148.5	2.19	0.562
C5	C6C7 R2	↗	1853147	144.6	146.8	2.65	1.20

Table V.2: Input data of hot process streams of Pre-Distillation Unit for Aspen Energy Analyzer.

ID	Process Stream		F (kg/hr)	T_{inlet} (ºC)	T_{outlet} (ºC)	Q (MW)	MCp (MW/ºC)
H1	C9^{+} CUT	↙	11,624	244.2	42.2	1.75	0.00866
				42.2	32.5	0.057	0.00588
H2	C8^{+} CUT	↙	110,274	202.7	202.6	0.00434	0.0434
				202.6	201.7	9.15	10.17
				201.7	130.7	5.25	0.0739
H3	C8^{+} CUT DIST	↙	19,465	130.7	108.7	0.303	0.0138
				108.7	32.5	0.798	0.0105
H4	BT CUT	↙	95,317	93.2	79.3	9.61	0.6914
				79.3	71.9	0.474	0.0641
H5	BT CUT DIST	↙	35,854	71.9	67.5	0.105	0.0239
H6	C5^{-} CUT	↙	13,985	67.2	64.6	0.019	0.00731
				64.6	58.1	1.31	0.202
				58.1	33.5	0.253	0.0103
H7	C5^{-} CUT	↙	4,740	33.5	32.5	0.0033	0.0033

Table V.3: Input data of cold process streams of Arosolvan Unit.

ID	Process Stream		F (kg/hr)	T_{inlet} (ºC)	T_{outlet} (ºC)	Q (MW)	MCp (MW/ºC)
C1	Aromatics Extracted	↗	24,480	50	59.5	0.0906	0.00954
				59.5	95	0.263	0.00741
				95	96	0.015	0.0150
				96	122.7	0.546	0.0204
C2	Solvent Glicol R2	↗	-	115	122	2.02	0.289
C3	Solvent Glicol R1	↗	-	115	116.2	1.45	1.21
C4	Extract Feed	↗	173,091	56.2	105.4	5.476	0.111
C5	Solvent (NMP+H2O)	↗	12,640	60.7	102.3	0.352	0.00846
C6	BT CUT	↗	11,283	31.5	72.5	0.275	0.00671
C7	Solvent (NMP+MEG) R1	↗	-	165.4	165.5	9.74	97.4
C8	T0252 BTM R1	↗	-	161.4	161.5	3.39	33.9
C9	Extract R2	↗	-	138	160.3	5.49	0.246
				160.3	160.4	0.24	2.40
C10	Extract R1	↗	-	138	140.5	1.61	0.644
C11	T0251 BTM R1	↗	-	132	133.4	1.02	0.729
C12	T0251 BTM R2	↗	-	132	132.4	5.08	12.70

Table V.4: Input data of hot process streams of Arosolvan Unit.

ID	Process Stream		F (kg/hr)	T_{inlet} (ºC)	T_{outlet} (ºC)	Q (MW)	MCp (MW/ºC)
H1	Solvent (NMP+MEG)	↙	148,979	165.4	150	1.61	0.105
				150	140	1.02	0.102
				140	134.6	0.546	0.101
				134.6	80.0	5.48	0.100
				80	76.9	0.275	0.089
				76.9	62.5	1.30	0.090
H2	C9 CUT	↙	417	161.4	103	0.015	0.000257
H3	Extract WNA	↙	25,356	138	126.3	1.45	0.124
H4	Toluene	↙	23,754	128.8	127.8	2.3	2.300
				127.8	109.7	0.272	0.015
H5	Toluene Dist	↙	13,482	109.7	75	0.263	0.008
				75	30.5	0.304	0.007
H6	Pure Water	↙	530	105.1	105.06	2.12	53.000
				105.06	72.4	0.138	0.004
H7	Benzene 2	↙	5,225	91.1	60	0.0906	0.003
				60	24.7	0.0944	0.003
H8	Benzene 1	↙	5,225	89.1	86	0.0389	0.013
				86	85.96	3.74	93.500
				85.96	75.4	0.207	0.020
H9	Extract Recycle Product	↙	180,683	72.8	62.2	0.119	0.011
				62.2	48.5	2.73	0.199
				48.5	28.1	0.306	0.015
H10	Pure Water Dist	↙	2,615	72.4	60	0.0233	0.002
H11	Light Non Aromatics	↙	12,971	60.7	33.1	0.236	0.009
H12	Aromatics Sat Glicol	↙	46,161	49.6	49.4	5.00	25.000
				49.4	30.5	0.434	0.023

Process streams operating conditions are defined as they enter and exit the heat exchanger network. For cold process streams, the enthalpy change is the total heat load required to heat the stream from its supply temperature to the target temperature. For hot process streams, the enthalpy change is the total heat load required to cold the stream from its supply temperature to the target temperature. For large temperature difference, supply and target temperatures must be segmented at different ranges of temperature (in this case, according to the results obtained for heat loads of the installed heat exchangers) to accurately portray MCp values of the process streams. For example, segmenting a stream becomes necessary when the heat capacity of a stream is not approximately constant over its temperature range across the heat exchanger network, mostly when dealing with large variations in heat capacity resulting from a phase change of a process stream.

Annex VI. Data Information Required to Estimate Bare Module Equipment Cost

Heat exchanger retrofit projects were evaluated economically using Bare Module Equipment Cost method to estimate the investment cost of new equipment. The total capital cost must have in consideration direct and indirect project expenses as the ones described in Table VI.1.

Table VI.1: Factor Affecting the Cost Associated with Evaluation of Capital Cost of Chemical Plants (Turton et al., 2018).

Factors Associated with the Installation of Equipment	Symbol	Comments
1. Direct project expenses		
(a) Equipment FOB cost	C_p	Purchased cost of equipment at manufacturer's site (FOB = free on board).
(b) Materials required for installation	C_M	Includes all piping, insulation and fire proofing, foundations and structural supports, instrumentation and electrical, and painting associated with the equipment.
(c) Labor to install equipment and material	C_L	Includes all labor associated with installing the equipment and materials mentioned in (a) and (b).
2. Indirect project expenses		
(a) Freight, insurance, and taxes	C_{FIT}	Includes all transportation costs for shipping equipment and materials to the plant site; all insurance on the items shipped; and any purchase taxes that may be applicable.
(b) Contractor's overhead	C_O	Includes all fringe benefits such as vacation, sick leave, retirement benefits, etc.; labor burden such as social security and unemployment insurance, etc.; and salaries and overhead for supervisory personnel.
(c) Contractor engineering expenses	C_E	Includes salaries and overhead for the engineering, drafting, and project management personnel on the project.
3. Contingency and fee		
(a) Contingency	C_{Cont}	A factor included to cover unforeseen circumstances. These may include loss of time due to storms, strikes, small changes in the design, and unpredicted price increases.
(b) Contractor's fee	C_{Fee}	This fee varies depending on the type of plant and a variety of other factors.
4. Auxiliary facilities		
(a) Site development	C_{site}	Includes the purchase of land; grading and excavation of the site; installation and hook-up of electrical, water, and sewer systems; and construction of all internal roads, walkways, and parking lots.
(b) Auxiliary buildings	C_{Aux}	Includes administration offices, maintenance shop and control rooms, warehouses and service buildings (e.g., cafeteria, dressing rooms, and medical facility).
(c) Offsites and utilities	C_{Off}	Includes raw material and final product storage, raw material and final product loading and unloading facilities, all equipment necessary to supply required process utilities (e.g., cooling water, steam generation, fuel distribution systems, etc.), central environmental control facilities (e.g., wastewater treatment, incinerators, flares, etc.), and fire protection systems.

Data for constants K_1, K_2 and K_3 corresponding to the year 2001 to estimate the purchase of new equipment (C_p^0) are indicated in Table VI.2.

Table VI.2: Data for constants to estimate purchase equipment cost (Turton et al., 2018).

Equipment Type	Equipment Description	K_1	K_2	K_3	Capacity, Units	Min Size	Max Size
Heat exchangers	Scraped wall	3.7803	0.8569	0.0349	Area, m^2	2	20
	Teflon tube	3.8062	0.8924	−0.1671	Area, m^2	1	10
	Bayonet	4.2768	−0.0495	0.1431	Area, m^2	10	1000
	Floating head	4.8306	−0.8509	0.3187	Area, m^2	10	1000
	Fixed tube	4.3247	−0.3030	0.1634	Area, m^2	10	1000
	U-tube	4.1884	−0.2503	0.1974	Area, m^2	10	1000
	Kettle reboiler	4.4646	−0.5277	0.3955	Area, m^2	10	100
	Double pipe	3.3444	0.2745	−0.0472	Area, m^2	1	10
	Multiple pipe	2.7652	0.7282	0.0783	Area, m^2	10	100
	Flat plate	4.6656	−0.1557	0.1547	Area, m^2	10	1000
	Spiral plate	4.6561	−0.2947	0.2207	Area, m^2	1	100
	Air cooler	4.0336	0.2341	0.0497	Area, m^2	10	10,000
	Spiral tube	3.9912	0.0668	0.2430	Area, m^2	1	100
Heaters	Diphenyl heater	2.2628	0.8581	0.0003	Duty, kW	650	10,750
	Molten salt heater	1.1979	1.4782	−0.0958	Duty, kW	650	10,750
	Hot water heater	2.0829	0.9074	−0.0243	Duty, kW	650	10,750
	Steam boiler	6.9617	−1.4800	0.3161	Duty, kW	1200	9400

Data for constants C_1, C_2 and C_3 corresponding to the year 2001 to estimate the pressure factor (F_P) are indicated in Table VI.3.

Table VI.3: Constants for Pressure factors F_p for process equipment (Turton et al., 2018).

Equipment Type	Equipment Description	C_1	C_2	C_3	Pressure Range (barg)
Heat exchangers	Scraped wall	0	0	0	$P<40$
		0.6072	−0.9120	0.3327	$40<P<100$
		13.1467	−12.6574	3.0705	$100<P<300$
	Teflon tube	0	0	0	$P<15$
	Bayonet, fixed tube sheet, floating head, kettle reboiler, and U-tube (both shell and tube)	0 0.03881	0 −0.11272	0 0.08183	$P<5$ $5<P<140$
	Bayonet, fixed tube sheet, floating head, kettle reboiler, and U-tube (tube only)	0 −0.00164	0 −0.00627	0 0.0123	$P<5$ $5<P<140$
	Double pipe and multiple pipe	0	0	0	$P<40$
		0.6072	−0.9120	0.3327	$40<P<100$
		13.1467	−12.6574	3.0705	$100<P<300$
	Flat plate and spiral plate	0	0	0	$P<19$
	Air cooler	0	0	0	$P<10$
		−0.1250	0.15361	−0.02861	$10<P<100$
	Spiral tube (both shell and tube)	0	0	0	$P<150$
		−0.4045	0.1859	0	$150<P<400$
	Spiral tube (tube only)	0	0	0	$P<150$
		−0.2115	0.09717	0	$150<P<400$
Heaters	Diphenyl heater, molten salt heater, and hot water heater	0 −0.01633	0 0.056875	0 −0.00876	$P<2$ $2<P<200$
	Steam boiler	0	0	0	$P<20$
		2.594072	−4.23476	1.722404	$20<P<40$

Data for constants B_1 and B_2 corresponding to the year 2001 to estimate bare module cost (C_{BM}) are indicated in Table VI.4.

Table VI.4: Constants for Bare Module Factor C_{BM} (Turton et al., 2018).

Equipment Type	Equipment Description	B_1	B_2
Heat exchangers	Double pipe, multiple pipe, scraped wall, and spiral tube	1.74	1.55
	Fixed tube sheet, floating head, U-tube, bayonet, kettle reboiler, and Teflon tube	1.63	1.66
	Air cooler, spiral plate, and flat plate	0.96	1.21
Process vessels	Horizontal	1.49	1.52
	Vertical (including towers)	2.25	1.82
Pumps	Reciprocating	1.89	1.35
	Positive displacement	1.89	1.35
	Centrifugal	1.89	1.35

Annex VII. Additional Information of Retrofit Design of Pre-Distillation Unit using Heuristic Rules

For fixed energy targets, retrofit design solutions were found using two retrofit methods: cross-pinch exchanger elimination method and pinch design method. In both cases, maximum re-use of the existing heat exchangers were considered.

Results obtained through Cross-Pinch Exchanger Elimination Method

The operating conditions resultant from stream matches using cross-pinch exchanger elimination method are presented in the next Tables VII.1 and VII.2.

Table VII.1: Operating data resulting from stream matches above pinch point using cross-pinch exchanger elimination method of Pinch Analysis for Pre-Distillation Unit.

Units	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m^2)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
NU-1	MP STEAM	-	200	199	0.837	161.7	51.5	52.0
	C6C7R1	C3	147	148.5				
NU-2	MP STEAM	-	200	199	0.687	190.3	36.5	35.85
	C8C9R2	C2	163.1	163.5				
NU-3	C8CUT	H22	176.6	162.4	0.903	1668	13.62	10
	C8C9R2	C2	152.4	163				
NU-4	C8CUT	H21	202.7	162.4	1.67	568.3	39.41	10
	C8C9R2	C2	152.4	163.3				
NU-5	C8CUT	H2	162.4	154.6	0.577	459.2	15.52	10
	C6C7R1	C4	144.6	146.9				
NU-6	C9CUT	H1	244.2	154.6	0.776	202.6	97.09	10
	C6C7R1	C4	144.6	147.1				

Table VII.2: Operating data resulting from stream matches below pinch point using cross-pinch exchanger elimination method of Pinch Analysis for Pre-Distillation Unit.

Units	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m^2)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
NU-7	C8CUT	H2	154.6	130.7	1.77	193.7	83.63	99.44
	REFORMATE	C1	31.26	70.97				
NU-8	C9CUT	H1	154.6	32.5	1.03	199.8	124.6	12.5
	CW	-	20	30				
NU-9	BTCUT TOP PROD	H4	93.2	71.9	10.08	1661	63.2	51.9
	CW	-	20	30				
NU-10	BTCUT DIST	H5	67.5	71.9	0.105	23.52	41.9	47.5
	CW	-	20	30				
NU-11	C5CUT TOP PROD	H6	67.2	33.5	1.58	481.7	37.2	13.5
	CW	-	20	30				

The purchased cost of the equipment resultant from stream matches using cross-pinch exchanger elimination method are presented in Table VII.3. For this case, it was considered shell and tube heat exchangers with floating head as it's the type that provides an easier maintenance. For heat transfer areas lower than 10 m^2, it was considered double pipe exchangers. The existing heat exchangers can be reused if its respective heat transfer area is not higher than 15 to 30% of the heat transfer area required for the new duty.

In this method, well allocated heat exchangers were left out of the study, which means that they were kept in the network. These are E0104 and E0107 with a total heat transfer area of 2377 m^2 in the subnetwork above pinch point and E0101 with a total heat transfer area of 33.2 m^2 in the subnetwork below pinch point. Air coolers were replaced by coolers as the aim is to evaluate costs without consuming air cooling but only cooling water. Moreover, the two coolers E0103 (5 m^2) and E0119 (222 m^2) could be reused in the network for the same stream matches, a total of 260 m^2 heat transfer area is re-used without any cost associated. Also, the reboiler E0102 (480 m^2) can be re-used and reallocated in the place of NU- 5 to perform a new duty.

Table VII.3: Heat transfer areas and respective purchased equipment cost for stream matches obtaining above pinch point for Pre-Distillation Unit using cross-pinch exchanger elimination method.

Subnetwork	Units	Heat Exchanger	Process Stream	A (m^2)	A_{reused} (m^2)	Over Capacity (%)	K_1	K_2	K_3	$log_{10}(Cp^0)$	Cp^0 (euros)
ABOVE PINCH POINT	NU-1	Floating Head	- / C3	161.7	0	0	4.8306	-0.8509	0.3187	4.51	28212
	NU-2	Floating Head	- / C2	190.3	0	0	4.8306	-0.8509	0.3187	4.55	31004
	NU-3	Floating Head	H22 / C2	1668	0	0	4.8306	-0.8509	0.3187	5.40	219904
	NU-4	Floating Head	H21 / C2	568.3	0	0	4.8306	-0.8509	0.3187	4.90	70699
	NU-5	Floating Head	H2 / C4	459.2	479.9	4.31	4.8306	-0.8509	0.3187	4.82	58664
	NU-6	Floating Head	H1 / C4	202.6	0	0	4.8306	-0.8509	0.3187	4.56	32213
Bellow Pinch Point	NU-7	Floating Head	H2 / C1	193.7	0	0	4.8306	-0.8509	0.3187	4.55	31338
	NU-8	Floating Head	H1 / -	199.8	0	0	4.8306	-0.8509	0.3187	4.56	31938
	NU-9	Floating Head	H4 / -	1661	0	0	4.8306	-0.8509	0.3187	5.40	218795
	NU-10	Floating Head	H5 / -	23.52	0	0	4.8306	-0.8509	0.3187	4.26	16127
	NU-11	Floating Head	H6 / -	481.7	0	0	4.8306	-0.8509	0.3187	4.84	61106
Total Heat Transfer Reused Area Above Pinch Point (m^2)					2857.1						
Total Heat Transfer Reused Area Below Pinch Point (m^2)					259.67						
Total Additonal Heat Transfer Area Above Pinch Point (m^2)					2790.9						
Total Additonal Heat Transfer Area Below Pinch Point (m^2)					2559.7						
Total Heat Transfer Area (m^2)					8467.4						

Data for the purchased equipment cost ($C_P{}^0$), at ambient operating pressure and using carbon steel construction material, is indicated in Annex VI. In addition, heat exchangers that are kept in the same position with the same function don't have any cost associated. Heat exchangers being reallocated to new stream matches and heat loads have an installation cost associated which corresponds to 20 % of a new equipment cost determined through Bare Module Equipment Cost. For new exchangers, total Bare Module Equipment Cost is considered. The Chemical Engineering Plant Cost Index of the year 2001 (CEPCI = 394) was assumed for all inflation adjustments. Using the values provided by Turton et al. (2018), CEPCI was updated using interpolation for 2018 (CEPCI = 591.3).

Bare cost module for the required equipment, including the installation cost of E0102 in place of NU-5 (CBM reuse) are presented in the next Tables VII.4 and VII.5.

Table VII.4: Bare Cost module for equipment above pinch point (2001) for Pre-Distillation Unit with cross-pinch elimination method.

Units	Heat Exchanger Type	Heat Exchanger	Cp^0 (dollar)	Fp	FM	B1	B2	FBM	CBM (euros)
NU-1	Floating Head	BES Vertical	32059	1	1	1.63	1.66	3.29	92818
NU-2	Floating Head	BES Vertical	35232	1	1	1.63	1.66	3.29	102004
NU-3	Floating Head	BES Vertical	249891	1	1	1.63	1.66	3.29	723485
NU-4	Floating Head	BES Vertical	80340	1	1	1.63	1.66	3.29	232599
NU-5	Floating Head	BES Vertical	69216	1	1	1.63	1.66	3.29	38601
NU-6	Floating Head	BES Vertical	36606	1	1	1.63	1.66	3.29	105981
Total Bare Cost module (euros) 2001				**1,295,489.57 €**					
Total Bare Cost module (euros) 2018				**1,944,220.77 €**					

Table VII.5: Bare Cost module for equipment below pinch point (2001) for Pre-Distillation Unit with cross-pinch elimination method.

Units	Heat Exchanger Type	Heat Exchanger	Cp^0 (dollar)	Fp	FM	B1	B2	FBM	CBM (euros)
NU-7	Floating Head	BES horizontal	35611	1	1	1.63	1.66	3.29	103102
NU-8	Floating Head	BES horizontal	36293	1	1	1.63	1.66	3.29	105074.7
NU-9	Floating Head	BES horizontal	248631	1	1	1.63	1.66	3.29	719836
NU-10	Floating Head	BES horizontal	18326	1	1	1.63	1.66	3.29	53057
NU-11	Floating Head	BES horizontal	69439	1	1	1.63	1.66	3.29	201039
Total Bare Cost module (euros) 2001				**1,182,109.68 €**					
Total Bare Cost module (euros) 2018				**1,774,064.60 €**					

Results obtained through Pinch Design Method for Retrofit Design

The operating conditions resultant from stream matches using pinch design method with maximum reuse of the existing heat exchangers are presented in the next Tables VII.6 and VII.7. The purchased cost of the equipment resultant from stream matches using cross-pinch exchanger elimination method are presented in the next Table VII.8.

Table VII.6: Operating data resulting from stream matches above pinch point using pinch design method of Pinch Analysis for Pre-Distillation Unit.

Exchangers	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m^2)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
HEATX-1	MP Steam	-	200	199	1.53	286	53.2	53.47
	C6/C7R2	C5	145.5	146.8				
HEATX-2	C8CUT	H2	202.7	202.6	0.349	60.93	57.14	57.32
	C6C7R2	C5	145.5	145.2				
HEATX-3	C8CUT	H2	202.6	201.9	6.82	1715	39.46	49.46
	C8C9R1	C2	163.1	152.4				
HEATX-4	C8CUT	H2	201.9	184.2	3.28	932.2	38.36	31.8
	C8C9R2	C3	163.5	152.4				
HEATX-5	C8CUT	H2	184.2	154.6	2.19	1084	35.7	10
	C6C7 R1	C4	148.5	144.6				
HEATX-6	C9CUT	H2	244.2	154.6	0.776	200	98.96	10
	C6C7R2	C5	145.2	144.6				

Table VII.7: Operating data resulting from stream matches below pinch point using pinch design method of Pinch Analysis for Pre-Distillation Unit.

Exchangers	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m^2)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
HEATX-7	C9 CUT	H1	154.6	121.7	0.285	40.94	83.63	51.16
	Reformate	C1	71	64.58				
HEATX-8	C8 CUT	H2	154.6	130.7	1.77	180.9	90.02	105.9
	Reformate	C1	64.58	24.8				
HEATX-9	C9 CUT	H1	121.7	32.5	0.746	176.9	91.73	12.5
	CW	-	20	30				
HEATX-10	C8 CUT DISTILLATE	H3	130.7	32.5	1.1	250.3	100.7	12.5
	CW	-	20	30				
HEATX-11	BT CUT TOP	H4	93.2	71.9	10.08	1661	63.2	51.9
	CW	-	20	30				
HEATX-12	BT CUT DISTILLATE	H5	71.9	67.5	0.105	23.52	41.9	47.5
	CW	-	20	30				
HEATX-13	C5 CUT TOP PROD	H6	67.2	33.5	1.58	481.7	37.2	13.5
	CW	-	20	30				
HEATX-14	C5 CUT DISTI	H7	33.5	32.5	0.033	4.67	3.5	12.5
	CW	-	20	30				

Bare cost module for the required equipment, including the installation cost of E0102 in place of NU-5 (CBM reuse) are presented in the next TablesVII.8 to VII.10. For the net heat source, E0102 and E0104 (HEATX-4), E0107 (HEATX-3), and E0108 (HEATX-5). For the net heat sink, the existing heat exchangers that can be re-used to minimize additional heat transfer area are E0103 (HEATX-14), E0109 (HEATX-20) and E0118 (HEATX-9).

Table VII.8: Heat transfer areas and respective purchased equipment cost for stream matches obtaining above pinch point for Pre-Distillation Unit pinch design method.

	Units	Heat Exchanger	Process Stream	Process Stream	A (m^2)	A_{reused} (m^2)	Over Capacity (%)	K_1	K_2	K_3	$log_{10}(Cp^0)$	Cp^0 (euros)
ABOVE PINCH POINT	HEATX-1	Reboiler	MP Steam C6/C7R2	- C5	286	0	0	4.8306	-0.8509	0.3187	4.66	40543
	HEATX-2	Reboiler	C8CUT C6C7R2	H2 C5	60.93	0	0	4.8306	-0.8509	0.3187	4.33	18691
	HEATX-3	Reboiler	C8CUT C8C9R1	H2 C2	1715	1881	8.8	4.8306	-0.8509	0.3187	5.46	254616
	HEATX-4	Reboiler	C8CUT C8C9R2	H2 C3	932.2	976	4.5	4.8306	-0.8509	0.3187	5.14	120107
	HEATX-5	Reboiler	C8CUT C6C7 R1	H2 C4	1084	1139	4.8	4.8306	-0.8509	0.3187	5.21	141804
	HEATX-6	Reboiler	C9CUT C6C7R2	H2 C5	200	0	0	4.8306	-0.8509	0.3187	4.56	31957
BELOW PINCH POINT	HEATX-7	Shell&Tube	C9 CUT Reformate	H1 C1	40.94	0	0	4.8306	-0.8509	0.3187	19370	17046
	HEATX-8	Shell&Tube	C8 CUT Reformate	H2 C1	180.9	0	0	4.8306	-0.8509	0.3187	34186	30084
	HEATX-9	Cooler	C9 CUT CW	H1 -	176.9	221.8	20.2	4.8306	-0.8509	0.3187	38761	34110
	HEATX-10	Cooler	C8 CUT DIST CW	H3 -	250.3	301.2	16.9	4.8306	-0.8509	0.3187	47826	42087
	HEATX-11	Cooler	BT CUT TOP CW	H4 -	1661	0	0	4.8306	-0.8509	0.3187	248631	218795
	HEATX-12	Cooler	BT CUT DIS CW	H5 -	23.52	0	0	4.8306	-0.8509	0.3187	18326	16127
	HEATX-13	Cooler	C5 CUT TOP PROD CW	H6 -	481.7	0	0	4.8306	-0.8509	0.3187	69439	61106
	HEATX-14	Cooler	C5 CUT DISTI CW	H7 -	4.67	4.67	0	4.8306	-0.8509	0.3187	25347	22306
Total Heat Transfer Reused Area Above Pinch Point (m^2)					3996.1							
Total Heat Transfer Reused Area Below Pinch Point (m^2)					527.7							
Total Additonal Heat Transfer Area Above Pinch Point (m^2)					546.9							
Total Additonal Heat Transfer Area Below Pinch Point (m^2)					2392.7							
Total Heat Transfer Area (m^2)					7463.4							

Table VII.9: Bare Cost module for equipment above pinch point (2001) for Pre-Distillation Unit with pinch design method.

Units	Heat Exchanger	Heat Exchanger TEMA	Cp^0	Fp	FM	B1	B2	FBM	CBM (euros)
HEATX-1	Reboiler	BES Vertical	46071	1	1	1.63	1.66	3.29	133385.2
HEATX-2	Reboiler	BES Vertical	21240	1	1	1.63	1.66	3.29	61492.7
HEATX-3	Reboiler	BES Vertical	289337	1	1	1.63	1.66	3.29	164594.7
HEATX-4	Reboiler	BES Vertical	136485	1	1	1.63	1.66	3.29	82839.52
HEATX-5	Reboiler	BES Vertical	161141	1	1	1.63	1.66	3.29	97245.36
HEATX-6	Reboiler	BES Vertical	36315	1	1	1.63	1.66	3.29	105139.4
Total Bare Cost module (euros) 2001				**644,697 €**					
Total Bare Cost module (euros) 2018				**967,536 €**					

Table VII.10: Bare Cost module for equipment below pinch point (2001) for Pre-Distillation Unit with pinch design method.

Units	Heat Exchanger	Heat Exchanger TEMA	Cp^0	Fp	FM	B1	B2	FBM	CBM (euros)
HEATX-7	Shell&Tube	BES horizontal	19370	1	1	1.63	1.66	3.29	56080.2
HEATX-8	Shell&Tube	BES horizontal	34186	1	1	1.63	1.66	3.29	98975.7
HEATX-9	Cooler	BES horizontal	38761	1	1	1.63	1.66	3.29	0.0
HEATX-10	Cooler	BES horizontal	47826	1	1	1.63	1.66	3.29	26742.9
HEATX-11	Cooler	BES horizontal	248631	1	1	1.63	1.66	3.29	719836.4
HEATX-12	Cooler	BES horizontal	18326	1	1	1.63	1.66	3.29	53057.4
HEATX-13	Cooler	BES horizontal	69439	1	1	1.63	1.66	3.29	201039.0
HEATX-14	Cooler	BES horizontal	25347	1	1	1.63	1.66	3.29	0.0
Total Bare Cost module (euros) 2001			**1,155,732 €**						
Total Bare Cost module (euros) 2018			**1,734,478 €**						

Annex VIII. Additional Information of Retrofit Design of Arosolvan Unit using Heuristic Rules

For fixed energy targets and operating costs, retrofit design solutions were found using two retrofit methods: cross-pinch exchanger elimination method and pinch design method. No viable solution was found using the first method. Data for the purchased equipment cost (C_P^0), at ambient operating pressure and using carbon steel construction material, is indicated in Annex VI. The same assumptions for the estimation of total investment cost considered before for Pre-Distillation Unit are now applied for Arosolvan Unit. The operating conditions resultant from stream matches using pinch design method with maximum reuse of the existing heat exchangers are presented in the next Tables VIII.1 and VIII.2.

The purchased cost of the equipment resultant from stream matches using pinch design method are presented in the next Table VIII.3 to VIII.6 for the subnetworks above and below pinch point, respectively.

Table VIII.1: Operating data resulting from stream matches above pinch point using pinch design method of Pinch Analysis for Arosolvan Unit.

Exchangers	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m²)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
HEATX-1	MP Steam	-	200	199	9.74	2861	34.5	33.6
	Solvent (NMP+MEG) R1	C7	165.4	165.5				
HEATX-2	MP Steam	-	200	199	3.39	891	38.5	37.6
	T0251 BTM R1	C8	161.4	161.5				
HEATX-3	MP Steam	-	200	199	5.73	1168	39.6	61
	Extract R2	C9	138	160.4				
HEATX-4	MP Steam	-	200	199	0.204	30.8	66.6	65.88
	T0251 BTM R1	C11	133.1	133.4				
HEATX-5	MP Steam	-	200	199	5.08	754.1	67.6	67
	T0251 BTM R2	C12	132	132.4				
HEATX-6	Solvent (NMP+MEG)	H1	165.4	150	1.61	911	24.9	12
	Extract R1	C10	138	140.5				
HEATX-7	Solvent (NMP+MEG)	H1	150	142	0.816	620.9	16.88	10
	T021 BRTM R1	C11	132	133.1				
HEATX-8	C9CUT	H2	161.4	142	0.005	2.77	29.4	10
	T0251 BTM R2	C12	132	132				

Table VIII.2: Operating data resulting from stream matches below pinch point using pinch design method of Pinch Analysis for Arosolvan Unit.

Exchangers	Streams	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q_{MATCH} (MW)	A (m^2)	ΔT_{HOT} (°C)	ΔT_{COLD} (°C)
HEATX-9	Solvent (NMP+MEG)	H1	142	133	0.915	252.6	19.27	82.96
	Aromatics Extracted	C1	50	122.7				
HEATX-10	Solvent (NMP+MEG)	H1	133	78.19	5.48	2211	27.54	21.99
	Extract pre-heat	C4	56.2	105.4				
HEATX-11	Extract WNA	H3	138	126.3	1.45	1173	16	9.33
	Solvent Glicol R2	C2	117	122				
HEATX-12	Toluene	H4	128.8	128.8	1.45	1100	12.6	13.78
	Solvent Glicol R1	C3	115	116.2				
HEATX-13	Toluene	H4	128.8	128.8	0.57	446.6	11.81	13.77
	Solvent Glicol R2	C2	115	117				
HEATX-14	Toluene	H4	128.8	123.7	0.252	80.28	26.47	63.06
	Solvent (NMP+H2O)	C5	60.68	102.3				
HEATX-15	Toluene	H4	123.7	109.7	0.2	34.07	51.24	67.06
	BT CUT	C6	72.5	42.64				
HEATX-16	Pure Water	H6	105.1	105.1	0.0747	11	62.46	73.6
	BT CUT	C6	31.5	42.64				
HEATX-17	Solvent (NMP+MEG)	H2	62.5	78.19	1.42	256	58.19	52.5
	CW	-	10	30				
HEATX-18	C9 CUT	H2	142	103	0.01	0.9375	122	93
	CW	-	10	30				
HEATX-19	Toluene DIST	H5	109.7	30.5	0.567	118.7	89.7	20.5
	CW	-	10	30				
HEATX-20	Pure Water	H6	105.1	72.4	2.18	245.9	85.1	62.4
	CW	-	10	30				
HEATX-21	Benzene 2	H7	91.1	24.7	0.185	50.8	71.1	14.7
	CW	-	10	30				
HEATX-22	Benzene 1	H8	89.1	75.4	3.99	564.4	69.11	65.4
	CW	-	10	30				
HEATX-23	Extract Recycle Product	H9	72.8	28.1	3.16	822.4	52.8	18.1
	CW	-	10	30				
HEATX-24	Pure Water Distillate	H10	72.4	60	0.0233	4.552	52.4	50
	CW	-	10	30				
HEATX-25	Light Non Aromatics	H11	60.7	33.1	0.236	75.95	40.7	23.1
	CW	-	10	30				
HEATX-26	Aromatics Sat Glicol	H12	49.6	30.5	5.43	1627	29.6	20.5
	CW	-	10	30				

Table VIII.3: Heat transfer areas and respective purchased equipment cost for stream matches above pinch point obtaining above pinch point for Arosolvan Unit pinch design method.

Units	Heat Exchanger Type	Process Stream	ID	A (m^2)	A_{reused} (m^2)	Over Capacity (%)	K_1	K_2	K_3	$\log_{10}(Cp^0)$	Cp^0 (dollar)	Cp^0 (euros)
HEATX-1	Reboiler	MP Steam	-	2861	2861	0	4.8306	-0.8509	0.3187	5.70	0	0
		Solvent (NMP+MEG) R1	C7									
HEATX-2	Reboiler	MP Steam	-	891	891	0	4.8306	-0.8509	0.3187	5.09	0	0
		T0251 BTM R1	C8									
HEATX-3	Reboiler	MP Steam	-	1168	1168	0	4.8306	-0.8509	0.3187	5.22	0	0
		Extract R2	C9									
HEATX-4	Reboiler	MP Steam	-	30.8	-	0	4.8306	-0.8509	0.3187	4.27	18628	16392
		T0251 BTM R1	C11									
HEATX-5	Reboiler	MP Steam	-	754.1	754.8	0	4.8306	-0.8509	0.3187	5.02	0	0
		T0251 BTM R2	C12									
HEATX-6	Reboiler	Solvent (NMP+MEG)	H1	911	911	0	4.8306	-0.8509	0.3187	5.10	0	0
		Extract R1	C10									
HEATX-7	Reboiler	Solvent (NMP+MEG)	H1	620.9	-	0	4.8306	-0.8509	0.3187	4.94	87134	76678
		T021 BRTM R1	C11									
HEATX-8	Reboiler	C9CUT	H2	2.77	-	0	4.8306	-0.8509	0.3187	4.52	32847	28905
		T0251 BTM R2	C12									
Total Heat Transfer Reused Area Above Pinch Point (m^2)				6585.8								
Total Additonal Heat Transfer Area Above Pinch Point (m^2)				654.5								
Total Heat Transfer Area (m^2)				7240.3								

Table VIII.4: Heat transfer areas and respective purchased equipment cost for stream matches above pinch point obtaining above pinch point for Arosolvan Unit pinch design method.

Units	Heat Exchanger Type	Process Stream	ID	A (m^2)	A_{reused} (m^2)	Over Capacity	K_1	K_2	K_3	$log_{10}(Cp^0)$	Cp^0 (dollar)	Cp^0 (euros)
HEATX-9	Shell&Tube	Solvent (NMP+MEG)	H1	252.6	0	-	4.8306	-0.8509	0.3187	4.63	42248	37178
		Aromatics Extracted	C1									
HEATX-10	Shell&Tube	Solvent (NMP+MEG)	H1	2211	0	-	4.8306	-0.8509	0.3187	5.55	354613	312060
		Extract pre-heat	C4									
HEATX-11	Reboiler	Extract WNA	H3	1173	0	-	4.8306	-0.8509	0.3187	5.22	166447	146474
		Solvent Glicol R2	C2									
HEATX-12	Reboiler	Toluene	H4	1100	1114.2	1.3	4.8306	-0.8509	0.3187	5.19	155123	136508
		Solvent Glicol R1	C3									
HEATX-13	Reboiler	Toluene	H4	446.6	0	-	4.8306	-0.8509	0.3187	4.81	65120	57306
		Solvent Glicol R2	C2									
HEATX-14	Shell&Tube	Toluene	H4	80.28	109.3	26.6	4.8306	-0.8509	0.3187	4.37	23231	20443
		Solvent (NMP+H2O)	C5									
HEATX-15	Shell&Tube	Toluene	H4	34.07	48.26	29.4	4.8306	-0.8509	0.3187	4.28	18839	16579
		BT CUT	C6									
HEATX-16	Shell&Tube	Pure Water	H6	11	0	-	4.8306	-0.8509	0.3187	4.29	19503	17163
		BT CUT	C6									
HEATX-17	Cooler	Solvent (NMP+MEG)	H2	256	315.6	18.9	4.8306	-0.8509	0.3187	4.63	42635	37519
		CW	-									
HEATX-18	Cooler	C9 CUT	H2	0.9375	0	-	4.8306	-0.8509	0.3187	4.85	71565	62977
		CW	-									
HEATX-19	Cooler	Toluene DIST	H5	118.7	130.3	8.9	4.8306	-0.8509	0.3187	4.44	27348	24066
		CW	-									
HEATX-20	Cooler	Pure Water	H6	245.9	0	-	4.8306	-0.8509	0.3187	4.62	41486	36508
		CW	-									
HEATX-21	Cooler	Benzene 2	H7	50.8	0	-	4.8306	-0.8509	0.3187	4.31	20253	17823
		CW	-									
HEATX-22	Cooler	Benzene 1	H8	564.4	0	-	4.8306	-0.8509	0.3187	4.90	79841	70260
		CW	-									
HEATX-23	Cooler	Extract Recycle Product	H9	822.4	907.4	9.4	4.8306	-0.8509	0.3187	5.06	114387	100660
		CW	-									
HEATX-24	Cooler	Pure Water Distillate	H10	4.552	5.49	17.1	4.8306	-0.8509	0.3187	4.41	25622	22547
		CW	-									
HEATX-25	Cooler	Light Non Aromatics	H11	75.95	0	-	4.8306	-0.8509	0.3187	4.36	22777	20044
		CW	-									
HEATX-26	Cooler	Aromatics Sat Glicol	H12	1627	2072	21.5	4.8306	-0.8509	0.3187	5.38	242542	213437
		CW	-									
Total Heat Transfer Reused Area Below Pinch Point (m^2)					4702.6							
Total Additonal Heat Transfer Area Below Pinch Point (m^2)					5032.2							
Total Heat Transfer Area (m^2)					9734.7							

Table VIII.5: Bare Cost module for equipment above pinch point for Pre-Distillation Unit with pinch design method.

Units	Heat Exchanger Type	Heat Exchanger TEMA	Cp^0	Fp	FM	B1	B2	FBM	CBM (dollar)	CBM (euros)
HEATX-1	Reboiler with floating head	BES Vertical	0	1	1	1.63	1.66	3.29	0	0
HEATX-2	Reboiler with floating head	BES Vertical	0	1	1	1.63	1.66	3.29	0	0
HEATX-3	Reboiler with floating head	BES Vertical	0	1	1	1.63	1.66	3.29	0	0
HEATX-4	Reboiler with floating head	BES Vertical	18628	1	1	1.63	1.66	3.29	13483	11865
HEATX-5	Reboiler with floating head	BES Vertical	0	1	1	1.63	1.66	3.29	0	0
HEATX-6	Reboiler with floating head	BES Vertical	0	1	1	1.63	1.66	3.29	0	0
HEATX-7	Reboiler with floating head	BES Vertical	87134	1	1	1.63	1.66	3.29	63067	55499
HEATX-8	Reboiler with floating head	BES Vertical	32847	1	1	1.63	1.66	3.29	23774	20922
Total Bare Cost module (euros) 2001			**88,286 €**							
Total Bare Cost module (euros) 2018			**132,496 €**							

Table VIII.6: Bare Cost module for equipment below pinch point for Pre-Distillation Unit with pinch design method.

Units	Heat Exchanger Type	Heat Exchanger TEMA	A (m^2)	A_{reused} (m^2)	Cp^0	Fp	FM	B1	B2	FBM	CBM (dollar)	CBM (euros)
HEATX-9	Shell&Tube	BES Vertical	252.6	0	42248	1	1	1.63	1.66	3.29	138996	122316
HEATX-10	Shell&Tube	BES Vertical	2211	0	354613	1	1	1.63	1.66	3.29	1166677	1026676
HEATX-11	Reboiler	BES Vertical	1173	0	166447	1	1	1.63	1.66	3.29	547611	481898
HEATX-12	Reboiler	BES Vertical	1100	1114.2	155123	1	1	1.63	1.66	3.29	102071	89822
HEATX-13	Reboiler	BES Vertical	446.6	0	65120	1	1	1.63	1.66	3.29	214246	188537
HEATX-14	Shell&Tube	BES Vertical	80.28	109.3	23231	1	1	1.63	1.66	3.29	15286	13452
HEATX-15	Shell&Tube	BES Vertical	34.07	48.26	18839	1	1	1.63	1.66	3.29	12396	10909
HEATX-16	Shell&Tube	BES Vertical	11	0	19503	1	1	1.63	1.66	3.29	64166	56466
HEATX-17	Cooler	BES Vertical	256	315.6	42635	1	1	1.63	1.66	3.29	28054	24687
HEATX-18	Cooler	BES Vertical	0.9375	0	71565	1	1	1.63	1.66	3.29	235448	207195
HEATX-19	Cooler	BES Vertical	118.7	130.3	27348	1	1	1.63	1.66	3.29	17995	15836
HEATX-20	Cooler	BES Vertical	245.9	0	41486	1	1	1.63	1.66	3.29	136490	120111
HEATX-21	Cooler	BES Vertical	50.8	0	20253	1	1	1.63	1.66	3.29	66632	58636
HEATX-22	Cooler	BES Vertical	564.4	0	79841	1	1	1.63	1.66	3.29	262677	231156
HEATX-23	Cooler	BES Vertical	822.4	907.4	114387	1	1	1.63	1.66	3.29	75266	66235
HEATX-24	Cooler	BES Vertical	4.552	5.49	25622	1	1	1.63	1.66	3.29	16859	14836
HEATX-25	Cooler	BES Vertical	75.95	0	22777	1	1	1.63	1.66	3.29	74938	65945
HEATX-26	Cooler	BES Vertical	1627	2072	242542	1	1	1.63	1.66	3.29	159593	140441
Total Bare Cost module (euros) 2001			**2,935,154 €**									
Total Bare Cost module (euros) 2018			**4,404,966 €**									

Annex IX. Additional information for HEN Synthesis of Pre-Distillation Unit using in Hybrid Methodology and Cross-Pinch Elimination Method

MILP was applied considering the case scenario defined only by data extracted of the inefficient zones of energy efficiency within the current HEN of Pre-Distillation Unit. The model required the definition of lower and upper bounds of the heat loads that could be transferred between process-to-process streams and process-to-utility streams in each subnetwork divided by pinch point location. The lower bounds for heat loads correspond to when no heat is being transferred between those streams. The upper bounds corresponds to the maximum heat load that can be transferred between streams. The upper bound levels defined are shown in Tables IX.1 and IX.2.

Table IX.1: Upper bounds used in MILP model for the remained subnetwork above pinch point case scenario of Pre-Distillation Unit.

UB (ij)	C6C7R1	C8C9R2
MP Steam	1486.4	1486.4
H1	764.8	764.8
H21	1766.1	1766.1
H22	1452.8	1452.8

Table IX.2: Upper bounds used in MILP model for the remained subnetwork below pinch point case scenario of Pre-Distillation Unit.

UB (ij)	Reformate	CW
H1	1042.2	1042.2
H21	246.5	246.5
H22	1471.2	1471.2
H3	798.0	798.0
H4	1750.0	10084.0
H5	105.0	105.0
H6	1578.7	1578.7
H7	3.3	3.3

The superstructures derived for the subnetworks above and below pinch point using MILP model are shown in Figures IX.1 and IX.3, respectively. Each stream superstructure has one input, one output, a number of heat exchangers equal to the matches in which the stream is involved, and all possible connections from input to the units, between each pair of units, and from the units to the output. Note that:

- Each input stream has a splitter that features of a number of outlet streams equal to the number of heat exchangers that are associated with this stream;
- Each outlet stream has a mixer that features of a number of inlet streams equal to the number of heat exchangers that are associated with this stream;
- Each exchanger has a mixer at its inlet and a splitter at its outlet;
- The mixer at the inlet of each heat exchanger is connected to the input splitter and the splitters of the other heat exchangers;
- The splitter at the outlet of each exchanger is connected to the output mixer and the mixers of the other heat exchangers.

By assigning flowrate heat capacities to all streams in the stream superstructure and selectively setting some of them equal to zero, the incorporation of many interesting structures can be verified. These include the alternatives of: i) parallel structure, ii) series structure, iii) parallel-series, iv) series-parallel, and v) by pass.

Stream Superstructures for Subnetwork above Pinch Point

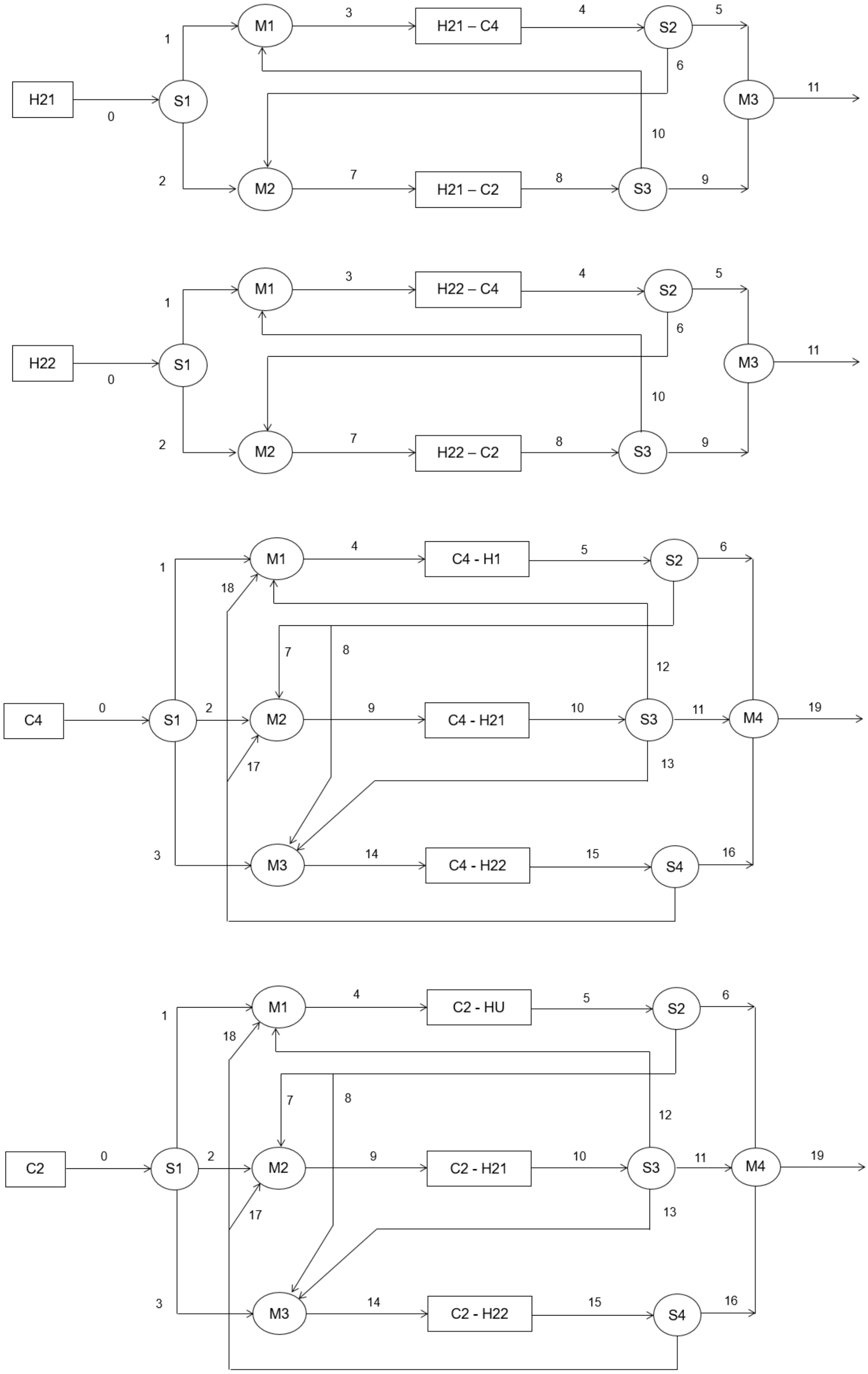
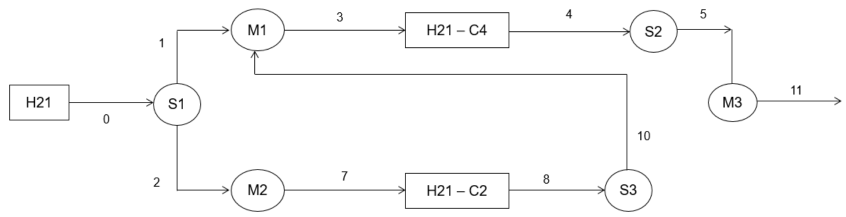
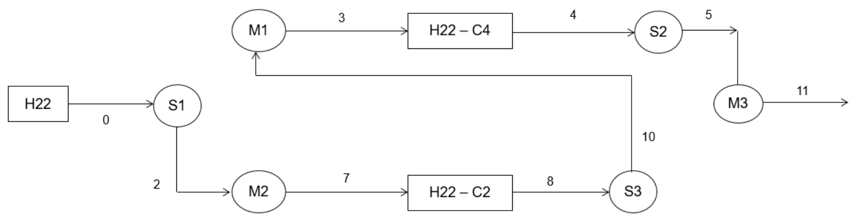


Figure IX.1: Streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network.

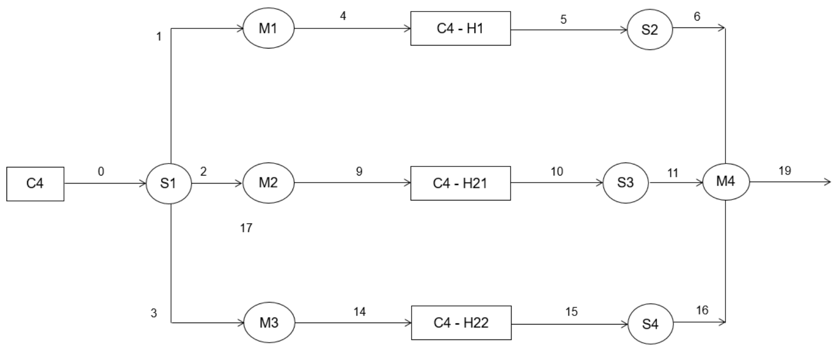
Stream Structures Solution for Subnetwork above Pinch Point



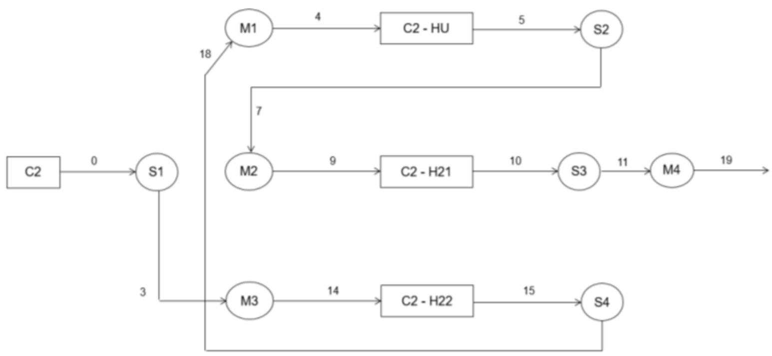
C8 CUT (H21)		
Stream	F (TON/HR)	T (°C)
0	15.438	202.7
1	0.419	202.7
2	15.019	202.7
3	15.438	201.686
4	15.438	154.6
5	15.438	154.6
7	15.019	202.7
8	15.019	201.66
10	15.019	201.66
11	15.438	154.6



C8 CUT (H22)		
Stream	F (TON/HR)	T (°C)
0	94.835	178.2
2	94.835	178.2
3	94.835	169.301
4	94.835	154.6
5	94.835	154.6
7	94.835	178.2
8	94.835	169.301
10	94.835	169.301
11	94.835	154.6



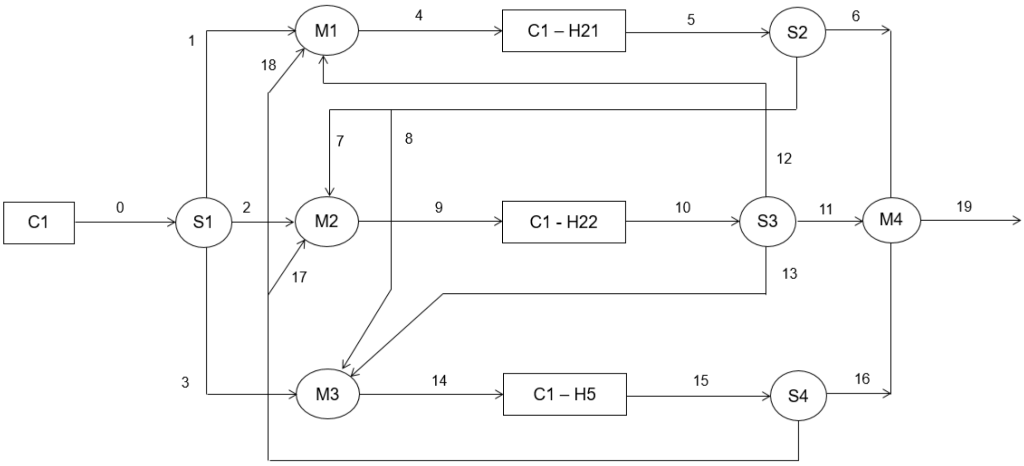
C6/C7R1 (C4)		
Stream	MCP (MJ/HR)	T (°C)
0	2021.539	144.6
1	705.965	144.6
2	480.234	144.6
3	835.34	144.6
4	705.965	144.6
5	705.965	148.5
6	705.965	148.5
9	480.234	144.6
10	480.234	148.5
11	480.234	148.5
14	835.34	144.6
15	835.34	148.5
16	835.34	148.5
19	2021.539	148.5



C8/C9R2 (C2)		
Stream	MCP (MJ/HR)	T (°C)
0	1063.784	152.4
3	1063.784	152.4
4	1063.784	154.254
5	1063.784	159.284
7	1063.784	159.284
9	1063.784	159.284
10	1063.784	163.5
11	1063.784	163.5
14	1063.784	152.4
15	1063.784	154.254
18	1063.784	154.254
19	1063.784	163.5

Figure IX.2: Results for streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network.

Stream Superstructure for Subnetwork below Pinch Point



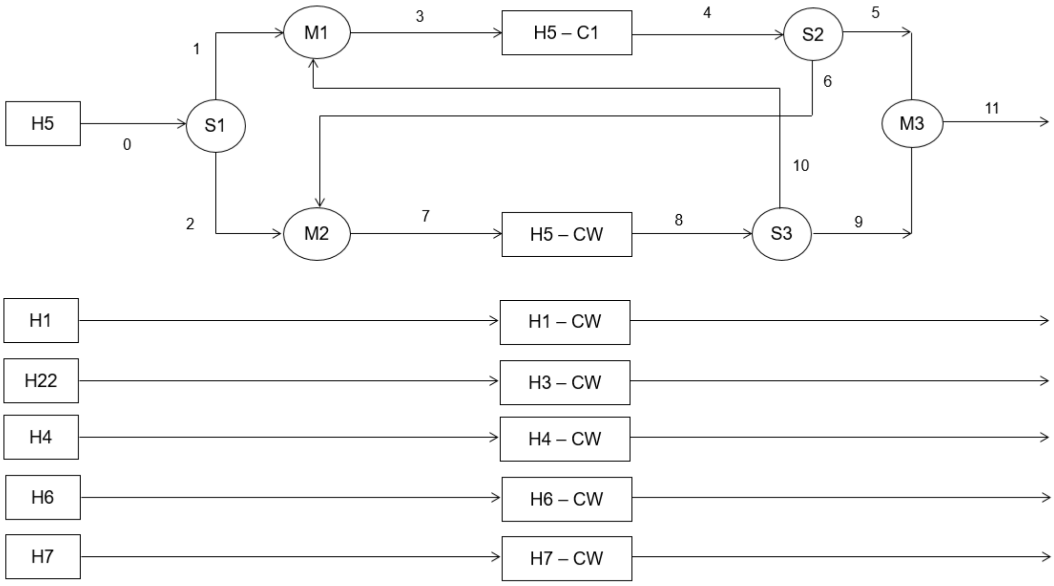
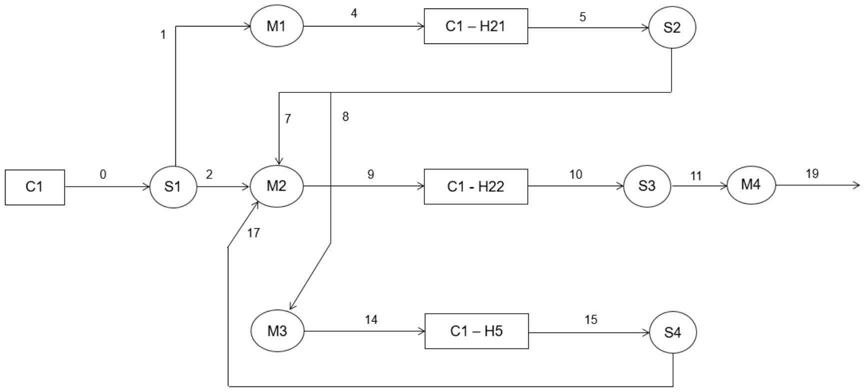
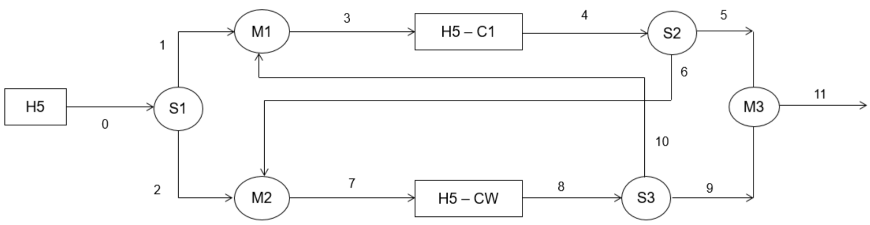


Figure IX.3: Streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network.

Stream Structure Solution for Subnetwork below Pinch Point



REFORMATE (C1)		
Stream	F (TON/HR)	T (^{o}C)
0	75.309	31.70
1	29.833	31.70
2	45.476	31.70
4	29.833	31.70
5	29.833	45.68
7	25.727	45.68
8	4.106	45.68
9	75.309	37.96
10	75.309	71.00
11	75.309	71.00
14	4.106	45.68
15	4.106	58.95
17	4.106	58.95
19	75.309	71.00



BT CUT (H5)		
Stream	F (TON/HR)	T (^{o}C)
0	35.859	71.90
1	11.004	71.90
2	24.855	71.90
3	33.405	68.95
4	33.405	67.50
5	22.400	67.50
6	11.004	67.50
7	35.859	70.55
8	35.859	67.50
9	13.459	67.50
10	22.4	67.50
11	35.859	67.50

Figure IX.4: Results for streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network.

The operating conditions resultant from stream matches using cross-pinch exchanger elimination method are presented in the next Tables IX.3 and IX.4.

Table IX.3: Operating data resulting from stream matches above pinch point using cross-pinch exchanger elimination method of Pinch Analysis for Pre-Distillation Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m^2)
NU-1	C9CUT	H1	244.2	154.6	764.8	38.2	200.0
	C6C7R1	C4	144.6	148.5			
NU-2	C8CUT1	H21	201.7	154.6	520.3	25.9	200.8
	C6C7R1	C4	144.6	148.5			
NU-3	C8CUT2	H22	169.3	154.6	905.0	14.7	613.6
	C6C7R1	C4	144.6	148.5			
NU-4	C8CUT1	H21	178.2	169.3	1245.8	40.8	305.6
	C8C9R2	C2	159.3	163.5			
NU-5	C8CUT2	H22	178.2	169.3	547.8	20.2	270.9
	C8C9R2	C2	152.4	154.3			
NU-6	STEAM	HU	200	199	1486.4	42.7	348.1
	C8C9R2	C2	154.3	159.3			

Table IX.4: Operating data resulting from stream matches below pinch point using cross-pinch exchanger elimination method of Pinch Analysis for Pre-Distillation Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m^2)
NU-7	C8CUT1	H21	154.6	130.7	246.5	103.9	23.7
	REFORMATE	C1	31.7	45.7			
NU-8	C8CUT2	H22	154.6	130.7	1471.2	88.1	167.0
	REFORMATE	C1	38	71			
NU-9	BTCUT2	H5	68.95	67.5	32.2	15.2	21.3
	REFORMATE	C1	45.7	58.95			
NU-10	C9CUT	H1	154.6	32.5	1042.2	50.5	206.3
	CW	CW	20	25			
NU-11	C8CUT3	H3	130.7	32.5	798.0	37.6	212.3
	CW	CW	20	25			
NU-12	BTCUT1	H4	70.55	67.5	10084.0	59.7	1689.7
	CW	CW	20	25			
NU-13	BTCUT2	H5	71.9	47.5	72.8	46.5	15.6
	CW	CW	20	25			
NU-14	C5CUT1	H6	67.2	33.5	1578.7	44.7	353.5
	CW	CW	20	25			
NU-15	C5CUT2	H7	33.5	32.5	3.3	10.4	3.2
	CW	CW	20	25			

Bare cost module for the required equipment, including the installation cost of E0102 in place of NU-5 (CBM reuse) are presented in the next Tables IX.5 and IX.6.

Table IX.5: Heat transfer areas and respective bare module cost for stream matches obtaining above pinch point for Pre-Distillation Unit using cross-pinch exchanger method.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
NU-1	C9CUT	H1	200.0	221.8	10	36315	1	1.63	1.66	3.29	23895	21028
	C6C7R1	C4										
NU-2	C8CUT1	H21	200.8	0	0	36407	1	1.63	1.66	3.29	119780	105407
	C6C7R1	C4										
NU-3	C8CUT2	H22	613.6	0	0	86182	1	1.63	1.66	3.29	283538	249513
	C6C7R1	C4										
NU-4	C8CUT1	H21	305.6	0	0	48335	1	1.63	1.66	3.29	159021	139939
	C8C9R2	C2										
NU-5	C8CUT2	H22	270.9	0	0	44341	1	1.63	1.66	3.29	145882	128376
	C8C9R2	C2										
NU-6	STEAM	HU	348.1	0	0	53303	1	1.63	1.66	3.29	175366	154322
	C8C9R2	C2										
Additional Area (m^2)			1739.0									
Re-used Area (m^2)			2599									
CBM $(EUROS)_{2001}$			798585									
CBM $(EUROS)_{2018}$			1198485									

Table IX.6: Heat transfer areas and respective bare module cost for stream matches obtaining below pinch point for Pre-Distillation Unit using cross-pinch exchanger method.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
NU-7	C8CUT1	H21	23.7	0.0	0.0	16130.4	1.0	1.63	1.66	3.29	53069	46701
	REFORMATE	C1										
NU-8	C8CUT2	H22	167.0	0.0	0.0	28729.0	1.0	1.63	1.66	3.29	94518	83176
	REFORMATE	C1										
NU-9	BTCUT2	H5	21.3	0.0	0.0	16111.8	1.0	1.63	1.66	3.29	53008	46647
	REFORMATE	C1										
NU-10	C9CUT	H1	206.3	0.0	0.0	32578.9	1.0	1.63	1.66	3.29	107185	94322
	CW	CW										
NU-11	C8CUT3	H3	212.3	301.2	29.5	33169.9	1.0	1.63	1.66	3.29	21826	19207
	CW	CW										
NU-12	BTCUT1	H4	1689.7	0.0	0.0	223353.9	1.0	1.63	1.66	3.29	734834	646654
	CW	CW										
NU-13	BTCUT2	H5	15.6	0.0	0.0	16346.5	1.0	1.63	1.66	3.29	53780	47326
	CW	CW										
NU-14	C5CUT1	H6	353.5	479.9	26.3	47471.3	1.0	1.63	1.66	3.29	31236	27488
	CW	CW										
NU-15	C5CUT2	H7	3.4	4.7	27.2	26785.2	1.0	1.63	1.66	3.29	17625	15510
	CW	CW										
Additional Area (m^2)			2124									
Re-used Area (m^2)			824									
CBM $(EUROS)_{2001}$			1027031									
CBM $(EUROS)_{2018}$			1541329									

Annex X. Additional information for HEN Synthesis of Pre-Distillation Unit using in Hybrid Methodology and Pinch Design Method for Retrofit Design

MILP was applied considering the case scenario of a grassroots case with maximum reuse of the existing heat exchangers. The upper bound levels defined and considered above and below pinch point are shown in Tables X.1 and X.2, respectively.

Table X.1: Upper bounds used in MILP model for the subnetwork above pinch point considering pinch design method of Pre-Distillation Unit.

UB (ij)	C6C7 R1	C6C7 R2	C8C9 R1	C8C9 R2
STEAM	1534.1	1534.1	1534.1	1534.1
C9CUT	764.8	764.8	764.8	764.8
C8CUT1	2190.0	2650.0	6815.0	3280.0

Table X.2: Upper bounds used in MILP model for the subnetwork below pinch point considering pinch design method of Pre-Distillation Unit.

UB (ij)	REFORMATE	CW
C9CUT	1042.2	1042.2
C8CUT1	1768.3	1768.3
C8CUT2	1101.0	1101.0
BTCUT1A	2053.0	10084.0
BTCUT2	105.0	105.0
C5CUT1A	1578.7	1578.7
C5CUT2	3.3	3.3

Stream Superstructures for Subnetwork above Pinch Point

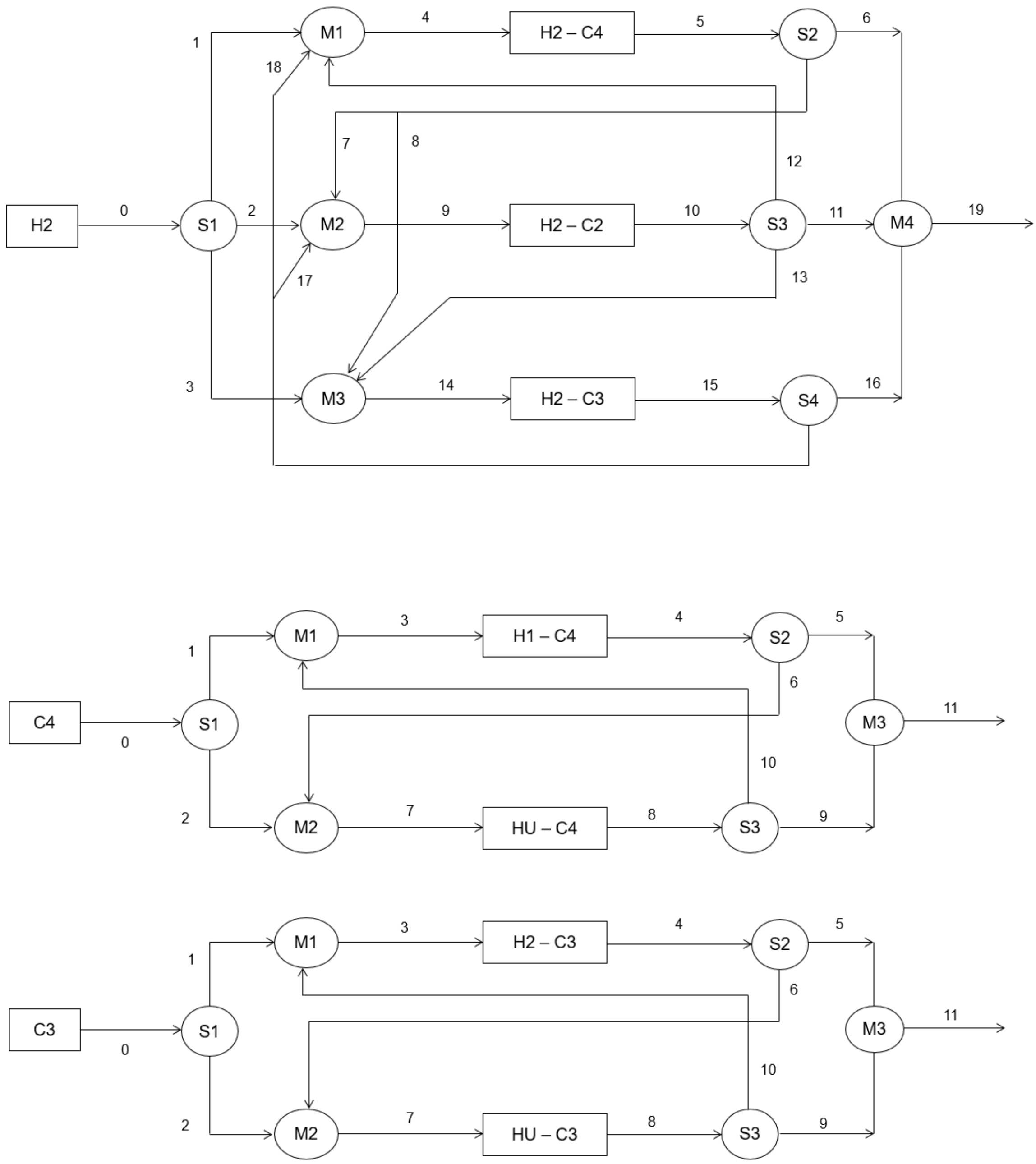
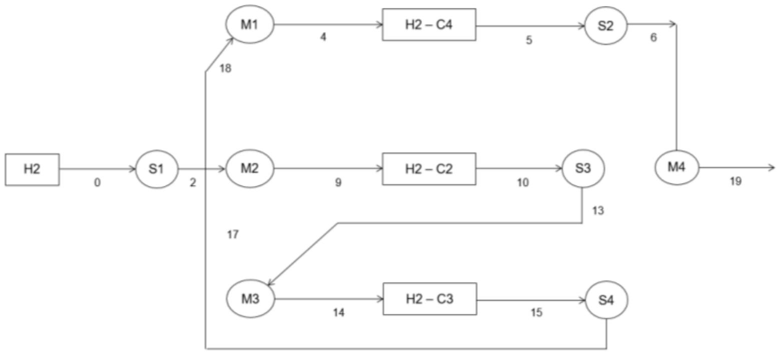
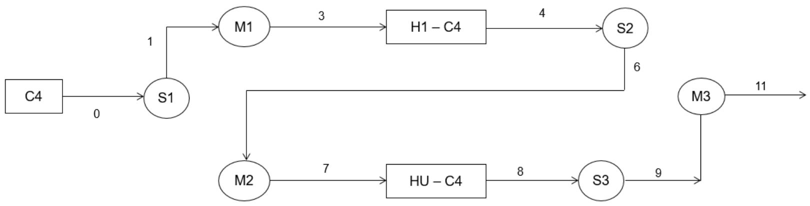


Figure X.1: Streams superstructure for HEN subnetwork above pinch point considering pinch design method for retrofit case.

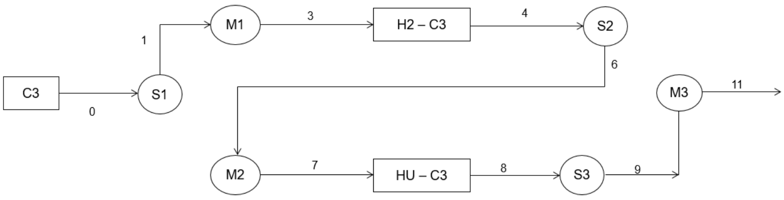
Stream Superstructures Solution for Subnetwork above Pinch Point



C8 CUT (H2)		
Stream	F (TON/HR)	T (°C)
0	110.273	202.7
2	110.273	202.7
4	110.273	190.423
5	110.273	154.6
6	110.273	154.6
9	110.273	202.7
10	110.273	201.905
13	110.273	201.905
14	110.273	201.905
15	110.273	190.423
18	110.273	190.423
19	110.273	154.6



C6/C7 R1 (C1)		
Stream	MCp (MJ/HR)	T (°C)
0	2021.539	144.6
1	2021.539	144.6
3	2021.539	144.6
4	2021.539	145.962
6	2021.539	145.962
7	2021.539	145.962
8	2021.539	148.5
9	2021.539	148.5
11	2021.539	148.5



C8/C9 R1 (C3)		
Stream	MCp (MJ/HR)	T (°C)
0	1063.784	152.40
1	1063.784	152.40
3	1063.784	152.40
4	1063.784	163.13
6	1063.784	163.13
7	1063.784	163.13
8	1063.784	163.50
9	1063.784	163.50
11	1063.784	163.50

Figure X.2: Results for streams superstructure for HEN subnetwork above pinch point considering pinch design method for retrofit case.

Stream Superstructure for Subnetwork below Pinch Point

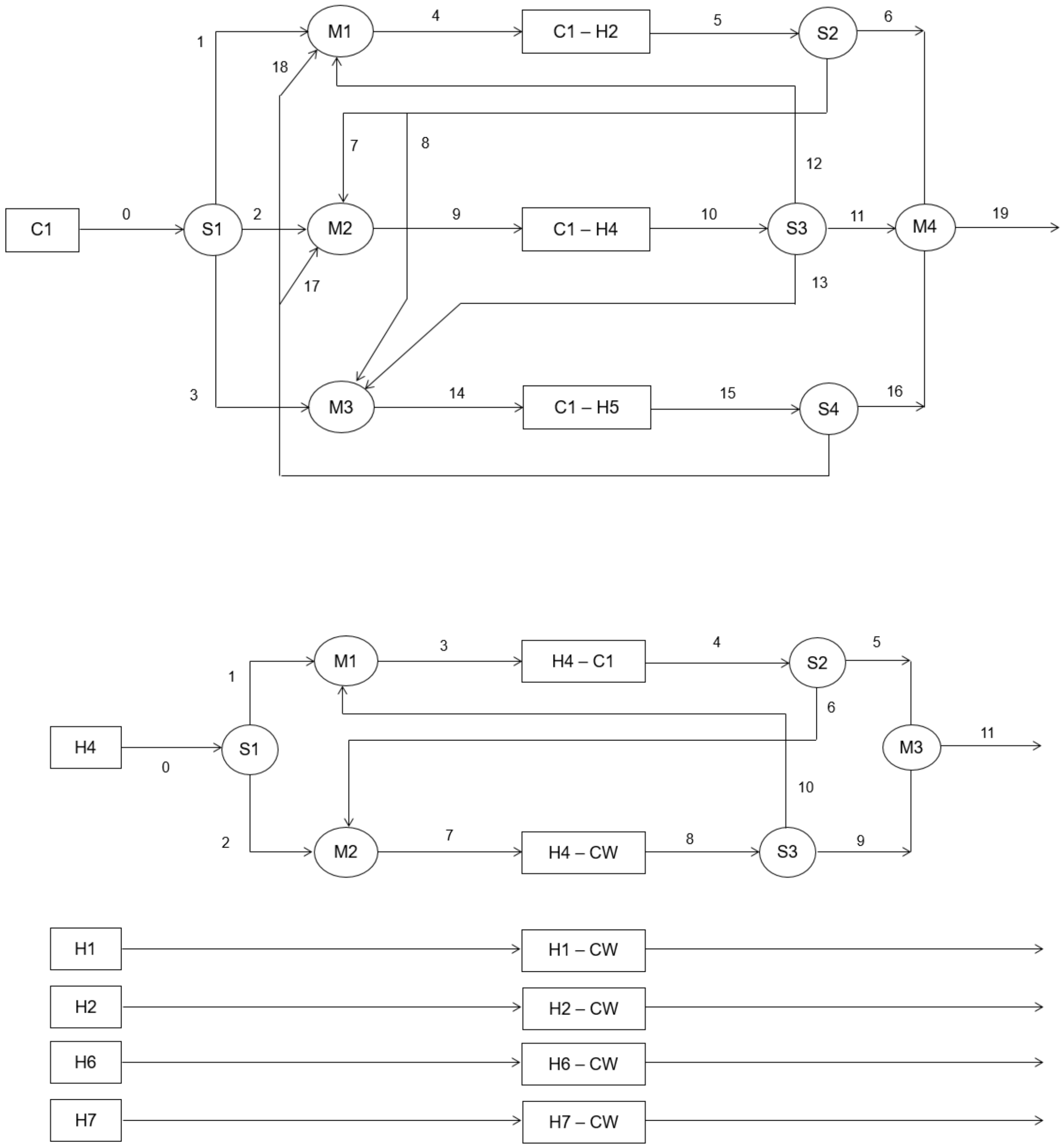
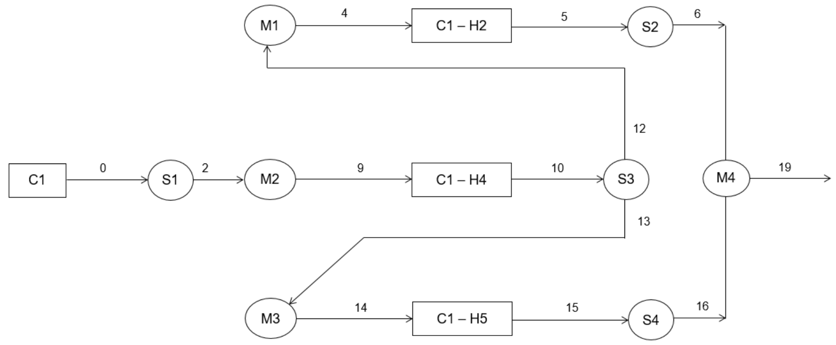
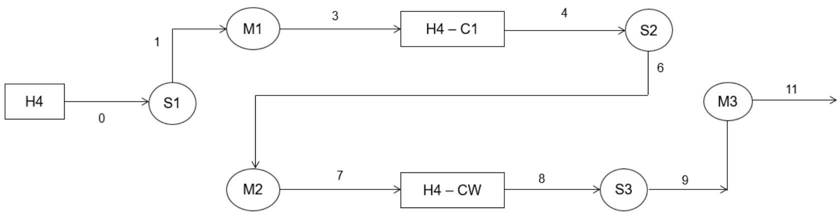


Figure X.3: Streams superstructure for HEN subnetwork above pinch point considering pinch design method for retrofit case.

Stream Superstructure Solution for Subnetwork below Pinch Point



REFORMATE (C1)		
Stream	F (TON/HR)	T (°C)
0	75.309	24.80
2	75.309	24.80
4	69.926	28.85
5	69.926	71.70
6	69.926	71.70
9	75.309	24.80
10	75.309	28.85
12	69.926	28.85
13	5.383	28.85
14	5.383	28.85
15	5.383	61.90
16	5.383	61.90
19	75.309	71.00



BT CUT (H4)		
Stream	F (TON/HR)	T (°C)
0	95.317	93.20
1	95.317	93.20
3	95.317	93.20
4	95.317	92.94
6	95.317	92.94
7	95.317	92.94
8	95.317	71.90
9	95.317	71.90
11	95.317	71.90

Figure X.4: Results for streams superstructure for HEN subnetwork below pinch point considering pinch design method for retrofit case.

The operating conditions resultant from stream matches using pinch design method with maximum reuse of the existing heat exchangers are presented in the next Tables X.3 and X.4. The purchased cost of the equipment resultant from stream matches using cross-pinch exchanger elimination method are presented in the next Tables X.5 and X.6.

Table X.3: Operating data resulting from stream matches above pinch point using pinch design method of Pinch Analysis for Pre-Distillation Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m^2)
HEATX-1	C9 CUT	H1	244.2	154.6	765.2	38.9	196.4
	C6C7 R1	C4	190.4	154.6			
HEATX-2	C8 CUT	H2	202.7	201.9	2649.9	22.9	1159.2
	C6C7 R2	C5	144.6	146.8			
HEATX-3	C8 CUT	H2	202.7	201.9	6818.0	44.4	1536.0
	C8C9 R1	C3	152.40	163.13			
HEATX-4	C8 CUT	H2	201.9	190.4	3168.4	38.4	825.9
	C8C9 R2	C2	152.4	163.1			
HEATX-5	STEAM	HU	200	199	1424.7	52.3	272.7
	C6C7 R1	C4	145.96	148.5			
HEATX-6	STEAM	HU	200	199	111.2	36.2	30.1
	C8C9 R2	C2	163.1	163.5			

Table X.4: Operating data resulting from stream matches below pinch point using pinch design method of Pinch Analysis for Pre-Distillation Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m^2)
HEATX-7	C8CUT1	H2	154.6	130.7	1768.3	92.1	192.1
	REFORMATE	C1	28.85	71.7			
HEATX-8	BTCUT1	H4	93.2	92.94	179.8	66.2	27.1
	REFORMATE	C1	24.8	28.85			
HEATX-9	BTCUT2	H5	71.9	76.5	105.0	42.9	24.5
	REFORMATE	C1	28.85	61.9			
HEATX-10	C9CUT	H1	154.6	32.5	1042.2	50.5	206.3
	CW	CU	20	25			
HEATX-11	C8CUT2	H2	130.7	32.5	1101.0	43.9	250.6
	CW	CU	20	25			
HEATX-12	BTCUT1	H4	92.94	71.9	9904.3	59.7	1659.6
	CW	CU	20	25			
HEATX-13	C5CUT1	H6	67.2	33.5	1578.7	25.2	626.6
	CW	CU	20	25			
HEATX-14	C5CUT2	H7	33.5	32.5	3.3	10.4	3.2
	CW	CU	20	25			

Table X.5: Heat transfer areas and respective bare module cost for stream matches obtaining above pinch point for Pre-Distillation Unit pinch design method.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
HEATX-1	C9 CUT	H1	196.4	0	0	35915.9	1	1.63	1.66	3.29	118163	103984
	C6C7 R1	C4										
HEATX-2	C8 CUT	H2	1159.2	0	0	164281.7	1	1.63	1.66	3.29	540487	475628
	C6C7 R2	C5										
HEATX-3	C8 CUT	H2	1536.0	1881	18.3	226510.0	1	1.63	1.66	3.29	149044	131158
	C8C9 R1	C3										
HEATX-4	C8 CUT	H2	825.9	1139	27.5	114872.0	1	1.63	1.66	3.29	75586	66515
	C8C9 R2	C2										
HEATX-5	STEAM	HU	272.7	0	0.0	44541.8	1	1.63	1.66	3.29	146542	128957
	C6C7 R1	C4										
HEATX-6	STEAM	HU	30.1	0	0	18587.2	1	1.63	1.66	3.29	61152	53814
	C8C9 R2	C2										
Additional Area (m^2)			1658.4									
Re-used Area (m^2)			3020									
CBM $(EUROS)_{2001}$			960057									
CBM $(EUROS)_{2018}$			1440816									

Table X.6: Heat transfer areas and respective bare module cost for stream matches obtaining below pinch point for Pre-Distillation Unit pinch design method.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
HEATX-7	C8CUT1	H2	192.1	221.8	13.4	35431.9	1.0	1.63	1.66	3.29	23314	20517
	REFORMATE	C1										
HEATX-8	BTCUT1	H4	27.1	33.2	18.3	18439.3	1.0	1.63	1.66	3.29	12133	10677
	REFORMATE	C1										
HEATX-9	BTCUT2	H5	24.5	0	0	18347.2	1.0	1.63	1.66	3.29	60362	53119
	REFORMATE	C1										
HEATX-10	C9CUT	H1	206.3	0	0	37021.0	1.0	1.63	1.66	3.29	121799	107183
	CW	CU										
HEATX-11	C8CUT2	H2	250.6	301.2	16.8	42021.8	1.0	1.63	1.66	3.29	27650	24332
	CW	CU										
HEATX-12	BTCUT1	H4	1659.6	0.00	0	248373.9	1.0	1.63	1.66	3.29	817150	719092
	CW	CU										
HEATX-13	C5CUT1	H6	626.6	0.00	0	87875.1	1.0	1.63	1.66	3.29	289109	254416
	CW	CU										
HEATX-14	C5CUT2	H7	3.4	4.7	27.2	30437.7	1.0	1.63	1.66	3.29	20028	17625
	CW	CU										
Additional Area (m^2)			2516.9									
Re-used Area (m^2)			560.9									
CBM $(EUROS)_{2001}$			1206961									
CBM $(EUROS)_{2018}$			1811360									

Annex XI. Additional information for HEN Synthesis of Arosolvan Unit using in Hybrid Methodology and Cross-Pinch Exchanger Elimination Method

MILP was applied considering the case scenario defined only by the data extracted of the inefficient zones of energy efficiency within the current HEN of Arosolvan Unit. The model required the definition of lower and upper bounds of heat loads that can be transferred between process-to-process streams and process-to-utility streams in each subnetwork. The upper bound levels defined and considered above and below pinch point are shown in Tables XI.1 and XI.2, respectively.

Table XI.1: Upper bounds used in MILP model for the remained subnetwork above pinch point case scenario of Arosolvan Unit.

UB (kW)	SOLVENT (NMP+MEG) R1	T0252 BTM R1	EXTRACT R2	T0251 BTM R1	T0251 BTM R2	SOLVENT GLICOL R2
MP Steam	9740	3390	5729.9999	1020	5080	923.4286
SOLVENT (NMP+MEG)	1020	1020	1020	1020	1020	923.4286
C9 CUT	8.3732	8.3732	8.3732	8.3732	8.3732	8.3732

Table XI.2: Upper bounds used in MILP model for the remained subnetwork below pinch point case scenario of Arosolvan Unit.

UB (kW)	AROMATICS EXTRACTED	SOLVENT GLICOL R2	CW
SOLVENT (NMP+MEG)	15	1096.5714	1309
C9 CUT	6.62669	6.62669	6.62669
TOLUENE	15	1096.5714	2572
TOLUENE DIST	15	304	304
PURE WATER	15	1096.5714	1903.007
BENZENE	15	1096.5714	3983.9
PURE BENZENE	15	94.4	94.4
EXTRACT RECYC PROD	15	1096.5714	3155
PURE WATER DIST	15	23.3	23.3
LIGHT NON AROMATICS	15	236	236
AROMATICS SAT GLI	15	1096.5714	5434

Stream Superstructures for Subnetwork Above Pinch Point

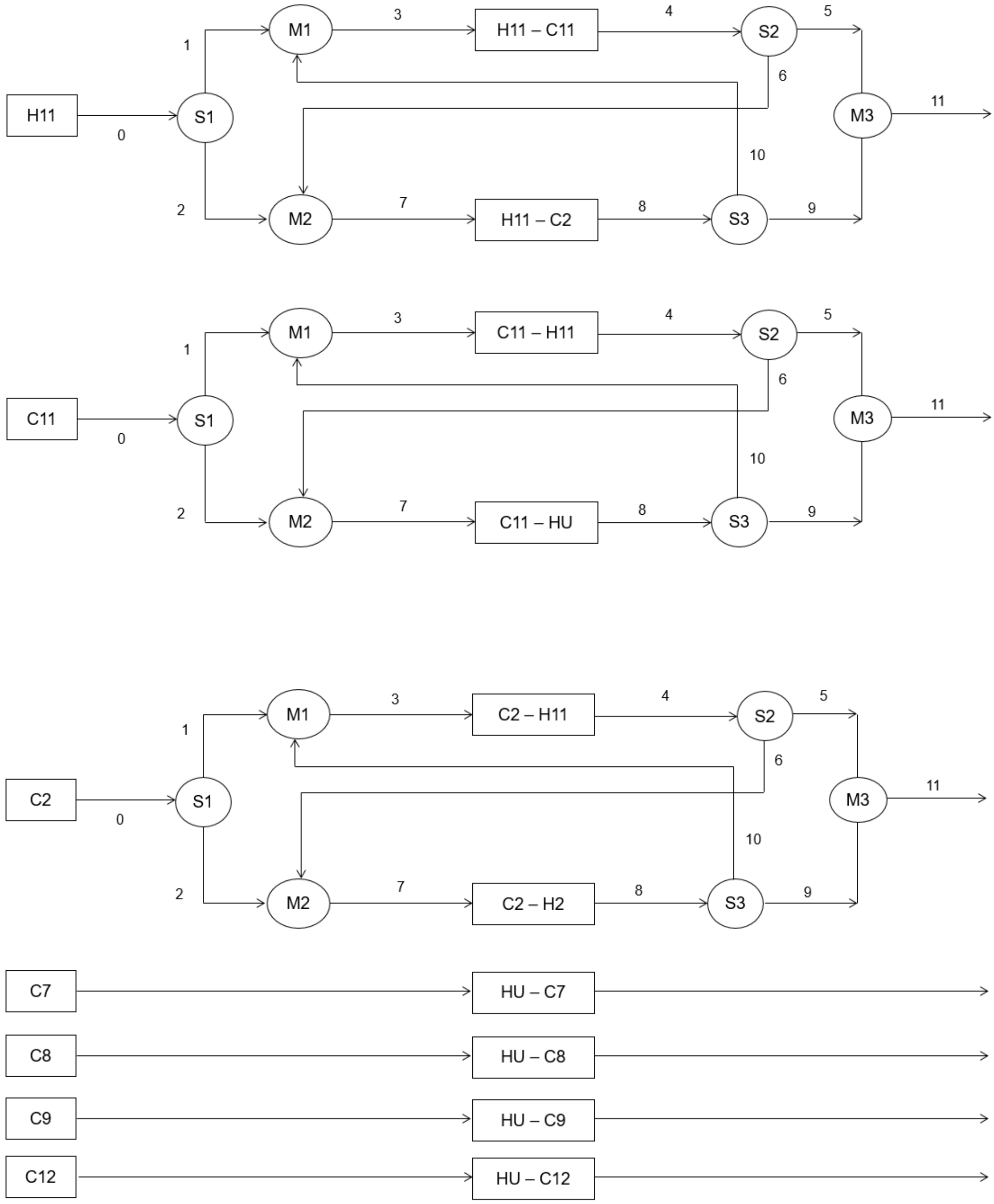
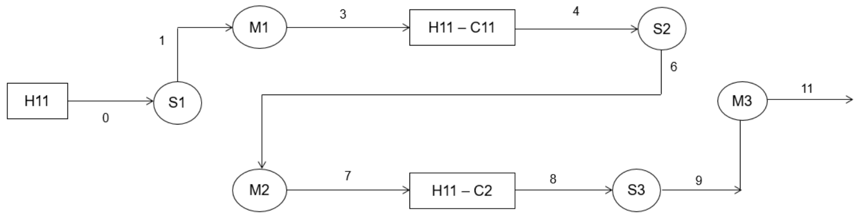
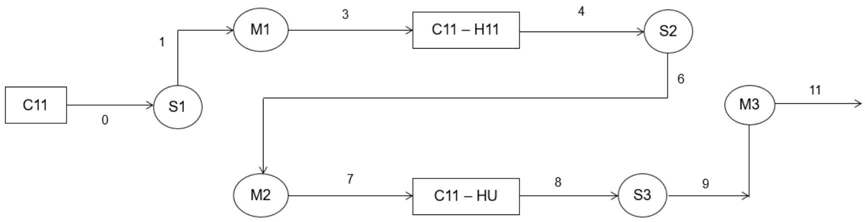


Figure XI.1: Streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network of Arosolvan Unit.

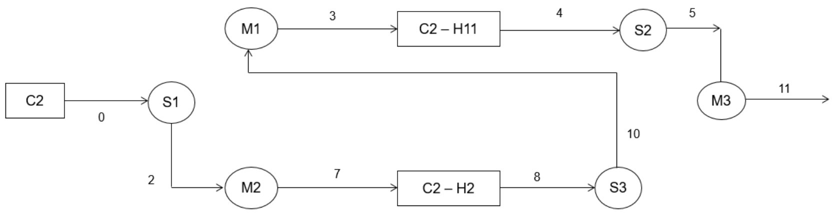
Stream Structures Solution for Subnetwork above Pinch Point



SOLVENT (NMP+MEG) (H21)		
Stream	MCp (MJ/HR)	T (°C)
0	367.200	150.00
1	367.200	150.00
3	367.200	150.00
4	367.200	148.97
6	367.200	148.97
7	367.200	148.97
8	367.200	140.00
9	367.200	140.00
11	367.200	140.00



T0251 BTM R1 (C11)		
Stream	MCp (MJ/HR)	T (°C)
0	2622.857	138.00
1	2622.857	138.00
3	2622.857	138.00
4	2622.857	139.26
6	2622.857	139.26
7	2622.857	139.26
8	2622.857	160.40
9	2622.857	160.40
11	2622.857	160.40



SOLVENT GLICOL R2 (C2)		
Stream	MCp (MJ/HR)	T (°C)
0	474.906	118.80
2	474.906	118.80
3	474.906	118.86
4	474.906	122.00
5	474.906	122.00
7	474.906	118.80
8	474.906	118.86
10	474.906	118.86
11	474.906	122.00

Figure XI.2: Results for streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network of Arosolvan Unit.

Stream Superstructure for Subnetwork below Pinch Point

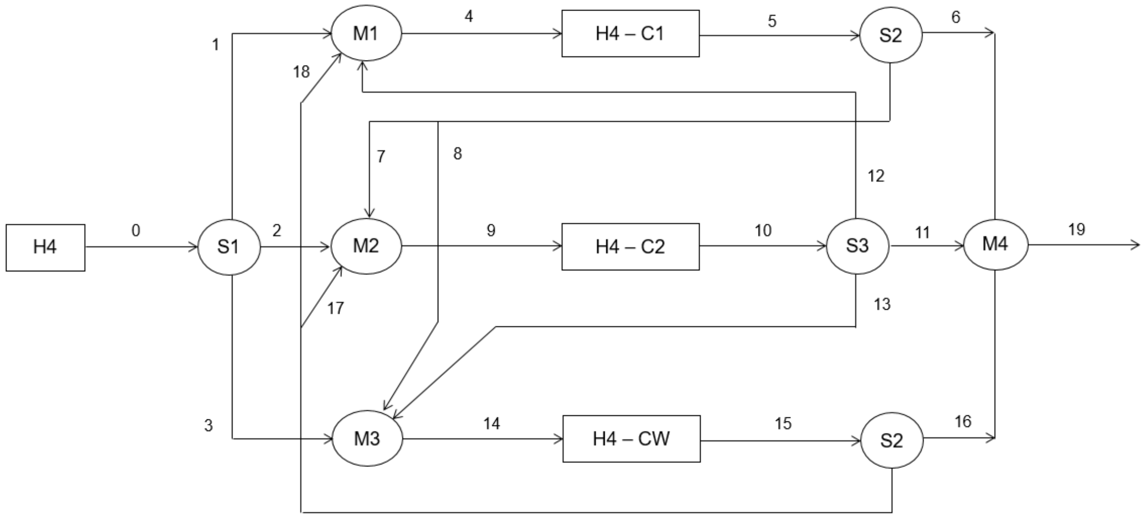
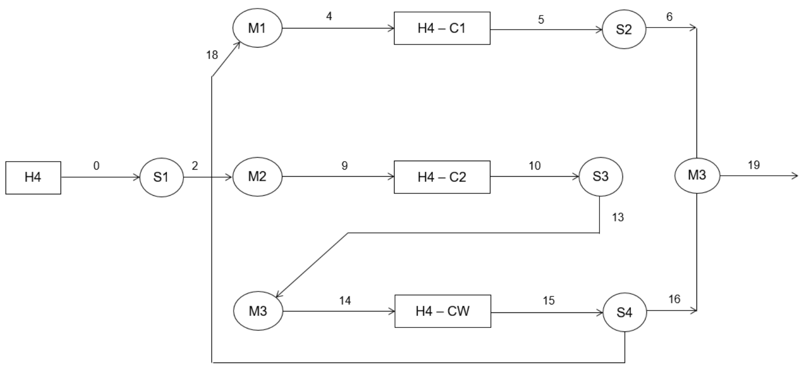


Figure XI.3: Streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network of Arosolvan Unit.

Stream Structure Solution for Subnetwork below Pinch Point



TOLUENE (H4)		
Stream	MCp (MJ/HR)	T (°C)
0	23.754	128.80
2	23.754	128.80
4	23.338	128.14
5	23.338	109.70
6	23.338	109.70
9	23.754	128.80
10	23.754	128.31
13	23.754	128.31
14	23.754	128.79
15	23.754	128.14
16	0.416	128.14
18	23.338	128.14
19	23.754	109.70

Figure XI.4: Results for streams superstructure for HEN subnetwork above pinch point considering inefficient zones of energy consumption network of Arosolvan Unit.

The operating conditions resultant from stream matches using pinch design method with maximum reuse of the existing heat exchangers are presented in the next Tables XI.3 and XI.4.

Table XI.3: Operating data resulting from stream matches above pinch point using hybrid methodology and cross-pinch exchanger elimination method for Arosolvan Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m²)
NU-1	SOLVENT(NMP+MEG)	H1	150	148.97	104.945	11.067	94.83
	T0251 BTM R1	C11	138.00	139.26			
NU-2	SOLVENT(NMP+MEG)	H1	148.97	140	915.055	24.458	374.13
	SOLVENT GLICOL R2	C2	118.8	118.86			
NU-3	C9CUT	H2	161.4	128.8	8.373	22.506	3.72
	SOLVENT GLICOL R2	C2	118.86	122			
NU-4	STEAM	HU	200	199	9740	49.55	1965.7
	SOLVENT (NMP+MEG) R1	C7	165.4	165.5			
NU-5	STEAM	HU	200	199	3390	53.55	316.5
	T0252 BTM R1	C8	161.4	161.5			
NU-6	STEAM	HU	200	199	5730	65.16	879.4
	EXTRACT R2	C9	138	160.4			
NU-7	STEAM	HU	200	199	915.055	68.121	134.3
	T0251 BTM R1	C11	139.26	160.40			
NU-8	STEAM	HU	200	199	5080	82.298	617.3
	T0251 BTM R2	C12	132	133.4			

Table XI.4: Operating data resulting from stream matches below pinch point using hybrid methodology and cross-pinch exchanger elimination method for Arosolvan Unit.

Unit	Matches (ij)	ID	T_{INLET} (°C)	T_{OUTLET} (°C)	Q (kW)	LMTD (°C)	A (m²)
NU-9	TOLUENETOP	H4	128.14	109.7	15.0	14.2	10.6
	AROMATICS EXTRACTED	C1	50	122.7			
NU-10	TOLUENE	H4	128.8	128.31	1096.6	11.6	947.3
	SOLVENT GLICOL R2	C2	115	122			
NU-11	TOLUENE	H4	128.79	128.14	1460.4	105.8	138.0
	CW	CU	10	20			
NU-12	SOLVENT (NMP+MEG) 3	H1	128.8	62.5	1309.0	47.2	277.2
	CW	CU	10	20			
NU-13	TOLUENE DIST	H5	109.7	30.5	304.0	27.7	109.9
	CW	CU	10	20			
NU-14	PURE WATE	H6	105.1	72.4	1903.0	58.8	323.8
	CW	CU	10	20			
NU-15	BENZENE TOP	H7	91.1	24.7	3983.9	59.8	666.7
	CW	CU	10	20			
NU-16	BENZENE 2	H8	89.1	75.4	94.4	18.0	52.5
	CW	CU	10	20			
NU-17	EXTRACT RECYCLE PROD	H9	72.8	28.1	3155.0	25.1	1256.8
	CW	CU	10	20			
NU-18	PURE WATER DIST	H10	72.4	60	23.3	43.7	5.3
	CW	CU	10	20			
NU-19	LIGHT NON AROMATICS	H11	60.7	33.1	236.0	23.8	99.0
	CW	CU	10	20			
NU-20	AROMATICS (SAT GLICOL)	H12	49.6	30.5	5434.0	17.5	3110.5
	CW	CU	10	20			

The purchased cost of the equipment resultant from stream matches using cross-pinch exchanger elimination method are presented in the next Tables XI.5 and XI.6.

Table XI.5: Heat transfer areas and respective bare module cost for stream matches obtained for subnetwork above pinch point using hybrid methodology and cross-pinch exchanger elimination method for Arosolvan Unit.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
NU-1	SOLVENT(NMP+MEG) T0251 BTM R1	H1 C8	94.83	0	0	24774.2	1.0	1.63	1.66	3.29	81507	71726
NU-2	SOLVENT(NMP+MEG) SOLVENT GLICOL R2	H1 C2	374.13	0	0	56383.4	1.0	1.63	1.66	3.29	185501	163241
NU-3	C9CUT SOLVENT GLICOL R2	H2 C2	3.72	0	0	28109.0	1.0	1.63	1.66	3.29	92479	81381
NU-4	STEAM SOLVENT (NMP+MEG) R1	HU C7	1965.69	2033.8	3.35	305607.8	1.0	1.63	1.66	3.29	201090	176959
NU-5	STEAM T0252 BTM R1	HU C8	316.53	0	0	49605.5	1.0	1.63	1.66	3.29	163202	143618
NU-6	STEAM EXTRACT R2	HU C9	879.38	891	1.30	122446.3	1.0	1.63	1.66	3.29	80570	70901
NU-7	STEAM T0251 BTM R1	HU C11	134.33	153.2	12.32	29051.4	1.0	1.63	1.66	3.29	19116	16822
NU-8	STEAM T0251 BTM R2	HU C12	617.27	754.8	18.2	86660.6	1.0	1.63	1.66	3.29	57023	50180
Additional Area (m^2)			789.2									
Re-used Area (m^2)			3832.8									
CBM $(EUROS)_{2001}$			774,828 €									
CBM $(EUROS)_{2018}$			1,162,833 €									

Table XI.6: Heat transfer areas and respective bare module cost for stream matches for subnetwork below pinch point obtained using hybrid methodology and cross-pinch exchanger elimination method for Arosolvan Unit.

Unit	Matches (ij)	ID	A (m^2)	A_{REUSE} (m^2)	Over Capacity (%)	Cp^0 (dollars)	FM	B1	B2	FBM	CBM (dollars)	Cp^0 (euros)
NU-9	TOLUENETOP AROMATICS EXTRACTED	H4 C1	10.6	0	0	19655	1.0	1.63	1.66	3.29	64663	56904
NU-10	TOLUENE SOLVENT GLICOL R2	H4 C2	947.3	0	0	132258	1.0	1.63	1.66	3.29	435128	382913
NU-11	TOLUENE CW	H4 CU	138.0	162.4	15.0	29457	1.0	1.63	1.66	3.29	19383	17057
NU-12	SOLVENT (NMP+MEG) 3 CW	H1 CU	277.2	0	0	45065	1.0	1.63	1.66	3.29	148263	130471
NU-13	TOLUENE DIST CW	H5 CU	109.9	0	0	26392	1.0	1.63	1.66	3.29	86829	76409
NU-14	PURE WATE R1 CW	H6 CU	323.8	0	0	50453	1.0	1.63	1.66	3.29	165989	146070
NU-15	BENZENE TOP CW	H7 CU	666.7	0	0	93162	1.0	1.63	1.66	3.29	306502	269721
NU-16	BENZENE 2 CW	H8 CU	52.5	0	0	20412	1.0	1.63	1.66	3.29	67155	59097
NU-17	EXTRACT RECYCLE PROD CW	H9 CU	1256.8	0	0	179767	1.0	1.63	1.66	3.29	591434	520462
NU-18	PURE WATER DIST CW	H10 CU	5.3	5.49	2.86	24012	1.0	1.63	1.66	3.29	15800	13904
NU-19	LIGHT NON AROMATICS CW	H11 CU	99.0	109.3	9.46	25216	1.0	1.63	1.66	3.29	16592	14601
NU-20	AROMATICS (SAT GLICOL) CW	H12 CU	3110.5	0	0	558015	1.0	1.63	1.66	3.29	1835868	1615564
Additional Area (m^2)			6755.3									
Re-used Area (m^2)			277.2									
CBM $(EUROS)_{2001}$			3,303,174 €									
CBM $(EUROS)_{2018}$			4,957,276 €									