Methodology for efficient use of thermal energy in the chemical and petrochemical industry

THÈSE N^{O} 8485 (2018)

PRÉSENTÉE LE 29 MARS 2018

À LA FACULTÉ DES SCIENCES ET TECHNIQUES DE L'INGÉNIEUR
GROUPE SCI STI FM
PROGRAMME DOCTORAL EN ENERGIE

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

POUR L'OBTENTION DU GRADE DE DOCTEUR ÈS SCIENCES

PAR

Elfie Marie MÉCHAUSSIE

acceptée sur proposition du jury:

Prof. J. Luterbacher, président du jury
Prof. F. Maréchal, Prof. G. M. Van Eetvelde, directeurs de thèse
Prof. S. Harvey, rapporteur
Dr B. Adams, rapporteur
Prof. D. Favrat, rapporteur

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Suisse
2018

Acknowledgements

This thesis would not have seen the light of day without the contributions of many people throughout these 4 years and 4 months.

First of all, I would like to deeply thank my thesis director, Prof. François Maréchal, and co-director, Prof. Greet Van Eetvelde. François, merci pour ta confiance, accordée dès les premiers instants où l'on a commencé à travailler ensemble, ainsi que d'avoir partagé ta passion pour l'étude et l'optimisation des systèmes énergétiques. Tes conseils et les nombreuses discussions que l'on a pu avoir tout au long de cette thèse m'ont beaucoup apporté au point de vue scientifique mais également personnel. Greet, je te remercie sincèrement de m'avoir offert cette opportunité. Ton support, ton investissement, et ton énergie à toute épreuve ont été des éléments essentiels pour le bon déroulement et la réussite de ce doctorat.

Besides my advisors, I would like to warmly thank the rest of my thesis committee: Prof. Simon Harvey, Dr. Bart Adams, Prof. Daniel Favrat, and the president of the jury, Prof. Jeremy Luterbacher. Thank you for thoroughly reviewing my thesis and providing me with pertinent comments.

I am very grateful to INEOS for granting me the trust and support to carry out this PhD thesis. I had the chance to travel across Europe and meet many great people in the framework of several energy studies, especially during the first three years. The technical knowledge and industrial experiences I gained on the way are of great value.

Thank you to all the energy managers and project coordinators that worked with the master students and myself and contributed to the smooth execution and success of the projects in France (to Bernard Descales, Marc Hanquet and Henri Amber), United Kingdom (to Dave Skeldon), Italy (to Claudio Mariottini), Netherlands (to Hak Maarten), Germany (to Falk Lindner), Canada (to Brad Campbell) and Belgium.

A special thought for the Antwerp/Gladbeck team, Tony De Roo, Markus Weber, Ralf Bonmann, and Marius Harrmann, with whom I had the privilege to collaborate with for several months.

Thank you to all the master students that contributed to this thesis: Julien Guenat, Akio Schoorl, Hélène Cervo, Matteo Latinov, Alessio Santecchia, Fran Jaksic and Simon Castres Saint Martin. A shout-out to Alessio and Hélène who started a PhD after successfully completing their master projects.

This thesis would not have been possible without the amazing people that are part of the Industrial Process and Energy Systems Engineering (IPESE) group.

Un grand merci aux deux secrétaires de l'IPESE, Brigitte dans les premiers temps puis Sylvie, avec qui j'ai eu le plaisir de collaborer (et de papoter) et qui ont fait et font un travail incroyable pour que le laboratoire tourne. Merci également à Cécile de s'être toujours assurée que je passe les différentes étapes de ma thèse sans anicroches.

J'aimerais remercier ici deux personnes en particulier. Stéphane, merci pour toute l'aide que tu m'as apportée ainsi que tes conseils durant le temps où l'on a bossé ensemble, et cela depuis le début sous le soleil aveuglant de Cologne jusqu'à tes derniers instants à l'EPFL. Le témoin n'aurait pas pu tomber entre de meilleures mains que celles d'Hélène. Malgré la distance, un grand merci pour ta motivation et tes encouragements sans faille. Je te suis très reconnaissante d'avoir relu l'entièreté de cette thèse!

A huge thank you to all the IPESE members for always bringing a nice and fun work environment: to Stefano (pour ton humour et tes questions existentielles), Sophia (for always having a story to tell), Victor (for your relaxed spirit), Maziar (you are the only one who can solve the energy trilemma), Dilan (for your kindness), Nils (I promise I was working when I was staring at the view from my desk), Paul (un temps mon compagnon de bureau), Alberto (aka le chasseur), Hür (the Osmose master), Raluca (the CO_2 network master), Ivan (for the best English pronunciation ever), Francesca (always a good fashion style), Sébastien (for sharing fonts with me), Alessio (the coffee drinker), Katie (for your easily identifiable laugh), but also to the people from the GEM lab with Priscilla (best Vivapoly decorator), Manuel, Giorgio, Guillaume, Hossein, and all the others! Une pensée également pour les anciens Jean-Loup, Matthias, Raman, Samuel, Ema, Lindsay, Tivi et Leandro.

Durant ces années de doctorat, si je n'étais pas au bureau, il y a de grandes chances que je fus sur une piste d'athlétisme. Mon club et mes entraineurs m'ont été d'une aide inestimable pour mener mes deux projets de front, sur la piste comme en dehors. Une dédicace spéciale à Etienne (et son chien Luxor) et Mahé (alias Mamel), avec qui j'ai partagé de longues minutes (heures?) de souffrance mais aussi de nombreux réconforts culinaires. Merci à Paul (la fusée de l'AEA), Piment (imbattable au bras de fer) et Karl (l'homme du 30m) pour avoir mis la bonne ambiance à l'entrainement. Je tiens à remercier également mes coachs: Antoine, pour avoir cru en mon potentiel sur 400m, et Brice, pour avoir toujours su me faire repousser mes limites et avoir pris soin de mes muscles pendant toutes ces années.

J'ai bien sûr une pensée pour tous mes amis, qui rendent la vie bien plus merveilleuse. Je remercie particulièrement Jenn et Raphi pour être toujours à mes côtés depuis mes années d'études à l'EPFL, ainsi qu'Ally, malgré les 5907 km qui nous séparent. Merci aussi à ma coloc préférée, Carole, pour tous les moments et fous rires partagés au Tunnel, sans oublier Lili et Bébou!

Un énorme merci à Marie et Rémi, pour m'avoir toujours encouragé et aidé dans ma double vie d'athlète et de doctorante.

Mes plus profonds remerciements vont à ma famille. A mes grands-parents et mes tantes, à mon frère Bertil et ma soeur Chloé, pour toujours être présents pour leur petite soeur, à mon adorable nièce Gladys, à QiaoWen, à Alban et enfin, à mes parents, Daniel et Agnès, pour toujours croire en moi et être là quoi qu'il arrive. La dernière personne que j'aimerais remercier, John, la vie n'aurait pas la même saveur si tu n'étais pas à mes côtés. Merci pour ton soutien constant durant ces années de thèse.

Lausanne, le 27 février 2018

Abstract

The current European energy regulation, aligned with the European Union energy strategy and targets for the next decade, requires large industrial companies to regularly assess their energy performance and implement energy efficiency improvement measures. In many cases, these energy reviews fulfil minimum criteria for energy audits set by the legislation and focus on the optimisation of the energy conversion units and utilities distribution. Opportunities for energy savings within production processes are missed, which can also lead to an inadequate hot and cold supply system. Existing methods for energy reviews in the petrochemical sector do not feature the holistic and systematic aspects required to deeply analyse and improve industrial sites down to the production units level. The lack of time and human resources, combined to the availability and reliability of data, are additional barriers preventing detailed studies to take place.

This thesis presents a comprehensive methodology to carry out detailed energy review of (petro)chemical plants, in accordance with energy management and auditing standards requirements. This methodology comprises three main steps: the energy consumption analysis, the targeting of the heat recovery potential and the identification and evaluation of energy saving opportunities to reach this target. A top-down approach is undertaken in the first step, with the objective of translating the raw energy consumption of the system into process units heating and cooling demand. In doing so the mass and energy flows are mapped and the efficiency of the entire energy chain is characterised in a structured way. The focus on the process requirements allows to understand how much, where and why energy is consumed. In this first step, guidelines and heuristic rules are defined to reduce the required time for data collection. A data consistency check in the form of key mass and energy balances ensures the validity of data and a good control of the energy flows of the system.

In the second step, a novel methodology for the definition of the minimum approach temperature in pinch analysis is presented. By considering the characteristics of each process hot and cold stream individually, together with the economic parameters of the system, the heat recovery potential is refined and the minimum energy consumption targets are closer to what can be achieved economically. From the results of the pinch analysis, the objective of the third step is to reach the energy targets through the identification of energy saving opportunities. A bottom up approach is defined to look for options starting from the process operating parameters and heat integration towards the optimisation of the energy conversion and distribution system. Waste heat recovery through heat pumping being a recurring identified opportunity, a heat transformer system is proposed, coupling a mechanical vapour compression cycle to an organic Rankine cycle. Integrated to the polyethylene slurry production, this system allows to recover the residual reaction heat and produce steam without importing electricity from the grid. In doing so the energy consumption is reduced by 50%.

The proposed methodology was developed, tested and refined on around 10 different petrochemical sites, enabling a comprehensive analysis of their energy performance and leading to the identification of promising energy saving opportunities to increase the energy efficiency of their production.

Keywords

Energy efficiency, energy review, methodology, petrochemical industry, pinch analysis, heat recovery targeting, energy performance indicators, data collection, heat transformer, waste heat recovery

Résumé

La législation européenne actuelle en matière d'énergie impose aux grands groupes industriels d'évaluer régulièrement leur performance énergétique, d'identifier les mesures adéquates permettant de l'améliorer, et de les mettre en oeuvre. Dans de nombreux cas, ces revues énergétiques répondent aux critères minimaux d'audits fixés par la législation et se concentrent sur l'optimisation des unités de conversion et de distribution d'énergie. Les opportunités d'économie d'énergie au niveau des procédés de production sont manquées, ce qui peut également conduire à un système de fourniture de chaud et de froid inadapté. Les méthodes existantes pour réaliser des revues énergétiques sur des sites pétrochimiques ne présentent pas les aspects holistiques et systématiques nécessaires pour analyser et améliorer en profondeur les sites industriels. Le manque de temps et de ressources humaines, combinés à la disponibilité et à la fiabilité des données, sont des obstacles supplémentaires qui empêchent de donner lieu à des études poussées.

Cette thèse présente une méthodologie complète pour effectuer un examen énergétique détaillé de sites pétrochimiques, en accord avec les exigences des normes de gestion de l'énergie et d'audit. Cette méthodologie comprend trois étapes principales : l'analyse de la consommation d'énergie, le ciblage du potentiel de récupération de chaleur et l'identification et l'évaluation des opportunités d'économie d'énergie pour atteindre cet objectif. Une approche descendante est utilisée en premier lieu, afin de traduire la consommation d'énergie brute du système en demande de chauffage et de refroidissement des procédés. Ce faisant, les flux de masse et d'énergie sont cartographiés et l'efficacité de la chaîne énergétique est caractérisée de manière structurée. Des lignes directrices et règles heuristiques sont fournies pour réduire le temps nécessaire à la collecte de données. Un contrôle de cohérence des données sous forme de bilans massiques et énergétiques est également introduit, assurant la validité des données.

Dans la deuxième étape, une nouvelle méthodologie pour la définition de la température minimale d'approche au niveau de l'analyse de pincement est présentée. En considérant les caractéristiques de chaque flux chaud et froid individuellement, ainsi que les paramètres économiques du système, le potentiel de récupération de chaleur est affiné et les objectifs de consommation d'énergie minimum sont plus proches de ce qui peut être atteint économiquement. Finalement, une approche ascendante est définie pour identifier les options permettant d'atteindre les objectifs énergétiques, en partant des paramètres de fonctionnement des procédés de production vers l'optimisation du

système de conversion de l'énergie. La récupération de la chaleur résiduelle par pompe à chaleur étant une opportunité identifiée de manière récurrente, un système de transformateur de chaleur est proposé, couplant un cycle de compression mécanique de vapeur à un cycle organique de Rankine. Intégré à la production de polyéthylène par le procédé "slurry", ce système permet de réduire la consommation d'énergie de 50% sans importer d'électricité du réseau.
La méthodologie proposée a été développée, testée et affinée sur une dizaine de sites pétrochimiques, permettant une analyse complète de leur performance énergétique, ainsi que l'identification d'opportunités d'économies d'énergie afin d'améliorer l'efficacité énergétique liée à leur production.

Mots-clefs
Efficacité énergétique, revue énergétique, méthodologie, industrie pétrochimique, analyse de pincement, intégration de chaleur, cibles énergétiques, indicateurs de performance énergétiques, collecte de données, transformateur de chaleur, récupération de chaleur perdue

Contents

Acknowledgements **iii**

Abstract (English/Français) **vii**

List of figures **xv**

List of tables **xix**

Glossary **xxi**

Nomenclature **xxiii**

Introduction **1**
European context . . . 1
Energy audits and energy management systems . . . 4
What is an energy review? . . . 5
Problematic and challenges . . . 6
Thesis objectives and outline . . . 8

1 Methodology for energy reviews **15**
1.1 Carrying out an energy review . . . 15
1.1.1 General guidelines . . . 15
1.1.2 Specific tools and techniques . . . 17
1.2 Proposed methodology . . . 21
1.2.1 Step 1: energy consumption analysis . . . 23
1.2.2 Step 2: targeting energy consumption reduction . . . 24
1.2.3 Step 3: achieving energy consumption reduction . . . 25
1.2.4 Pinch analysis at the core of the methodology . . . 26
1.3 Conclusion . . . 27

2 Energy consumption analysis **29**
2.1 Black box characterisation . . . 30
2.1.1 System's boundaries . . . 30

2.1.2 Energy vectors distribution . . . 32
2.1.3 Energy vectors comparison . . . 33
2.1.4 Energy baseline . . . 36
2.2 From black box to process flowsheet representation . . . 40
2.2.1 Site map . . . 40
2.2.2 Process block flow diagram . . . 42
2.2.3 Process flowsheet . . . 42
2.2.4 Choosing the level of detail . . . 44
2.3 Data gathering . . . 45
2.3.1 Dual representation . . . 46
2.3.2 Streams classification . . . 47
2.3.3 Minimum data set . . . 48
2.3.4 Heuristic rules . . . 52
2.4 Data validation . . . 54
2.4.1 Data reconciliation . . . 54
2.4.2 Data consistency check . . . 55
2.5 Key performance indicators . . . 61
2.6 Conclusion . . . 64

3 Targeting heat recovery **67**
3.1 Pinch analysis and energy review . . . 67
3.2 Generating the energy profile . . . 68
3.2.1 Current process-utility profile . . . 68
3.2.2 Level of detail refining . . . 69
3.3 Energy consumption targeting . . . 73
3.3.1 Importance of the targeting step . . . 73
3.3.2 ΔT_{min} selection in pinch analysis . . . 74
3.3.3 Parameters impacting the thermo-economic trade-off . . . 75
3.3.4 Parameters estimation . . . 78
3.3.5 Economic indicator for decision criteria . . . 84
3.3.6 Heat exchanger choice and technical limitations . . . 85
3.3.7 Single heat exchange example . . . 86
3.3.8 Consequences for pinch analysis . . . 88
3.4 Methodology proposition for ΔT_{min} definition . . . 88
3.4.1 Theoretical basis . . . 89
3.4.2 Corrected profiles generation procedure . . . 90
3.4.3 Impact of parameters . . . 92
3.5 Application on two examples . . . 93
3.5.1 Scenario 1 . . . 95

3.5.2 Scenario 2 99
3.5.3 Impact on heat pumping potential and utility integration 103
3.5.4 Discussion 105
3.6 Conclusion 106

4 Reaching the energy consumption target 107
4.1 Bottom-up approach 107
4.1.1 Onion diagram for the identification of energy saving opportunities 108
4.2 Example on a case study 110
4.2.1 Process operating parameters 112
4.2.2 Process direct heat integration 114
4.2.3 Heat pumping 116
4.2.4 Energy conversion 119
4.2.5 Summary 121
4.2.6 Sensivity analysis 122
4.3 Study of a new heat transformer 124
4.3.1 Heat pumping technologies overview 125
4.3.2 System description 127
4.3.3 Integration with polymer production 128
4.3.4 Perspectives 133
4.4 Conclusion 135

Conclusions and perspectives 137
Main results summary 137
Future perspectives 144

A List of streams depending on the level of details 147

B Scenarios 1 & 2 list of streams 151

C Calculation details for EnSO's evaluation 155

D Vali models of the heat transformer 157

References 159

Curriculum Vitae 171

List of Figures

1 Global context for industrial energy efficiency improvement in Europe. *(*)EnMS = Energy Management System* 1
2 Key requirements of an energy review as defined in ISO 50001. 5
3 Representation of the main approaches for energy reviews according to the level of detail and time required. 7
4 Overview of the main petrochemical processes studied in the thesis. 10

1.1 Venn diagram of the different tools and techniques that can be used during an energy review 17
1.2 Detailed overview of methodology and open questions. 22
1.3 Example of daily production and monthly averages. 23
1.4 Example of (a) hot and cold composite curves and (b) corresponding grand composite curves. 27

2.1 Schematic representation of possible system boundaries 30
2.2 Mass and energy flows to consider at the system's boundary, when applicable 31
2.3 Energy content of the condensation of 1 ton of steam according to the pressure level (condensates = 1.5 bar and 100°C). 33
2.4 Example of the energy consumption according to production per energy vector (daily values). 36
2.5 Example of the specific energy consumption according to production per energy vector (daily values). 37
2.6 Multi-period representation of a production profile (a) and typical period distribution over the study period (b). 38
2.7 Site map representation 41
2.8 Example of process unit decomposition into main blocks 42
2.9 Example of process flowsheet. 43
2.10 Black, grey and white box grand composite curves of a production unit 45
2.11 Key questions of the data gathering step. 46
2.12 Dual representation of a black box and a grey box cold process stream with the corresponding utility. 46

2.13 Energy balance around a distillation column. 50
2.14 Procedure to collect data. 50
2.15 Comparison between full and Pareto streams definition 53
2.16 Mass and energy flows involved in the key balances of the data consistency check . . . 55
2.17 Example of a Sankey diagram at the site level (LPS = low pressure steam, HW = hot water) 56
2.18 Example of a Sankey diagram 60
2.19 Example of an industrial site KPI's map. 62
2.20 Key questions of the data gathering step. 65

3.1 Example of a total site profile. 69
3.2 GCC according to the level of detail for the streams definition. 70
3.3 MER hot and cold according to the level of detail. 71
3.4 Number of cold (top), hot (middle) and total (bottom) streams in black, grey and white boxes representations according to the level of detail. 72
3.5 Parameters influencing the choice of ΔT_{min} for a counter-current heat exchanger . . . 77
3.6 Evolution of the natural gas price in France and Germany between 1979 and 2014 (including taxes) [1]. *NB: missing price data in 2001 for Germany.* 80
3.7 (a) Turton et al. module cost estimates for a fixed tube heat exchanger (CS/CS) operating under ambient pressure conditions (b) cost estimates comparison on the same type of exchanger. 84
3.8 ΔT_{min} distribution (nb. evaluations = 100'000) 87
3.9 Scatter plot of the corresponding payback times. 87
3.10 Example of corrected profiles for a hot (left) and a cold (right) stream 89
3.11 Procedure to generate the corrected T-H profiles of all streams 91
3.12 Graphical representation of the main parameters at a given temperature point along the procedure. 92
3.13 (a) Influence of the heat transfer coefficient U (in $W/m^2 °C$) and (b) of the payback time constraints on the corrected profile of a hot stream. 93
3.14 (a) $\Delta T_{min}/2$ and (b) $\dot{Q}_{min}$ variation according to the overall heat transfer coefficient and different economic conditions. 93
3.15 Composite curves for S1.A (a) and S1.B (b). 95
3.16 Streams involved in HEN redesign above the pinch point for S1.A (a) and S1.B (b). . . . 97
3.17 Streams involved in HEN redesign below the pinch point for S1.A (a) and S1.B (b). . . . 98
3.18 Composite curves for S2.A (A) and S2.B (B). 99
3.19 Streams involved in HEN retrofit above the pinch point for S2.A (a) and S2.B (b). 101
3.20 Streams involved in HEN retrofit below the pinch point for S2.A (a) and S2.B (b). 102
3.21 Different scenarios for heat pump and utility integration for S1.A (a) and S1.B (b). LPS and MPS are respectively for low and middle pressure steam. 104

4.1 (a) Typical onion diagram for chemical process design (derived from [2]) and (b) modified onion diagram for the identification of EnSO's. 109
4.2 (a) Total site profile and (b) grand composite curve of the case study. 111
4.3 Utility system in place in the case study. 111
4.4 Distillation column without (initial) and with feed preheating. 113
4.5 Initial heat exchangers configuration. 115
4.6 Redesign of the heat exchangers configuration. 116
4.7 Zoom on the process GCC with heat pumping integration possibilities: (a) MVR or (b) close HP cycle with multi-products stream and (c) MVR with single product condensing stream. 117
4.8 Implementation of mechanical vapour recompression on a distillation column. 118
4.9 Updated GCC including the mechanical vapour recompression. 118
4.10 Corrected temperature and Carnot integrated composite curve of the system with (a&c) the initial natural gas boiler and (b&d) a gas turbine with lower steam pressure levels. 120
4.11 Caption for LOF 121
4.12 Sensitivity analysis results for the feed preheating (top), heat exchanger network redesign (middle) and mechanical vapour recompression (bottom). Results for 1000 evaluations. 123
4.13 Grand composite curves of the HPDE slurry process when the initial cooling water and real reaction temperatures are considered. 124
4.14 Overview of active waste heat recovery technologies for heat and electricity production (from [3]). The two highlighted technologies are the ones involved in the proposed heat transformer. 125
4.15 P-T representations of an (a) absorption heat pump, (b) absorption heat transformer, (c) ORC-HP and (d) of the proposed heat transformer (reversed ORC-HP). 126
4.16 T-s diagrams of (a) the ORC-HP cycle, (b) proposed heat transformer 127
4.17 Schematic representation the heat transformer. 128
4.18 T-s diagrams of a (a) wet fluid, (b) dry fluid and (c) isentropic fluid, and the effect of isentropic expansion or compression from the saturated vapour state. 128
4.19 Schematic representation the heat transformer integrated with the HDPE slurry process, using hexane as working fluid. 129
4.20 Integrated composite curves of the hexane heat transformer with the rest of the system130
4.21 Schematic representation of the integrated open cycle heat transformer using water. . 132
4.22 Integrated composite curves of the open heat transformer. 133
4.23 Key requirements of an energy review as defined in ISO 50001 and link to the steps of the methodology. 138
4.24 Overview of methodology and thesis contributions 139
4.25 Results of the application of the methodology on different industrial sites. 144

D.1 Vali model of the integrated heat transformer with hexane as working fluid. 157
D.2 Vali model of the open version of heat transformer with water as working fluid. 158

List of Tables

1 Scope of the audit and penalties for non compliance in France, Germany, Belgium and the United Kingdom. . . . 3

2.1 Energy consumption breakdown based on Best Practice Technologies of the production processes of key petrochemicals. . . . 32
2.2 Final energy consumption calculations 34
2.3 Yearly production and energy baseline 39
2.4 Comparison between the study year and the energy baseline 40
2.5 Complementary data collection for process stream definition 51

3.1 MER results for each level of detail 71
3.2 Typical overall heat transfer coefficients for tubular heat exchanges, involving common (petro)chemical species and utilities. . . . 79
3.3 Overview of widely used cost estimates for heat exchangers. . . . 82
3.4 Best and worst cases parameter values. . . . 86
3.5 Probability distribution functions for the selected uncertain parameters. . . . 86
3.6 Utilities description for both scenarios 94
3.7 Other cost parameters 94
3.8 MER results - S1 95
3.9 Penalising heat exchanges for S1 96
3.10 Pairs of streams involved in heat recovery of S1.B above the pinch. . . . 97
3.11 Pairs of streams involved in heat recovery of S1.B below the pinch. . . . 98
3.12 MER results - S2 100
3.13 Penalising heat exchanges for S2 100
3.14 Pairs of streams involved in heat recovery of S2.A above the pinch. . . . 101
3.15 Pairs of streams involved in heat recovery S2.B below the pinch. . . . 102
3.16 Scenario 1 heat pump integration schemes 104

4.1 Pinch analysis results (T_{pinch} = 89.5°C). . . . 110
4.2 Energy prices and economic parameters 112
4.3 Penalising heat exchangers, total = 6 MW. . . . 112

4.4 Thermo-economic analysis of the feed preheating 113
4.5 Thermo-economic analysis of the heat exchanger network redesign. 116
4.6 Thermo-economic analysis of the mechanical vapour recompression. 117
4.7 Summary of the energy saving opportunities. 121
4.8 Summary of the energy saving opportunities. 122
4.9 Comparison of system COP with AHT examples. 131
4.10 Heat transformer COP and pressure levels for different working fluids. 133

A.1 Streams definition for the grey box level. 147
A.2 Streams definition for thegrey box Pareto level. 148
A.3 Streams definition for the white box level. 149
A.4 Streams definition for the optimum box level. 150

B.1 Scenario 1 - hot streams 151
B.2 Scenario 1 - cold streams 152
B.3 Scenario 2 - hot streams 152
B.4 Scenario 2 - cold streams 153

C.1 Feed preheating new heat exchanger. 155
C.2 Heat exchanger network redesign. 155
C.3 Mechanical vapour recompression 156

Glossary

benchmarking: procedure of comparing an industrial system's performance to the Best Practice Technologies.

best practice technologies (BPT): specific energy consumption (i.e. GJ/ton of product) of the best performing economically viable processes currently in operation at industrial scale.

best practices reference documents (BREF): series of documents available for different industrial sectors (http://eippcb.jrc.ec.europa.eu/reference/). Each document gives information on a specific industrial sector in the EU, on the techniques and processes used in this sector, current emission and consumption levels, techniques to consider in the determination of the best available techniques and emerging techniques.

energy audit: systematic procedure with the purpose of obtaining adequate knowledge of the existing energy consumption profile of a system, identifying and quantifying cost-effective energy savings opportunities, and reporting the findings [4].

energy baseline: quantitative reference providing a basis for comparison of energy performance. It reflects a specified period of time used for calculation of energy savings, as a reference before and after implementation of energy performance improvement actions [5].

energy management: set of interrelated or interacting elements to establish an energy policy and energy objectives, and processes and procedures to achieve those objectives [5].

energy review: determination of the organisation's energy performance based on data and other information, leading to identification of opportunities for improvement [5]. In this thesis, it also includes the generation of the energy baseline and the definition of key performance indicators.

system's boundaries: physical or site limits and/or organisational limits as defined by the organisation [5].

Nomenclature

Abbreviations

AHP	Absorption heat pump
AHT	Absorption heat transformer
BPT	Best practice technology
COP	Coefficient of performance
CW	Cooling water
CS	Carbon steel
EED	Energy Efficiency Directive
EnMS	Energy management system
EnSO	Energy saving opportunity
EU	European Union
FH	Floating head
FT	Fixed tube
GCC	Grand composite curve
HDPE	High density polyethylene
HEN	Heat exchanger network
HEN	Heat exchanger
HHV	Higher heating value
HP	Heat pump
HT	Heat transformer
HTC	Heat transfer coefficient
HW	Hot water
IC	Investment cost
KPI	Key performance indicator
LHV	Lower heating value
LMTD	Logarithmic mean temperature difference
LPS	Low pressure steam
MVC	Mechanical vapour compression

MER	Minimum energy requirements
MPS	Middle pressure steam
NPV	Net present value
OC	Operating cost
ORC	Organic Rankine cycle
PBT	Payback time
SEC	Specific energy consumption
SS	Stainless steel
TC	Total cost
TDHP	Thermally driven heat pump
TDHT	Thermally driven heat transformer
TSA	Total Site Analysis

Symbols

A	Area	[m^2]
c_p	Heat capacity	[kJ/kg°C]
ΔT	Temperature difference	[°C]
$\dot{E}$	Electrical flow	[kW]
h	Enthalpy	[kJ/kg]
i	Interest rate	[%]
$\dot{m}$	Mass flow	[kg/s]
n	Lifetime	[y]
P	Pressure	[bar]
$\dot{Q}$	Heat flow	[kW]
s	Entropy	[kJ/kg°C]
T	Temperature	[°C]
U	Overall heat transfer coefficient	[$W/m^2 {}^\circ C$]

Indices

a	ambient
c	cold
$cond$	condensation
$desup$	desuperheating
$evap$	evaporation
h	hot
in	inlet
lm	logarithmic mean
max	maximum
min	minimum
o	reference
out	outlet
p	pinch
rec	recovered
$subc$	subcooling
tot	total

Introduction

Overview

- Why is industrial energy efficiency so important in Europe?
- What are the main challenges for increasing energy efficiency in industrial companies?
- Contributions and outline of the thesis.

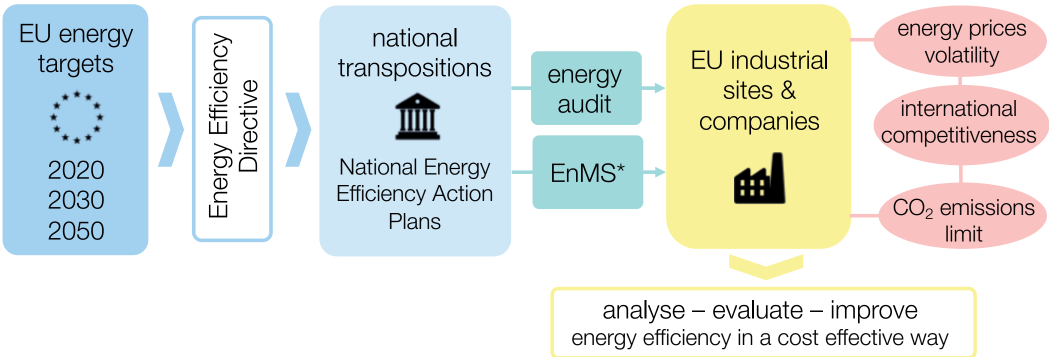


Figure 1 – Global context for industrial energy efficiency improvement in Europe.
(*)EnMS = Energy Management System

European context

European Union energy targets

Around 10 years ago, in order to fight against climate change and increase energy security, the European Union launched its Climate and Energy Package to reach energy targets defined for 2020. Three objectives were set and agreed upon by Member States, with the goal of moving Europe to a highly energy efficient and a low carbon economy. The three targets, also known as the 20/20/20 targets aim a 20% reduction in Europe greenhouse gas emissions compared to 1990 levels, 20% of energy produced from renewable sources, and 20% reduction of primary energy consumption for 2020 [6].

Early 2014, the European Commission went further and released preliminary energy targets for 2030, as a prolongation of the 2020 climate and energy package. The European Union established its commitment to a domestic emissions reduction target of at least 40% by 2030, defined an EU-wide binding target for renewable energy of at least 27% in the energy mix and an improvement in energy efficiency of at least 27% [7].

At the 2015 Climate Change Conference in Paris, Europe committed itself to contributing to limiting the global rise in temperature to only 1.5°C [8]. Following this ambitious decision, the energy efficiency target for 2030 has been extensively negotiated to be better in line with the overall objective in terms of global warming limitation. While a proposition of 30% came up in November 2016 [9], on January 17th, 2018, the European Parliament in plenary sitting endorsed a 35% binding EU target for energy efficiency and indicative national ones [10].

The 2030 objectives are defined as intermediate targets, having in mind even more ambitious ones for 2050 in order to reduce carbon footprint and secure the European energy system by this time, with a 80 to 95% reduction of greenhouse gas emissions as compared to 1990 levels [11]. This timeline, with a clear tightening of the ambitions and targets, enforces and demonstrates the will of Europe to move towards a low-carbon economy, but also put additional pressure on the main energy consuming sectors that are buildings, transport and industry.

Energy Efficiency Directive

The Energy Efficiency Directive 2012/27/UE (EED) [4] was released in December 2012, amending some earlier European directives related to energy by introducing new legally binding measures covering the whole energy chain, from its conversion to end-use consumption. The EED was originally drawn up to reach the 20% EU target for the reduction of energy consumption by 2020, as this target was unlikely to be met according to projections by the time.

The Energy Efficiency Directive is the reference document defining the actual European regulation for energy efficiency. It establishes a common framework of legally binding measures for the promotion of energy efficiency within the European Union at all stages of the energy chain, from the transformation of energy to its final consumption, in order to reach its 2020 and 2030 objectives and to pave the way for further energy efficiency improvements beyond that date.

The main EED requirement impacting large industrial companies is the need for regular assessment of their energy performance (Article 8), either through energy audits and/or implementation of an energy management system (e.g. ISO 50001 standard [5]). Europe strategy for industrial energy consumption is therefore aligned with the International Energy Agency which has recognised industrial energy efficiency as a key element to be able to reach energy consumption and greenhouse gases emissions targets [12].

Minimum criteria for good quality energy audits have been defined in the appendix of the EED, such as being based on up to date energy consumption data and providing a reliable picture of the energy performance and opportunities to save energy. Penalties have to be put in place in case of non-compliance to the Article 8 of the directive.

The transposition within Member States national legislation had to be effective by June 2014. While the basic requirements from the EED are embedded into national transpositions, the scope of the audit and the potential sanctions for non-compliance may differ widely across EU Member States. Table 1 highlights some of these disparities for four European countries [13].

Table 1 – Scope of the audit and penalties for non compliance in France, Germany, Belgium and the United Kingdom.

	France	**Germany**	**Belgium (Flanders)**	**United Kingdom**
Scope of audit	at least 65% of company's energy consumption for the 1st audit, at least 80% for the next ones	at least 90% of the total energy usage; audit has to comply with DIN EN 16247-1 (basis for ISO 50002)	detailed overview of the energy consumption to determine improvement points in a reliable manner	at least 90% of the total energy usage, in compliance with ESOS regulations
Penalties	formal notice indicating a delay for compliance, 2) fine of an amount capped at 2% of the previous annual turnover 3) the rate might be increased from 2% to 4% for repeated infringement	sanction might be up to 50'000€ per offence	administrative and criminal sanctions ((temporary) closing order, fine up to 250'000€ multiplied by the inflation coefficient (6), 1 month to 2 years of imprisonment)	financial penalty from 5'000£ to 50'000£ depending on the failure, with additional 500£ per day until obligation is met

In order to be consistent with the new energy efficiency target for 2030 defined in January 2018 and the overall European Union energy strategy, the directive was already reviewed and updated [14] and will continue to be. While the focus was originally put on the energy efficiency assessment, it is now also on the implementation of energy saving opportunities as part of energy efficiency improvement plans as well as the energy consumption monitoring.

Whether it is in view of energy management system certification or part of an energy audit, the energy consumption should be analysed and understood, the energy performance evaluated and energy saving opportunities generated and quantified. This process is found in both energy auditing procedures and energy management systems and is called "**energy review**" in the international standard for energy management systems ISO 50001.

Energy audits and energy management systems

According to the International Organisation for Standardisation, an energy management system is a ”set of interrelated or interacting elements to establish an energy policy and energy objectives, and processes and procedures to achieve those objectives” [5]. The worldwide reference in terms of energy management systems is the ISO 50001 standard.

The core of the technical part of ISO 50001 is the energy planning phase, where the **energy review** is carried out, the **energy baseline** established and **key performance indicators** are defined and calculated (*NB: The energy baseline and key performance indicators are complementary to the energy review. In the rest of the thesis, the term "energy review" will refer to these three elements together*). Energy objectives should also be established according to the company's energy policy and achieved following an action plan, pushing further towards continuous improvement and the implementation of opportunities to save energy.

An energy audit is defined by the EED as a ”systematic procedure with the purpose of obtaining adequate knowledge of the existing energy consumption profile of a system, identifying and quantifying cost-effective energy savings opportunities, and reporting the findings” [4].

Contrary to energy management system, it is a punctual event, to be repeated regularly. There is no single agreed-upon definitions for the different types of energy audits. Three categories can be found depending on the scope, the system's boundaries and the level of detail required [15]:

- Walk-through audit (type I): lowest level of detail for energy audit that can be used as input for more detailed ones. This type of audit corresponds to a rapid survey of the plant based on energy inputs and energy bills, aiming at quantifying losses and identifying low-hanging fruits opportunities and housekeeping measures.
- Intermediate audit (type II): more detailed analysis of the plant's energy consumption, analysing and quantifying the energy efficiency of system and identifying low investment energy saving opportunities.
- Detailed/comprehensive audit(type III): highest level of detail for energy audits. These audits are based on detailed calculations and analysis at the level of subsystems. Benchmarking against best practices is carried out and a long list of improvements options are generated, from low investment opportunities to major retrofitting schemes.

In general, the more detailed an energy audit is, the longer and more expensive it is. From one day for a walk-though audit, it can take up to several months for the last type of audit. The ISO 50002 standard [16] defines the minimum set of requirements to carry out an energy audit from the opening to the closing meeting, with general guidelines at each step (e.g. data collection, site visit, energy performance analysis, reporting) and can be used as a support for the energy review of ISO 50001.

What is an energy review?

The energy review is defined in the ISO 50001 standard [5] as the "determination of the organisation's energy performance based on data and other information, leading to identification of opportunities for improvement".

Its key steps and requirements are summarised in Figure 2, in addition to the generation of the energy baseline and key performance indicators included in the energy planning phase and which are closely linked to the energy review itself.

The first step is to analyse the current energy consumption and identify the energy sources (i.e. energy vectors). The energy baseline needs to be generated. It is defined as a "quantitative reference providing a basis for comparison of energy performance" and is used for the evaluation of energy savings opportunities. The second step goes a step further and look at the end-use consumption. The objective is to map the energy flows to identify the areas of significant energy use and the influencing factors acting on the energy consumption (e.g production load, product purity, external temperature).

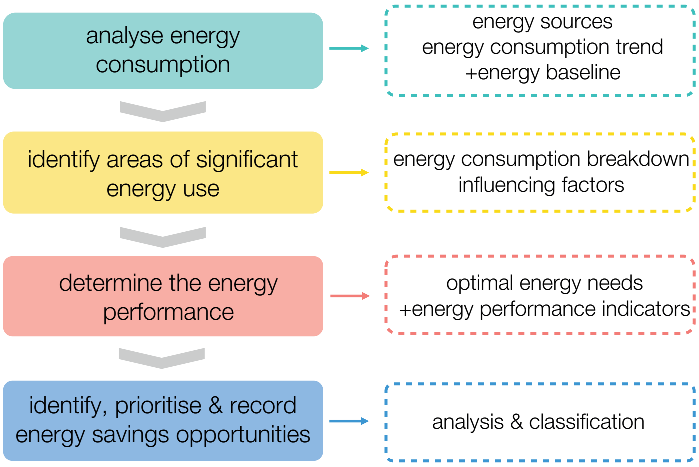


Figure 2 – Key requirements of an energy review as defined in ISO 50001.

Once energy consumption is understood and detailed, the use of key performance indicators allows to analyse and quantify the energy performance. Finally, energy savings opportunities are identified, evaluated and prioritised based on the energy performance analysis.

Although the Energy Efficiency Directive does not impose a specific level of detail for energy audits, the increasing energy efficiency targets and Europe long term energy strategy would suggest to go towards deep and detailed energy audits of type III.

Problematic and challenges

European (petro)chemical industry

This thesis focuses on the chemical and petrochemical industry. This sector is responsible for 19% of Europe's industry final energy consumption [17]. 80% of manufacturing costs of petrochemicals are related to feedstock (85% of European crackers use naphta as main feedstock) and energy [18]. The European petrochemical industry faces a hard challenge in staying competitive with the United States, the Middle East and Asia. The shale gas boom across the Atlantic caused US gas prices to fall by two third between 2008 and 2012, while naphta prices rose by 19% [19]. The recent drop in crude oil prices decreased the difference in terms of feedstock between Europe and the US but not with the Middle East.

In this highly competitive context, topped with increasing European and national regulations to limit industrial CO_2 emissions and energy consumption, the European chemical and petrochemical industry still needs to operate successfully. In this regard, developing and implementing cost-effective ways to assess their energy performance and evaluate the possibility for improvement are of major importance, since it would at the same time decrease operating costs for the same production level and enable industrial companies to more easily cope with European regulations.

Significant energy savings in the chemical and petrochemical sector are reported to be still possible [20]. However, a gap, known as the energy efficiency gap, remains between the available solutions and the actual implementation in industrial companies.

Even if a lot of documentation is available and mature techniques are in place, many companies seem to lack appropriate methods to effectively master energy efficiency in their production system [21]. Part of this gap can be explained by barriers to cost-effective investment, such as market-related or behavioural and organisational-based barriers, but also to technical and methodological issues on how to evaluate, control and continuously improve their energy performance [22, 23]. The two last issues are therefore related to the energy review itself and are partly due to the use of the wrong approach to the analysis, with no comprehensive methodologies.

When investigating further the industry needs identified in the literature, it can be found the need for suitable key performance indicators, the use of real-time data, the improvement of the reliability of data, effective tools for cost-analysis of energy savings options, or also innovative ways of simulating and visualising energy efficiency [21, 24].

Other issues observed from practical experience, are the lack of time and people dedicated to the task and the availability and reliability of data. The first observation varies from one industrial site to another. Very often, the energy manager is also in charge of other daily operations related to the production, which overshadow or delay energy management duties. The process of analysing the energy efficiency of an industrial site, followed by the identification and implementation of the energy saving opportunities, from the preliminary estimates to the final design and operation, involves various trades. This interdisciplinary aspect can sometimes also be a barrier for energy efficiency improvement but is a key element for a successful energy management.

In addition to this, measurements are often lacking to be able to properly characterise the energy performance of industrial systems, and any measurement or assumption is subject to errors and uncertainty. It is challenging to find suitable ways to check the validity of results and work with a consistent set of data.

Improving industrial energy efficiency

Improving energy efficiency of an industrial site means to deeply analyse the energy consumption, understanding and quantifying first the real energy requirements. Too often energy studies and audits aiming at improving the energy performance of an industrial system are carried out at a too low level of detail. Whether this is done on purpose to fulfil minimum requirements or due to resources constraints (e.g. money, time, skills, not enough data), it usually results in improvements related to standalone standard practices, replacement of equipment or maintenance and control. Such "surface" optimisation leads to investment in equipment that might not be needed if the system would be studied to understand for which purpose energy is being consumed in a first place, and carefully integrated when possible.

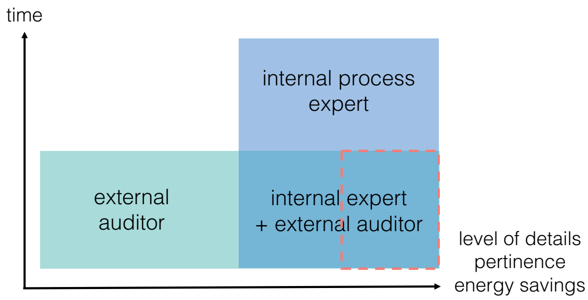


Figure 3 – Representation of the main approaches for energy reviews according to the level of detail and time required.

Putting aside the level of detail, there are two general approaches for the energy review of an industrial system, depending on who is carrying out the analysis:

1) External auditor: external energy auditors and consultants will have a limited time for the study, with an understanding of the system based on provided internal documents and information. In this case the top-down approach is preferred, starting from an overview of the energy consumption of the industrial system and gradually entering into the details of the process. A general or more specific methodology can be followed, depending on the auditors/consultants expertise and on the scope of the review. Often, the output of such analysis is based on best practices reference documents related to the production processes and utilities in place. As a result, improvements are usually made at the level of the utility system, without understanding the real energy requirements of the processes due to the lack of time and process knowledge. Data validation might also be difficult for the same reasons.

2) Internal process expert: on the other side, the energy review can be carried out internally, by a team of engineers and/or specialised workers. In this case data gathering and energy consumption mapping can be done at the highest level of detail, sometimes with the help of existing models of the system (simulation). This approach has the advantage of screening the entire industrial system and benefits from the knowledge of the internal auditors. However, it requires the involvement of employees dedicated to the task, which might be an issue in some companies with limited human resources. Also, having a good knowledge of the system under study and a full access to information is not enough to carry out a proper energy review. Necessary analytic skills related to energy efficiency improvement might be lacking.

Usually, the more detailed the energy review, the higher the cumulated sum of potential energy savings and the pertinence of findings, coming at the expense of a higher time required for the analysis. This observation is depicted on Figure 3, which also shows that the best results are obtained from a combination of these two general approaches, i.e. an informed external auditor that works together with internal process experts. This corresponds to finding the right trade-off between the realisation of highly detailed energy reviews and the associated time and complexity.

Thesis objectives and outline

The goal of this thesis is to contribute to the closing of the energy efficiency gap and thereby try to answer to part of the industry needs presented above. This is done in two ways:

- the generation of a global methodology for energy reviews (**Chapter 1**), in line with existing standards and regulations, leading to a comprehensive analysis of the energy performance of industrial systems and enabling the identification of energy savings opportunities covering the whole energy chain.

- at each step of the methodology, problematic and challenges with existing approaches are raised and guidelines, tools and/or methods are proposed to solve these issues (**Chapters 2,3 and 4**).

Research methodology

The thesis focuses on the chemical and petrochemical sector. It is partly based on the PhD thesis from Stéphane Bungener entitled "Energy efficiency and integration in the refining and petrochemical industries" [25]. While the latter provides a methodology to identify energy efficiency solutions in the utility networks of large refining and petrochemical clusters, this thesis has a stronger focus on the global approach to energy reviews in the framework of energy audits and energy management systems, applicable from small to large production sites. These two theses are therefore complementary and references to Stéphane Bungener's work are made throughout the thesis.

The research development was made considering the actual state-of-the-art related to methodologies and specific tools/techniques to carry out energy reviews in the process industry. Existing limitations of the literature as well as industry specific constraints were established, and answers to the resulting research questions were developed and validated in the industrial context.

Ten petrochemical sites were studied as part of the thesis, covering 11 different production processes displayed as color boxes in Figure 4. Such diversity helped to develop, refine and validate the proposed methodology so that the maximum aspects of the energy review are taken into account, and resulted in significant applied experience which was transformed into heuristics rules included in the methodology.

Thesis scope

The proposed methodology can be applied to any **small to large size** chemical and petrochemical production sites, featuring **continuous** processes and a **significant thermal power consumption** (i.e. heating and cooling demands).

While the thesis scope targets increased energy efficiency, the methodology can easily be integrated to other actions related to complementary policies and regulations that are forcing change of industrial processes. Reduced on-site emissions of greenhouse gases are linked to both cleaner heat and power production and higher energy efficiency, since less fossil energy is consumed for the same output. Indicators in place for CO_2 emissions can be merged with the ones generated for energy efficiency, according to their level of application, and energy saving opportunities can be evaluated and prioritised also based on CO_2 emission reduction. Turbomachinery is accounted for in the methodology since it can consume a significant amount of steam to produce the mechanical work driving compressors or pumps. Its replacement by electrical devices, as well as other aspects covered in the thesis scope such as heat pumping, fit into Europe's move towards an increased electrification of the industry sector [26]. Finally, the methodology is still valid even with a switch to renewable or recycled feedstocks. Energy will still remain the driver for the production processes to take place.

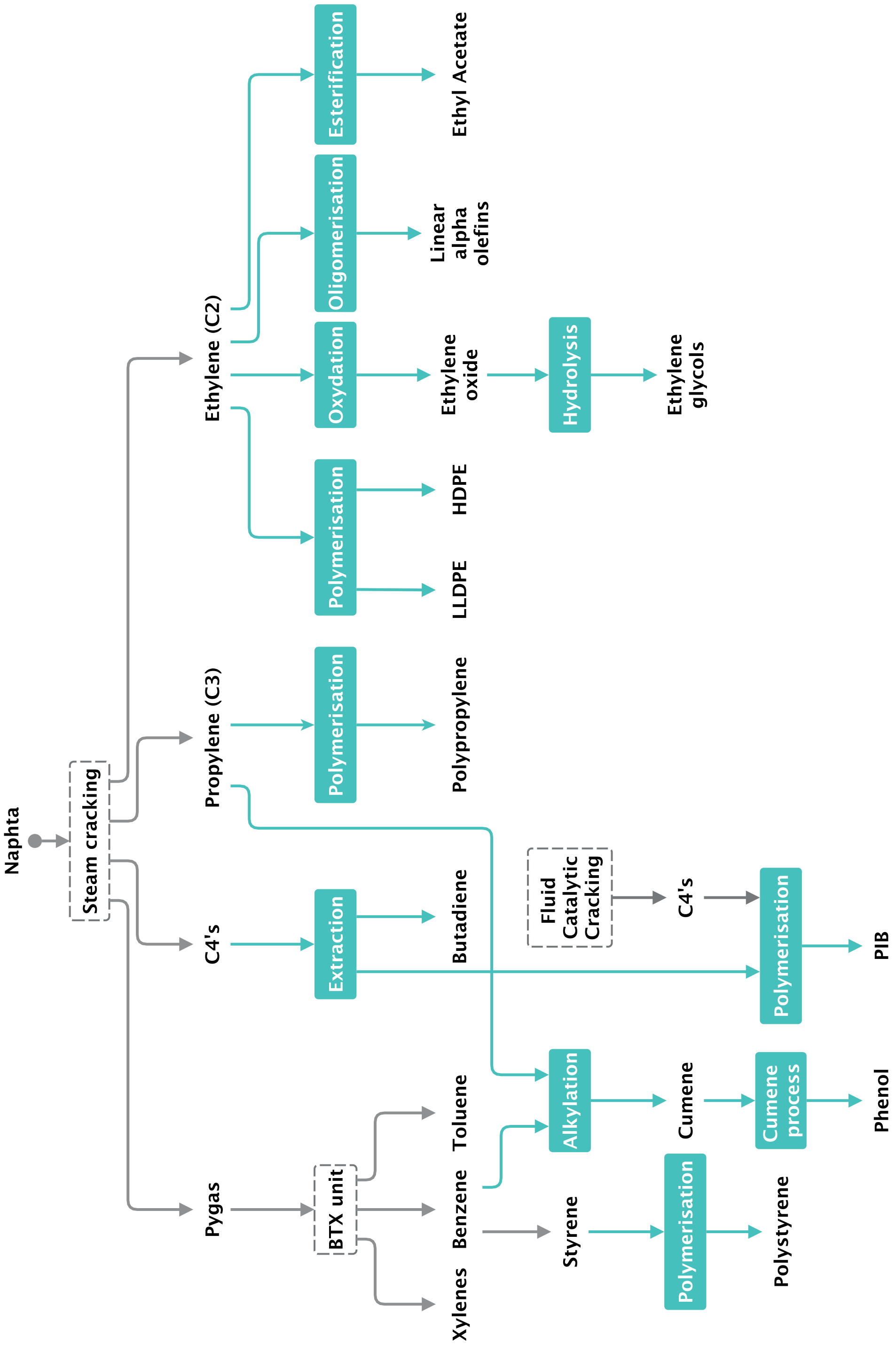


Figure 4 – Overview of the main petrochemical processes studied in the thesis.[1]

[1] Polystyrene being produced via batch processing, the described methodology was only partly applied and validated in this case, since the representation of the heating and cooling demands requires another approach in comparison to continuous processes.

Chapter 1: Methodology for thermal energy reviews

The research question of the first chapter can be expressed as follows:

How to carry out an energy review covering the whole energy chain and enabling the identification of energy savings opportunities at an adequate level of detail?

Existing guidelines and standards for energy audits and energy management systems are first investigated, together with the tools and techniques which can be used at the different steps. Strengths and limitations of existing documentation are discussed and the lack of detailed and systematic methodologies for energy reviews in the petrochemical sector is pointed out.

In order to help filling this gap, a detailed methodology is proposed, which includes the basic requirements for the energy review while enabling the generation of energy savings opportunities down to the level of detail of the production processes. The proposed methodology is composed of 3 main steps, following the logic of analysing-targeting- and achieving energy efficiency, which is similar to what is defined in energy management standards:

1. Energy consumption analysis: at this step the raw energy consumption of the system is gradually translated into process requirements, in order to understand where and why energy is consumed. In doing so, the entire energy chain is characterised (i.e. energy conversion, distribution and end-use consumption). The required data to analyse the system energy efficiency and identify improvement opportunities is collected and validated to ensure working with a consistent set of data along the analysis.
2. Targeting heat recovery: the second step aims at targeting the energy consumption reduction potential through the application of pinch analysis. The actual energy consumption is compared to the minimum energy requirements of the system, targeting the potential for heat recovery. The grand composite curve of the system gives information on the temperature-enthalpy profile of the process heating and cooling requirements.
3. Reaching the energy consumption target: based on the results of the previous steps, energy saving opportunities are identified, with the objective of getting as close as possible to the minimum energy requirements target and improve the utility system. A bottom-up approach is followed, starting from the process operating parameters towards the energy conversion and distribution system. Each opportunity is evaluated via a thermo-economic analysis to estimate its profitability.

The first chapter of this thesis goes through the main steps of the methodology. Tools and techniques used at each substep are indicated, together with the expected outcomes. In doing so, existing key questions and challenges are raised which will be tackled in the following three chapters, each corresponding to one of the steps of the methodology.

Chapter 2: Energy consumption analysis

How to analyse and characterise the efficiency of the entire energy chain down to the end-use consumers in a reliable manner, while keeping the required time for data collection at an acceptable level?

Starting from the characterisation of the system boundaries, this chapter presents a systematic approach to translate the raw energy consumption of the site into the end-use consumption down to the equipment level. The objective is to understand where and why energy is consumed and prepare the input for pinch analysis, which is carried out in the second step.

At the level of the system boundaries definition, this chapter introduces the importance of working with energy and exergy units rather than financial or mass quantities to compare energy vectors. A method to define the energy baseline is presented, making use of multi-period analysis on the production combined with the specific energy consumption of the site.

Several levels of details for the site representation are defined, allowing to progressively zoom in the system until the process flowsheet level. This approach helps to understand how energy is converted, distributed and delivered to the end use consumers. It also allows to structure the analysis and the data collection. The latter being usually the most time-consuming step, heuristic guidelines and rules are defined to reduce the required time and complexity of data gathering.

In order to ensure the consistency of data when data reconciliation cannot be applied, a set of key mass and energy balances at different levels of the energy consumption chain is presented. This consistency check ensures that the major mass and energy flows of the system are reliably quantified and points towards areas were more investigation is required. Finally, a set of key performance indicators is proposed at the same levels as for the consistency check, to evaluate the energy efficiency of the system.

Chapter 3: Targeting energy consumption reduction

How to generate economically feasible minimum energy consumption targets in pinch analysis, with the minimum level of detail for streams definition?

Once the process heating and cooling requirements are defined in the form of a list of hot and cold streams, pinch analysis can be carried out. In this methodology, the default level of detail for process energy requirement representation is the "grey box" level, which considers only the process streams exchanging with utilities.

This chapter discusses first the influence of the level of detail for streams definition on the minimum energy requirements and the shape of the grand composite curve. It is shown on an example that for the same minimum heating and cooling demands, corresponding to the highest level of detail for streams definition (i.e. "white box" or full pinch analysis), only a third of the streams needs to be detailed at this level. Although the optimum trade-off for streams definition cannot be known in advance, the default list of streams can be refined by going further in the process details at specific temperature locations.

One main concept in pinch analysis is the performance target ahead of design. The heat cascade on the process hot and cold profiles leads to the determination of the minimum heating and cooling demands of the system. These targets are depending on the definition of the minimum temperature difference ΔT_{min} of the system. This chapter shows that existing methods for the definition of the ΔT_{min} in existing industrial systems are often not adapted and can lead to serious over- or underestimation of minimum energy consumption targets.

A novel way of defining the contribution of each stream to the minimum approach temperature, prior to the heat cascade, is then presented and tested on two case studies. As a result, more economically realistic energy consumption targets are obtained through a more accurate temperature correction of streams and pinch point location.

Chapter 4: Reaching the energy consumption target

How to generate energy savings opportunities in a systematic way from the production process to the integration of utilities and how to properly evaluate their profitability? What are the available technologies to recover waste heat?

From the results of the two first steps of the methodology, the last step aims at generating and evaluating a list of energy saving opportunities (EnSO's) to improve the energy efficiency of the site, thereby decreasing its energy consumption and CO_2 emissions. A bottom-up approach is introduced, derived from the onion diagram for chemical processes design, which defines optimisation layers for the generation of EnSO's in a systematic way. A case study is used to illustrate the identification of EnSO's from the process operating parameters to the optimisation of the energy conversion and utility system.

A thermo-economic analysis is carried out for each opportunity, estimating its profitability. The uncertainty on the capital costs and the main parameters influencing the operating cost savings is briefly studied, showing how the economic indicators used for decision criteria and risk evaluation are varying according to different sets of economic parameters.

Finally, this chapter highlights the potential for heat pumping in chemical processes, especially when exothermic reactions are taking place. It introduces a new heat transformer system and shows how its integration to a polymerisation process can reduce the steam consumption by 50 to 60%.

1 Methodology for energy reviews

Chapter overview:

- What are the available guidelines and techniques to carry out an energy review?
- What are the remaining challenges?
- Description of the proposed methodology.

1.1 Carrying out an energy review

1.1.1 General guidelines

When carrying out energy audits or energy reviews as part of energy management systems, the first interface for general definition and structure is provided by international standards. The International Standard Organisation has published several standards in both fields (ISO 50001 [5] and ISO 50002 [16]), to help beginners and practitioners in their approach as well as to harmonise definitions and general expectations in energy audits and energy management systems.

These standards were defined to be applicable to all types of organisation, and all forms of energy usage. Not only they provide support by detailing the different steps and expected outcomes, they also enable fair competition and comparison between service providers. The main drawback of these standards in applied situation is the lack of details on the methods and tools to analyse, evaluate and improve the energy efficiency.

To tackle this issue, complementary guidelines were established, either by chemical and petrochemical associations (IPIECA [27]) and councils (Cefic [28]), government bodies [29, 30], or energy-related international and national agencies [31, 32]. These handbooks and guides cover the whole process of the energy review and provide additional information on the scientific methods that can be applied.

Too often in these guidelines, the level of detail stops at the utility system and the efficiency of equipment, without looking at the energy recovery potential at the level of the process itself or understanding if the utilities in place are optimised with respect to the end-use energy requirements. Aspects related to the data availability and collection, as well as its validation, are either forgotten or briefly mentioned although it is of major importance to ensure to work with a consistent set of data. It is also hard to identify a clear methodology with well-defined and connected steps being able to be applied directly.

In the scientific literature, several case studies of energy audits are available, whether it is on utility systems, specific consumption types [33] or on entire production plants [34]. In these works, the focus is more on the description of the energy systems under consideration and on the applied results, rather than on the methodology and tools used to do so. Most of the time, the focus is put on electricity rather than thermal power. No specific works have been found related specifically to the chemical and petrochemical sector.

Two papers present innovative and global energy efficiency improvement methodologies that can be employed to carry out detailed and systematic energy reviews. Petek et al. [35] proposes a holistic approach combining the concepts of Cleaner Production, Total Site Integration and Energy Efficiency Optimisation in order to maximise energy efficiency improvement and environmental performance of industrial systems. While the literature review and the description of the different techniques mentioned in the methodology is quite extensive, the focus is more on case studies and resulting energy saving opportunities rather than on a clear methodology and detailed explanations on the practical application of the approach.

Drumm et al. [36] presents a Structured Efficiency System for energy (STRUCTese), developed internally at Bayer as an energy management tool to continuously improve the energy efficiency of their plants. Key steps of the continuous improvement cycle are presented as well as an innovative way to determine and represents the energy losses from the theoretical energy optimum to the current energy consumption. Improvement opportunities are generated through checklists, best practices and brainstormings, and make use of different optimisation levels. The optimisation levels considered in the energy efficiency analysis start from the end-use individual consumers towards the utility integration, passing by operational and process design improvement. The application of this global and systematic approach on a specific plant resulted in a significant decrease of the overall specific energy consumption. Details on the techniques applied at each step are however not provided, the focus of the paper being more on the energy management system itself.

It can already be seen here that there is a lack of a clear methodology to carry out detailed energy review of (petro)chemical systems. Although methods, tools and techniques exist and are well-documented a major limitation is the level of detail of the analysis. A methodology embedding all the requirements of the energy review and made of key and logical steps screening reliably the entire energy chain down to the end-use consumers is missing.

1.1.2 Specific tools and techniques

Among the different tools which can be used during an energy review, recurring ones are presented in Figure 1.1, depending on the stage at which they can be applied. Three usage categories can be defined: the energy consumption analysis, the energy efficiency improvement and the energy monitoring. Some tools and techniques are specific to a single category while others can be assigned to two or all of them.

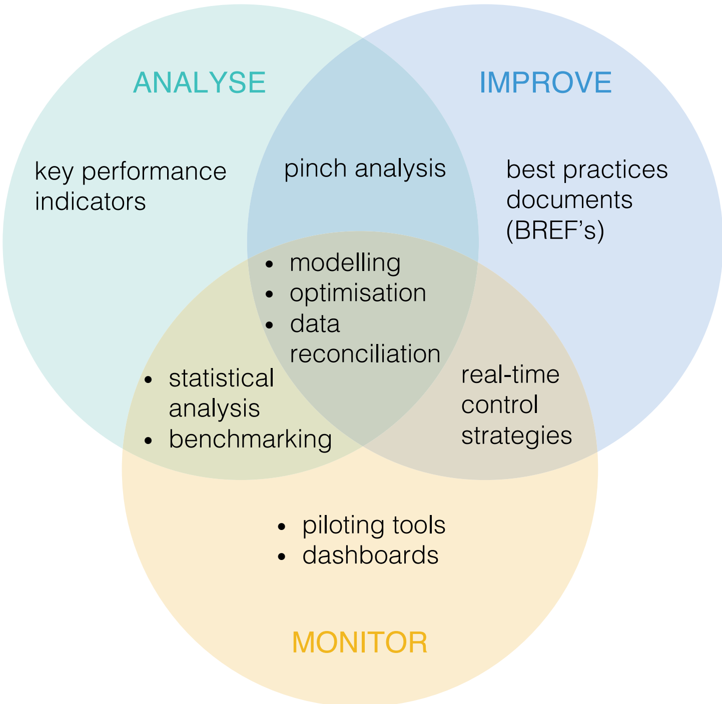


Figure 1.1 – Venn diagram of the different tools and techniques that can be used during an energy review

Modelling and data reconciliation techniques can be used at all stages of the energy review since they allow working with a validated and consolidated set of data, which is of major importance for the accuracy and reliability of the analysis. Depending on the size of the system, the availability of data and the study scope, modelling and data reconciliation can be applied to the whole system or to smaller subparts like utility networks. Aspen Plus® and Belsim Vali are two powerful flowsheeting software that can be used for modelling and simulation of chemical industrial systems with the possibility of applying data reconciliation.

One major limitation with modelling and data reconciliation, in addition to the availability of data, is the availability of these software internally, with employees with the necessary time and skills to use them. Building reliable models can be quite complex and requires a significant amount of time. When data reconciliation cannot be applied it is difficult to find in the literature other approaches to check the consistency of data in petrochemical sites.

Mixed Integer Linear (MILP) and Non Linear Programming (MINLP) are mathematical programming techniques used for solving optimisation problems involving both continuous and discrete variables. Process integration [37], heat exchanger network generation [38] and energy supply optimisation [39] are examples of problems that can be efficiently addressed using MILP. MINLP can be used to address these problems and when non-linearity cannot be overcame.

ANALYSE

Internal benchmarking can be used for similar plants within the company in order to compare their respective performances, or in view of energy consumption monitoring. It can be applied at the plant and subunit levels [40] or at the level of the different energy vectors [41]. It has the advantage of applying a consistent methodology, avoiding boundary and calculation details issues, since the same methodology is applied to each system.

Most of the time benchmarking is carried out externally. Without external benchmarks a company may lack information and understanding on the grounds of the best performance, currently achieved or theoretical. External benchmarking is usually applied on the entire production process based on the specific energy consumption (SEC) indicator, where the energy performance of the plant is measured as the quantity of final or primary energy required to produce one unit of good [42]. SEC's from Best Practice Technologies (BPT), defined according to the best performing economically viable processes currently in operation at industrial scale, can be used for comparison [20].

While the SEC of an industrial system is useful for energy consumption monitoring purposes, it does not give information on how efficiently energy is used. Also comparison with BPT's to compare the energy performance should be done with care, since calculations details are hard to obtain and assumptions might be different from one value to another.

More complex methods for internal benchmarking can be found in [43, 44], where the industrial system energy consumption is decomposed and a system of equations is developed, including linear relationships between subsystems energy consumptions and factors impacting their consumption. In this way energy consumption benchmarking is carried out at the same time at the site and subsystem levels.

The specific energy consumption ratio is part of the so-called Key Performance Indicators (KPI's). Energy efficiency KPI's are used to evaluate the evaluate the energy performance of a system, establish targets and track improvement. A wide range of KPI's was developed in the literature to characterise the energy and environmental performance of industrial systems at different levels (e.g. sector, plant) [45, 46]. They are generally classified in four main groups: thermodynamic, physical-thermodynamic (e.g. SEC), economic-thermodynamic, and economic [47]. In the context of the energy consumption analysis the three first categories are of interest for the energy review.

Among the KPI's related to energy efficiency in the cited papers, only a few are suitable for energy management application since they are mostly applied at the overall industrial sector or plant scale and do not report information on how efficiently energy is used within the plant. The MORE European research project [48] made a significant contribution in the definition of indicators related not only to the energy use but also resources and water consumption. A large number of indicators were developed for different industry sectors, from the site-level down to the equipment level for real-time monitoring and optimisation of resource efficiency.

Another comprehensive method to develop a set of specific KPI's for improving energy efficiency was also found in the literature [49], but its application is more adapted to the manufacturing industry in particular rather than the (petro)chemical industry.

Finally, relationships between energy consumption and influencing factors can be generated through multivariable linear regression analysis on archived data, to identify factors influencing the energy consumption (e.g. production load, external temperature, product purity, reflux ratio, catalyst age). This statistical method allocates coefficient to each factor which may affect the energy consumption to generate a linear relationship linking all variables. Such relationships can be used for both energy consumption analysis and monitoring as it corresponds to an extension of the SEC indicator.

IMPROVE

When it comes to energy efficiency improvement, the level of detail of the energy review will define the tools and techniques to use.

Best practices documents, the so-called BREFs, are the reference documents in industry. The 32 BREFs were developed under the Industrial Emissions Directive and covers all the industry sectors, as well as waste treatment and energy use. The important ones for energy performance in the (petro)chemical industry are the BREF on Energy Efficiency [50], Refining of Mineral Oil and Gas [51], Large Volume Organic Chemical Industry [52], and the production of Polymers [53].

While the former covers industrial efficiency at the level of the entire energy chain (e.g. combustion, steam network, heat exchanges), the three others are related to best practices of the chemical processes (i.e. equipment, waste, emissions) which is also linked to the energy consumption.

Depending on the production processes and utility systems included in the perimeter, a checklist can be prepared based on these best practices and improvement propositions can subsequently be made if the actual system differs from what could be attained. The advantages of best practices documents are numerous.

They cover a wide range of production processes and utility systems and are based on observed operation and performance of existing facilities, making them economically viable. Also a large number of the presented best practices imply low-investment and/or low-risk actions, mainly related to maintenance and control and widely spread equipment layout. These solutions are often readily implemented in industry as they correspond to “low-hanging fruits”, with short payback times. More complex energy efficiency options involving heat recovery and process integration are recommended but only briefly described. These options do however provide the highest potential for energy consumption reduction [54].

For energy reviews with a higher level of detail and carried out on industrial systems consuming a significant amount of thermal power, which is the case for the chemical and petrochemical sector, pinch analysis is the method of choice for the improvement of energy efficiency. Pinch analysis on single production units can help identify direct and/or indirect heat recovery opportunities through optimised heat exchanges between process streams.

Total Site Analysis (TSA) is the application of pinch analysis to large industrial sites or even clusters, extending the potential for energy and resources flow optimisation and industrial synergies. Based on the process requirements in terms of heating and cooling demands and the existing utilities, TSA identifies heat recovery opportunities and targets cogeneration potential through the modification and/or optimisation of the utility system.

Two major problems can be identified with the use of pinch analysis in the framework of energy reviews. First, depending on the size of the system, a pinch analysis requires a significant amount of time, especially if the analysis is carried out at the highest level of detail. Second, the minimum thermodynamic targets obtained applying the traditional approach are often under or overestimated, raising feasibility issues at the level of the engineering work.

Once opportunities are identified, thermo-economic analysis has to be carried out to evaluate the profitability and financial risk of the implementation. On one side the investment linked to the implementation is estimated and on the other side the operating cost savings are determined. At this level, it is important of being aware of the impact of the different parameters involved in these two terms (e.g. interest rate, utility costs, cost estimates) and how they influence the decision making.

MONITOR

Most of the tools and techniques already described above can be applied for energy consumption monitoring. The purpose of monitoring is to ensure that the daily operation takes place under predefined optimal conditions through the regular collection of information on energy use, and determine when and why energy consumption is deviating from the expected behaviour.

The optimal set points for energy efficiency can be defined based on energy consumption models, generated at the level of the energy consumption analysis and benchmarking. From the past behaviour of the plant, models for energy consumption, corresponding to average or minimum observed consumption according to the plant production and other key energy use drivers, can be used to define the optimal conditions. Online [55] and "enhanced" [56] data reconciliation can be used to reconcile measurements and close mass and energy balances according to the uncertainty of sensors, even on systems with low instrumentation level and poor redundancy. When the reconciled measurements deviate from their expected values (i.e. decreasing reconciled accuracies), anomalies such as wrong plant operation or heat exchanger fouling can be detected.

The CoPro European project [57], started in November 2016, aims to "develop and demonstrate methods and tools for process monitoring and optimal dynamic planning", which will likely integrate such units energy consumption and production models. This project complements the MORE European project previously cited [48], for which the goal was to develop key performance indicators to "monitor resource efficiency during daily operations and to influence the operational decisions such that the plant efficiency is optimised".

The proposed methodology being mostly focused on analysing and improving the energy consumption, tools and techniques specific to monitoring are not covered in this thesis.

1.2 Proposed methodology

Thanks to the analysis of the literature, it can be seen that while methods and tools which can be used at some point to study the energy performance of an industrial system exist and are well documented, a comprehensive energy review methodology specific to the (petro)chemical industry and including a logical combination of these tools is missing in the literature. This thesis is contributing to fill this gap by proposing a methodology reducing the limitations of existing ones.

The proposed methodology comprises three main steps, following the energy review process. The core of the methodology is the pinch analysis, carried out at the level of the 2^{nd} step, which allows to determine and locate the potential for energy efficiency improvement at the deepest level of detail.

The overview of the methodology is schematically represented on Figure 1.2. Each main step is detailed with its substeps, for which the colored title represents the name of the substep and the

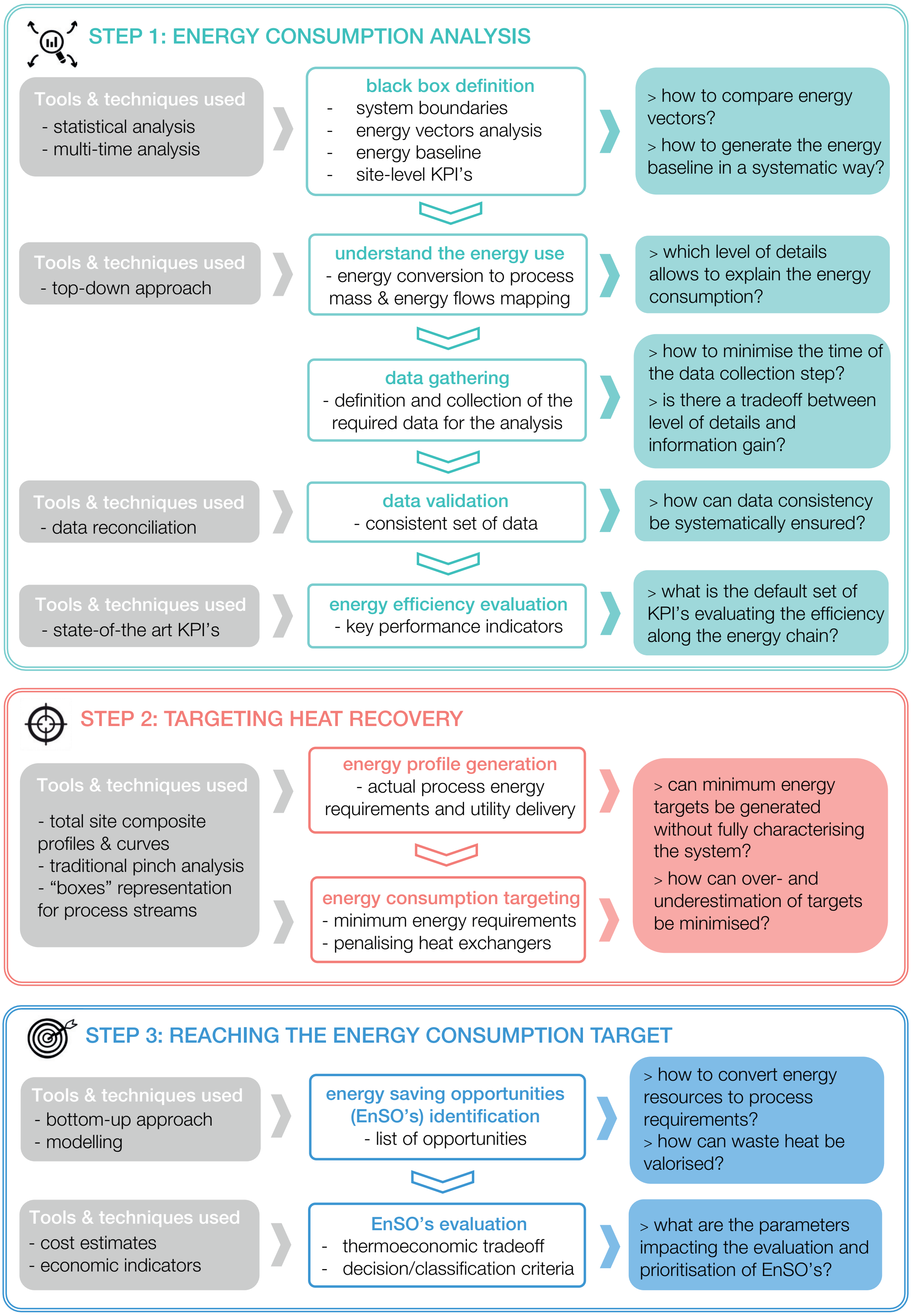


Figure 1.2 – Detailed overview of methodology and open questions.

black text below being the expected outcomes of the substep. The existing tools and techniques which are applied at each substep are displayed on the left in grey and the challenges and open questions raised in this chapter are highlighted in the colored boxes on the right.

1.2.1 Step 1: energy consumption analysis

The first step of the methodology aims at defining the real energy requirements of the system, following a **top-down approach**.

The system is first studied as a black box, establishing the system boundaries and defining the main chemicals and energy vectors entering and leaving the plant. This step is important to understand the raw energy consumption supporting the production and the interactions of the site with its surroundings (e.g utility contracts, industrial symbiosis). The study of the energy vectors entering the plant indicates the distribution of the energy consumption, provided that a clear basis for comparison is defined. Measuring units for common energy vectors are often different (e.g. tons, normal cubic meter, cubic meter, kilowatthour, megajoule), raising the issue of the basis for energy vectors comparison.

At this level, the energy baseline needs to be generated, representing the reference energy consumption of the system. It is based on a selected time period, typically a year, and derived from the analysis of the energy consumption and the production rate, as well as other factors significantly impacting the consumption (e.g. outdoor temperature). Clear guidelines for the generation of an energy baseline are difficult to find in the literature. Also, the use of monthly of weekly averages should be avoided since it can lead to fictive operation modes not reflecting typical production scenarios. This can be seen on Figure 1.3 (days 60-185 and 245-340), where averages for the months combining both shutdown and high production periods result in productions lower than what is observed normally.

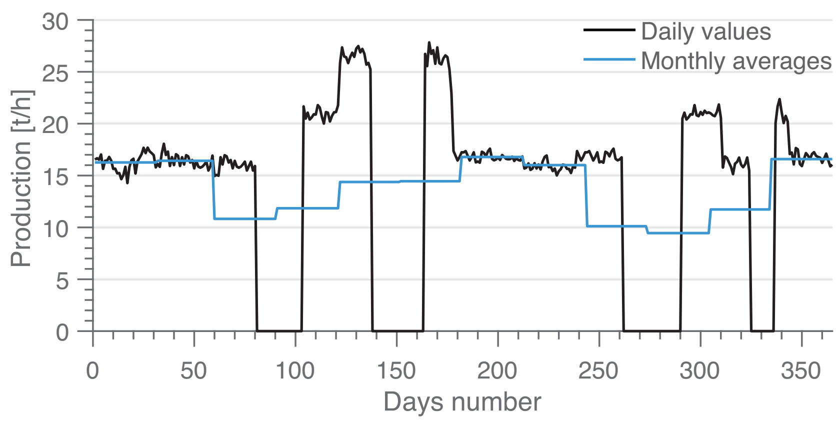


Figure 1.3 – Example of daily production and monthly averages.

Once the black box level is characterised, the mass and energy flows are mapped, gradually entering into the site details in order to spot where and why energy is consumed. A clear top-down decomposition is required at this stage to structure the data acquisition and understand the connections between the industrial system components.

Data gathering is then carried out and is typically the most time-consuming step. The three basic questions to be answered at this step are who? what for? and how much? With the objective of reducing the complexity and time required to collect the required data without losing information to be able to identify energy saving opportunities, several questions arise: how to minimise and simplify the data collection step? can a trade-off between level of detail and information gain be found, and what is the associated level of detail?

Once the required raw data to come up with the list of streams is acquired, it needs to be validated to ensure that it is consistent in terms of mass and energy balances, and that results can be trusted. The use of data reconciliation on the conversion units, the utility networks (e.g. steam network, hot oil network) and processes is highly recommended and is the method of choice to correct and validate data. However, it might be difficult to be used depending on the available time, skills and access to the right platform or software. In this regard, other strategies need to be developed to ensure the validity of the collected data and locate areas where inconsistencies are occurring.

Finally, the energy efficiency of the system is evaluated thanks to key energy performance indicators. From the existing KPI's in the literature, not all are suitable for (petro)chemical sites and the level of detail of the analysis, and the single specific energy consumption indicators is not enough to characterise an entire plant. A set of KPI's, giving information on the energy efficiency at each step of the energy chain is required.

Thanks to the first step, not only the list of streams serving as input to the pinch analysis of the second step is generated, but the whole analysis procedure allows to characterise the entire energy chain, from its conversion to end-use consumption. At the same time, the site measurements are checked and missing or malfunctioning sensors can be spotted.

1.2.2 Step 2: targeting energy consumption reduction

In the second step, total site graphical representations are first generated to obtain the hot and cold composite curves of both process and utility streams, leading to the hot and cold total site profiles of the site. These profiles show the temperature levels and heat loads of the system's requirements and how heat is supplied to and removed from the process.

Pinch analysis is then carried out on the process streams to determine the minimum energy requirements of the system. When the number of process units is high, as in large industrial clusters, direct heat integration is rarely viable as the involved process streams might be located far away from each other and belong to different process units. In this case, total site pinch analysis is more adapted, but pinch analysis on individual or dependent process units should be carried out at the same time, to evaluate the potential for both direct and indirect heat recovery at the unit and site level (i.e. through the intermediate utility system). In this thesis, almost all the studied industrial systems were composed of 1 to 2 process units, making pinch analysis suitable.

Several levels of details exist to represent the process energy requirements. The black box level represents process requirements as its actual utility consumption, the grey box level considers also only the process streams interacting with the utility system but looks at the temperature level of the heating/cooling, and finally the white box level characterises the entire real process energy requirements. The lighter the color the higher the level of detail and the more complex the analysis. Again with the objective of reducing the complexity and time of the energy review, without missing opportunities, we can ask ourselves if minimum energy consumption targets can be generated without fully characterising the system, and how to do it.

A recurring observation when pinch analysis is carried out on existing industrial systems is that minimum energy requirements are often under or overestimated, when further engineering calculations are done to actually design and implement heat recovery schemes. This is mainly due to the traditional definition of a key assumption in pinch analysis, which is the minimum temperature difference between the hot streams and cold streams profiles of the system (ΔT_{min}). A better understanding of the signification of ΔT_{min} and control of the influencing parameters implied in its determination would allow a better targeting of the minimum energy consumption of the system.

1.2.3 Step 3: achieving energy consumption reduction

Based on the results of the pinch analysis, the third step aims first at generating energy saving opportunities. A **bottom-up approach** is followed, starting from process modifications, direct heat integration, indirect heat integration, heat pumping to finally utility integration and optimisation. This approach allows to generate a full list of options to increase the energy efficiency of the system in a systematic way, starting from the core of the process.

Petrochemical processes have the characteristic of being usually exothermic, thereby releasing heat at different temperature levels depending on the chemical process. Sometimes this heat cannot be recovered to heat up cold process streams and is evacuated through the cooling system as waste heat. Heat pumping opportunities and the development of innovative technologies to do so are promising options to valorise waste heat.

Each identified energy saving opportunity is then evaluated by carrying out a thermo-economic analysis, estimating the investment cost of the modifications and the expected operating cost savings. Economic indicators such as the payback time, net present value or internal rate of return can be used as classification criteria. At this level, it is important to be aware of how parameters used in this analysis influence the selected economic indicators. Natural gas prices variations, a CO_2 tax introduction, or uncertainty on cost estimates can drastically change the risk and profitability of the different options.

1.2.4 Pinch analysis at the core of the methodology

Pinch analysis being the centerpiece of the methodology, the basic principles of this technique and the resulting graphical representations are presented in this section. Complementary information and details on its application on existing industrial systems are provided in Chapter 3.

The first developments of the pinch analysis date from the early 80's with Linnhoff and Flower [58]. For more than forty years, heat integration based on pinch analysis and mathematical programming has received continuous attention and significant developments were made in the field [59].

Pinch analysis is a systematic methodology based on thermodynamic and economic principles which targets the maximum heat recovery via counter-current heat exchanges that can be realised in a given system.

In any chemical process, streams have to be heated up or cooled down. Each stream is defined by its heat load and its starting and target temperatures. Another key parameter to define is the minimum temperature difference (ΔT_{min}), representing the trade-off between energy savings resulting from heat integration and the investment cost linked to the heat exchange area to install.

Once the ΔT_{min} is defined, each hot and cold process stream is corrected, either by respectively decreasing or increasing their temperatures by their contribution to the minimum temperature difference, represented by $\Delta T_{min}/2$.

Heating and cooling requirements of individual process streams are then summed up to generate the so-called hot and cold composite curves of the system, showing at which temperatures heat has to be removed and supplied to the system. These curves are then shifted horizontally until they touch each other at the pinch point. Example of composite curves in real and corrected temperature domains can be seen on Figure 1.4 (a).

The hot and cold utility consumption targets (i.e. minimum hot (MERH) and cold (MERC) energy requirements) as well as the maximum heat recovery potential can be read on the curves. The difference between the actual utility consumption and the minimum energy requirements is caused by penalising heat exchangers within the system. These are explained by a bad positioning of a utility (i.e. hot utility below the pinch point and cold utility above) or the transfer of heat across the pinch.

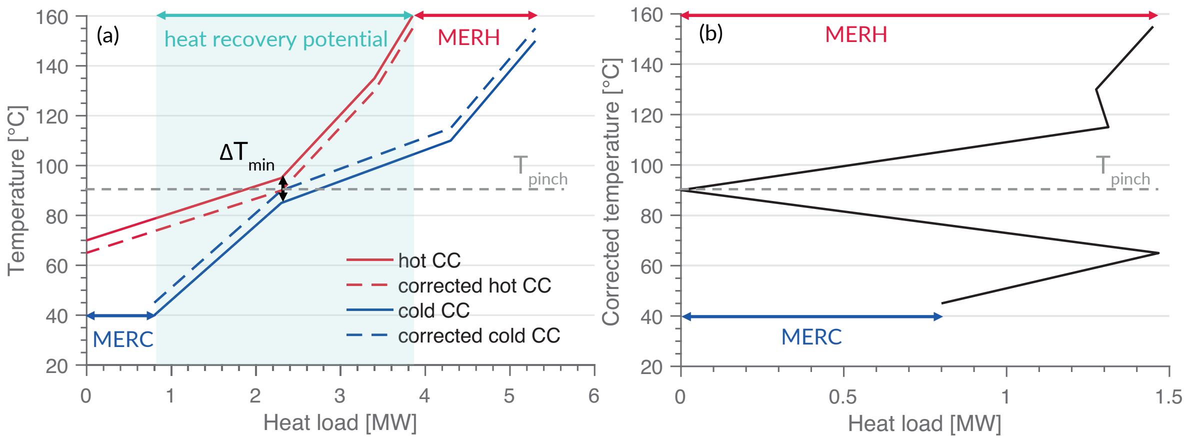


Figure 1.4 – Example of (a) hot and cold composite curves and (b) corresponding grand composite curves.

The grand composite curve (GCC), represented on Figure 1.4 (b), gives information on the heat loads and temperature levels of the utilities to optimally supply the rest of the energy requirements and highlights opportunities for heat pumping.

1.3 Conclusion

This first chapter brings an answer to the following research question:

How to carry out an energy review covering the whole energy chain and enabling the identification of energy savings opportunities at an adequate level of detail?

by proposing a global methodology for energy reviews in the (petro)chemical sector, which covers all the requirements of the existing standards and enables the generation of energy savings opportunities starting from the process itself to the optimisation of the utility system, in a reliable manner.

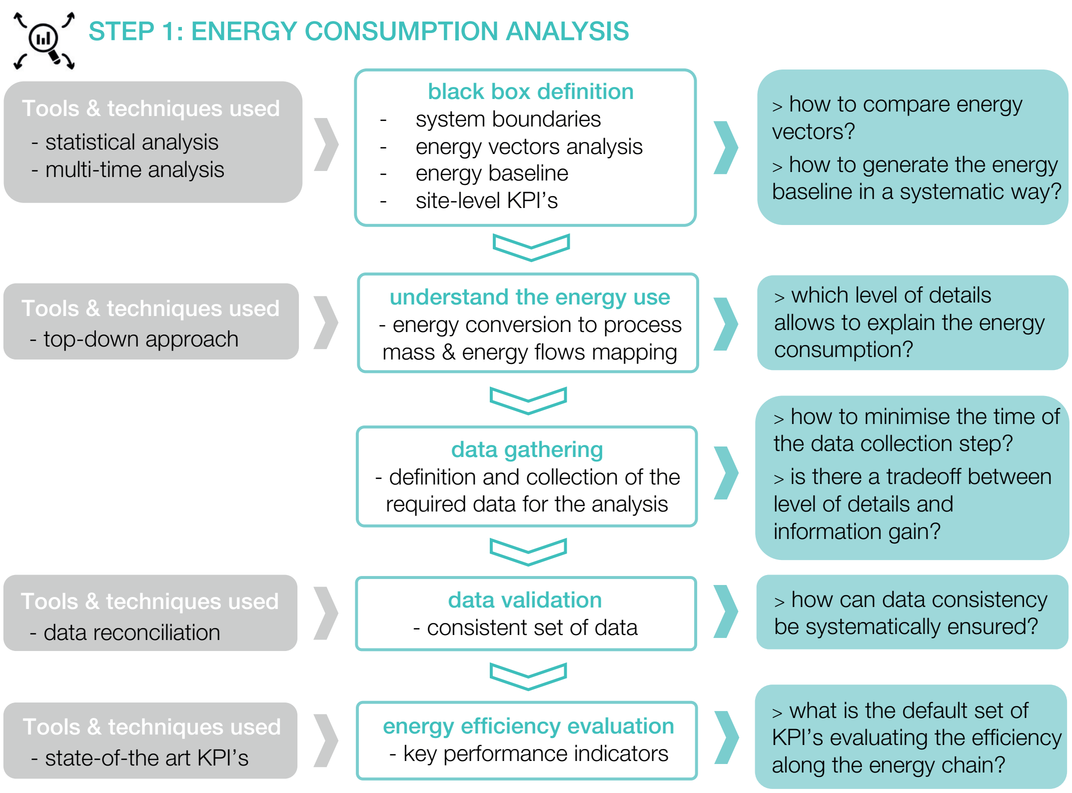
This methodology comprises three main steps: 1) the energy consumption analysis 2) the energy consumption reduction targeting and 3) and the achievement of the energy consumption reduction. It makes use of state-of-the-art tools and techniques, with pinch analysis at the core, that are used at particular points along the methodology.

At each substep of the methodology open questions and challenges were raised and will be investigated in the next three chapters of this thesis, corresponding to the three main steps of the methodology, with the aim of providing answers and close the gap and limitations found in the literature.

2 Energy consumption analysis

Chapter overview:

> From site raw energy consumption to detailed analysis of energy performance and process units requirements.



2.1 Black box characterisation

2.1.1 System's boundaries

The energy audit scope, as defined in the ISO 50002 standard [16], is the "extent of energy uses and related activities to be included in the energy audit". It corresponds to the energy consumption share of the business entity which has to be covered by the energy audit, according to each member state's legislation.

When carrying out an energy review on a (petro)chemical site, several cases can be faced depending on the limits of the business entity, as depicted in Figure 2.1.

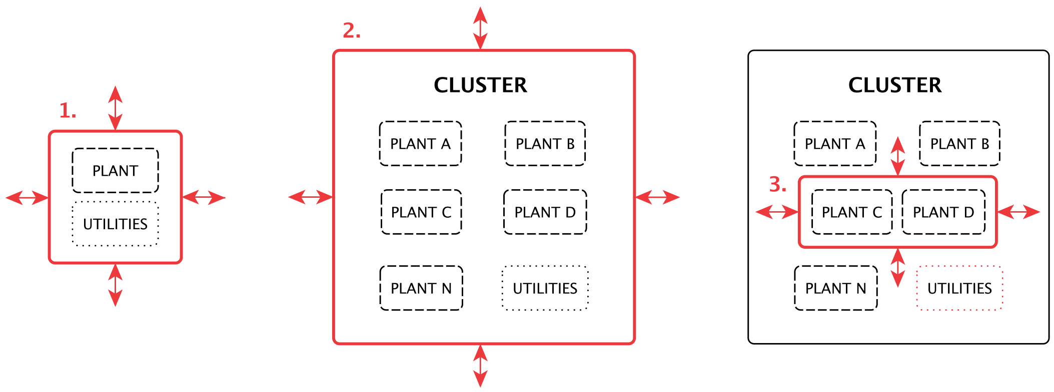


Figure 2.1 – Schematic representation of possible system boundaries

Case 1 features a standalone plant, producing one or two main chemicals and having its own utility system in place. Case 2 is similar except for the size of the site. Many related and/or independent production units compose the system, forming an industrial cluster with its central utility system. The last case is when the system under study is part of such cluster, but with the utility system outside the boundaries. In this case, the site is directly importing its hot and cold utilities (e.g. steam, cooling water) from another business entity.

The results of an energy review strongly depend on the choice and definition of the system's boundaries. Compared to case 1 and 2, in case 3 opportunities for direct or indirect heat recovery with neighbouring production units can be missed. The utility system being outside of the boundaries, it is audited separately, without including the real energy requirements of the end-use consumers and heat integration potential if the entire cluster would be studied as a whole.

This can result in oversized investments and suboptimal configuration of the energy conversion and distribution system. It is important to comment at this point that, in terms of energy efficiency, taking the legal entity boundaries is therefore not the best approach, and finding the optimum scope for an energy analysis is not always straightforward.

Once the perimeter has been established, mass and energy flows entering and leaving the system's boundaries should be identified. Figure 2.2 shows the main flows to consider at the black box level, corresponding to the limits of system. Horizontal flows represent the material flows related to the chemical production itself.

Reactants and co-reactants enter the system, undergo chemical and physical transformations, to finally leave as useful products and by-products. Vertical flows entering the system are mass and energy flows required to support the production. These are energy vectors linked to the system's hot and cold utilities. The exiting vertical arrows correspond to mass and energy flows resulting from the process unit operations. Among them can be found waste streams from the process, either to be treated in a waste treatment plant, or waste fuels which can be valorised in boilers or sold to neighbouring businesses. If the process is exothermic, excess heat can be exported in the useful form of steam or a hot fluid.

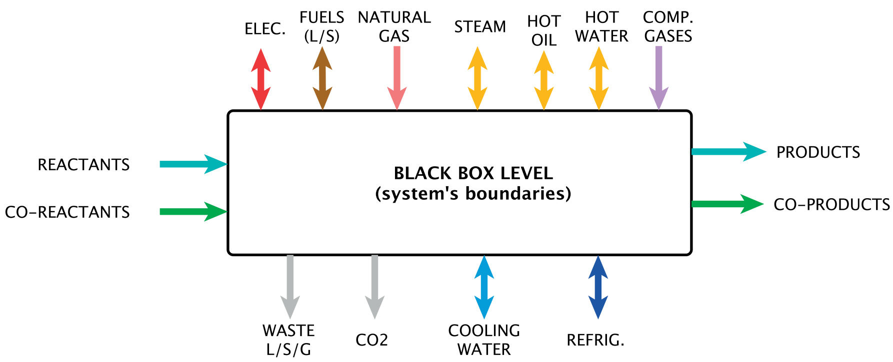


Figure 2.2 – Mass and energy flows to consider at the system's boundary, when applicable

The goal of the energy review is to quantify the energy consumption of the system with respect to the production, breakdown the energy consumption to identify the main consumers, and finally identify and propose energy savings opportunities to reduce the energy consumption and CO_2 emissions and increase the energy efficiency. The objective of these opportunities is to reduce the size of the vertical flows related to waste or primary fuel consumption, for the same level of the horizontal ones.

The remaining waste mass and energy flows leaving the system's boundaries are important to characterise since they offer potential for industrial symbiosis and waste heat valorisation. For example, a waste product stream could perhaps be of interest for a neighbouring industrial site, or waste heat could be recovered through a steam line or hot water network. It is therefore important to understand the interactions of the system with its surroundings and the flows crossing its border.

2.1.2 Energy vectors distribution

Listing and characterisation of the energy vectors entering and leaving the system allows a better understanding of the energy consumption and the quantities and temperature levels at stake. Among energy vectors can be found electricity, any type of fuels (e.g. gaseous, liquid, solid), steam, hot fluids, but also compressed gases if their pressure is high enough compared to atmospheric conditions.

In the literature, when petrochemical processes are evaluated in terms of their energy consumption, it is often expressed in final energy consumption of electricity, fuel and steam. The end-use consumption of these three vectors is however not detailed.

Table 2.1 shows the final energy consumption breakdown for Best Practice Technologies of most of the processes displayed in Figure 4 and other key petrochemical products (relative values calculated from [60]). Relative and not absolute values are shown to highlight the energy consumption distribution. It can be seen that for all processes, except polymers, steam alone is already responsible for a large share of the final energy consumption.

If we assume that fuel is also converted to hot utility, fuel and steam combined sum up to more than 90% of the final energy consumption for the same processes, except for ethylene oxide (still significant with 76%). Although the share of energy consumption which has to be investigated in the framework of energy audits differs across Member States, the minimum scope varies between 80% and 95% of the total final energy consumption.

Table 2.1 – Energy consumption breakdown based on Best Practice Technologies of the production processes of key petrochemicals.

Studied processes	Electricity [%]	Fuel [%]	Steam [%]	Fuel+ Steam [%]
Butadiene (C4 separation)	7	0	93	93
Cumene	0	43	57	100
Ethylene glycol	4	18	78	96
Ethylene oxide	24	76	0	76
Phenol	6	0	94	94
HDPE	47	0	53	53
LLDPE	20	0	80	80
Polypropylene	90	0	10	10
Polystyrene	44	56	0	56
Other important processes	Electricity [%]	Fuel [%]	Steam [%]	Fuel+ Steam [%]
Acetaldehyde [ref Neelis]	8	0	92	92
Acetone	2	0	98	98
Aromatics extraction	5	0	95	95
Ethanol	3	0	97	97
Ethylbenzene	3	0	97	97
Styrene	0	0	100	100

These observations show the importance of thermal power consumption in petrochemical processes and corroborates the focus of this thesis on hot utilities. Electricity is sometimes consumed for heating purposes, which is the case for polymer extrusion, where pellets are gradually melted via the absorption of heat provided by barrel heaters and through mechanical work [61]. In other types of processes, it is however mostly consumed to drive mechanical devices (e.g. pumps, compressors, blowers and fans), where it is sometime replaced by steam in turbomachinery. Production of electricity and steam is linked in cogeneration units and within steam networks via back-pressure turbines between steam pressure levels. These two energy vectors can therefore be highly interconnected.

2.1.3 Energy vectors comparison

Proper comparison between energy vectors entering the system's boundaries is ensured through the careful definition of energy flows and the use of homogeneous physical units. Several comparison bases are used to study the energy vectors distribution.

Economic units: a first mistake is made when energy vectors are compared on the basis of economics and on their share in the energy bill. The variability of energy prices according to the energy vector type and site location can lead to various energy cost distributions for the same energy consumption pattern, and hide the true order of magnitude for each vector. Operating costs should enter into play at the level of the identification and evaluation of energy efficiency opportunities, not at the level of the energy consumption analysis.

Mass units: another mistake is to use mass quantities. This is valid for fuels but more especially for steam consumption. Because it is how it is measured, steam is too often characterised by tons no matter what its pressure and temperature levels are. Figure 2.3 shows the energy content of 1 ton of saturated steam, from 1 to 80 bar.

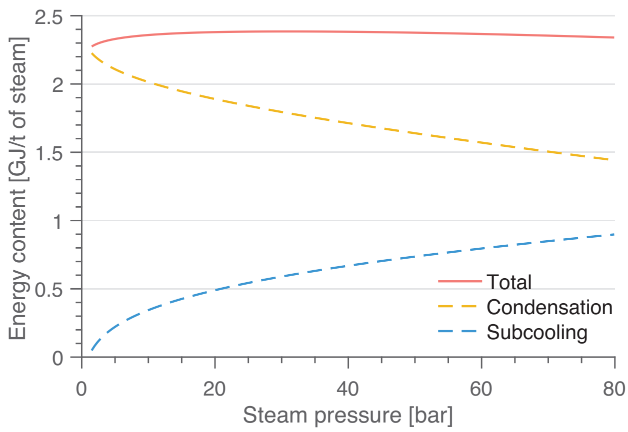


Figure 2.3 – Energy content of the condensation of 1 ton of steam according to the pressure level (condensates = 1.5 bar and 100°C).

Although the total energy content from saturated vapor to condensate is not varying much according to the steam pressure, the distribution between the condensation and subcooling varies drastically. Steam condensation occurs at constant temperature with a high heat transfer rate, this is why it is used for process heating. The energy content in the subcooling can be used for lower pressure flash steam production or to heat up streams at lower temperatures. The lower is the steam pressure the higher is the energy released during the condensation phase compared to the subcooling phase, but the lower is the saturation temperature.

Energy units: more generally one ton of steam cannot be compared with one ton of natural gas. Energy vectors should then all be characterised using energy units for proper comparison. The question arising at this point is the choice between final and primary consumption.

Final energy consumption corresponds to the quantity of energy entering the system's boundaries (i.e. electricity and fuels). Table 2.2 shows the calculation of the final energy consumption for the most common energy vectors, from what it typically measured. Steam and hot fluid do not correspond to final energy since the final energy consumption is at the level of the fuel that is burnt to generate these two energy vectors. However, considering the fact that these flows can enter directly the system boundaries (i.e. energy conversion outside the system), the corresponding heat flows are associated to final energy consumption in this case.

Mass or volumetric flowrates ($\dot{m}, \dot{V}$) of fuels and imported heating fluids are usually measured. T_{cond} corresponds to the return temperature of condensates. If condensates are not valorised and returned to the steam generation system, this reflects in additional cost linked to make-up water preheating. For common fuels, the lower heating value (LHV) can easily be found in the literature [62]. For other fuels such as waste fuels, these values can be derived from the atomic composition, using for example the Dulong's formula [63] originally developed for coal, or modified versions of the formula proposed more recently for gas, liquid and solid fuels [64] and biomass-based fuels [65].

Table 2.2 – Final energy consumption calculations

Energy vector	Measured	Required data	Final energy [kW]
Electricity	$\dot{Q}_{elec}$ [kW]	-	$\dot{Q}_{elec}$
Natural gas, $_{\text{ng}}$	$\dot{m}$ [kg/s], ($\dot{V}$) [m^3/s]	LHV [kJ/kg]	$\dot{Q}_{ng} = \dot{m}_{ng} LHV_{ng}$
Waste fuel, $_{\text{wf}}$	$\dot{m}$ [kg/s], ($\dot{V}$) [m^3/s]	LHV [kJ/kg]	$\dot{Q}_{wf} = \dot{m}_{wf} LHV_{wf}$
Steam, $_{\text{s}}$	$\dot{m}$ [kg/s], T [°C], P [bar]	$T_{in}, T_{sat}, T_{cond}$	$\dot{Q}_s = \dot{m}_s \cdot (h_{in} - h_{cond})$
Hot fluid, $_{\text{hf}}$	$\dot{m}$ [kg/s], T [°C], P [bar]	c_p [kJ/kg°C]	$\dot{Q}_{hf} = \dot{m} c_p \cdot (T_{in} - T_{out})$

Primary energy considers the efficiency in the energy resources exploitation, including the conversion and distribution losses in the production of the final energy. Once the final energy consumption is calculated, primary energy consumption can be determined by applying conversion factors to the final consumption of the different energy vectors. Conversion factors are determined depending on how the energy vectors are produced (e.g energy mix, type of conversion unit, fuel consumption).

In [66], conversion factors of respectively 40% and 90% are used to calculate the primary energy consumption related to the final consumption of electricity and heat at the European level.

The energy mix drastically varying from country to country and with renewable energy being more and more present, there is a need to define suitable conversion factors at the national and even regional levels with regard to primary energy, if this basis for comparison is to be used.

In the framework of energy audits and energy management, final energy consumption is the most convenient way of comparing energy vectors, since the energy flows can be directly measured and monitored. This is how energy consumption is expressed in this thesis.

Exergy units: the exergy of a heat transfer or an energy quantity is defined as the maximum amount of work that would ideally be possible to obtain from each energy unit transferred or stored, using reversible cycles with the atmosphere as hot or cold source (at the temperature T_a).

Exergy is used to quantify at the same time the quantity and quality of different energy vectors. It enables the comparison of different energy conversion systems with the aim of minimising the consumption of primary energy by maximising thermodynamic efficiency.

Exergy losses of the heat and refrigeration supply to an industrial site, from the system's boundaries to the end-use consumers can be calculated at several levels of the energy chain. For example, exergy losses in boilers are calculated by the difference between the fuels exergy and the heat exergy of the hot fluid (i.e steam or hot oil). The temperature difference between these intermediate energy carriers and the production process streams determine the exergy losses at the level of the end-use consumption.

According to Borel and Favrat [67], the exergy value of a fuel is defined as $\underline{\Delta} k^0$, defined for standard conditions P^0 and T^0 (often P^0 = 1 atm, T^0 = 25°C). This parameter introduces the coenthalpy k, which is a derivative state property combining enthalpy h and entropy s ($k = h - T_a \cdot s$). Exergy values of common fuels are available in [67].

The heat exergy $\dot{E}_{qi}$ is equal to the heat quantity $\dot{Q}_i$ multiplied by the Carnot factor. The exergy of a heat source can then be calculated thank to Equation 2.1. According to this equation, the higher is the temperature of the heat source, the higher is the work production potential.

$$\dot{E}_{qi} = \left(1 - \frac{T_a}{T_{lm,i}}\right) \cdot \dot{Q}_i \qquad \text{with} \quad T_{lm,i} = \frac{T_{in,i} - T_{out,i}}{\ln(T_{in,i}/T_{out,i})} \tag{2.1}$$

The exergy losses of a heat exchange $\dot{L}_{ht}$ can be determined by Equation 2.2, as the difference between the exergy of the hot source and the resulting heated stream:

$$\dot{L}_{ht} = \dot{E}_{q,hot} - \dot{E}_{q,cold} \tag{2.2}$$

2.1.4 Energy baseline

Specific energy consumption

Once final and/or primary energy consumption is calculated, its variation with the site production can be investigated. An example for a production site can be seen on Figure 2.4, where the total final energy consumption is plotted against the yearly production, with the details at the level of the energy vectors (i.e. middle and low pressure steam and electricity). Linear regressions can be fitted on each data set, together with the corresponding coefficient of determination (R^2).

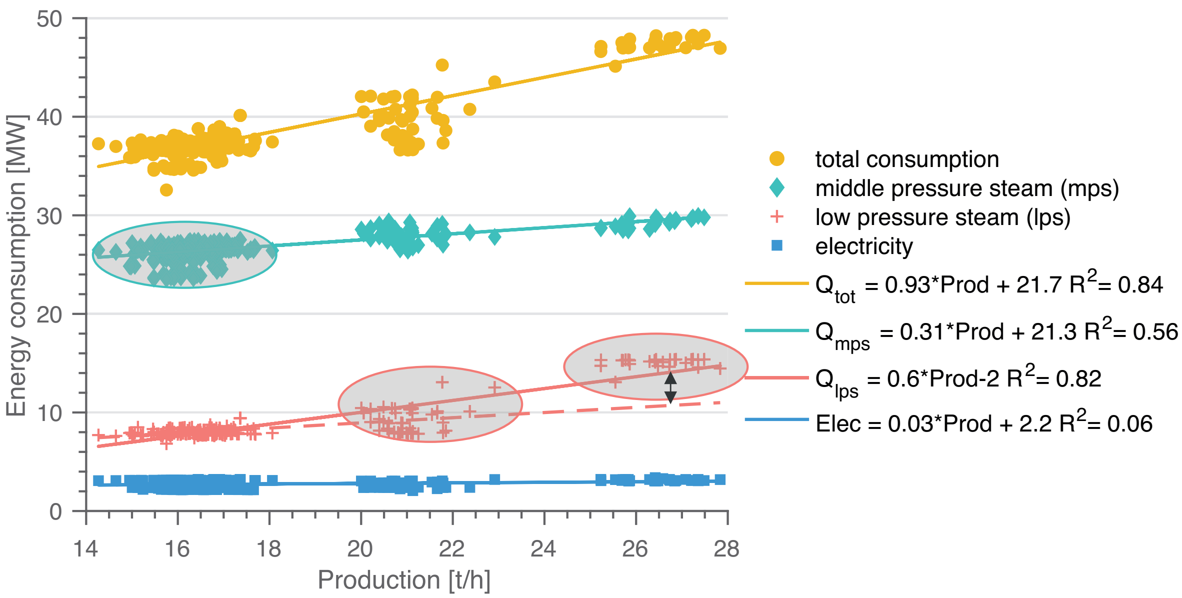


Figure 2.4 – Example of the energy consumption according to production per energy vector (daily values).

From the example, it can be seen first that the consumption of electricity is very small compared to the steam usage. The steam consumption at the two pressure levels are then the main components of the total energy consumption. Although the low pressure steam consumption has the best R^2, it can be seen that if a linear regression is carried out only for the points corresponding to low and medium production, the resulting trend line would be much lower for high production points, compared to what is actually observed.

As for the middle pressure steam, a large vertical variation is observed at low production meaning that for a specific production rate its consumption varies significantly (around 4MW). These two aspects should be analysed in details, by investigating which parts of the plant and/or which final consumers are responsible for this behaviour.

The specific energy consumption (SEC), introduced in Chapter 1, is then calculated at each level (i.e. site and per energy vector) to serve as internal or external benchmark. Logarithmic trend lines where generated for electricity, middle pressure steam and the total energy consumption, showing the effect of the part load.

Results are shown on Figure 2.5. The coefficient of determination for the SEC according to the production is the same as in Figure 2.4 for the total energy consumption. However, results are drastically different at the level of the specific steam consumption.

While the R^2 of the middle pressure steam SEC indicates a good correlation (R^2 =0.92), the SEC for the low pressure steam is not following the expected decreasing trend with the production. On the contrary, it is higher at higher production rate. This observation adds up to the previous one and should also be explained by entering into the site details.

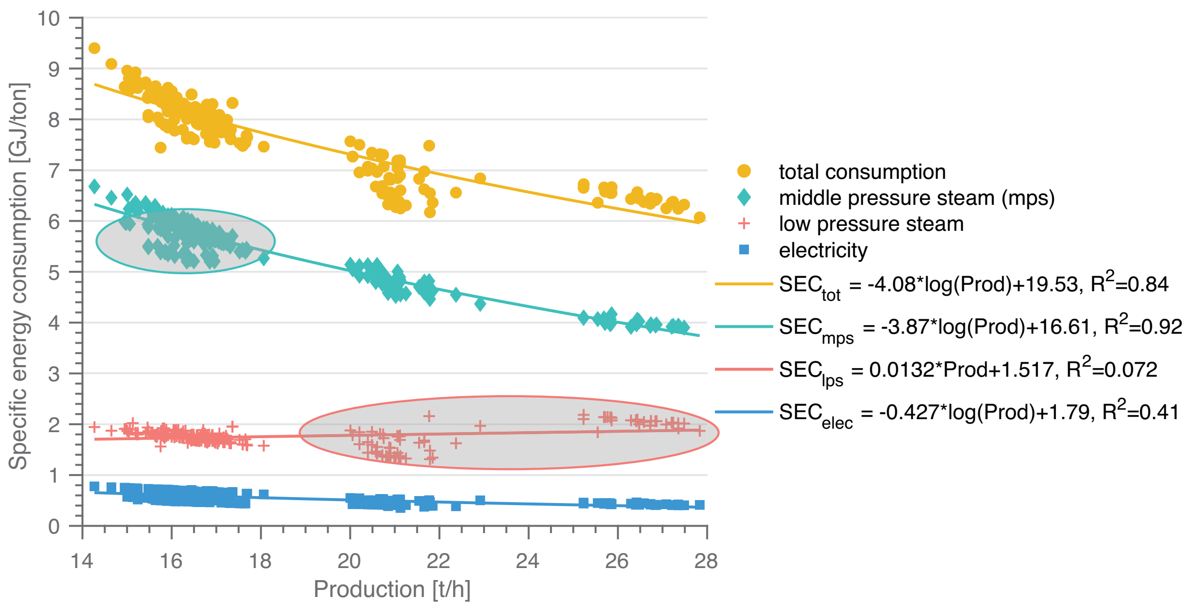


Figure 2.5 – Example of the specific energy consumption according to production per energy vector (daily values).

More generally, the evolution of the energy consumption and the specific energy consumption with the production are two good indicators at the site level. They can be used to define reference lines corresponding to best and average "business as usual" situations. While the latter will serve for energy baseline generation, the former indicates the best points at which the plant was already operated for different production rates and can be used as energy targets.

When modifications are made to the production units and impacting the energy consumption, the specific energy consumption model(s) has to be updated.

Multi-period analysis

The recommended study period length for an energy review is minimum one year. An entire year is long enough to encompass several production modes and shutdowns and allows to see the effect of seasons on the energy consumption. While the analysis of the energy performance and benchmarking can and should be carried out on a daily basis, it is more difficult to do so when carrying out a pinch analysis and generating engineering solutions to improve energy efficiency, due to the large amount of data to treat and analyse.

However, yearly or monthly averages do not reflect the real behaviour of the industrial system and can result in "fictive" operation scenarios. Also, high and low production periods are not visible. In order to successfully study the different operation modes, it is necessary to reduce the study period into a number of base case scenarios, each representing a typical plant operation. In this way, the data size is reduced but the variability of the system is still taken into account.

This multi-period analysis depends on the number of units in the system and the variation of their production rates. When the plant comprises a single or two related plants operating simultaneously, the multi-period profile is generally easy to generate. Figure 2.6 (a) shows the decomposition of such production profile in 13 periods, each corresponding to a typical operation scenario. Production values correspond to the same example as in the previous section (Figure 2.4 and 2.5).

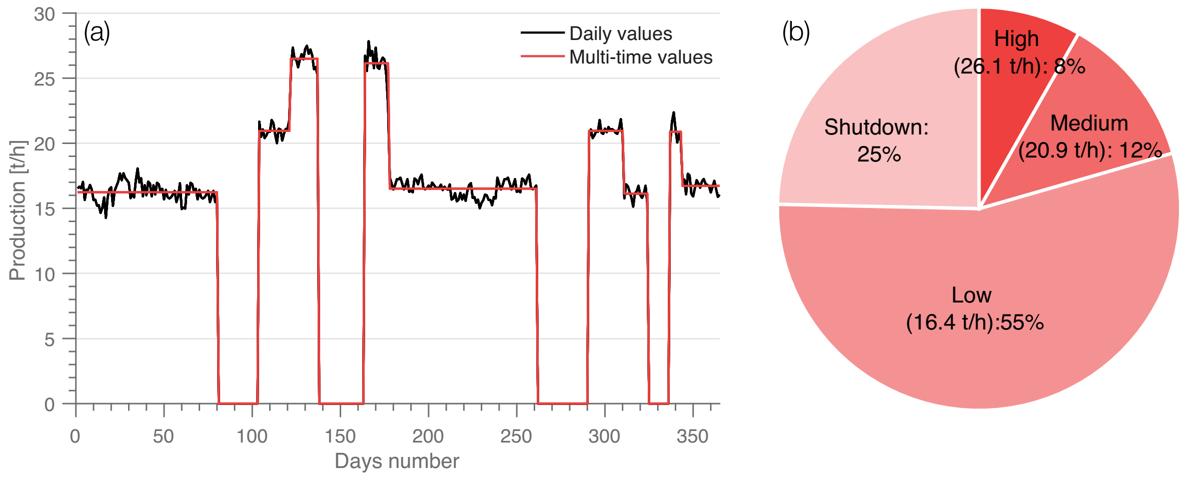


Figure 2.6 – Multi-period representation of a production profile (a) and typical period distribution over the study period (b).

In this specific case, 4 production regimes are identified (e.g zero, low, medium and high production) with averaged productions very close to each other for periods belonging to the same production regime. Instead of oscillating around only three values, the plant production can vary more significantly. In this case, several production ranges are defined, covering the full plant production spectrum, and each period can be assigned to the range within which it is located. Additionally to the multi-period definition, the study year can also be represented according to the share of the production ranges as it can be seen on Figure 2.6 (b).

For systems with a large number of units, as it is the case when studying industrial clusters, the identification of a limited number of periods is more difficult. In this case, mathematical programming and optimisation techniques can be selected, as it is presented in [68], where a genetic evolutionary algorithm is used to find the best solution for multi-period decomposition based on two objectives: the minimisation of the standard deviation between the averaged and real profiles and the respect of the zero flow days.

This methodology has been applied on a large industrial cluster where a Total Site Analysis was previously carried out without considering multi-period analysis [69]. The results highlighted the importance of this approach for more accurate investment sizes with, among other, recommendation for a larger boiler capacity than previously calculated.

Generating the energy baseline

The evaluation of any project aiming at improving the energy efficiency of a system has to take into account the duration and capacity level of plant operations. The analysis of the energy consumption of the system over the year defines how energy consumption varies according to the production rate (section 2.1.4). The multi-period analysis defines the production model of the plant over the same year. By putting the two together, it is possible to generate the energy baseline, which will be used to evaluate energy saving opportunities.

From the multi-period decomposition, Table 2.3 shows the averaged values of the plant production and energy consumption for each typical production regimes, which are then considered for the energy baseline. The comparison between averaged values on a daily basis for the study period and the energy baseline is provided in Table 2.4.

Table 2.3 – Yearly production and energy baseline

Operation mode	Production [t/h]	MPS [t/h]	LPS [t/h]	Electricity [kW]	[hours/y]
High production	26.1	44.6	21.3	2983	701
Medium production	20.9	42.2	16.4	2827	1051
Low production	16.4	40.1	12.2	2692	4818
Shutdown	0	0	0	0	2190

The energy baseline using the multi-period decomposition shows results close to the daily values of the study year, showing the good representation of the plant's behaviour with the multi-period approach. The latter has the advantage of simplifying the analysis, considering a limited number of scenarios, each corresponding to a real operation mode of the plant. As a result, the energy profile of the plant can be generated for the different scenarios (i.e. via pinch analysis) and the accuracy of the design and evaluation of energy saving opportunities is improved compared to the use of yearly or monthly averages.

Table 2.4 – Comparison between the study year and the energy baseline

	Production [kt/y]	**MPS** [kt/y]	**LPS** [kt/y]	**Electricity** [GWh/y]
Energy baseline	119.3	268.8	90.9	18.0
Study year	120.3	269.9	92.0	18.1

The energy baseline defines the future operating conditions of the system. It has first to be approved internally and match the expected future operating conditions of the plant. If higher production rates are expected in the near future, the energy baseline should be adapted to take it into account.

2.2 From black box to process flowsheet representation

Starting from the black box and the global energy consumption of the site, the goal is to track the energy flows down to the process level and the final energy use, thereby understanding where and why energy is consumed. When the utility system is part of the system's boundaries, the energy conversion flows should be considered, together with the utilities distribution network.

This section gradually details the site representation from the black box perspective to the process block flow diagram and flowsheet, which enables the complete mapping of the energy flows. It takes over and complete the approach presented in [70] for chemical sector virtual profile generation.

2.2.1 Site map

The site map decomposes the industrial system into its major sections. They can be divided in three main categories: process units, production support units, and utility units.

Process units are responsible for most of the thermal energy end-usage as well as production when chemical reactions taking place are exothermal. In the site map representation, each individual process unit is detailed in terms of reactants, products and co-product flows as well as other smaller material streams to close the mass balance. Energy vectors entering and leaving the units are drawn.

Utility units encompass all units required to convert and distribute hot and cold utilities. Among them are found the energy conversion units (e.g. boiler, cogeneration unit), directly delivering heat to the process or converting fuels to intermediate energy carriers, and the distribution system of these intermediate carriers (e.g steam network with the different steam headers and back-pressure steam turbines). On the cold utility side, cooling towers and cooling water network are drawn, together with potential refrigeration systems.

Production support units are all the other components of the site. Among them are found workshops and offices, the production support system providing air, inert gases or basic chemicals to the process, the flaring system and the storage tanks.

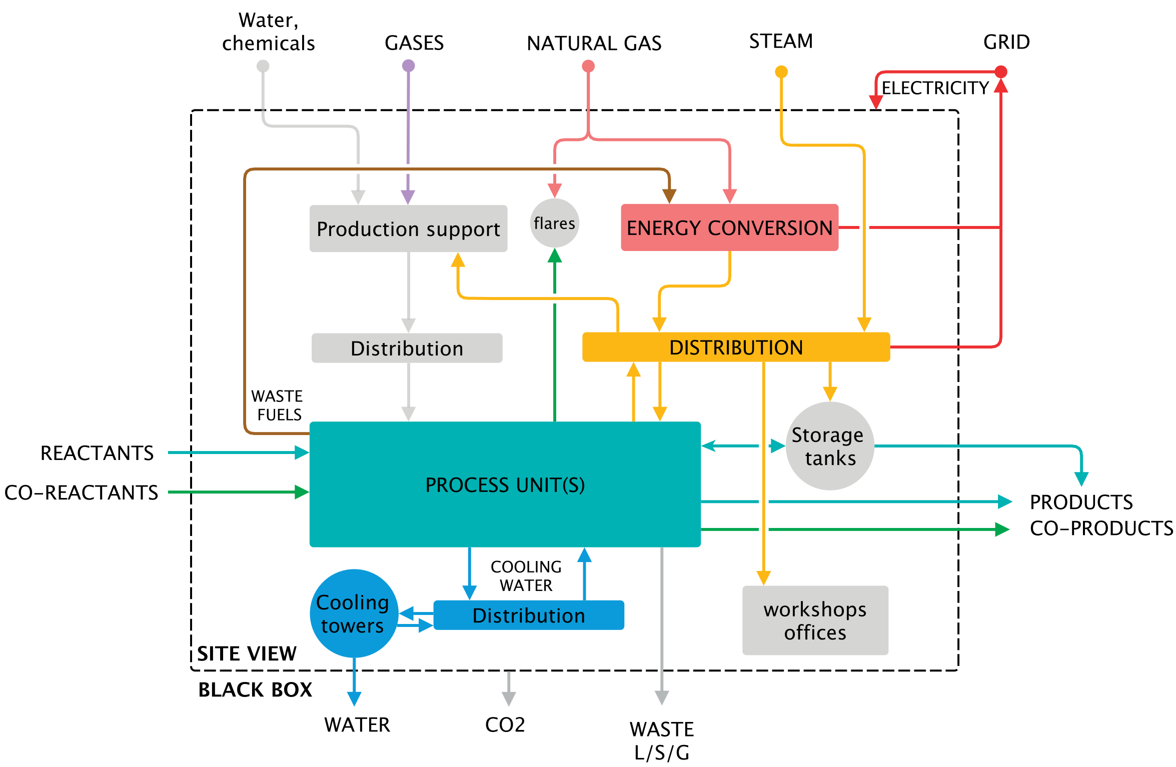


Figure 2.7 – Site map representation

Connections between the utility units and the process and production support units have to be drawn to map all the energy flows of the system and track energy conversions and heat transfers within the system. A simplified example of a site map can be seen in Figure 2.7.

2.2.2 Process block flow diagram

At the level of the site map, details on the final usage of this energy, meaning to which purpose it is consumed, is unknown. The next level of representation zooms inside the process units, to decompose each one of them into interconnected blocks representing their main transformative operations.

As represented in Figure 2.8, these blocks can be reactants mixing and preparation step, followed by the reaction itself, then a recovery step where all the main unreacted chemicals are extracted and recycled back, and finally a separation step to recover the main product(s). Other transformative steps can be for example absorption, distillative extraction, CO_2 capture or cleaning.

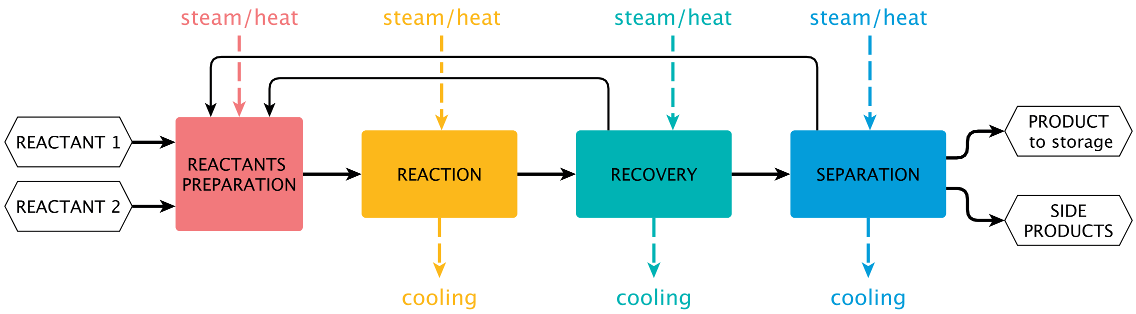


Figure 2.8 – Example of process unit decomposition into main blocks

These blocks are usually straightforward and readily defined and accepted internally. Main product and energy flows entering and leaving each block have to be connected at this step. When using this representation, the "grey box level" is targeted, meaning that the process requirements are defined at the interface between process and utility stream. Existing process-process integration is left out of the analysis.

2.2.3 Process flowsheet

For industrial systems composed of only one or two production units, the mass and energy flows mapping can be carried out at another deeper level, called the process flowsheet. Instead of stopping at the process block flow diagram level and only targeting final energy consumption use, process-process integration is also looked at. Therefore, mass flows inside each block are connected to the major pieces of equipment and all heat exchangers are mapped and connected to their surrounding pieces equipment.

This level of detail is used for white box analysis, which is the level of detail for traditional unit pinch analysis. Translation of Figure 2.8 to the detailed view is shown on Figure 2.9.

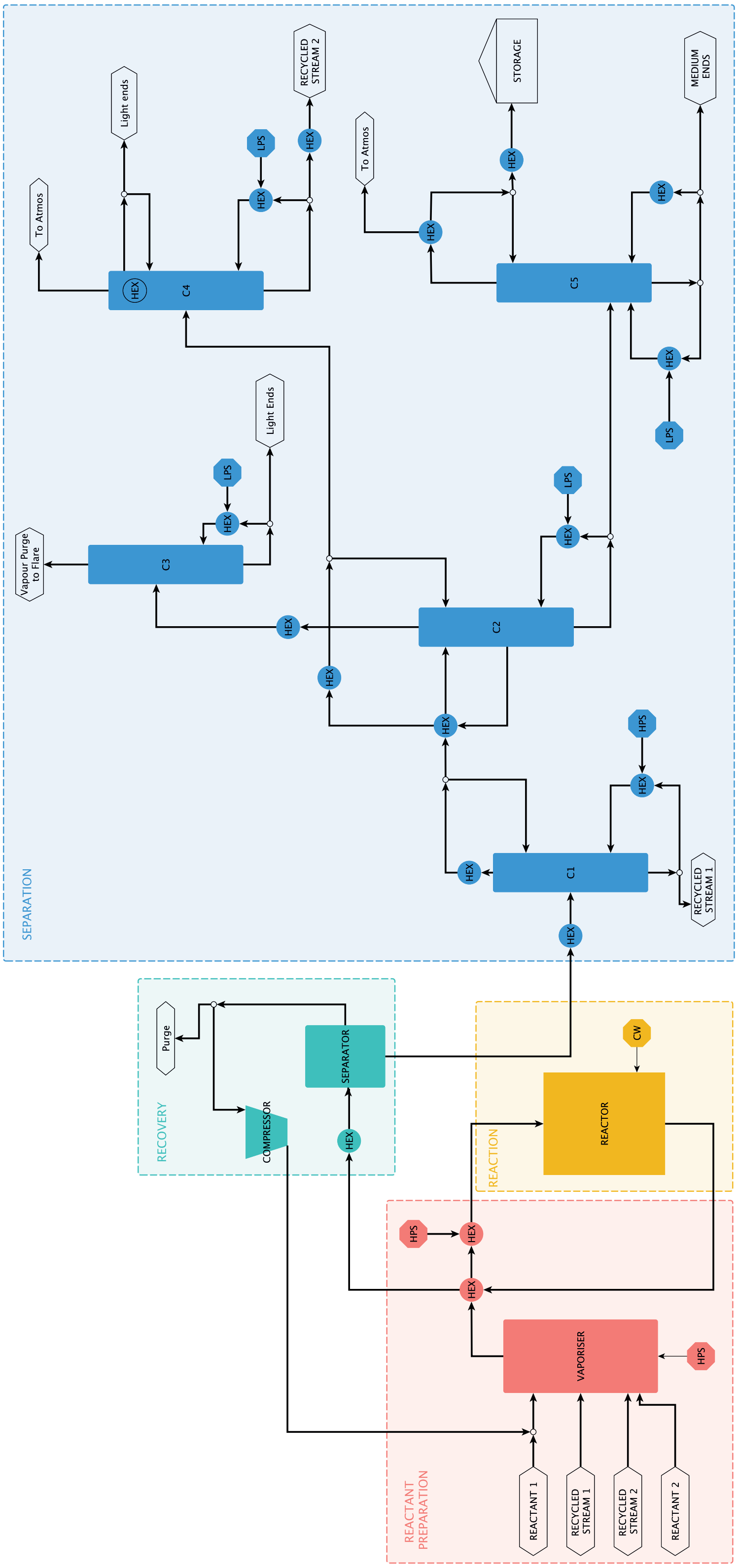


Figure 2.9 – Example of process flowsheet.

2.2.4 Choosing the level of detail

The choice in the level of detail of the energy review will dictate the list of streams in the pinch analysis of the system. Depending on the expected level of detail of the analysis and the system constraints, the energy requirements can be represented in several ways. Practitioners usually consider three categories for streams definition [71]: black boxes, grey boxes and white boxes.

A **black box** defines the energy requirement of a stream as its utility consumption itself. A 1000 kW consumption of steam at 4 bar will be represented by an horizontal segment at the saturation temperature of water at this same pressure (144°C). Choosing the black box representation means that the current utility consumption is fixed and cannot be changed, but the heat load is still taken into account in the analysis. Most of the time black boxes are either smaller utility consumers, processes for which the utility profile cannot be modified or consumers for which data is missing. Showing the actual temperature and heat loads of the hot and cold utilities consumption and/or production, the black box representation only allows optimisation on the actual utility flows and the identification of cogeneration potential between the existing steam pressure levels.

The **grey box** representation goes a step further and considers the temperature level of the process streams exchanging with utilities. Only process streams which are heated up or cooled down by utilities are included in the analysis. The previous 4 bar steam consumption will be translated into the real temperature requirements of the process stream, which might be heating from 100°C to 115°C, while the heat load stays identical. When switching to grey box representation, the utility system can be modified and optimised so that it better fits the process curve while maximising the cogeneration potential. The grey box level also allows the identification of direct and indirect heat recovery schemes and highlight opportunities for heat pumping.

The **white box** representation corresponds to a traditional pinch analysis, where all the hot and cold energy requirements of the system are considered, thereby also looking at process-process heat integration and non-isothermal mixings. Depending on the size and complexity of the system under study, a significant amount of data and a simulation model are needed for this type of representation. Compared to the grey box level, additional findings to improve the energy efficiency concerns mostly process-process heat integration redesign and the removal of non-isothermal mixings, involving modifications of the actual heat integration due to penalising or not optimal heat exchanges configurations.

Figure 2.10 shows for the same system the grand composite curves obtained when using the three types of representation. The switch from black box to grey box shows only a slight potential for heat recovery but it reveals the temperature profile of the heating and cooling demands of the system, allowing the identification of opportunities for heat pumping. The white box level, corresponding to the full characterisation of the system, brings 4MW of additional heat recovery, at the expense of a bigger time spent on data gathering and streams definition.

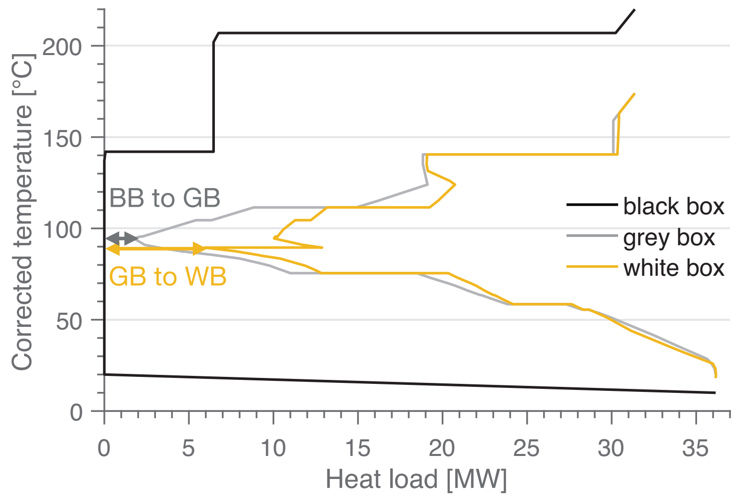


Figure 2.10 – Black, grey and white box grand composite curves of a production unit

The grey box representation of the energy requirements is usually more suitable when carrying out an energy review on systems larger than a single process unit and allows to greatly reduce the complexity and size of data to collect.

Not only the data gathering step is much longer and difficult in white box situation, but in the end the proposed modifications will rarely be viable in retrofit situation, due to diverse constraints like safety issues, space limitation, streams too far from each other, which will also lead to economically infeasible modifications. The grey box level mostly targets heat recovery schemes through intermediate utility systems, allowing greater flexibility and site operability, while still enabling the identification of direct process heat integration potential.

For these reasons, **the grey box level is selected as the default level of detail for this methodology**. It can be applied for small systems to large clusters. In the former case, the actual process-process heat integration can always be checked with respect to the process pinch point, to verify if heat exchangers are correctly placed and not penalising. Inversely, in certain cases, the number of utility consumers can still be very high and grey box data can also be missing for some streams. In these situations, it can be judicious to switch to black box representation.

2.3 Data gathering

The targeting of minimum energy requirements and heat recovery opportunities is only possible once the full set of hot and cold streams is defined, which is usually the most time-consuming step even at the grey box level. Indeed, the complexity of large industrial systems, the significant data size and the lack of time are some of the barriers preventing large companies from carrying out site-wide energy integration studies [72].

This section provides guidelines and heuristic rules to reduce the time required for the data collection step, properly define the main types of heat flows commonly found in industrial systems and simplify the acquisition of the input data for pinch analysis. This section is an extension of a conference paper [73] of the thesis author, in which complementary information on the graphical representation of each type of stream can be found.

Figure 2.11 – Key questions of the data gathering step.

The goal of the data gathering step is to answer to the three key questions displayed on Figure 2.11 that are: who are consuming energy, to which purpose and how much?

2.3.1 Dual representation

The dual representation shows the same heat requirement at two different levels: from the utility and process stream perspectives. At the grey box level of detail, it means that for each process stream, the corresponding current utility stream is defined. It allows to generate the corresponding process and utility hot and cold composite curves of the actual system while ensuring that the energy balance is closed.

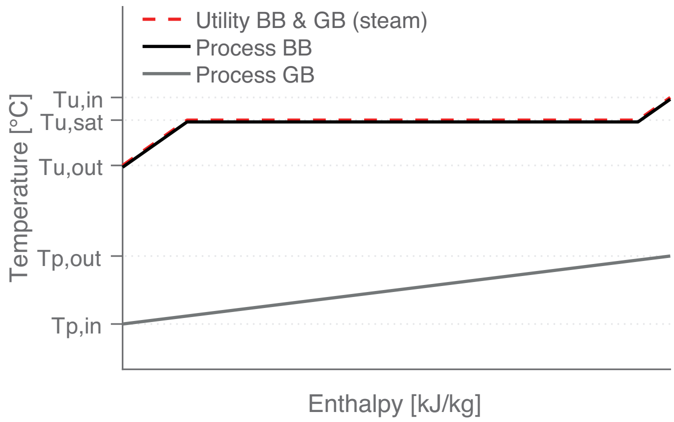


Figure 2.12 – Dual representation of a black box and a grey box cold process stream with the corresponding utility.

The dual representation depends on the stream box color as it can be seen on Figure 2.12. For a same utility stream, here steam heating, the equivalent process requirement will vary. The process requirement of a black box stream corresponds to its utility consumption profile, whereas at the grey box level the real temperature-enthalpy profile of the process is represented, that is heating from $T_{p,in}$ to $T_{p,out}$.

Contrary to black boxes, grey boxes require additional data collection and calculations to properly define the process side of the heat exchange, corresponding to the real process thermal requirements, which depends on the stream type.

2.3.2 Streams classification

The main types of heating and cooling demand encountered in the (petro)chemical industry are:

- **Heaters and coolers:** simple heating or cooling without phase change can be represented by a heat load segment going from the initial to the target temperature, assuming a constant heat capacity.
- **Reboilers and condensers:** heat exchangers usually found respectively at the bottom and at the top of distillation columns (sometimes on the side) for evaporation or condensation. As soon as a phase change is taking place during the heat exchange, the phase change temperature enthalpy profile is determined by the stream composition.
  - one major compound: the stream is represented by a horizontal segment at the saturation temperature of the main compound at the stream pressure. If desuperheating or superheating and/or subcooling or preheating is required, additional temperature-enthalpy segments should be added to the stream.
  - several compounds: the phase change profile cannot be approximated by a straight line since it is likely that the different chemical species have different saturation temperatures. Depending on the stream composition, different methods can be used such as the true boiling point for hydrocarbon mixtures or other specific thermodynamic methods to generate the phase change profile of the stream.
- **Steam injection:** steam is directly injected inside the process. Injected steam is mostly used for separation purposes (stripping, desorption, venting) but also for cracking (refineries), cleaning or water heating. The representation of a stripping stream corresponds to the production of steam from the ambient temperature to the saturation temperature of the minimum pressure allowed by the system.
- **Reactors cooling:** most of the petrochemical reactions are exothermic and release heat. Reactors cooling is carried out either through water cooling or though the production of steam if the temperature is high enough.
- **Building heating:** buildings on a plant are often heated up by the same utility system as the plant itself. Depending on the location and the size of buildings, the energy consumption for heating might be non-negligible.

Three special cases not corresponding to a pure process utility consumption but to the steam network should be added in the curves to account for other important utility flows:

- **Tracing/storage:** Steam is used to maintain a fixed temperature in the distribution pipes, so that process streams do not degrade or start condensing when being transported from one point to another or stored in intermediate tanks. The process stream corresponds to the minimum temperature required.
- **Cogeneration:** the production of electricity by back-pressure turbines within the steam network as well as the different pressure level between which the expansions occur should be noted to be included in the total site profile.
- **Distribution losses:** Lack of maintenance and poor insulation are responsible for losses through steam traps and leaks. Depending on the system, steam losses can be significant. Quantified heat losses within utility systems should be included as well since they contribute to the optimisation potential of the site. In this case the process side is represented by a segment at the ambient temperature.

2.3.3 Minimum data set

In any industrial system, the size of data available to control and check the chemical and physical operations taking place within the site boundaries is gigantic. This section aims at defining the minimum data set to collect to be able to carry out the next steps of the methodology. In this way, the optimum time is spent on data collection without losing information.

Conversion units

At the level of the energy conversion, the minimum data to collect is related to the calculation of the efficiency of conversion units (e.g. boilers, cogenerating units). The following information is required:

- Lower heating value(s) (LHV[kJ/kg]) of fuels
- Mass flow ($\dot{m}$ [kg/s]) or volumetric flow ($\dot{V}$ [m^3/s]) of fuel(s) .
- Temperature (T [°C]), pressure (P [bar]) and $\dot{m}$ of intermediate energy carrier(s).
- Temperature of the fumes (T_{fumes} [°C])
- Inlet and outlet conditions of turbines (T and P) and electricity production ($\dot{E}_{prod}$ [MW]).

If available, additional data such as the excess air, fumes composition and blowdown rate should be collected to further investigate energy losses.

Steam network

The steam network is a key component of almost all (petro)chemical sites. In order to characterise it properly, the following measurements should be collected:

- P and T of each steam header at different points to check for pressure changes and heat losses.
- $\dot{m}$, P and T at each steam consumer and producer level.
- $\dot{m}$, P and T at the inlet and outlet of each letdown and steam turbine.
- P and T of condensates at the outlet of the heat exchangers.
- Inlet and outlet water/steam conditions (T and P) for flash drums and flash steam mass flow.
- $\dot{m}$ of steam venting.

While steam consumed and produced by the production unit(s) are generally well measured, it is seldom the case for the condensates system. In this case, assumption can be made on the pressure drop and subcooling level.

Process streams

According to the type of stream, data should be collected to be able to properly define it and prepare the input for the pinch analysis. Within a pair of process and utility streams, each stream is characterised by a minimum number of four parameters: the heat load of the heat exchange (the same for both streams), the initial temperature T_{in}, the target temperature T_{out} and the contribution to the minimum temperature difference $\Delta T_{min}/2$.

Temperature information of process streams are most of the time measured or easily found in design data or via discussions with operators. Regarding the heat load of the heat transfer, the grey-box approach allows to calculate it either from the utility or the process side. When data on utility flows and thermodynamic properties are available, it is easier to calculate the heat load from the utility side. The best case is to have access to validated measurements on mass flows, temperatures and pressures of the utility streams. If not, mass and energy balances can be calculated using other measurements to determine directly the heat load or the missing parameters required to calculate it.

A good example of the use of mass and energy balances are distillation columns. Figure 2.13 shows the main parameters involved in the calculation of the energy balance around the column.

When feed (F), distillate (D) and bottom (B) flows have approximately the same temperature, the overall energy balance can be expressed by Equation 2.3. The sum of the heat flows 'in' (i.e. reboiler (R) and preheater (PH) heat load) should equal the sum of the heat flows 'out' (i.e. condenser (C), top (TC) and bottom (BC) coolers). In the case where inlet and outlet flows have a different temperature and/or there are no coolers, the individual stream enthalpies should be considered and the overall

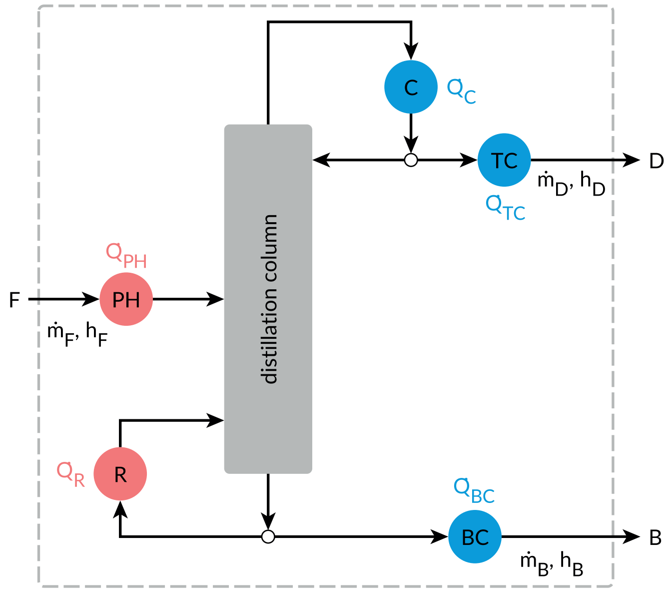


Figure 2.13 – Energy balance around a distillation column.

energy balance is written as Equation 2.4.

$$\dot{Q}_{PH} + \dot{Q}_R = \dot{Q}_C + \dot{Q}_{TC} + \dot{Q}_{BC} \tag{2.3}$$

$$\dot{Q}_{PH} + \dot{Q}_R + \dot{m}_F h_F = \dot{Q}_C + \dot{m}_D h_D + \dot{m}_B h_B + (\dot{Q}_{TC}) + (\dot{Q}_{BC}) \tag{2.4}$$

When no measurements are available and/or if sensors are malfunctioning, design data can be used, either directly or applying linear interpolation from the design reference flow. The last option is to make an educated guess.

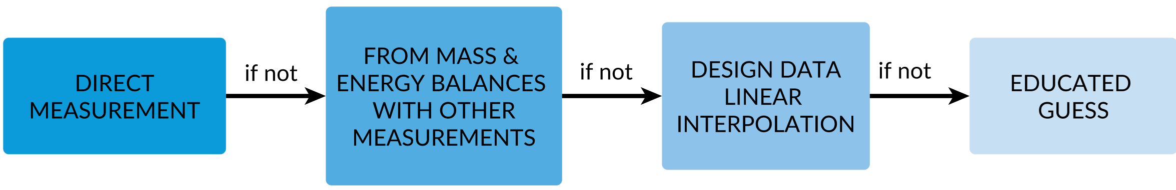


Figure 2.14 – Procedure to collect data.

This procedure, schematically represented on Figure 2.14, is to be followed for each required information. When one or several parameters are missing and cannot be recovered or calculated, complementary data should be collected on the process side to determine the stream heat load. Large chemicals databases (e.g NIST WebBook [74]) and modelling software [75, 76] can be very useful at this stage, facilitating calculations. In specific cases, additional data can also be required to properly define and graphically represent process streams, summarised in Table 2.5.

Table 2.5 – Complementary data collection for process stream definition

Type	Additional data
Phase-change heaters/coolers	T_{evap},T_{cond},TBP's
Injection	P_{min}, $\Delta T_{superheating}$
Tracing/Storage	P_{min}, T_{min}
Building heating	Area, HDD , T_{inside}
Reactor cooling	$X_{reaction}$, $\Delta H_{reaction}$

In the case where evaporation or condensation occurs in heat exchangers, the stream phase-change temperature has to be known. When a stream is mainly made of a single component, the phase transition is represented as a straight line at the evaporation temperature. However, if the stream is composed of a mixture of components having different boiling points, the condensation can take place over a wide temperature range.

Depending on the stream composition, several thermodynamic methods can be applied to approximate the temperature-enthalpy profile of the evaporation [77]. In the refining industry, the true boiling point (TBP) method is an efficient way to determine thermal properties of hydrocarbon streams, which may be made up of millions of components. TBPs give the fraction of fluid evaporated or condensed according to the temperature, over the whole phase transition temperature range.

The minimum pressure for steam injection (P_{min}), based on the required overpressure, and the level of superheating ($\Delta T_{superheating}$) should be determined. Tracing and storage heat requirements are based on the product temperature and the minimum steam pressure (P_{min}, T_{min}). For these two heat flows, the objective is to establish the minimum requirements of the process stream by questioning the real requirements, rather than describing what is currently done.

Instead of representing building heating as a black box requirement, the heat demand can be determined according to the external temperature, the surface to be heated and the buildings insulation. Standards can be found on indoor temperature criteria according to the geographical location and the heating degree-day (HDD) method [78] can be used to calculate the required energy demand. Choosing to represent building heating as a grey box enables the identification of heat recovery opportunities at low temperatures.

Finally, the cooling load of reactors can be determined based on the heat of reaction ($\Delta H_{reaction}$) and reaction conversion ($X_{reaction}$), or through the heat evacuated by the cooling system, a simple calculation in the case of a well-measured water cooling.

The minimum temperature difference for heat exchange (ΔT_{min}) is an important parameter in pinch analysis, as it has a direct impact on the heat recovery potential and associated investment costs. In a heat exchange, each stream contributes to the minimum temperature difference ($\Delta T_{min}/2$). Depending on the type of stream (e.g. gaseous, liquid, phase-changing stream) and other parameters (e.g. utilities cost, heat exchanger type), different $\Delta T_{min}/2$ can and should be attributed. A comprehensive analysis on the definition and impact of the ΔT_{min} on the results is provided in Chapter 3.

2.3.4 Heuristic rules

For large systems and/or when scarce information is available, the following set of heuristic rules can be applied at the data collection step.

Pareto principle or "cut-off" criterion

Although the higher the details the better the analysis, a trade-off can be found between the amount of data to collect and the quality of the results. The application of the Pareto principle, or 80/20 rule, reduces the data size while keeping a high information level. This principle states that in general 80% of the effect is explained by 20% of the cause.

Applied to the energy consumption analysis, it means that data collection on final consumers can be stopped after having identified and characterised at least 80% of the consumers for each utility, in decreasing order. The streams for which the cumulative sum is below or equal to 80% are defined as grey boxes and the rest of the streams as black boxes.

The comparison between the grand composite curves of a system when the Pareto principle is applied and when all the streams are characterised as grey boxes is illustrated on Figure 2.15. For this example, the minimum energy requirements are similar in both cases. Yellow areas correspond to grey-box streams not included in the streams required to reach at least 80% of the total hot and cold utility consumption, which were then transformed to black-boxes. The application of the Pareto principle for process integration can also be found in a previous thesis from Damien Müller [79], focused on the food industry.

This cut-off criterion of 80% can of course be adjusted, depending on the size of the process unit and the availability of data. For process units with a manageable number of streams the limit can easily be set to 90%, and all energy consumers can even be characterised. The grey-box Pareto representation of the heating and cooling demand is not unique and depends on the availability of data.

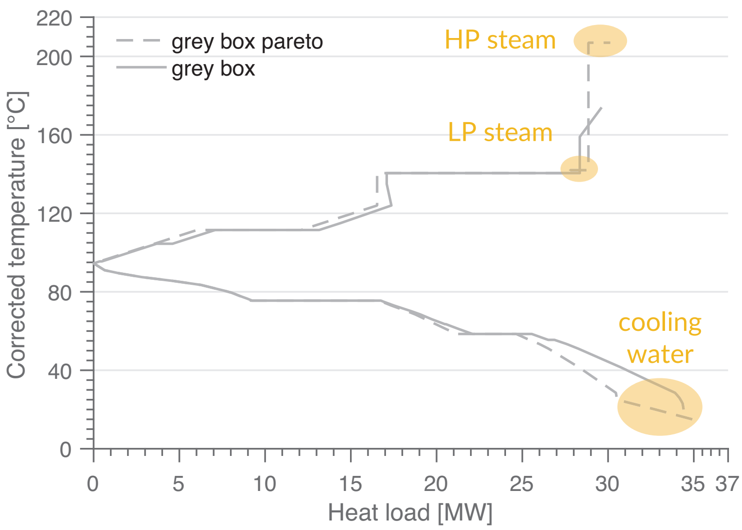


Figure 2.15 – Comparison between full and Pareto streams definition

Defining such cut-off criterion will prevent spending too much time on the smallest consumers, often poorly monitored, which would anyway not be worth considering for heat recovery schemes in retrofit situations. It is however important to keep in mind here that small consumers defined as black box will have an impact at the level of the utilities integration and optimisation.

Hot process streams targeting

Process streams cooling is in the majority of cases carried out by a cooling water network, cooled down by cooling towers. When collecting data to define process hot streams it is often difficult to have access to information on the utility side to calculate the heat load, although these are in reality the possible opportunities for heat recovery.

Cooling water flow measurements and temperatures are often missing, and a first screening rarely allows to obtain 80% of the consumption from utility flow measurements. In this case, other calculation means like mass and energy balances, modelling techniques or the use of design values can be used to reach the Pareto limit.

In the case where limited information is available on both process and utility side a screening can be applied on hot process streams regarding their potential for heat recovery. Streams with temperature higher than 80-90°C, large heat transfer coefficient (phase change) and large heat loads have to be characterised first, since they feature a priori interesting properties for heat recovery.

Low temperature and/or small heat load streams and streams for which modifications or heat integration with another process stream would be consider dangerous or unlikely due to size/location constraints should be characterised last.

2.4 Data validation

Once the required minimum data set has been collected, the next step is the data validation. Indeed, as soon as the level of detail is quite high, with an analysis looking for opportunities from low to significant investment costs and risk taking, it is of major importance to work with consolidated and validated data. Data reconciliation is a powerful method to do so when enough data and time is available. In case of missing data or when faced with too large and complex systems, a set of key mass and energy balances to carry out at the different level of the site map representation has been developed to ensure working with reliable data.

2.4.1 Data reconciliation

When the redundancy of measurements and parameters in the system allow it, data reconciliation techniques can be used to correct the data set while ensuring the consistency of the reconciled values [80].

Measurements from process control sensors (e.g. temperature, mass flow, pressure measurements) are subject to systematic, random and gross errors. Systematic errors have the same magnitude and sign and are due to the limitation of equipment. Random error are statistical fluctuations in the measured data due to the precision limitation of sensors and can therefore be treated with by statistical methods. Gross errors are caused by non random events (e.g. instrument malfunctioning, corrosion, solid deposit) and can differ greatly from the average measurements under the same process conditions. They should be detected and removed before carrying out data reconciliation.

Data reconciliation is a technique that is used to improve measurements by adjusting the measured values so that they satisfy the system constraints. In any industrial system the variables are linked together through physical constraints, material and energy conservation laws and constitutive equations. If enough measurements are available, they can be reconciled using the redundancy of the system, coming from the combination of the model constraints and the measurements themselves.

Data reconciliation has been found to be very powerful when applied to industrial systems, with examples on a gas pipeline [81], a steam turbine power plant [82] or a multi-fuel fired boiler [83], resulting in improved system knowledge and system performance control.

Models can be developed for the entire system or for smaller subparts like process units and utility system. Data reconciliation on steam networks allows to close mass and energy balances around the utility system, from the conversion units to the end-use consumers, including letdowns, turbines and losses quantifications. Practical application of data reconciliation of steam networks in refineries and petrochemical sites can be found in this technical report [84].

The use of data reconciliation is highly recommended and was carried out for almost all case studies during this thesis. It was also covered in the PhD thesis of Stéphane Bungener [25] via its application on the steam network of a large petrochemical cluster, and is therefore not investigated further here.

2.4.2 Data consistency check

When data or time is missing or when the lack of proper programming skills and software does not allow the use of data reconciliation, it is however still possible to check the consistency of the data set through a set of **key mass and energy balances** to be carried out at different levels in the system. Figure 2.16 shows an example of the main mass and energy flows at the level of site map, providing a visual basis for the equations presented in this subsection.

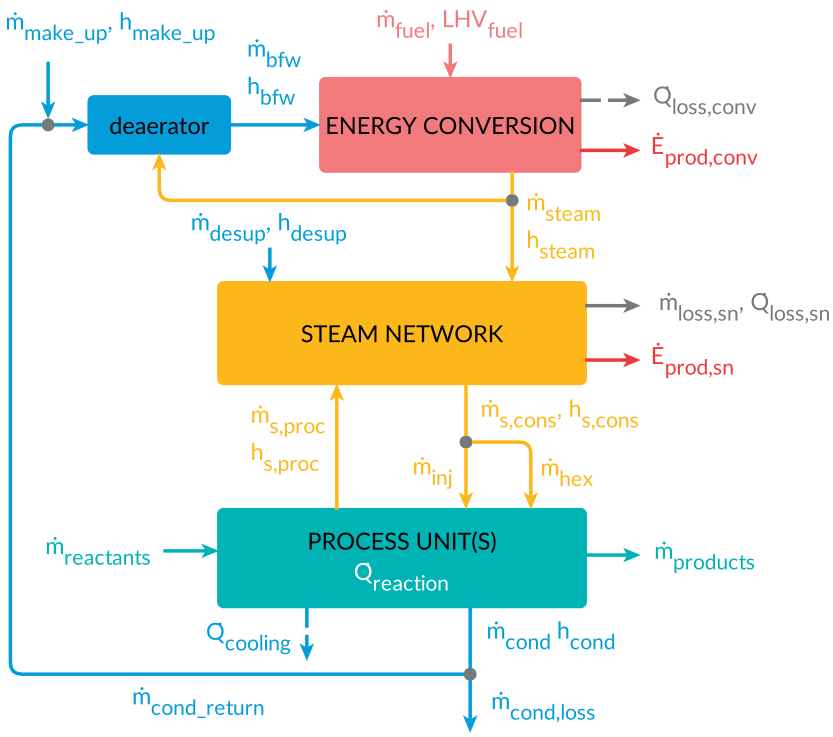


Figure 2.16 – Mass and energy flows involved in the key balances of the data consistency check

The objective of these balances is to minimise the system inconsistencies. Imbalances will be inevitable and will occur between what comes in and out of the system. These imbalances are in reality composed of errors (i.e. coming from raw measurement and assumptions) and real losses, which can then be identified and quantified. Areas were more investigation is required are pointed out, in order to understand where the losses come from and if they can be recovered. Once data is validated and balances explained, energy saving opportunities can be sought.

Site level:

At the site-level it is important to calculate the global energy balance, which can be expressed by Equation 2.5 as the sum of the energy entering the system ($\dot{Q}_{in}$) being equal to the energy leaving the system ($\dot{Q}_{out}$) and the heat losses ($\dot{Q}_{losses}$) .

$$\dot{Q}_{in} = \dot{Q}_{out} + \dot{Q}_{losses} \tag{2.5}$$

Taking an example of an industrial system with a natural gas boiler, a steam export, back-pressure steam turbines, an exothermic process, and water cooling (cold and hot water), the previous equation becomes Equation 2.6.

$$\dot{m}_{fuel} \cdot LHV_{fuel} + \dot{Q}_{reac} = \dot{E}_{out} + \dot{Q}_{steam} + \dot{Q}_{cooling} + +\dot{Q}_{HW} + \dot{Q}_{losses} \tag{2.6}$$

where:

$\dot{m}_{fuel}$ = mass flow of fuel [kg/s]
LHV_{fuel} = lower heating value of fuel [kJ/kg]
$\dot{Q}_{reac}$ = heat of reaction [kW]
$\dot{E}_{out}$ = exported electricity [kW]
$\dot{Q}_{steam}$ = exported steam [kW]
$\dot{Q}_{cooling}$ = cooling water load [kW]
$\dot{Q}_{HW}$ = exported hot water [kW]

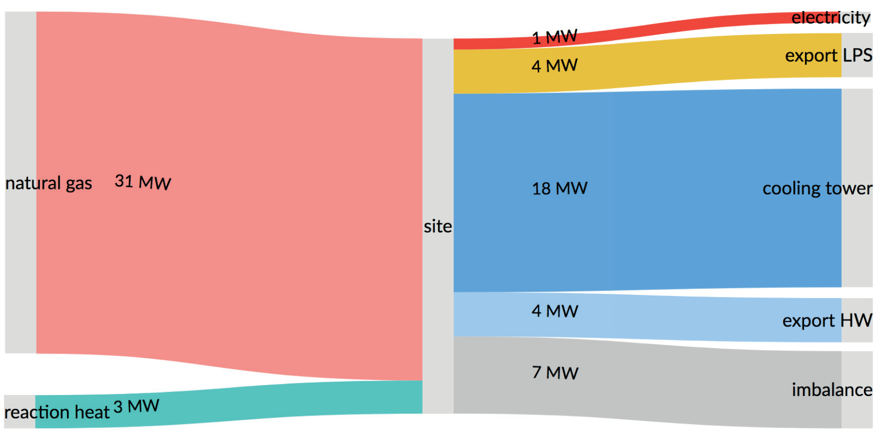


Figure 2.17 – Example of a Sankey diagram at the site level (LPS = low pressure steam, HW = hot water)

This energy balance is represented on a Sankey diagram (Figure 2.17), where the order of magnitude for each energy flow and the energy losses can be seen. The 21% imbalance (7 MW) at the level of the global energy balance has to be explained, and therefore the energy chain needs to be decomposed to understand where and why losses occur in the system.

Conversion units:

Energy conversion units such as boilers or cogeneration units convert final energy and/or waste fuels into secondary energy carriers (e.g. steam, hot oil) and electricity in case of cogeneration. These units are important to characterise as they can show potential for energy efficiency improvement which are well documented in the literature and in best practices documents [50].

The energy balance around energy conversion units, displayed in equation (2.7), seeks to determine the efficiency of the conversion and quantify the energy losses.

$$\dot{m}_{fuel} \cdot LHV_{fuel} = \dot{m}_{steam}(h_{steam} - h_{bfw}) + \dot{Q}_{loss,conv} + \dot{E}_{prod,conv} = \dot{Q}_{hu} + \dot{Q}_{loss,conv} + \dot{E}_{prod,conv} \tag{2.7}$$

where:

$\dot{m}_{fuel}$ = mass flow of fuel [kg/s]
LHV_{fuel} = lower heating value of fuel [kJ/kg]
$\dot{m}_{steam}$ = mass flow of steam [kg/s]
h_{steam} = enthalpy of superheated steam [kJ/kg]
h_{bfw} = enthalpy of boiler feed water [kJ/kg]
$\dot{Q}_{loss,conv}$ = conversion losses (e.g. fumes heat, radiative losses) [kW]
$\dot{E}_{prod,conv}$ = cogenerated electricity [kW]

If an intermediate carrier other than steam is generated as hot utility, like hot oil, then the useful heat produced becomes $\dot{Q}_{hu} = \dot{m}_{fluid} \cdot c_{p,fluid} \cdot (T_{out} - T_{in})$.

The direct method is the easiest way to quickly determine the efficiencies of conversion units. It calculates the ratio between the useful energy coming out over the input energy. The difference between the inlet and outlet energy flows corresponds to losses in the system, about which no details are however available when using the direct method.

The indirect method is more fastidious and requires additional measurements. It can be used complementarily to the direct method, if efficiency results are far from what is expected or from traditionally observed results. It focuses on the losses and aims at calculating each of them individually.

Major sources of losses are the heat losses in the flue gases and the heat losses through radiation and convection. Other loss sources and detailed explanations on the direct and indirect method calculations can be found in [85].

Steam network:

The steam network is usually the centerpiece of the utility system, connecting energy conversion units to the final consumers. If poorly designed, insulated or maintained, the steam distribution system can be a significant source of losses.

Both mass (Equation(2.8)) and energy (Equation(2.9)) balances around the overall network and around each distribution header allow to evaluate the quality of the distribution efficiency and helps in the identification of the nature and location of losses. It also ensures that consumers and/or producers are not forgotten in the analysis. Care should be taken since an apparent surplus in steam inlet compared to steam outlet can hide unaccounted consumers, additionally to pure mass losses.

Depending on the size, age, design and maintenance of the steam network, losses can vary greatly from one site to another. Major causes for heat and mass losses are poor and insufficient insulation, malfunctioning steam traps and steam leaks. Best practices on steam network operation and maintenance can be found in [50].

Equation (2.10) is the application of Equation (2.9) on the steam network box of Figure 2.16.

$$\sum_{i=1}^{nin} \dot{m}_i = \sum_{j=1}^{nout} \dot{m}_j + \dot{m}_{losses} \tag{2.8}$$

$$\sum_{i=1}^{nin} \dot{m}_i \cdot h_i = \sum_{j=1}^{nout} \dot{m}_j \cdot h_j + \dot{Q}_{losses} \tag{2.9}$$

$$\dot{m}_{steam} h_{steam} + \dot{m}_{s,proc} h_{s,proc} + \dot{m}_{desup} h_{desup} = \dot{m}_{s,cons} \cdot h_{s,cons} + \dot{E}_{prod,sn} + \dot{Q}_{loss,sn} \tag{2.10}$$

where:

nin = total number of inlet flows
$nout$= total number of outlet flows
$\dot{m}_{losses}, \dot{Q}_{losses}$ = mass [kg/s] and heat [kW] losses of the perimeter
$\dot{m}_{s,proc}, h_{s,proc}$ = mass flow [kg/s] and enthalpy [kJ/kg] of steam produced by process units
$\dot{m}_{desup}, h_{desup}$ = mass flow [kg/s] and enthalpy [kJ/kg] of water for desuperheating

$\dot{m}_{s,cons}, h_{s,cons}$ = mass flow [kg/s] and enthalpy [kJ/kg] of steam to process
$\dot{E}_{prod,sn}$ = cogenerated electricity [kW]
$\dot{Q}_{loss,sn}$ = steam network heat losses [kW]

Equation (2.11) encompasses both steam network and process units boxes of Figure 2.16. It provides insights on the condensates return rate, since all the condensed steam should theoretically be returned to the conversion units.

$$\dot{m}_{steam} + \dot{m}_{s,proc} + \dot{m}_{desup} = \dot{m}_{cond,return} + \dot{m}_{inj} + \dot{m}_{loss,sn} + \dot{m}_{cond,loss} \tag{2.11}$$

where:

$\dot{m}_{cond,return}$ = mass flow of condensates return [kg/s]
$\dot{m}_{inj}$ = mass flow of injected steam [kg/s]
$\dot{m}_{cond,return}$ = mass flow of condensate losses [kg/s]

A last point to consider at the level of the steam network are the flash units, where a decrease in pressure causes a fraction of hot condensates to evaporate. The higher the condensate flow temperature, the higher the vapour fraction. These units are typically found between steam pressure levels, to maximise the use of steam. Condensates temperature at the outlet of heat exchangers and inlet of flash units should be checked to investigate if the current system is well designed and the production of flash steam is optimised.

Process units:

Energy balances around each process unit should also be verified. A typical energy balance is displayed in equation (2.12). This equation states that the heat supplied to the process streams, either through hot utilities or internal heat generation, should be equal to the sum of the exported heat and the heat evacuated via cold utilities. When material flows entering and leaving the process unit have different temperatures, their contribution has to be included in the energy balance.

$$\dot{Q}_{in} + \dot{Q}_{reac} = \dot{Q}_{out} + \dot{Q}_{cooling} \tag{2.12}$$

where:

$\dot{Q}_{in}$ = heat supplied to process units [kW]
$\dot{Q}_{reac}$ = heat of reactions [kW]
$\dot{Q}_{out}$ = heat exported by process units [kW]

$\dot{Q}_{cooling}$ = heat removed by cold utilities [kW]

$$\dot{Q}_{in} + \dot{Q}_{reac} + \sum_{i=1}^{nin} \dot{m}_i \cdot h_i = \dot{Q}_{out} + \dot{Q}_{cooling} + \sum_{j=1}^{nout} \dot{m}_j \cdot h_j \tag{2.13}$$

In the case of Figure 2.16 the heat balance can be translated as follows:

$$\underbrace{\dot{m}_{hex} \cdot \left(h_{s,cons} - h_{cond}\right) + \dot{m}_{inj} \cdot h_{s,cons}}_{\dot{Q}_{in}} + \dot{Q}_{reac} = \dot{Q}_{cooling} + \underbrace{\dot{m}_{s,prod} \cdot \left(h_{s,prod} - h_{demin}\right)}_{\dot{Q}_{out}} \tag{2.14}$$

where:

$\dot{m}_{hex}$ = mass flow of steam to heat exchangers
$h_{s,cons}$ = enthalpy of steam at the inlet of process units
h_{cond} = enthalpy of condensates
h_{demin} = enthalpy of water for process steam production

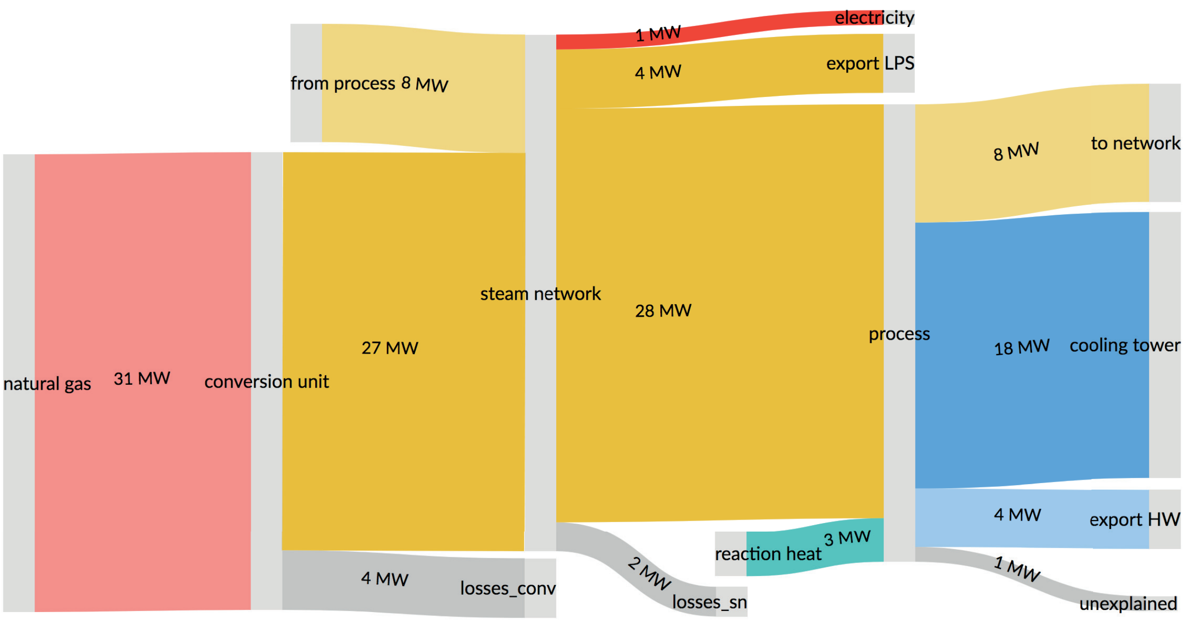


Figure 2.18 – Example of a Sankey diagram

Additional energy flows should be added in equation (2.12) when relevant. Sometimes part of the steam consumed by process units serve to drive turbomachinery. In this case the electricity generated to drive the associated devices (e.g. pumps, compressors), should be taken into account in the heat balance. Finally if important heat losses to the environment have been identified (e.g. ambiant cooling), they should be included in the equation.

Energy flows from the set of key mass and energy balances presented above can be visualised via the use of a Sankey diagram, like the one provided on Figure 2.18. Losses at the level of the conversion units and the steam network can be seen, as well as potential imbalance around the process units, often due to uncertainty on the heat of reaction and process cooling.

These balances do not correct measurements contrary to data reconciliation. However, they are used to check for inconsistencies and spot the areas where additional investigation is required, by going more into the details of subunits and locate losses and/or identify malfunctioning sensors. Generally, it was found that 5% to 10% of imbalance is acceptable for smaller to larger systems.

2.5 Key performance indicators

Key performance indicators are quantifiable measurements to establish actual performance and evaluate progress towards specific goals, and are thus extensively used in energy management systems. Energy efficiency KPI's are used to evaluate the energy efficiency of the system, establish targets, and follow the energy performance improvement through effective monitoring.

To evaluate the energy efficiency of an industrial site, it is important to generate a set of relevant and representative performance indicators as already pointed out in section 1.1.2. Indeed, an industrial site is composed of several subsystems that have different purposes and energy consumption types. A single performance indicator is not enough to describe the energy efficiency of such complex sites, therefore suitable metrics to identify inefficiencies within a plant's energy usage are needed.

A significant contribution in the development and implementation of real-time resource and energy efficiency indicators was brought by the MORE European project [48]. This project targeted the optimisation of daily operations. At the level of the analysis of the energy consumption to identify ways of improving the energy efficiency of a system, the level of detail and number of indicators defined are maybe too important and would be more suitable at the monitoring step, which was the objective of the project.

In order to evaluate the energy efficiency of an industrial system, it is required to be able to characterise it at a global level, but also decompose the overall energy efficiency into its main components, corresponding to the different energy conversion steps until the final end-usage.

Starting from the site-level, Figure 2.19 shows an example of a KPI's map, covering the energy chain from the conversion to the end-use consumption. The proposed energy efficiency related KPI's are common indicators applicable to all (petro)chemical sites. Additional indicators, specific to particular production processes or sites should be developed and added to the map.

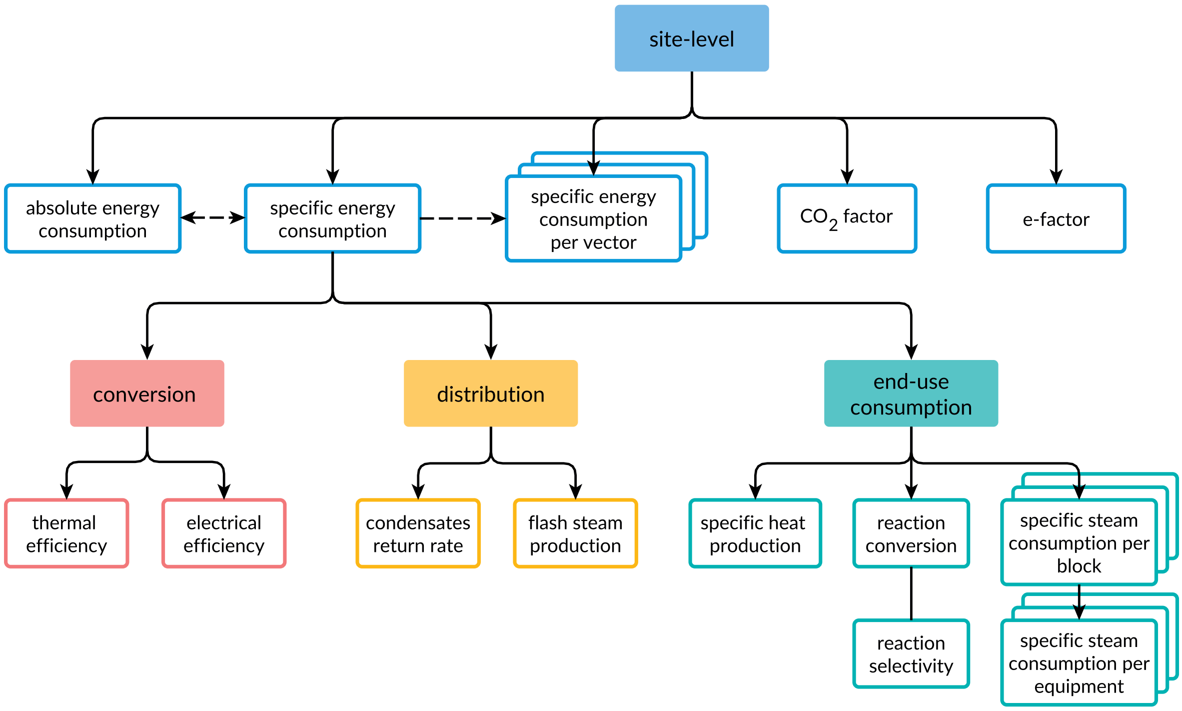


Figure 2.19 – Example of an industrial site KPI's map.

Overall plant: Apart from the overall and energy vector specific energy consumptions already introduced in section 2.3.1, other site-level sustainability indicators can be used such as the e-factor (Equation (2.15)) representing the waste produced per ton of useful output (kg of waste/kg of product) or the CO_2 factor (Equation (2.16)) showing the CO_2 emissions with respect to the production (tons of CO_2/kg of product). The absolute energy consumption should also be monitored alongside the specific energy consumption.

$$\text{e-factor} = \frac{m_{waste}}{\text{1 ton of product}} \tag{2.15}$$

$$CO_2 \text{ factor} = \frac{m_{CO2}}{\text{1 ton of product}} \tag{2.16}$$

Conversion units: The KPI's for energy conversion units mainly relate to the conversion efficiency.

Thermal and electrical efficiencies are most of the time calculated by the direct method, which is the ratio of the useful energy over the input energy. The total efficiency is calculated by summing these two efficiencies. This indicator has the advantage of being simple to evaluate since it requires few parameters for computation and few instruments for monitoring. It gives a good overview of the efficiency of fuel conversion but does not provide insight on what differs from normal behavior if the value is lower than typical efficiencies or how to improve it.

$$\eta_{th} = \frac{\dot{Q}_{hu}}{\dot{m}_{fuel} \cdot LHV_{fuel}} \tag{2.17}$$

$$\eta_{elec} = \frac{\dot{E}_{prod}}{\dot{m}_{fuel} \cdot LHV_{fuel}} \tag{2.18}$$

$$\eta_{tot} = \eta_{th} + \eta_{elec} = \frac{\dot{Q}_{hu} + \dot{E}_{prod}}{\dot{m}_{fuel} \cdot LHV_{fuel}} \tag{2.19}$$

NB: when the input fuel to the conversion units is a mix of fuels, the conversion efficiency according to the share of the different fuels should also be calculated, to determine the impact of the mix.

Steam network: The energy distribution efficiency is mainly related to the condensates return rate calculated by Equation (2.20). Indeed, the more condensates are returned, the less water make-up is needed. Since water make-up has a much lower temperature than condensates, it would require more energy to bring it to the steam thermodynamic properties. Also costs due to fresh water import and deionization treatment are decreased when steam is produced on-site.

$$\text{condensates return rate} = 100 - \frac{\dot{m}_{makeup}}{\dot{m}_{steam}} \cdot 100 \tag{2.20}$$

A decrease in the condensates return rate might be explained by several factors:

- increase of injected steam
- discarded condensates
- steam starting to condense causing losses through steam traps
- purges within units
- piping leakage

The pure losses of the steam distribution network are calculated by subtracting the amount of injected steam to the condensates not returned:

$$\text{network losses} = 100 - \frac{\dot{m}_{makeup} - \dot{m}_{inj}}{\dot{m}_{steam}} \cdot 100 \tag{2.21}$$

Process units: By defining and regularly evaluating the specific consumptions of the different processes or blocks, it is possible to identify the locations explaining the value and the variations of the overall specific steam consumption.

For each process and/or block, a reference flow has to be defined for the calculation of the specific steam consumption. The same can be done for the export of steam from the process with the specific steam production indicator.

Specific steam consumption/production indicators depend mostly on the chemical production but also on other parameters related to the operation itself, product specification (e.g. purity), raw material properties or also catalyst age. These influencing factors and their respective impacts should be studied in details as part of energy consumption monitoring.

The reaction conversion (X) and selectivity (S) are two important indicators since their variations are closely linked to the energy consumption. If the conversion is lower then recycled streams are bigger, which might cause a higher utility consumption, and steam production from the reaction is lower. The same goes with selectivity, which also has an impact on the distillation columns utility consumption.

2.6 Conclusion

The second chapter of this thesis corresponds to the first step of the methodology for energy review presented in Chapter 1. The main research question it is aiming to answer is the following:

How to analyse and characterise the efficiency of the energy chain down to the end-use consumers, in a suitable and reliable manner, while keeping the required time for data collection and complexity of the analysis at an acceptable level?

At the level of the black box, corresponding to the system's boundaries, **guidelines and recommendations** to properly quantify the energy flows crossing the limits of the system and establish the energy baseline were provided.

To characterise and evaluate the energy efficiency from the site raw energy consumption down to the final use of energy, a **top-down approach** was followed with well-defined intermediate level of detail (i.e. black box, site map, process block flow diagram and process flowsheet). This approach allows to gradually enter into the site details, track mass and energy flows, to ultimately understand where and why energy is consumed and how efficiently it is done.

The data gathering step is traditionally the most time-consuming step in such energy study. It is highly dependent on the size of the system and the number of sources and availability of data. However, when the required data is properly defined in advance, the time for data collection can be drastically reduced. The ultimate objective of the data gathering step is to obtain the process heating and cooling requirements.

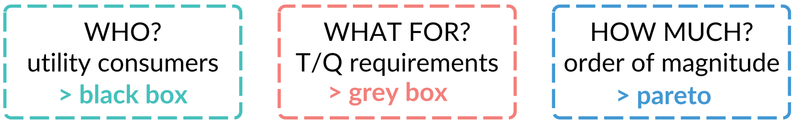


Figure 2.20 – Key questions of the data gathering step.

Having this in mind, this chapter introduced **strategies and heuristic** rules to answer to the key three questions preparing the input for the pinch analysis: who are the energy consumers? what is the energy used for? and how much each end-usage is consuming? The first question corresponds to the black box level of detail, identifying the energy consumers. To answer to the second question, the real requirements of the process need to be characterised and therefore the grey-box level of detail is required. Finally, based on the recurring observation that the largest share of the energy consumption is often explained by a small number of consumers, the use of the Pareto principle to prioritise the streams characterisation allows to reduce the time and complexity of the streams definition, without losing too much information for the next steps of the analysis.

In order to ensure the validity of data, a **consistency check** was defined in the form of a set of key mass and energy balances to be carried out at the site-level, but also for each main entity at the level of the site map (i.e. energy conversion units, steam network, process units). These balances are of major importance to master energy flows across the site. They allow to estimate losses and therefore identify the areas where further investigation is required.

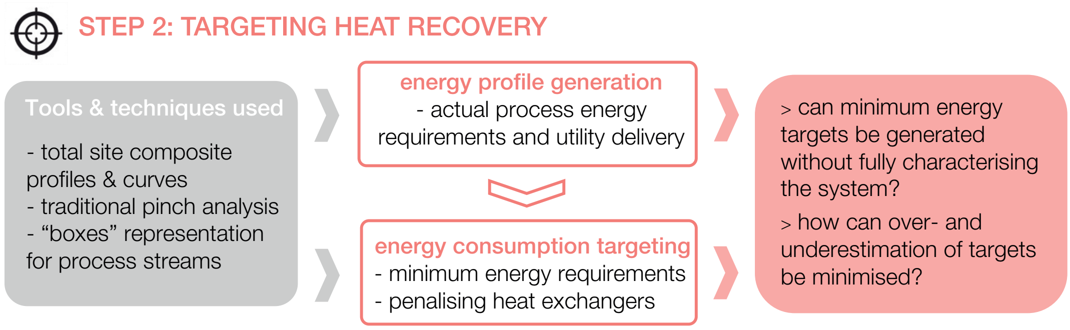
Finally, in order to evaluate the energy efficiency of the system, a set of **key performance indicators** was proposed at the same levels as for the consistency check. These indicators are used for the energy consumption analysis and should also be used for monitoring purposes.

The next step of the methodology aims at targeting the minimum energy requirements of the system, based on the analysis of the first step and the list of process hot and cold streams.

3 Targeting heat recovery

Chapter overview:

> From actual energy consumption analysis to heat integration potential targeting.



3.1 Pinch analysis and energy review

As defined in [59], heat integration based on pinch analysis "examines the potential for improving and optimising the heat exchange between heat sources and sinks in order to reduce the amount of external heating and cooling, together with the related cost and emissions". It is a powerful method largely used to improve heat integration within industrial sites or clusters with significant thermal power consumption [86, 87].

Originally applied to single processes, pinch analysis was extended on entire industrial sites via the so-called Total Site Analysis (TSA). TSA accounts for heat recovery between subsystems through intermediate utilities and thereby overcome constraints linked to direct heat integration between different production units. Since its first introduction and definition in the 1990's [88], significant theoretical developments [89, 90] and practical applications contributed to the robustness and versatility of TSA.

Issues related to the practical implementation were also tackled. Among them can be found the integration of geographical and/or operational and security constraints in the optimisation problem formulation through the use of restricted matches [91, 92] and the consideration of multi-periods [93, 69] allowing the generation of a set of profiles accounting for different operational modes of production units.

When applied in the framework of energy reviews, pinch analysis from a single process to total site analysis has several advantages. First, it provides insights on the temperature enthalpy profile of the industrial system, showing at which temperatures heat is supplied to and removed from the process, including the order of magnitudes of the heat exchanges. This observation might seem evident but often on-site people are not aware of these information.

Secondly, pinch analysis provides targets for energy consumption reduction, via the difference between the minimum energy requirements resulting from the heat cascade and the actual energy consumption. This potential corresponds to the penalising heat exchangers with respect to the system pinch point. The redesign of the heat exchanger network will aim at getting closer to the minimum energy consumption targets while respecting different constraints (e.g. economic, safety, technical, restricted matches).

Third, the grand composite curve of the system provides information on the real temperatures and heat loads to be delivered by the utility system, highlighting as well heat pumping opportunities.

On the basis of the heat cascade results, different strategies can be followed. If potential for process integration is low, focus will be put on the utility system optimisation or heat pumping integration if applicable. If there is a significant potential for heat recovery, then redesign of the new heat exchanger network (HEN) can be carried out either using pinch techniques, mathematical programming or hybrid methods (combinations of both approaches). The different techniques and problem formulation to redesign the HEN are not investigated in details in this thesis.

NB: Extensive reviews of the heat exchanger network retrofitting methodologies and their applications can be found in [94] as well as in [59], together with more general information on process integration.

3.2 Generating the energy profile

3.2.1 Current process-utility profile

In the first step of the methodology, the full list of streams at the grey-box level (i.e. default level of detail) is obtained with the dual representation presented in section 2.3.1. Before determining the utility and energy consumption targets, it is interesting to generate the actual energy profile of the industrial system, through the use of the so-called hot and cold total site profiles. The hot total site profile shows how heat is removed from the process and inversely for the cold site profile.

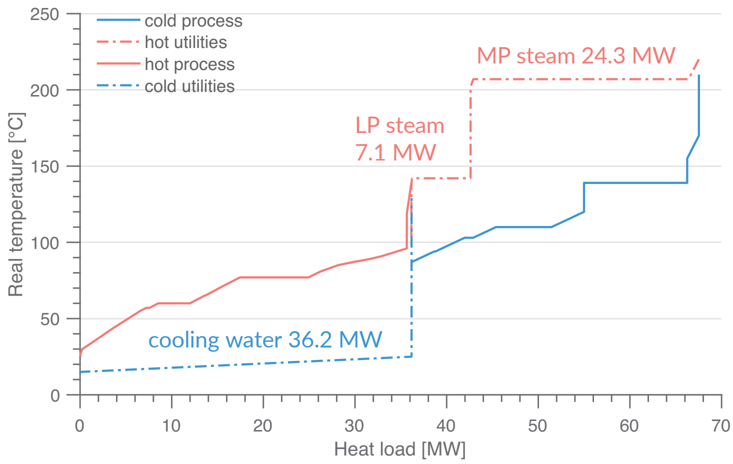


Figure 3.1 – Example of a total site profile.

Such graphical representation can be seen on Figure 3.1 for a reference case study which will be used in this section and in Chapter 4. In this case study, heating is provided by steam at two pressure levels (middle pressure steam (MPS) at 18 bar and low pressure steam (LPS) at 4 bar) and cooling is realised with cooling water. The grey box list of streams can be found in Appendix A.

At this level of the energy review and for this specific example, several observations can be made:

- the grey box level shows only a small potential for heat integration (direct or indirect), the temperatures of the cold composite curve being higher than the ones of the hot composite curve.
- increasing the level of detail might lead to additional heat recovery opportunities
- the steam pressure levels could be optimised to better match the cold composite curve.
- there is a potential for hot water production if neighbouring areas have use of it.

Generally speaking, the total site profile helps to visually understand the existing heat transfer between the process and the utility steams. It gives preliminary information on the potential for direct and indirect process integration and utility optimisation.

3.2.2 Level of detail refining

From the default level of detail, which is the grey box level with or without the application of the Pareto principle introduced in section 2.3.4 (applied depending on the system size and availability of data), the refining of the list of streams is highly recommended and is investigated in this section.

Let's say that for the same industrial system as in Figure 3.1, the complete list of the heat transfer requirements at all the levels of representation is available (i.e. black box (BB), grex box with Pareto principle (GBP), full grey box (GB) and white box (WB)). The white box level will give the minimum energy requirements of the system, corresponding to the maximum heat recovery potential.

However, the highest the level of details, the hardest it is to modify and integrate the system, mainly explained by economical and topological constraints. The goal of the list of streams refining is to be able to unveil the white box streams of interest. To highlight this, another representation of the same industrial system is added, called OPT, which corresponds to the optimum level of detail for each stream which leads to the same minimum energy requirements as the white box level, but with the minimum number of streams defined at this level.

The grand composite curves and the corresponding hot and cold energy requirements can respectively be seen on Figure 3.2 and Figure 3.3. Details on the pinch point and the heat penalty compared to the MER from the white box level are displayed in Table 3.1. The full list of streams for each case is available in Appendix A.

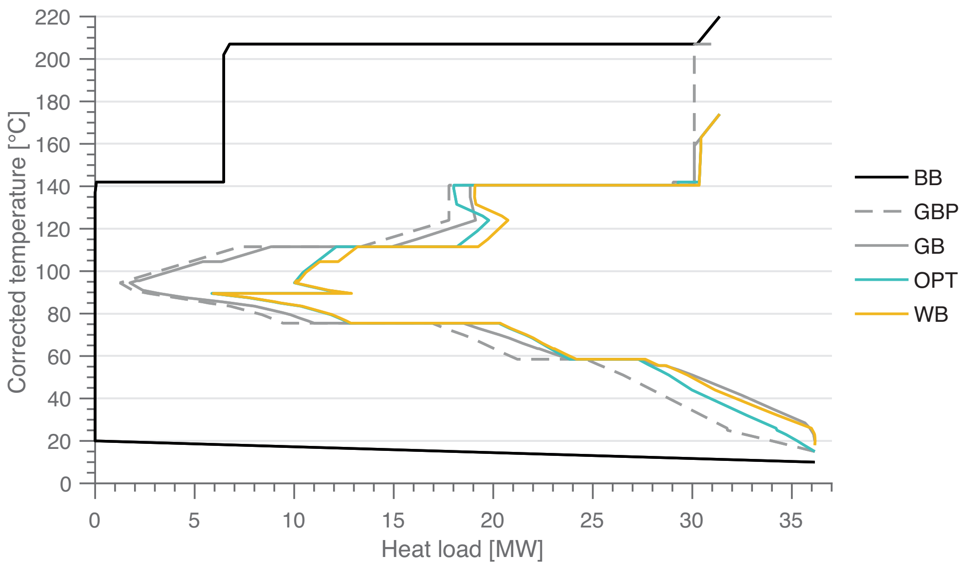


Figure 3.2 – GCC according to the level of detail for the streams definition.

The actual energy consumption of the system corresponds to the black box energy requirements, i.e. 31.4 MW of hot utility (steam) and 36.2 MW of cold utility (cooling water). Switching from the black box to the grey box level through the application the Pareto principle allows to identify a potential for heat recovery of 1.24 MW, which corresponds to stream 'HEAT2_1', consuming a hot utility below the pinch point located at 94°C in corrected temperature.

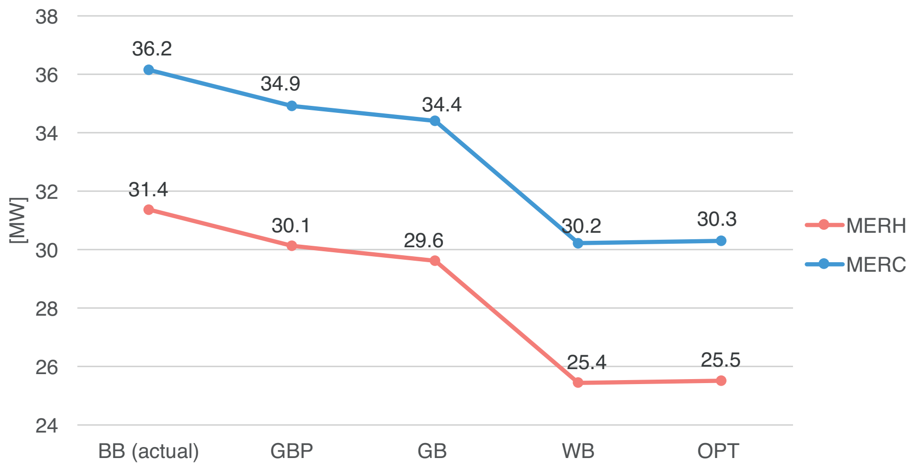


Figure 3.3 – MER hot and cold according to the level of detail.

Table 3.1 – MER results for each level of detail

	Black box	Grey box pareto	Grey box	White box	Optimum MER WB
Pinch point [°C]	-	94.5	94.5	89.5	89.5
ΔGB [MW]	5.9	4.7	4.2	0	0.07

The full grey box level shows very similar minimum energy requirements (MER) than the Pareto one, but additional 500 kW could theoretically be recovered, coming from a hot black box stream ('RECYCLING') turned into a grey box and consuming a cold utility above the pinch. These two streams are the only penalising streams at the grey box level, with a total amount of 1.7 MW.

Increasing the level of detail to the deepest level (white box), the difference between the actual energy consumption and the MER is now of 5.9 MW. Characterising fully the heating and cooling requirements of the entire process allows then to identify an additional heat penalty of 4.2 MW. The pinch point is also changed by 5°C (from 94.5°C to 89.5°C), showing a fair approximation from the grey box level.

Finally, for the optimal case "OPT", the grand composite is the same than the white box one in terms of MER, but the shape is slightly different due to the temperature definition of streams.

Figure 3.4 details the number of streams per level of representation (i.e. black, grey and white). The top and bottom graphs show the results respectively for the cold and hot streams, while the bottom graph is for the total number of streams. It can be seen that the total number of streams for the WB and OPT cases is identical, but the number of streams being defined as white boxes is only one third. The two other thirds are represented by black and grey streams.

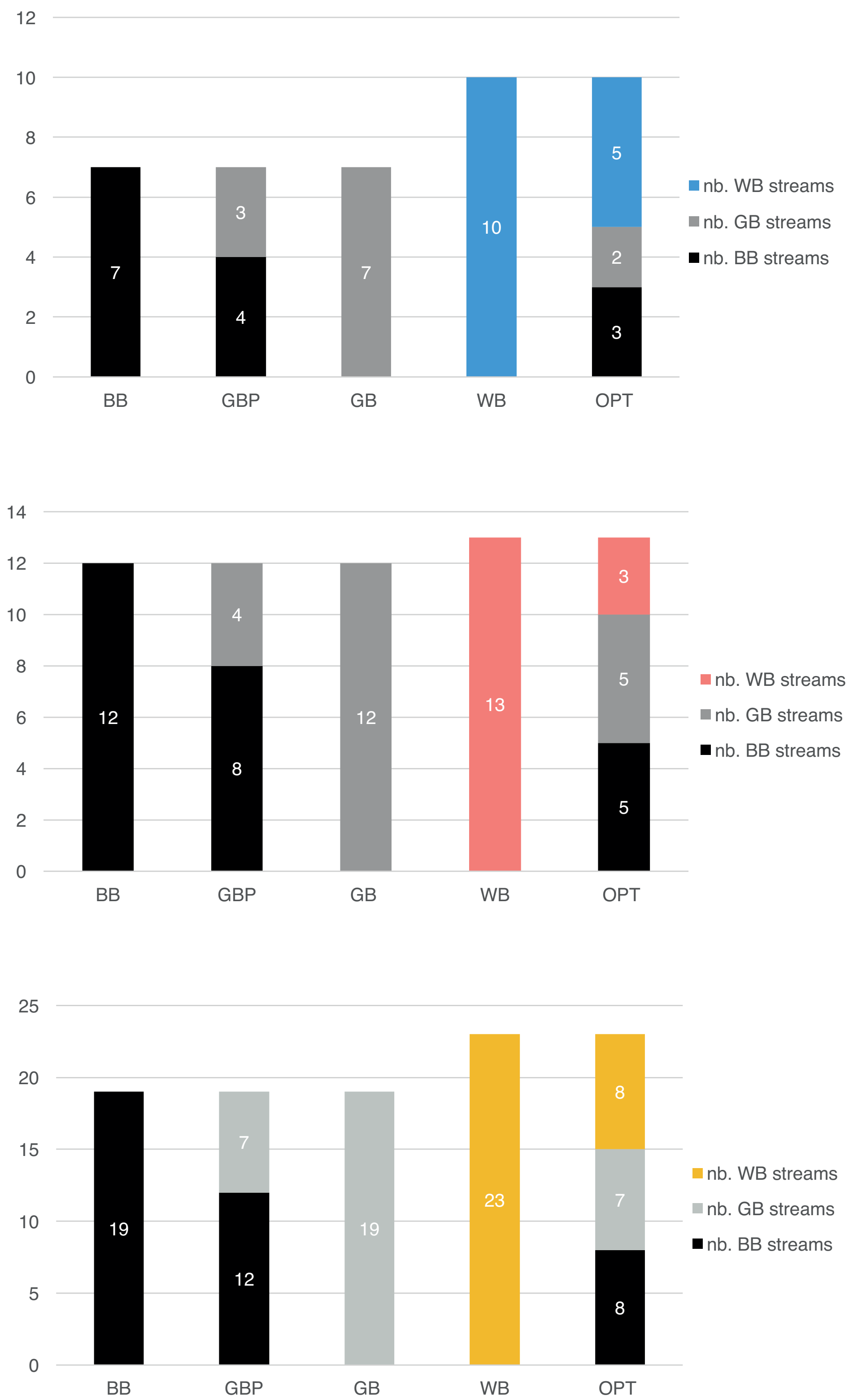


Figure 3.4 – Number of cold (top), hot (middle) and total (bottom) streams in black, grey and white boxes representations according to the level of detail.

By further investigating how to go from the default (pareto) grey box level to the optimum case, it was found that the white box streams to be defined correspond to 3 distinct heat recovery schemes involving 5 cold streams and 3 hot streams. Among these 3 systems, one is responsible for 95% of the information gain going from grey to white level. The hot and cold streams involved in this existing heat recovery system have the following properties: 1) both are crossing the pinch point 2) both have a significant heat load.

The last aspect was already raised in section 2.3.4 for grey box hot process streams targeting at the data gathering phase, and is therefore still valid for this phase of composite curves refining towards the white box level. The first aspect leads to the generation of other heuristic rules adding up to the previous ones, once the pinch analysis at the default grey box level is carried out:

- identify and include in the list white box streams in the area of the pinch point (+/- 20°C), with a heat load at least equal to 300-500 kW (these are typical observed values, they depend in reality on the thermodynamic and economic properties of the system).
- for systems with a large number of process units, convert potential black boxes to grey boxes in the same area.

The white box being the highest level of detail and requiring a significant amount of data collection time for large systems, it is seldom possible to reach such deep investigation. It is also obvious that the optimum level of detail for all the streams are not known from beginning of the analysis. However, starting from the grey box level, the list of streams can be gradually extended depending on the shape of the composite and grand composite curves and the pinch point location. In this way, additional information on heat recovery and heat pumping opportunities can be gained, without spending too much additional time on data collection.

The importance of allowing several representations for process streams definition is also raised and demonstrated mathematically in a recent paper on retrofit process integration based on MILP [95]. It was shown in this work that bringing flexibility in the energy requirement representation provides preliminary design suggestions and reduces the number of streams to be considered for the heat exchanger network retrofit.

3.3 Energy consumption targeting

3.3.1 Importance of the targeting step

One main concept in pinch analysis, as pointed out in [96] is the performance target ahead of design. The minimum approach temperature ΔT_{min} is therefore a key input parameter. When considering a single heat exchange, it corresponds to the smallest temperature difference between the hot and the cold stream. The higher it is the lower is the required heat exchange area, and consequently the lower the investment cost. On the other hand, the recovered heat load is smaller, leading to higher operating costs to supply the remaining energy requirements. The minimum approach temperature is then a trade-off to be explored depending on the variables influencing the calculations.

Applied to larger systems like process units, the minimum approach temperature locates the temperature levels where the heat exchanges between the hot and cold streams are the most difficult. The so-called pinch point divides the system into independent heat sink and heat source profiles across which heat should not be transferred.

Assumptions made at the level of the heat cascade and the ΔT_{min} definition will then directly impact the results of the targeting step, which will influence the decisions in terms of energy savings opportunities.

3.3.2 ΔT_{min} selection in pinch analysis

In existing industrial systems, heat exchanger network modifications are only economically viable if the operating costs saving linked to the heat recovery compensates the capital expenditure of the redesign, so that the payback time do not exceed a certain limit. Companies are asking for payback times lower than a year, with a higher limit usually around 3 years. When pinch analysis is applied in the framework of energy reviews, it is needed to be able to obtain appropriate consumption targets and avoid or minimise a posteriori engineering calculations leading to economically infeasible solutions.

Too often a single ΔT_{min} is defined for the entire system, usually based on typical values. Such values are for instance available in [97], derived from the fact that similar retrofit projects featuring similar cost conditions are likely to result in similar ΔT_{min} values. Although thermodynamically correct, since similar processes have similar heat transfer properties, it is not straightforward for the other parameters influencing the ΔT_{min}. This is especially true regarding utility costs, with the high price variability of natural gas.

Examples of the use of a single ΔT_{min} in the literature can be found in [98], [99] and [100], where pinch analysis and heat exchanger redesign is respectively applied on the production of ethylbenzene (ΔT_{min} = 10°C), in the food industry (ΔT_{min} = 5°C) and in an ethanol production plant (ΔT_{min}= 7°C).

Using typical values without considering the economic and thermodynamic specificities of the system can lead to serious overestimation or underestimation for heat recovery potential as well as non-optimal heat recovery schemes. This can be seen in [101] for a single process unit and in [102] in Total Site Analysis, where results in terms of internal heat recovery and utility integration can vary significantly according to the ΔT_{min} assumption (+18% and -25% for two process units in the case study).

The first observation is that gas, liquid and evaporating/condensing streams have very distinct heat transfer properties, directly impacting the required area for the heat exchange and consequently the cost of the heat exchanger. The use of stream specific $\Delta T_{min}/2$ according to the physical state can be found in several case studies in the literature ([91, 103]). Although more accurate, the choice for the individual $\Delta T_{min}/2$ are most of the time also based on typical values without considering the other parameters influencing the heat recovery trade-off calculations. Indeed, the cost of utilities, the interest rate and operating time are some of the parameters having an impact on the heat recovery potential which may differ significantly from country to country, and from site to site.

The first analytical method to analyse and improve the HEN of existing industrial systems was developed by [86], via the targeting and design approach. Trade-off between investment and operating costs, including payback period specification is included in the determination of the optimum ΔT_{min} for the retrofit through the use of the so-called area efficiency [104].

In this method, supertargeting is first carried out over a wide range of ΔT_{min} to generate the grass root curve of the minimum heat exchange area according to the corresponding energy costs. This line serves as reference for comparison with the actual area efficiency, given by the existing area divided by the actual energy consumption. The area-energy cost curve can then be translated into an investment cost-energy cost curve, and according to the constraints set on the payback time, an optimum ΔT_{min} of the system can be determined. Examples of application of the area efficiency on existing industrial processes can be found in [105, 106].

The major limitation when using the area efficiency comes from the use of pairs of pseudo single hot and cold streams resulting from the vertical splitting of the composite curves. In reality these pseudo single streams can be made of several streams, having different heat transfer characteristics as well as particular constraints for the choice in heat exchanger (e.g. material, pressure). The use of only one hot and one cold utility for operating costs calculations is a second limitation. Several utilities having different prices can be used to supply the energy requirements of the process. It may be less economically attractive to recover heat in a temperature interval where a hot utility price is particularly low, thereby increasing the minimum approach temperature difference and reducing the exchange area to maintain a sufficiently low payback time. The area efficiency also implies to have access to the area of all the existing heat exchangers, which can be difficult to obtain in practice.

3.3.3 Parameters impacting the thermo-economic trade-off

Provided that initial and target temperatures of a hot and a cold stream are overlapping and the use of a counter-current heat exchanger to maximise the heat recovery, the heat transfer between the two streams will be determined by the minimum approach temperature of the heat exchange. This parameter is usually selected from the analysis of the trade-off between the capital costs linked to the installation of the required heat exchange area and the resulting decrease in operating costs [107], with the objective of minimising the total costs.

Along this optimisation solving problem, schematically represented and summarised in Figure 3.5, several parameters are influencing the calculations. These parameters can be classified in 3 distinct categories: process, site, and equipment related.

Process stream parameters impact the required heat exchange area and consequently the capital cost of the heat exchange at several levels. For a range of ΔT_{min}, the corresponding recovered heat load can be determined ($\dot{Q}_{rec}$). The initial and final temperatures of both streams ($T_{h,in/out}$, $T_{c,in/out}$) will influence the temperature gradient along the heat exchanger, expressed by the logarithmic mean temperature difference (LMTD). The streams composition and flow characteristics will determine the overall heat transfer coefficient (U), representing the rate of heat transfer on a section of the heat exchanger. The required heat exchange area A can be calculated using Equation 3.1, and serves as the reference parameter to estimate the cost of the heat exchanger installation.

$$A = \frac{\dot{Q}_{rec}}{U \cdot LMTD} \qquad \text{where} \quad LMTD = \frac{(T_{h,in} - T_{c,out}) - (T_{h,out} - T_{c,in})}{\ln \frac{(T_{h,in} - T_{c,out})}{(T_{h,out} - T_{c,in})}} \tag{3.1}$$

The streams properties will have an impact on the material of the heat exchanger as well as the operating pressure (P). Once this is fixed together with the choice of the heat exchanger type, the capital cost (IC) of the heat exchanger can be determined. At this stage of the analysis, preliminary cost estimates are used, generated through statistical analysis on observed equipment and installation costs versus heat exchange area. In this work **cost laws from Turton et al.** [108] are used for all cost estimation.

The operating costs depend on the recovered heat load ($\dot{Q}_{rec}$) and site parameters. Utility costs and operating time will determine the yearly operating cost savings (OC) resulting from the heat exchanged between the two streams. For proper comparison, the investment cost of the heat exchanger has to be annualised using an annualisation factor involving the interest rate (i) and the lifetime (n) of the project. These two parameters are also site-related.

Depending on the company's financial practices and investment strategy, one or several economic indicators can be selected for the final decision on the chosen ΔT_{min}. The minimisation of the total costs (TC) is the most common objective for this particular problem. However, restrictions on the payback time (PBT) can also be used and combined with the minimisation of the total costs. This optimisation problem, combining the total cost minimisation constrained by the payback time, can be expressed by Equation 3.2 and will be referred to as "**P1**" in the rest of the chapter.

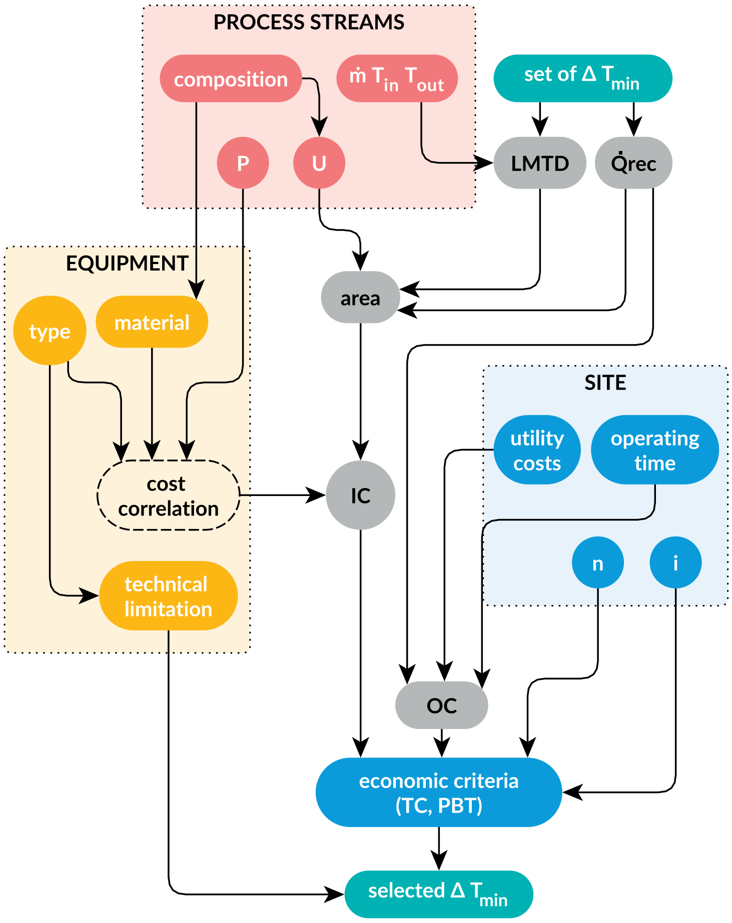


Figure 3.5 – Parameters influencing the choice of ΔT_{min} for a counter-current heat exchanger

$$\min_{\Delta T_{min}} \left[\underbrace{\frac{i(1+i)^n}{(1+i)^n-1}\cdot\left(\frac{I_t}{I_{t,ref}}\cdot 10^{k_1+k_2 log(A)+k_3(log(A))^2}\cdot C_{BM}\cdot e\right)}_{IC} + \underbrace{\left(\dot{Q}_{tot}-\dot{Q}_{rec}(\Delta T_{min})\right)\cdot t_{op}\cdot c_{ut}}_{OC} \right] \tag{3.2}$$

$$s.t \quad A = \frac{\dot{Q}_{rec}(\Delta T_{min})}{U\cdot\dfrac{\Delta T_{min}-\Delta T_{high}}{\ln\dfrac{\Delta T_{min}}{\Delta T_{high}}}} \tag{3.3}$$

$$C_{BM} = b_1 + \left(b_2\cdot F_m\cdot 10^{c_1+c_2 log(P)+c_3 log(P)^2}\right) \tag{3.4}$$

$$\frac{IC}{\dot{Q}_{rec}(\Delta T_{min})\cdot t_{op}\cdot c_{ut}} - PBT_{max} \leq 0 \tag{3.5}$$

$$\Delta T_{min} \geq 1.5 \tag{3.6}$$

where:

$I_t, I_{t,ref}$ = cost index values for the current and reference year [-]
k_1, k_2, k_3 = purchase cost coefficients of the chosen heat exchanger [-]
C_{BM} = Bare module factor [-]
e = currency exchange rate [€/$]
t_{op} = operating time [h]
c_{ut} = utility cost [€/MWh]
ΔT_{high} = temperature difference at the other end of the heat exchanger [°C]
b_1, b_2 = Bare module cost coefficients [-]
F_M = material factor (CS/CS = 1, CS/SS = 1.8, SS/SS = 2.7) [-]
c_1, c_2, c_3 = coefficients to determine the pressure factor [-]

3.3.4 Parameters estimation

For a given heat recovery scenario, in a given plant, many parameters have a single fixed value. Compositions and temperatures of process streams are known, as well as the required operating pressure. For the equipment related variables, the material and heat exchanger type are fixed according to the heat exchange characteristics. Finally, the lifetime and interest rate are site-related parameters that are usually established internally by the financial department. The other parameters are subject to more uncertainty.

Throughout the year, it is common for an industrial site to have one or several plant shutdowns, which are periods where production is stopped. It can be due to different reasons, e.g. maintenance purposes, refurbishment or process modifications. Although the operating time can vary from one year to another, a typical operating time, based on past and projected operation can be derived. This is part of the energy baseline generation, addressed in Chapter 2.

The overall heat transfer coefficient depends on the final design of the heat exchanger but needs to be estimated beforehand. Cost estimation methods are based on empirical statistical analysis and are therefore given with accuracy ranges. Uncertainty is finally also at the level of utility costs, with fluctuations of natural gas price. Each of these aspects is investigated in the next subsections.

Overall heat transfer coefficient

The overall heat transfer coefficient represents the rate of heat transfer on a section of the heat exchanger, expressed in $[W/m^2K]$. It is a composite term which can be expressed by Equation 3.7, as the sum of the contributions of the individual film heat transfer coefficients of the two fluids (h_{cold} and h_{cold}), the thermal resistance of the heat exchanger wall, involving the wall thickness (e)

and thermal conductivity (λ), and the resistance due to the fouling on both sides (R_f).

$$\frac{1}{U} = \frac{1}{h_{cold}} + \frac{e}{\lambda} + \frac{1}{h_{hot}} + R_f \tag{3.7}$$

Most of the time, the wall resistance is negligible compared to the contribution of other terms. With highly conductive metals such as copper (386 W/m°C), two orders of magnitude can separate the wall resistance to the individual film heat transfer contribution. For materials with lower thermal conductivity like carbon steel (45 W/m°C), stainless steel (16 W/m°C) or nickel (90 W/m°C), and depending on the wall thickness, it is closer to a one order of magnitude difference. For very low conductivity materials and/or thick walls due to specific chemicals handling or a large pressure difference between the two sides, the wall resistance can have a significant impact of the overall heat transfer coefficient. A fouling factor is added to account for heat transfer resistance due to corrosion products or the accumulation of dirt [109].

Table 3.2 – Typical overall heat transfer coefficients for tubular heat exchanges, involving common (petro)chemical species and utilities.

	Hot fluid	**Cold fluid**	**U [W/m^{2}C]**
Heat exchangers	water	water	800 - 1500
	organic solvents	organic solvents	100 - 300
	light oils	light oils	100 - 400
	heavy oils	heavy oils	50 - 300
	gases (p=atm)	gases (p=atm)	5 - 35
Coolers	organic solvents	water	250 - 750
	light oils	water	350 - 700
	heavy oils	water	60 - 300
	gases	water	20 - 300
Heaters	steam	organic solvents	500 - 1000
	steam	light oils	300 - 900
	steam	heavy oils	60 - 450
	steam	gases	30 - 300
Condensers	aqueous vapours	water	1000 - 1500
	organic vapours	water	700 - 100
	refinery hydrocarbons	water	400 - 550
Vaporisers	steam	aqueous solutions	1000 - 1500
	steam	light organics	900 - 1200
	steam	heavy organics	600 - 900

The overall heat transfer coefficient can be obtained by calculating or estimating each term in Equation 3.7. If the design of the heat exchanger is known and data is available to characterize streams, calculations are straightforward. If parameters are missing, typical values for fouling factors, film or directly overall heat transfer coefficients are available in the literature [110, 111].

It is however difficult to find detailed databases for both film and overall heat transfer coefficients, due to the many parameters involved (i.e. fluids density, viscosity, velocity, thermal conductivity, specific heat, and heat exchanger type, fouling factor, wall thickness, thermal conductivity of metal). This often results in large ranges for the heat transfer coefficients even for the same type of fluids or heat exchanges, as it can be seen in Table 3.2 (values from [111]). Acceptable estimations can be determined combining typical values from literature and observed values derived from existing heat exchangers with similar features.

Operating costs

Another parameter to be estimated in the ΔT_{min} determination procedure is the cost of utilities. Depending on the temperature levels of the hot and cold streams, the corresponding utilities which should be consumed in the case where there is no recovery is easy to identify, especially in retrofit situations. These utilities are often intermediates (e.g steam, hot oil, refrigerant), for which the cost is principally linked to the consumption of final energy sources like natural gas, coal or electricity.

The major energy source for heating in the (petro)chemical industry is natural gas and future variations of its price are hard to predict. Evolution of the natural gas price in France and Germany between 1979 and 2014 (data derived from IEA energy prices and taxes [1]) is visible on Figure 3.6.

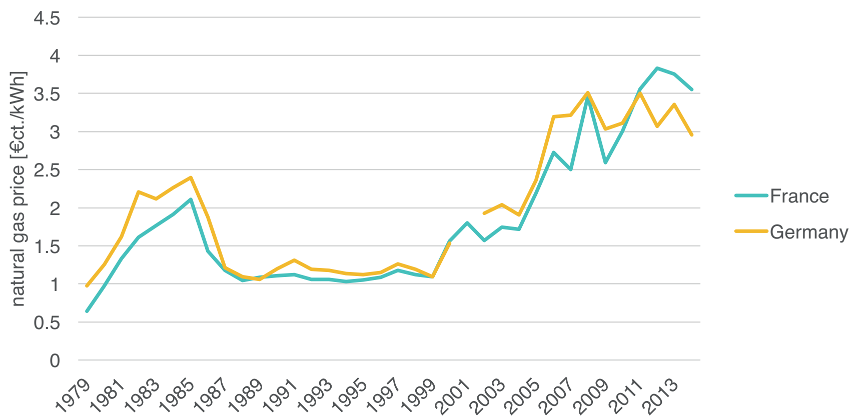


Figure 3.6 – Evolution of the natural gas price in France and Germany between 1979 and 2014 (including taxes) [1]. *NB: missing price data in 2001 for Germany.*

Different strategies can be used to account for natural gas price in the ΔT_{min} trade-off calculations, such as taking an average value based on market observations or predictions, using forecasts from authorities in the field or applying uncertainty models. Several scenarios can also be developed as it is done in Nemet et al. [112], with projections made on monthly basis over the project lifetime.

Investment cost estimation

According to Turton et al. [108], there are 5 classes of capital cost estimates, depending on the level of project definition and the purpose of the estimate: detailed estimates, definitive estimates, preliminary estimates, study estimates, and order-of-magnitude estimates. Although wording and number of classes may vary according to other authors [110], such classification is widely accepted by practitioners.

When carrying out a pinch analysis, whether it is on existing or design cases, not enough details are available at the targeting stage on the matches and characteristics of heat exchangers to go below preliminary cost estimates. This type of cost estimates has a typical accuracy of **+/- 25%**.

Several cost estimation methods have been generated to estimate the preliminary purchase cost of a heat exchanger, all developed around correlations based on a reference parameter which is its area. They differ in the way the purchase cost (free on board cost, f.o.b) of the heat exchanger is expressed and on the factors used to account for indirect and additional expenses linked to the installation. Purchase cost are expressed according to 3 formulation categories:

1. log based (ln or log10): $log(PC) = k_1 + k_2 \cdot log(A) + k_3 \cdot log(A)^2$
2. power law: $PC = a \cdot A^b$
3. power law with fixed contribution: $PC = a + b \cdot A^c$

From the purchase cost of the heat exchanger, based on the cheapest material and atmospheric operating conditions, its final total cost is determined through factorial costing or module costing methods. These factors take into account direct (heat exchanger material, operating pressure and temperature) and indirect costs (instrumentation, piping, insurance, overhead, engineering expenses). A contingency factor, accounting for unforeseen circumstances, can also be taken into account. Costs related to auxiliary facilities are left out since they are more related to grass root situations and total plants rather than the installation of a single or several heat exchangers.

Table 3.3 presents six methods which can be used for preliminary cost estimates, often cited in costing reviews or related work in the literature [113, 114]. References are provided for further investigation since only a brief summary is provided in this thesis. A recent review on cost estimation methods can be found in [115], were the author discusses traditional and novel and more detailed costing methods, applicable for design and preliminary cost estimates.

All of these correlations have been developed based on surveys carried out over a certain period of time, usually within a month or a year. Observed prices according to the type and characteristics of the heat exchangers lead to the generation of trends, linking the investment cost to the area of the heat exchangers. Apart from the quantifiable factors associated with the installation of the heat exchanger, additional factors influence the quality and accuracy of the resulting cost functions.

Table 3.3 – Overview of widely used cost estimates for heat exchangers.

Authors	**Reference year**	Reference cost C_p (CS, Patm)	**ISBL cost C^1**	**Cost factors**	**Comments**
Turton [108]	2001	$10^{k_1+k_2 \cdot log(A)+k_3 \cdot log(A)^2}$	$C_p \cdot (B_1 + B_2 f_p f_m)$	direct and indirect costs	wide range of HEX types and material, cost facors are well detailed
Sinnot [116]	2007	$a + b \cdot (A)^n$	$C_p \cdot [(1 + f_{pip}) f_m + (f_{er} + f_{el} + f_i + f_s + f_l)]$	direct and indirect costs	limited S&T types (U tube and double pipe), no effect of the pressure
Smith [117]	2000	$32800 \cdot (A/80)^{0.68}$	$C_p \cdot [(1 + f_{pip}) f_m f_p f_T + (f_{er} + f_{el} + f_i + f_{dec})]$	direct and indirect costs	based on a single reference cost, all shell and tube the same
Seider [110]	2006	$e^{k_1+k_2 \cdot ln(A)+k_3 \cdot ln(A)^2}$	$f_p f_m f_l \cdot C_p$	f.o.b cost only	from mix of methods and correlations, no factors for direct & indirect costs
Corripio [118]	1995	$e^{8.551-0.30863 \cdot ln(A)+0.06811 \cdot ln(A)^2}$	$f p f m f d \cdot C_p$	f.o.b cost only	old reference, similar to Seider [110] no factors for direct and indirect costs
Hall [119]	1982	$a + b \cdot (A)^n$	material, pressure and temperature accounted in C_p coefficients	f.o.b cost only	very old, only for small HEX (up to 140m2), all shell and tube the same

[1] InSide Battery Limits: ISBL cost does not take into account auxiliary facilities cost. Since we are looking at a cost of a heat exchanger, it is assumed that all other facilities apart from what is needed to install the equipment is already here.

Among them can be found the variability of manufacturers profit margins or differences in design and fabrication quality. Location also plays a role. Most equipment cost data were developed in US dollar, on a US Gulf Coast basis. Application of the correlations and factors in a different location, with a different currency, implies first the variability of the currency exchange rate but also other aspects such as the availability of labor and the efficiency of the work force in the specific region or country [110]. Location factors can be applied in these situations, although they are also subject to variability over time.

Since correlations were developed at a certain point of time and cost is not static, cost indexes are used to update prices taking into account inflation. Commonly used indexes are the Chemical Engineering Plant Cost Index and the Marshall & Swift equipment cost index.

From Table 3.3, whereas cost factors linked to direct and indirect costs are extensively detailed in Turton [108], Sinnot [116] and Smith [117], it was not the case for Seider [110], Corripio [118] and Hall [119], which make the comparison between the six methods difficult. Additionally, Sinnot is providing cost data for a limited number of shell & tubes heat exchangers (only U-tube and double pipe) and Smith and Hall present a single reference cost for all shell & tubes. The Turton cost data has the advantage of a large diversity in the type of heat exchangers available and the cost factors involved in the direct and indirect costs calculations, which can make it tunable.

Initially introduced by Guthrie in the late 1960s [120] and developed by Ulrich [121], this method is used to estimate the cost of a new plant, from the purchase cost of of each piece of equipment. It can then be used to estimate the cost of installing a new heat exchanger.

The module costing technique details 4 different costs: the purchase cost of the equipment, the bare module cost (accounting for material, operating conditions, installation and other indirect costs), the total module cost (accounting for contingency and fee) and the grass root cost (accounting for auxiliary facilities, i.e. green field construction). The total module cost referring to the cost of making small modifications to an existing facility, it is the best suited to estimate the cost of heat exchangers installation. The method and data provided in Turton [108] are selected in this paper for preliminary cost estimation.

Figure 3.7(a) shows these four costs for a reference heat exchanger as well as the expected accuracy for the total module cost, while the comparison with other cost estimates of Table 3.3 can be seen on Figure 3.7(b). Other comparisons between capital cost methods [114] and programs [122] can be found in the literature for common shell and tube heat exchanger types (floating head and/or fixed tube), also showing large disparities between the methods.

Despite similar trends in the capital cost according to an increasing area, the first thing to note is that capital cost can differ significantly from one method to another. This highlights the disparity that could be obtained in results when applying two different methods. In both cited references, the module costing method by Turton leads to capital costs in the upper cost range and in the same range as most of the common other methods.

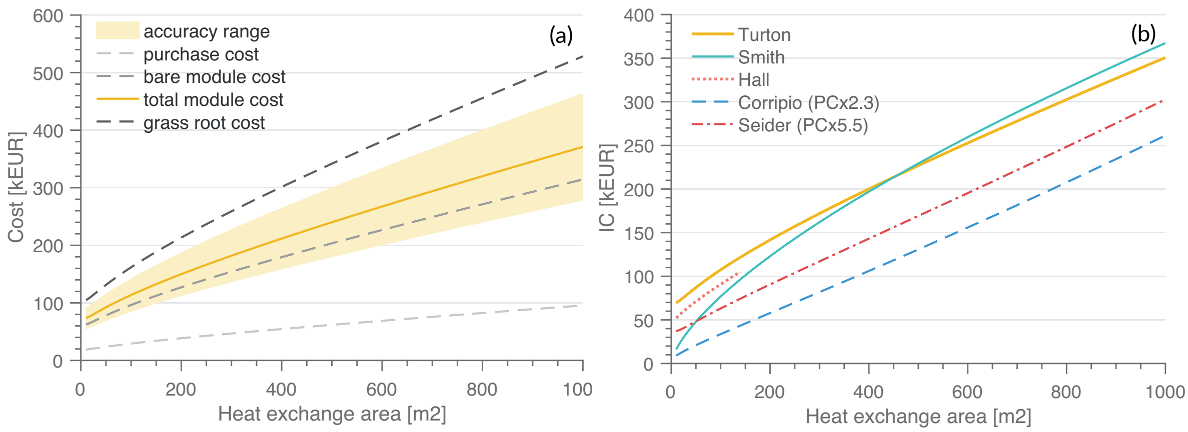


Figure 3.7 – (a) Turton et al. module cost estimates for a fixed tube heat exchanger (CS/CS) operating under ambient pressure conditions (b) cost estimates comparison on the same type of exchanger.

Other alternatives in applied industrial situations can be the use of scaling factors from the cost of similar heat exchangers or the use of internal cost data derived from internal observations and surveys. This would have the advantages of reflecting the real installation costs with respect to the type of industry and plant location. To be noted that Aspen Capital Cost Estimator™, part of the Aspen Engineering Suite, seems to be one of the most detailed and accurate method currently available for equipment preliminary cost estimation.

3.3.5 Economic indicator for decision criteria

Increasing heat recovery through process integration implies investing a certain amount of money to buy and install the new heat exchange area and generate benefits in the form of operating cost savings. The decision on the ΔT_{min} and the final design of the heat exchanger is usually made based on specific criteria. In any companies, financial indicators are used to compare investment projects by calculating their profitability and evaluate risks. Depending on the internal practices and strategy, different indicators can be selected to decide whether or not investing. The total cost (TC), payback time (PBT) and net present value (NPV) are the most common methods used for investment decision.

The payback time is the ratio of the investment cost over the operational cost savings. When margins are low and competition is hard, as in the European (petro)chemical sector, companies are reluctant to implement energy saving opportunities with a payback time larger than 1.5 - 2 years. They even ask for the investment to pay for itself within the same year.

Depending on the situation different ΔT_{min} candidates can have a very similar or a very different PBT, highlighting the possible degree of freedom in the decision. In order to choose "the best" ΔT_{min} among the different possibilities the minimisation of the total cost over the potential candidates can guide the selection. The total cost is the sum of the operating costs and the annualised investment cost. The minimisation of total costs is a typical optimisation problem in design projects were the use of the payback time as decision constraint would make less sense.

The NPV can be used to determine the profitability of the investment. When the annual income does not vary over the project lifetime, as it is usually the case with heat exchanger network installation, the NPV can be expressed by Equation 3.8, as being the difference between the present value of the yearly operating cost savings and the present value of the investment.

$$NPV = \frac{(1+i)^n - 1}{i(1+i)^n} \cdot OC_{savings} - IC \qquad (3.8)$$

For a project to be profitable the NPV has to be positive. Different project scenarios with similar payback time can be compared in terms of NPV, as the indicator of their profitability. However, the time value of money having little influence in industry due to the small payback times required, the latter is often enough as decision criteria.

3.3.6 Heat exchanger choice and technical limitations

The investment cost of a heat exchanger will depend on its type and characteristics. Shell and tubes heat exchangers already show differences depending on their design (e.g. U-tube, fixed tube, floating head, kettle vaporiser). Also, although this type is widely used in the chemical and petrochemical industry, other heat exchanger types can be preferred for particular applications (e.g. viscous liquids, particular alloys). While flat-plate heat exchanger are more commonly used in the food industry, their application to petrochemical processes in increasing. The purpose of the heat exchanger and the process streams characteristics will dictate the heat exchanger type, but also the choice for the material of construction and the operating pressure.

The heat exchanger annualised investment cost and associated yearly operating costs being calculated, the minimisation of the sum yields to the optimum ΔT_{min} . However, beyond this thermo-economic analysis, technical limitations might prevent the obtained ΔT_{min} to be practically achieved. It is found in literature [121] that each type of heat exchanger has approach temperature limitations, that might prevent the implementation of the optimum heat recovery. It seems that shell and tube heat exchangers are limited by a difference of minimum 5°C due to fouling tendencies whereas flat plate could go down to 2°C. However, the reasons for these limitations are not well documented and should theoretically be able to be circumvented with an increased heat exchange area.

3.3.7 Single heat exchange example

This subsection illustrates how the minimum approach temperature can vary with a simple example of a counter-current heat exchanger. A hot stream is to be cooled down from 130°C to 100°C with a heat load of 800 kW. Heat can be recovered by heating up a cold stream of the same heat load, starting at the temperature of 100°C. Apart from these temperatures and heat loads, all the other parameters involved in the determination of the maximum heat recovery between these two streams (see Figure 3.5) can vary between upper and lower limits.

When these two extreme values are used for all parameters, two scenarios are obtained. The "best case" scenario corresponds to the best conditions for heat recovery, with the combination of parameter extreme values leading to the smallest ΔT_{min}. The "worst case" scenario is the opposite. "Best" and "worst" case parameters values are displayed in Table 3.4.

Table 3.4 – Best and worst cases parameter values.

	Best case	**Worst case**	**Units**
Cold stream outlet T	100	130	[°C]
Overall HTC	1000	50	[kW/m^{2}C]
Pressure	1	50	[bar]
Operating time	8500	6000	[h/y]
Utility cost	30	10	[€/MWh]
Interest rate	5	10	[%]
Project lifetime	30	10	[y]
HEX type	fixed-tube (FT)	floating head (FH)	[-]
HEX material	carbon steel (CS)	stainless steel (SS)	[-]

When the minimisation of total cost of the installation of a heat exchanger is carried out, the ΔT_{min} corresponding to the best case conditions corresponds to the lower limit set for the temperature difference between the hot and the cold stream of **1.5°C**. On the contrary, when all the worst case parameters are considered, the obtained ΔT_{min} is of **40.5°C**.

In reality, as mentioned in section 3.3.4, when the same problem is applied in an existing plant for a specific heat exchanger, most of the parameters are fixed. When only uncertain parameters are allowed to vary, it is possible to narrow the variation range of ΔT_{min}. Table 3.5 shows the probability distribution functions used for the uncertain parameters.

Table 3.5 – Probability distribution functions for the selected uncertain parameters.

Overall HTC [kW/m^{2}C]	normal dist.	$\mu = 400$	$\sigma = 30$
Operating time [h/y]	normal dist.	$\mu = 7250$	$\sigma = 50$
Utility cost [€/MWh]	random dist.	min = 17	max = 25

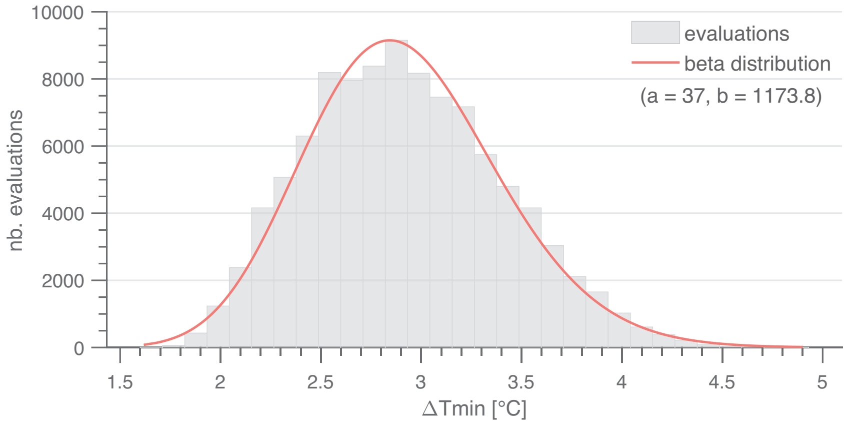


Figure 3.8 – ΔT_{min} distribution (nb. evaluations = 100'000)

The fixed parameters are given a value corresponding to the central point between the upper and lower limits from Table 3.4. The heat exchanger is a floating head shell & tube made of CS for the shell and SS for the tubes. The ΔT_{min} results for random 100'000 evaluations can be seen on Figure 3.8, spread around the expected value of 2.9°C when everything is fixed at central values. The distribution follows a beta probability distribution function, often applied to model the behaviour of random variables limited to a finite interval, which is the case for the utility cost.

Payback times corresponding to the ΔT_{min} distribution are represented on Figure 3.9. Since the optimisation problem was solved without setting a limit on the payback time, many evaluations are outside the economic feasibility corresponding to a payback time below 3 years. For these points, the minimisation of the total costs does not fulfil the PBT condition.

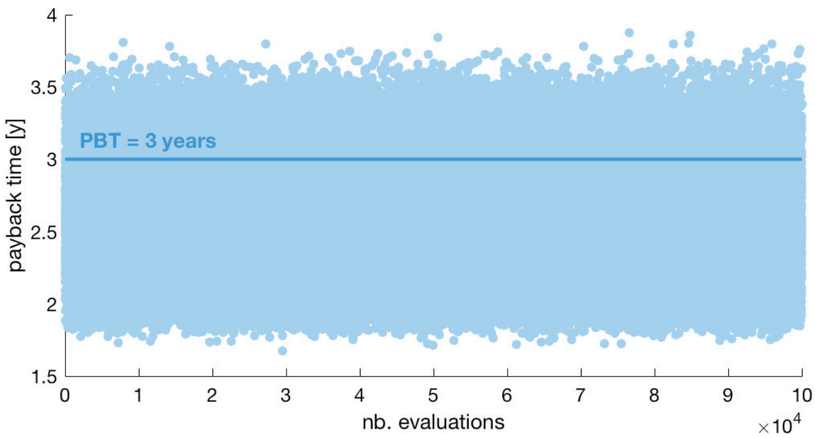


Figure 3.9 – Scatter plot of the corresponding payback times.

3.3.8 Consequences for pinch analysis

Several observations can be derived from this simple example:

- The use of a uniform ΔT_{min} applied to all streams should be avoided. This statement seems intuitive but too often practitioners tend to overlook the impact on the minimum approach temperature assumption on the energy consumption targeting step, where a uniform ΔT_{min} can lead to serious over- or underestimations.
- A contribution to the minimum approach temperature should be defined for each hot and cold process stream. Using a set of typical $\Delta T_{min}/2$ for each thermodynamic state (gas, liquid and phase change) is a first step, but values are most of the time selected based on what is currently observed and accepted, without carrying out a deeper analysis specific to the industrial system under study.
- While the minimisation of total costs being the commonly used decision criteria, in existing industrial systems a limit is usually put on the payback time. Depending on the streams characteristics and the values of each parameters, it can be that no ΔT_{min} fulfils the maximum payback time allowed and these streams will in the end not be considered for heat recovery schemes.

Starting from the list of process hot and cold streams, it is not possible to know where the pinch is going to be and which heat exchanges will be "pinched". The application of the simple procedure described in section 3.3.3 is of course not an option since it is only applicable for a single pair of streams. However, a better definition of the hot and cold process streams through individual analysis of their contribution to the ΔT_{min}, and considering all parameters involved in the thermo-economic trade-off, would allow a better targeting of the potential for heat integration and avoid over- and under-estimations.

The latter can have a non-negligible impact on decision making for energy management, especially if the objective of the pinch analysis is to obtain a first screening for improvement potential and heat integration opportunities, before launching follow-up projects. In order to try to tackle this issue, the proposed methodology revisits one of the core assumption of pinch analysis, which is the definition of the minimum approach temperature of the system.

3.4 Methodology proposition for ΔT_{min} definition

This section presents a novel methodology revisiting one of the core assumption of pinch analysis, the definition of the ΔT_{min}. It differs from traditional approaches involving the use of the area efficiency for the determination of the ΔT_{min}, while still considering the thermo-economic trade-off resulting from the physical and financial characteristics of the system. The proposed methodology is first presented theoretically step by step and results of its application on two examples are shown.

3.4.1 Theoretical basis

The pinch point divides a thermal system in two distinct parts: a heat sink located above the pinch and a heat source below. Above the pinch point, the integration of hot streams with cold streams to be heated up is to be maximised, in order to avoid the consumption of a cold utility and the creation of penalties. Inversely, below the pinch, the cold streams should be heated up by streams requiring cooling instead of consuming a hot utility. The most critical heat exchanges are the pinched ones, for which one end is located at the level of the pinch point.

Instead of making use of traditional approaches and correct each stream with a constant ΔT_{min}, this methodology defines for one stream after the other its temperature-enthalpy profile directly in corrected temperatures, according to its thermodynamic characteristics, its heat exchanger requirements and the economic parameters of the site.

To do so, a virtual pinch point is varied along the temperature range of each stream, starting from its initial temperature. This virtual pinch point will define at each step the maximum heat recovery, corresponding to an infinite heat exchange area. Then, a corresponding mirror stream is defined having the exact same heat transfer properties and slope, except that the initial and final temperatures are reversed to account for counter current heat exchanges.

This virtual stream is moved with increasing minimum temperature difference. The optimal ΔT_{min} is found at each temperature step according to the economic objectives, being in this paper the minimisation of total costs while fulfilling a **maximum payback time of 3 years**. The obtained corrected temperature-enthalpy profiles of a hot and a cold stream can be seen in Figure 3.10.

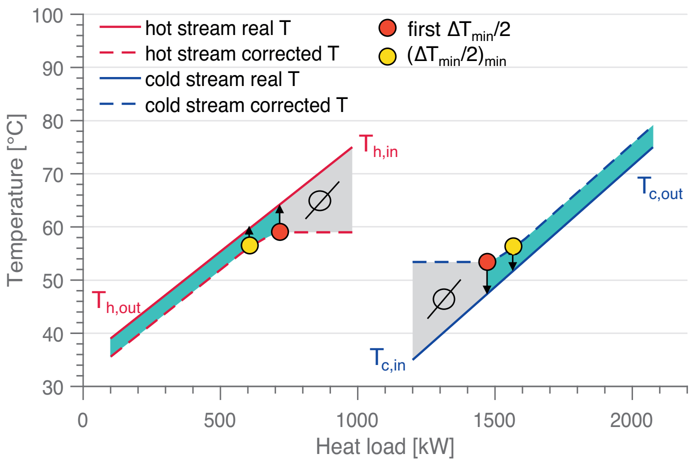


Figure 3.10 – Example of corrected profiles for a hot (left) and a cold (right) stream

Taking as an example the hot stream on the left on the Figure 3.10, the virtual pinch point is varied starting from its initial temperature $T_{h,in}$ towards the ambient temperature. At first, the heat load above the pinch is too small to be recovered in an economically interesting way. The investment cost linked to the installation of a heat exchanger is too important compared to the operating costs savings to be able to get below the required payback time. This is observed until a certain temperature where a first ΔT_{min} fulfilling the economic constraint is found.

In between the first evaluation point and the latter one, the stream profile is corrected as a flat line at the corrected temperature at which a first minimum approach temperature is obtained. This comes down to say that, considering the characteristics and constraints of the system, this heat load, which is called $\dot{Q}_{min}$, is in reality available for recovery when the pinch point temperature is at least below a certain value. Progressing down the hot stream, the optimum ΔT_{min} is decreasing until a minimum value. This transition zone is due to the increasing heat load available above the pinch point. The remaining part of the stream is corrected using the minimum $\Delta T_{min}/2$.

For some streams, the entire heat load can correspond to $\dot{Q}_{min}$, and the heat recovery would be economically feasible only with a large correction. If this correction is too big and the corrected temperature is higher or lower than the utility that the stream is consuming or can consume (+/- $\Delta T_{min}/2$ of utility), the stream is transformed to black box representation. In this way it is still accounted in the heat balances but it reflects only the temperature levels of the utility it consumes.

3.4.2 Corrected profiles generation procedure

The generation of corrected profiles can be schematically represented by Figure 3.11. The same procedure is used for the total number of streams *ns*, represented by the outside loop. The inside loop corresponds to the evaluation of each stream *s* at each temperature $T_{p,i}$ starting from the initial temperature of the stream $T_{in,s}$, until the total heat load of the stream Q_s is reached.

At each temperature step $T_{p,i}$, corresponding to a potential pinch point, the optimisation problem P1 (Equation 3.2) is solved for a given maximum heat recovery $(Q_{rec,max})_{i,s}$. Figure 3.12 shows the main parameters involved in the procedure. The generation of corrected profiles can easily be automated and they can be directly integrated in the heat cascade mathematical formulation.

In order to be able to calculate the thermo-economic trade-off, all parameters depicted on Figure 3.5 have to be defined. An additional parameter to decide on is the temperature step along each stream. It can be the same for each stream, for example 0.5°C, or be fixed by linearising the temperature range of the stream according to a certain number of evaluations.

One of the interesting features of the proposed methodology is the possibility to have flexibility in the heat exchanger characteristics. If a stream requires a specific type of heat exchanger, if a particular material should be used or if the operating pressure is high, the cost estimation method can take into account these specificities already at the targeting stage.

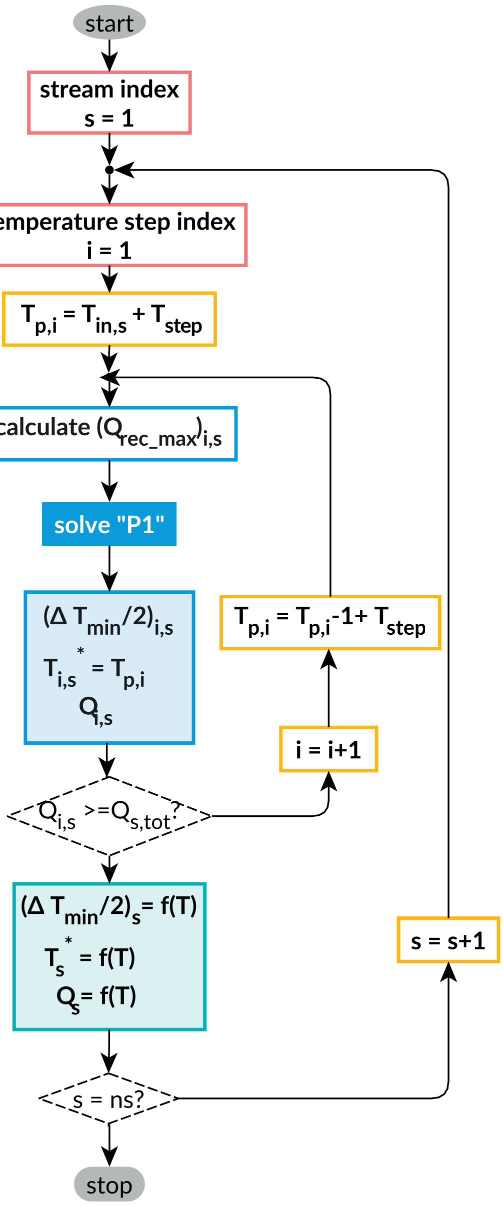


Figure 3.11 – Procedure to generate the corrected T-H profiles of all streams

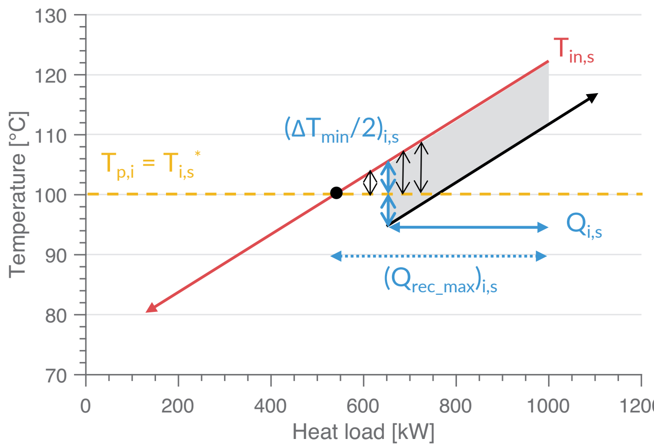


Figure 3.12 – Graphical representation of the main parameters at a given temperature point along the procedure.

There is also the possibility to consider several utilities having different costs. For example, a site can use several pressure levels for steam, each having its own cost and temperature range for heating. If the temperature range of a cold stream is located over several hot utility temperature ranges, when the corrected profile is determined the operating costs are varying depending on which utility would be saved.

3.4.3 Impact of parameters

Figure 3.13 (a) shows the influence of the overall heat transfer coefficient on the shape of a hot stream corrected profile. It can be seen that with a decreasing coefficient, the temperature correction is increasing, making the heat available at a lower temperature in the heat cascade for this hot stream example. The minimum heat load for which heat recovery becomes profitable is also getting bigger, due to the lower heat transfer rate and consequently the higher heat exchanger area required. The impact on the maximum payback time can be seen on Figure 3.13 (b).

The variation of the corrected profile according to the overall heat transfer coefficient can more globally be observed on Figure 3.14 (a), showing the variation of the minimum $\Delta T_{min}/2$ and heat recovery load $\dot{Q}_{min}$ (b) and for 4 different sets of economic parameters.

The three first scenarios have the same payback time constraint but the operating time and utility price are gradually increased (from low to high operating cost savings). The last scenario, represented by the red crosses, is a variation of the scenario featuring a high operating time and utility price, but with a limit on the payback time set to 2 years.

It can be seen that when larger savings are resulting from heat recovery, both $\dot{Q}_{min}$ and $\Delta T_{min}/2$

are decreasing for given overall heat transfer coefficient. The inverse behavior is observed when the payback time constraint is stronger. It is also interesting to note that for overall heat transfer coefficient in the upper range (700-1300 W/m^2°C), results slightly vary, compared to coefficients in the lower range (50-400 W/m^2°C). Uncertainty on low overall heat transfer coefficient will then have higher impact, which is the case for gaseous streams or heavy organics products.

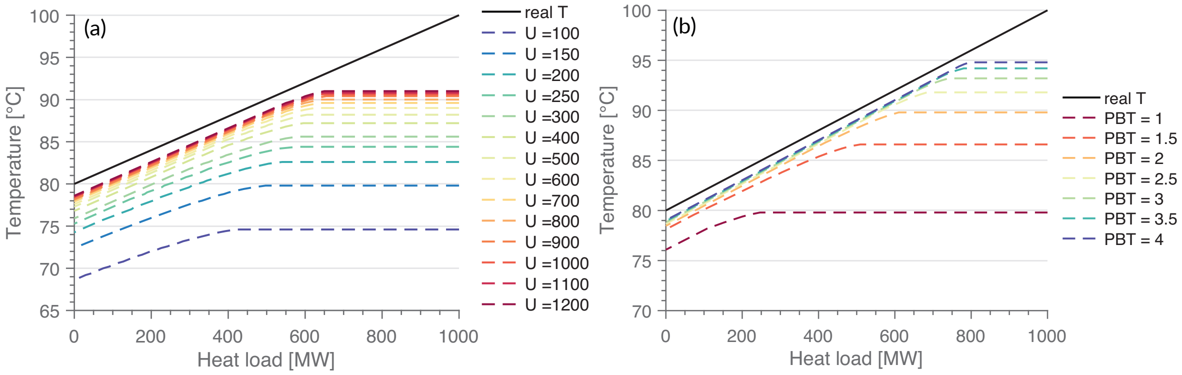


Figure 3.13 – (a) Influence of the heat transfer coefficient U (in W/m^2°C) and (b) of the payback time constraints on the corrected profile of a hot stream.

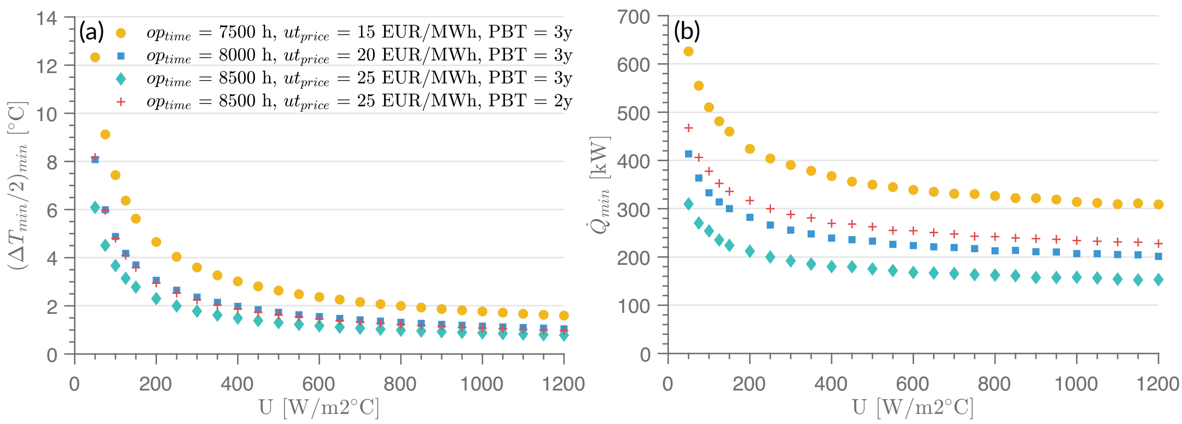


Figure 3.14 – (a) $\Delta T_{min}/2$ and (b) $\dot{Q}_{min}$ variation according to the overall heat transfer coefficient and different economic conditions.

3.5 Application on two examples

The described methodology has been applied on two industrial system scenarios S1 and S2, both featuring a large production site composed of two plants operating simultaneously and importing utilities. In both scenarios, the actual process requirements are represented by 17 hot streams and 11 cold streams, for which the heat load, temperatures and heat transfer coefficients vary from one scenario to the other. Heat is removed from the process through a cooling water network, and steam is delivered to cold process streams at two pressure levels (3 bar (LPS) and 10 bar (MPS)).

The list of streams for S1 and S2 are available in Appendix B. Details on the utilities and parameter sets involved in the calculations are displayed in Table 3.6 and Table 3.7.

Scenario 1: S1 features favorable economic parameters encouraging process integration. Utilities cost are rather high and the cheapest type of shell & tube heat exchanger is considered for all streams (carbon steel fixed tube sheet, operating at low pressure), pushing the investment costs and operating cost savings respectively in the lower and upper range.

Scenario 2: compared to S1, utilities cost, the operating time and the project lifetime are lower and the interest rate is higher. In S2, the heat exchanger type (fixed-tube FT or floating head FH), material (shell side/tube side: CS/CS, SS/SS) and operating pressure are defined for each stream.

Table 3.6 – Utilities description for both scenarios

Utility	**Pressure [bar]**	**Tin [°C]**	**Tout [°C]**	**Cost S1 [€/MWh]**	**Cost S2 [€/MWh]**
LP steam	3	133	133	20	16
MP steam	10	180	180	23	18
Cooling water	2	20	30	0.1	0.1

When the proposed methodology is applied to the list of streams, the corrected profile of each stream is generated and the heat cascade is carried out directly in corrected temperatures. Results can then be compared with a reference situation for which a uniform ΔT_{min} of 5°C is used. Reference cases will be called **S1.A** and **S2.A** respectively for scenario 1 and 2, and corrected cases resulting from the application of the proposed methodology **S1.B** and **S2.B**.

Table 3.7 – Other cost parameters

Parameter	**S1**	**S2**	**Units**
Heat exchanger type	fixed-tube	varying	[-]
Heat exchanger type pressure	2	varying	[bar]
Heat exchanger material	CS/CS	varying	[-]
CEPCI reference (2001)	397	397	[-]
CEPCI (2016)	541.7	541.7	[-]
currency exchange rate	0.86	0.86	[€/$]
Operating time	8000	7500	[h/y]
Lifetime	20	15	[y]
Interest rate	8	9	[%]

3.5.1 Scenario 1

MER and penalising heat exchanges

Hot and cold composite curves for scenario 1 can be seen in Figure 3.15 with Table 3.8 summarising the hot and cold minimum energy requirements for both cases, compared to the actual consumption. In the reference case, potential for heat recovery amounts to 9.4MW whereas in the new case, with the application of the proposed methodology, this potential equals to 12.3MW.

Table 3.8 – MER results - S1

	Actual consumption	**S1.A** ($T_p = 101°C$)	**S1.B** ($T_p = 91.7°C$)	**Difference**
MERH [MW]	24.1	14.7	11.8	+2.9
MERC [MW]	27.4	17.9	15.1	+2.9

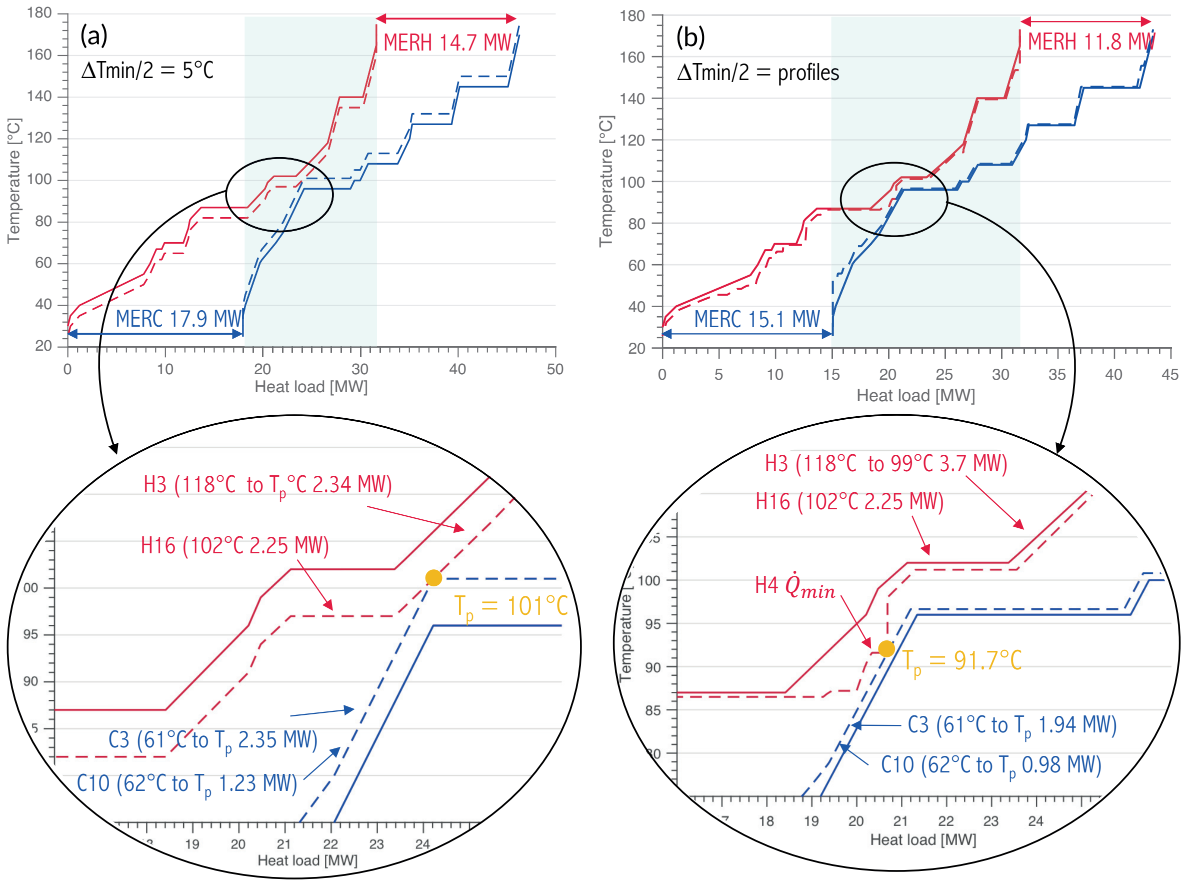


Figure 3.15 – Composite curves for S1.A (a) and S1.B (b).

For this first scenario, the use of a single ΔT_{min} for each stream, without taking into consideration the physical and cost specificities of the system, leads to an underestimation of the potential for heat recovery of 30% at the targeting step.

When a uniform typical ΔT_{min} is used, the pinch is located at 101°C. It is caused by cold stream C7, which corresponds to a reboiler at 96°C in the real temperature domain. Condensing hot stream H16 is located under the pinch point. Using the proposed methodology, the $\Delta T_{min}/2$ of H16 is lower and the stream is now located above the pinch point, enabling its integration with C7. The pinch point is at a lower temperature of 91.7°C, created by the flat heat load of H4 corresponding to $\dot{Q}_{min}$ (344 kW).

Table 3.9 – Penalising heat exchanges for S1

Stream	**S1.A [kW]**	**S1.B [kW]**	**Difference [kW]**
H3	2337	3700	+1363
H12	2590	2590	0
H14	82	0	-81
H16	0	2250	+2250
C2	900	900	0
C3	2348	1944	-404
C10	1229	984	-245
C11	(cf. H3)	(cf. H3)	0
total	9486	12368	+2882

As a result, 2.9 MW of additional penalising heat load is found, coming from the decrease of the pinch point and the better overlapping of the hot and cold composite curve in the pinch area. Table 3.9 details the penalising heat exchanges for S1.A and S1.B. The latter shows higher heat recovery potential although streams C3 and C10 are less penalising since the pinch point is as a lower temperature. This is due to the entire integration of hot stream H3 and H16 above the pinch.

Impact on direct heat integration

Once the pinch point of the system is determined, hot and cold streams belonging to the heat sink and source can be generated. Figures 3.16 (a) and (b) show the streams involved above the pinch point, respectively for cases S1.A and S1.B, where hot streams are penalising and have to be cooled down using cold streams. Streams are depicted in the real temperature domain for sake of simplicity and clarity. Indeed, the segmentation of the streams in the corrected domain for S1.B is more difficult to represent in such diagram.

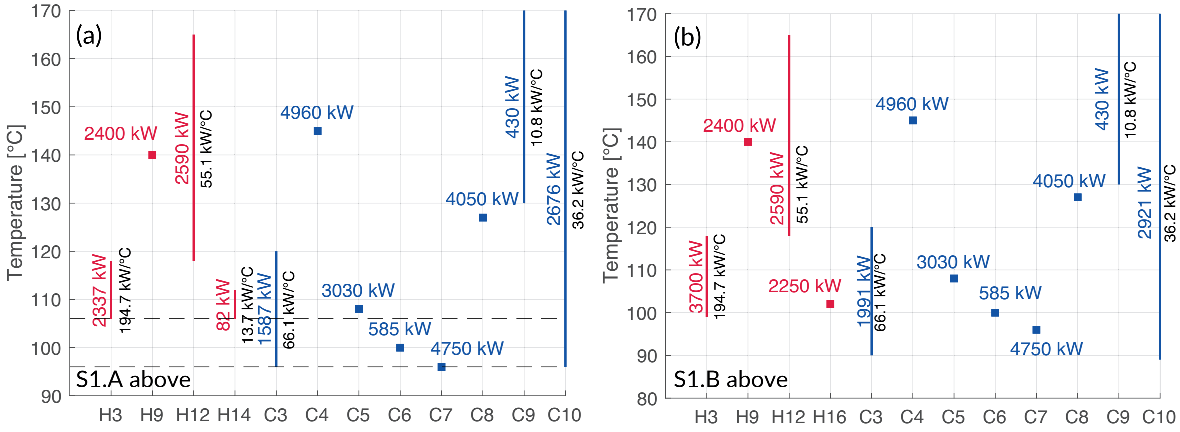


Figure 3.16 – Streams involved in HEN redesign above the pinch point for S1.A (a) and S1.B (b).

Table 3.10 – Pairs of streams involved in heat recovery of S1.B above the pinch.

Streams	Load [kW]	U [W/m^2°C]	A [m^2]	IC [kEUR]	OC [kEUR/y]	PBT [y]
H16 - C7	2250	545	688	386	360	1.1
H3 - C7	2500	600	540	333	400	0.83
H3 - C5	1200	720	259	224	192	1.2
H12 - C5	1830	327	246	219	293	0.75
H12 - C3	760	255	48	121	140	0.87

The first difference, as mentioned previously, is the presence of H16 and H3 entirely above the pinch in S1.B. The second difference is that H14 is not penalising nor crossing the pinch as it is the case in S1.A. This stream is associated with a rather low heat transfer coefficient (270 W/m2°C), leading to a larger $\dot{Q}_{min}$ and therefore a temperature correction below the pinch point. To be noted that H9 is already integrated with C8 (see list of streams) and this heat exchange is not penalising.

Table 3.10 shows one option for the heat exchangers involving the penalising hot streams for S1.B above the pinch , when the proposed methodology is applied. For both H3 and H16, although the heat recovery approach temperature is smaller than the 10°C in scenario S1.A, the payback times of their heat integration with cold streams are below the 3 years constraint, making the heat recovery economically acceptable considering the system's characteristics.

Figure 3.17 (a) and (b) shows the streams involved below the pinch point, respectively for cases S1.A and S1.B, where cold streams are penalising and have to be heated up using hot streams. H3 and H16 are no longer available in S1.B, reducing the choice for pinch streams connections. The integration below the pinch should then also be studied to check if the economic constraint is still satisfied. To be noted that C1 is already integrated with H10, and this heat exchange is not penalising.

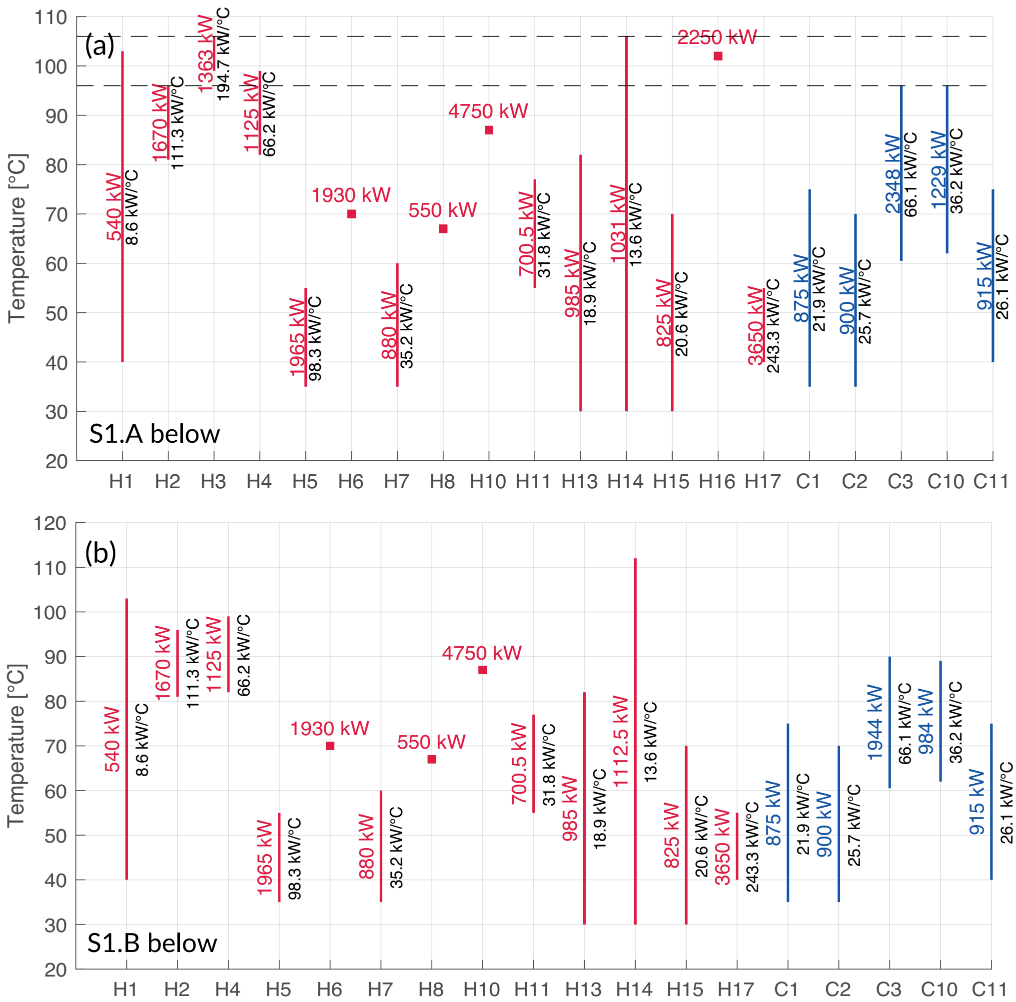


Figure 3.17 – Streams involved in HEN redesign below the pinch point for S1.A (a) and S1.B (b).

Table 3.11 – Pairs of streams involved in heat recovery of S1.B below the pinch.

Streams	Load [kW]	U [W/m^2°C]	A [m^2]	IC [kEUR]	OC [kEUR/y]	PBT [y]
C3 - H2	1070	255	639	368	197	1.9
C10 - H2	600	40	22	250	110	2.3
C3 - H4	874	445	79	139	161	0.9
C10 - H10	384	480	41	117	71	1.7
C11 - H10	915	343	104	153	146	1
C2 - H11	700	343	218	207	112	1.8
C2 - H17	200	462	14	100	32	3.1

For a heat exchanger to be placed below the pinch, the slope ("$\dot{m}c_p$") of the hot stream should be bigger than the one of the cold streams. A possible heat exchanger network redesign is presented in

Table 3.11. This example shows that, despite the lower temperature gradients for the heat exchanges and the lower number of available hot streams at high temperature, heat recovery targets are possible to meet in an economic way, thanks to the lost cost of the heat exchanger and favorable utility cost conditions.

3.5.2 Scenario 2

MER and penalising heat exchanges

Composite curves for S2 can be seen in Figure 3.18. In the reference situation S2.A, hot and cold composite curves in the corrected temperature domain are very close to each other in the area around the pinch point. However, the application of the methodology drastically changes the temperature levels at which the heat is available within the same area, thereby changing the pinch temperature.

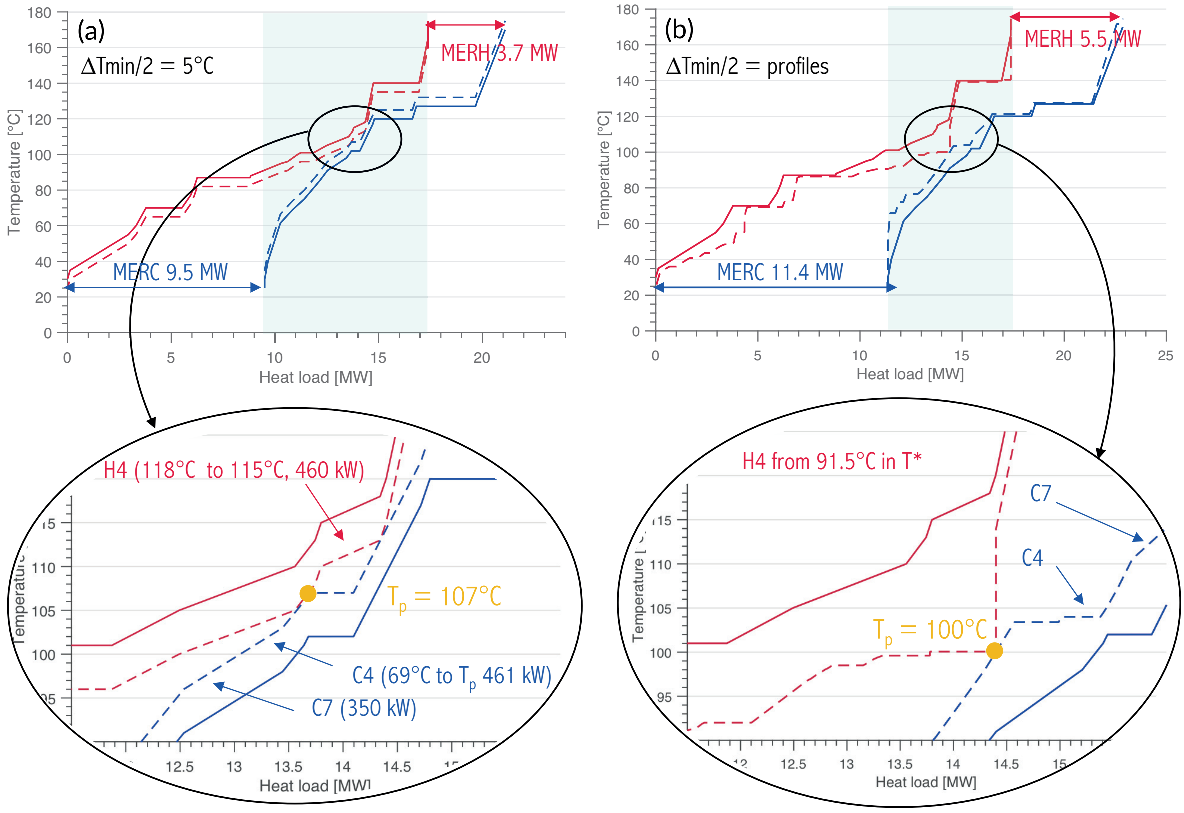


Figure 3.18 – Composite curves for S2.A (A) and S2.B (B).

In the reference case, potential for heat recovery amounts to 5.2MW whereas in the new case, with the application of the proposed methodology, this potential equals to 3.4MW. For this second scenario, the use of a single ΔT_{min} for each stream, without taking into consideration the physical and cost specificities of the system, leads to an overestimation of the potential for heat recovery of 35% at the targeting step.

Table 3.12 – MER results - S2

	Actual consumption	**S2.A** (T_p = 107°C)	**S2.B** (T_p = 100°C)	**Difference**
MERH [MW]	8.9	3.7	5.5	-1.8
MERC [MW]	14.8	9.5	11.4	-1.8

The $\Delta T_{min}/2$ is for the majority of streams higher than 5°C coupled with a larger $\dot{Q}_{min}$ load. Good examples are streams H4 and C4. When the methodology is applied, H4 and C4 are entirely located respectively below and above the pinch point in corrected temperatures, both being therefore not penalising. This is not the case in S2.A with the constant ΔT_{min}, for which H4 is entirely above and C4 partly below, thereby creating a heat penalty.

The pinch point being lower in the corrected situation, penalties of streams C3, C7 and C10 are also lower. For this scenario, this results in an overestimation of approximately 1.7 MW of the potential for heat recovery when a uniform ΔT_{min} is used (Table 3.12 and Table 3.13).

Table 3.13 – Penalising heat exchanges for S2

Stream	**S2.A [kW]**	**S2.B [kW]**	**Difference [kW]**
H1	136	0	-136
H3	35	0	-35
H4	460	0	-460
H12	781	781	0
H14	85	0	-85
C2	390	390	0
C3	962	869	-93
C4	461	0	-461
C7	350	0	-350
C10	1098	954	-144
C11	415	415	0
total	5173	3409	-1764

Impact on direct heat integration

Figures 3.19 (a) and (b) show the system above the pinch point respectively for S2.A and S2.B cases. Compared to S2.B, 4 additional hot streams are located above the pinch in the reference case. H1, H3 and H14 are "pinched" streams and they all have a relatively small heat load.

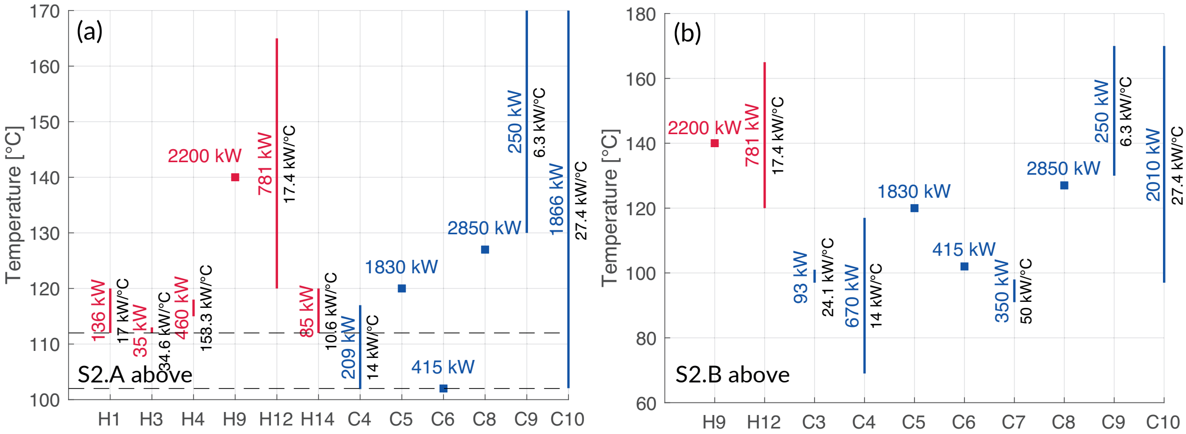


Figure 3.19 – Streams involved in HEN retrofit above the pinch point for S2.A (a) and S2.B (b).

Table 3.14 – Pairs of streams involved in heat recovery of S2.A above the pinch.

Streams	Load [kW]	U [W/m^2°C]	A [m ^{2}]	IC [kEUR]	OC [kEUR/y]	PBT [y]
H1 - C6	136	498	20	84	18	4.6
H3 - C6	35	422	8	96	5	20.3
H4 - C6	460	325	98	161	62	2.6
H14 - C6	85	411	15	85	11	7.4
H12 - C10	781	238	163	147	105	1.4

If S2.A is studied first, it is easy to show that hot pinch streams H1, H3 and H14, would never be economically integrated with cold pinch streams (C4, C6 and C10). If the analysis is carried out for each pinch stream together with C6 (best cold stream in term of U and LMTD) payback times are always much higher than 3 years, as it can be seen in Table 3.14.

In the corrected case only H9 and H12 are located above the pinch, and H9 is already correctly integrated with respect to the pinch point. The integration of H12 with C10, as it is the case in the reference case, leads to a payback time of 1.4 years.

Figures 3.20 (a) and (b) show this time the system below the pinch point. The major differences between S2.A and S2.B are that in the first case streams C4 and C7 are found below the pinch point, while they are both located above in S2.B. C4, although being heated up from 69°C to 125°C, does not appear in the list of streams below the pinch point due to its large $\dot{Q}_{min}$ making it available only above the pinch. The same behavior is observed for C7, also located entirely above the pinch in the corrected temperature domain. H4 heat load is available entirely below the pinch in S2.B while it was above in S2.A. Finally, a decrease in cold streams penalties is observed due to the lower pinch point as well as an increase of the heat of the hot streams available below the pinch, since most of the high temperature hot streams below the pinched are not crossing it in S2.B.

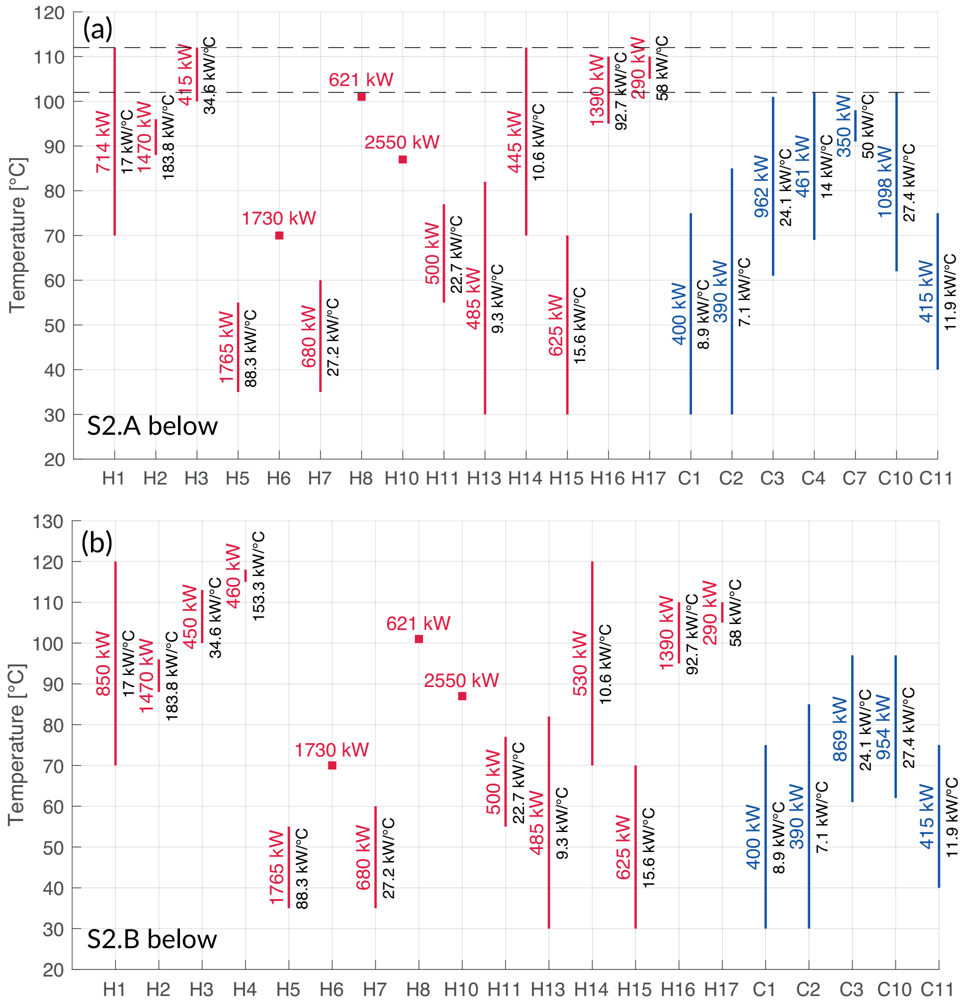


Figure 3.20 – Streams involved in HEN retrofit below the pinch point for S2.A (a) and S2.B (b).

Table 3.15 – Pairs of streams involved in heat recovery S2.B below the pinch.

Streams	Load [kW]	U [W/m^2°C]	A [m ^{2}]	IC [kEUR]	OC [kEUR/y]	PBT [y]
C3 - H4	460	240	68	141	62	2.3
C3 - H3	409	290	38	122	55	2.2
C10 - H16	954	2630	157	144	129	1.1
C2 - H14	390	284	32	119	47	2.6
C11 - H1	415	388	21	74	50	1.5

In S2.A, pinch cold streams are C3, C4 and C10 and pinch hot streams are H1, H3 and H14. When applied, the number of streams and "$\dot{m}c_p$" rules of the pinch design method cause extensive stream splitting, leading to smaller areas and a larger number of connections, which are both more expensive than a single larger heat exchanger.

Although not a pinch stream, both initial and target temperature of C7 are close to the pinch point, making the heat integration with this hot stream also difficult. In the subsystem created by these 7 streams, the best scenario would be the integration of C7 with H16, which results in a payback time of already 4.3 years.

As it was the case above, the corrected situation features generally larger minimum approach temperatures for the heat recovery of the most critical streams, leading to lower heat exchanger areas and lower investment costs. In S2.B, C7 and C4 are no longer present in the system below the pinch and an additional back up is available for heating up the pinch cold streams with H4.

3.5.3 Impact on heat pumping potential and utility integration

The ΔT_{min} definition at the targeting stage has also an impact on indirect heat integration and utility system optimisation. A good example is the evaluation of heat pumping opportunities from the heat cascade results.

Taking as an example scenario 1, the smaller $\Delta T_{min}/2$ for phase change streams compared to a constant $\Delta T_{min}/2 = 5$°C brings H16 above the pinch where it forms a self-sufficient pocket. In the reference case S1.A, this same stream would be the best candidate for heat pump integration, in order to supply part of C7 heat load. However, in the corrected scenario, heat pumping would then take place between H10 and C7.

Not only the ΔT_{min} definition changes the temperature levels of the cycle, which might as well change the fluid choice, but also the streams interacting with the heat pump. In turn this has an impact on utility integration and optimisation, depending on the identified heat pumping opportunities.

Such possibilities are summarised in Table 3.16 with the corresponding integrated composite curves for all situations on Figure 3.21. In cases S1.A HP1 and S1.B HP1, a single heat pump is evaluated while in cases S1.A HP2 and S1.B HP2, two heat pumping stages are considered. The term $\dot{Q}_{out}$ corresponds to the heat delivered above the pinch point.

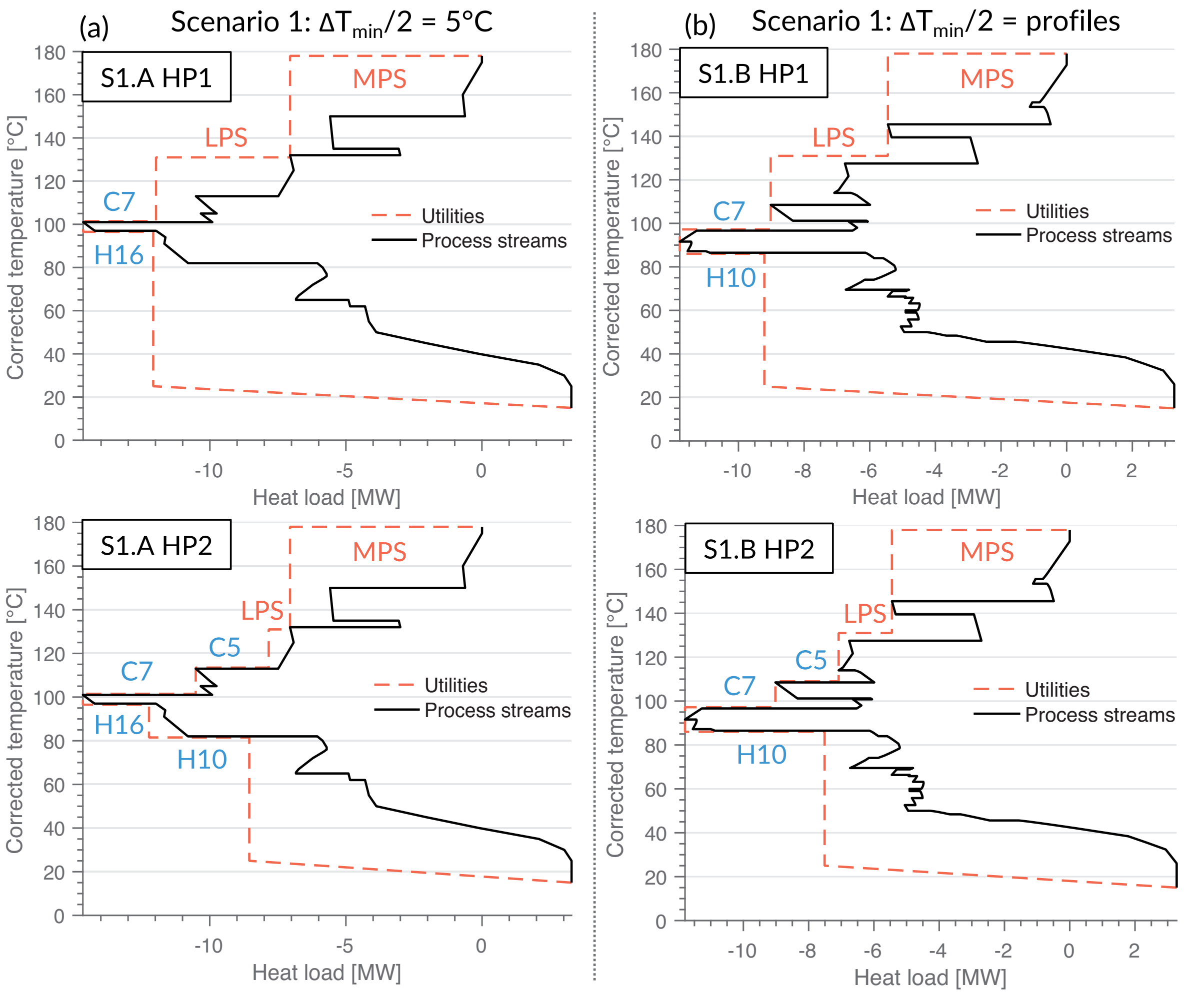


Figure 3.21 – Different scenarios for heat pump and utility integration for S1.A (a) and S1.B (b). LPS and MPS are respectively for low and middle pressure steam.

Table 3.16 – Scenario 1 heat pump integration schemes

	S1.A HP1	S1.A HP2	S1.B HP1	S1.B HP2
LP steam [MW]	4.9	0.8	3.6	1.7
MP steam [MW]	7.1	7.1	5.5	5.5
HP1 streams	H16/C7	H10/C7	H10/C7	H10/C7
HP1 Q_{out} [MW]	2.7	4.1	2.9	2.9
HP1 COP [-]	25.9	9	14.4	14.4
HP2 streams	-	H16/C5	-	H10/C5
HP2 Q_{out} [MW]	-	2.7	-	1.9
HP2 COP [-]	-	10.7	-	8.1
$E_{in,tot}$ [MW]	0.10	0.71	0.20	0.44

3.5.4 Discussion

One of the main advantages of this methodology is that targets for heat recovery are closer to a realistic economical optimum than when using a single ΔT_{min} or typical values for $\Delta T_{min}/2$, chosen without any optimisation considering the characteristics of the system under study. Compared to the area efficiency approach, this methodology allows the use of different cost laws for individual streams if need be and the possibility to account for different utility prices according to the temperature levels of streams. Flexibility is also enabled, in the sense that the user can specify its own economic objectives, heat exchangers costs and define its own set of parameters.

Another advantage is that calculations are relatively easy and quick to implement, which is of major importance when carrying out energy reviews in the framework of energy audits or energy management in industry. In these situations, being able to obtain realistic potential for energy consumption reduction, without complex methods requiring significant computing resources and advanced skills, is a main asset.

Beyond the refining of the ΔT_{min} definition, an interesting aspect of the approach is the calculation of the parameter $\dot{Q}_{min}$ and the temperature at which it is found for each stream. This approach allows a pre-screening of streams through a better definition of the temperature-enthalpy profiles of streams, according to the thermo-economic trade-off of the system.

Using pairs of identical parallel streams in the corrected profile generation implies two things. Neglecting the wall resistance in Equation 3.7, the individual stream contribution can be determined by dividing the ΔT_{min} profile in two, thereby allowing to obtain the contribution of each stream to the minimum temperature difference according to the temperature of the stream $\Delta T_{min}/2 = f(T_{real})$.

Secondly, by considering parallel streams the LMTD (being equal to ΔT_{min}) is the smallest possible, meaning that the results for the minimum approach temperature are located at the upper boundaries. This aspect can be modified according to the user's preferences. For example, a flat stream can be used rather than a parallel stream, leading to slightly lower approach temperatures.

The main drawback is the division of each stream profile in many segment, which might cause problems in heat cascade calculations. This also leads to "fictive" segments corresponding to $\dot{Q}_{min}$ and the transition zone until it reaches the $\Delta T_{min}/2$. As a result the composite and grand composite curves directly obtained are more difficult to read.

A simplification can be to divide the stream profile in two segments only ($\dot{Q}_{min}$ and a constant $\Delta T_{min}/2$). However, in doing so the transition area is lost, resulting is a slight overestimation or underestimation of $\dot{Q}_{min}$.

3.6 Conclusion

This third chapter aims to answer to the following research question:

How to generate economically feasible minimum energy consumption targets in pinch analysis, with the minimum level of detail for streams definition?

It discusses first the influence of the level of detail for streams definition on the minimum energy requirements and the shape of the grand composite curve. An example is used to show how for the same minimum heating and cooling demands, corresponding to the "white box" level of detail for streams definition, only a third of the process requirements needs to be detailed at this level. Although the optimum trade-off for streams definition cannot be known in advance, **the default list of streams can be refined by following heuristic rules**, targeting process streams in the area of the pinch point.

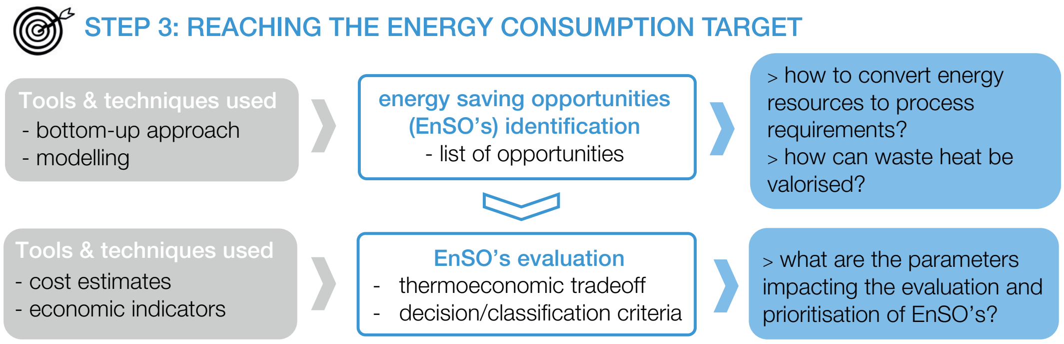
This chapter shows that existing methods for the definition of the ΔT_{min} in existing industrial systems are often not adapted and can lead to serious over- or underestimation of minimum energy consumption targets. The proposed methodology differs from traditional approaches involving the use of the area efficiency for the determination of the ΔT_{min}, while still considering the thermo-economic trade-off resulting from the characteristics of the system. Instead of generating a single optimum ΔT_{min}, each stream is characterised individually, thereby enabling the use of several equipment cost laws and utility costs depending on the system under study and the temperature levels of the streams.

With a better approximation of the contribution to the minimum approach temperature of each stream along its temperature, the heat recovery between process streams is refined and small penalising heat exchanges which would not be profitable are either highly corrected or transformed to black boxes. This approach has the advantage of refining the targeting step and providing **more reliable energy integration targets** at the early stage, prior to the generation of the heat exchanger network.

4 Reaching the energy consumption target

Chapter overview:

> From the minimum energy consumption target to the list of energy saving opportunities.



4.1 Bottom-up approach

At this point, the hot and cold utility consumption of the system is mapped, verified and translated into process requirements. The heat removal and heat supply to the process can be seen on the total site profile, and the maximum heat recovery potential is determined via the pinch analysis on the process streams. The difference between the actual and minimum energy requirements is explained by the penalising heat exchangers.

Building on these results, the objective of this last step is to generate a list of energy saving opportunities (EnSO's), aiming to reach the heat recovery target and look at the energy conversion technologies to satisfy the remaining process heating and cooling requirements. It is important to adopt a no-taboo strategy at this stage and list all possible modifications that would increase the overall energy efficiency. Opportunities can be missed if they are disregarded too fast based on preconceptions or a priori constraints. The goal is to generate a full list of options, from the deepest level of detail corresponding to the process itself, to the energy conversion and distribution system.

Each opportunity is evaluated with a thermo-economic analysis, which determines its profitability estimating on one side the capital expenditure linked to the capital cost of the modification, and on the other side the operating cost savings. Both sides of the economic analysis are subject to uncertainty and so are the resulting economic indicators selected for decision making. Sensitivity analysis has to be carried out on the main uncertain parameters to understand how they influence the thermo-economic analysis results.

Since energy efficiency improvement is linked to carbon dioxide emissions reduction, CO_2 emissions taxes should also be taken into account in the analysis. Finally, in some countries, subsidies are put in place to help companies finance the implementation of energy efficiency projects with medium to long payback times, which are often responsible for large energy savings. It is for example the case for cogeneration units.

This chapter presents first the procedure for the generation of energy saving opportunities, in the form of an onion diagram representing the ordered optimisation layers. A case study is then used to show an example of energy efficiency improvements identified at several levels and a simple sensitivity analysis on each option is carried out to demonstrate the impact of the economic parameters.

4.1.1 Onion diagram for the identification of energy saving opportunities

The optimisation layers for chemical process design are traditionally represented by an onion diagram, which consists of consecutively embedded circles starting from the first layer of optimisation.

A typical onion diagram for process design can be seen on Figure 4.1 (a) [123], derived from the first reported one from Linnhoff et al. [2] where the compression and expansion layer was included in the heat recovery layer.

The optimisation of the energy consumption of existing industrial systems can also be represented by an onion diagram. Figure 4.1 (b) shows the optimisation layers that are defined in this thesis to generate the list of energy saving opportunities:

1. **Process technology:** modifications at the level of the chemical process technology itself. Examples are new technology switching, replacement of existing reactors with more efficient ones and unit debottlenecking.
2. **Process operating parameters:** modifications of operating conditions (e.g. temperature, pressure, reflux ratio) to increase energy efficiency. Such opportunities are often found at the

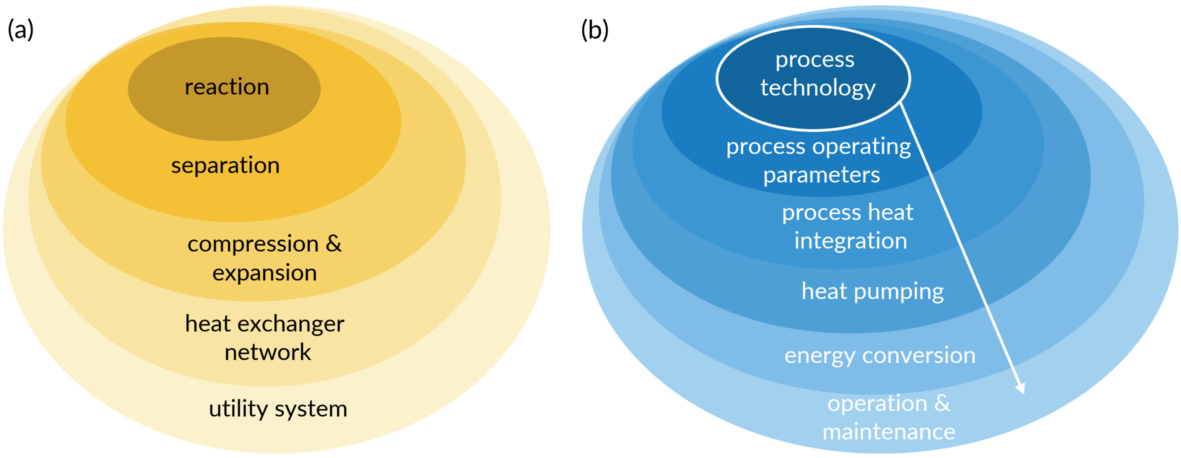


Figure 4.1 – (a) Typical onion diagram for chemical process design (derived from [2]) and (b) modified onion diagram for the identification of EnSO's.

level of the separation step, with the optimisation of distillation columns operation. Examples can be pressure modification to enable direct process integration and optimisation of the reflux ratio to reduce reboiler and condenser heat loads.

3. **Process heat integration:** penalising heat exchangers resulting from the pinch analysis heat cascade are removed through the redesign of the heat exchanger network, and direct or indirect heat recovery schemes are generated to get as close as possible to the minimum energy requirements.

4. **Heat pumping:** depending on the shape of the grand composite curve, heat pumping opportunities can be identified, involving the increase in temperature of a heat source below the pinch and lifting it above the pinch to supply heat to cold streams. Several technologies exist for heat pumping (i.e) mechanical vapour recompression (open cycle), one/several -stage(s) heat pumps and absorption heat pumps.

5. **Energy conversion:** the remaining process heating and cooling requirements have to be supplied by the utility system. Again based on the grand composite curve and process requirements, the energy conversion units can be optimised or replaced to better match the process energy profile. Examples can be the installation of a gas turbine, the optimisation of boiler operation, the optimisation of the steam network (maximisation of electricity cogeneration, flash steam production, condensates return), or the integration of an organic Rankine cycle to produce electricity from the waste heat.

6. **Operation and maintenance:** the last level of energy efficiency optimisation relates to the determination of optimal operation set points and the development of proper maintenance

routines, especially at the level of the steam network (e.g. status checks on insulation and steam traps, identification of leaks) and heat exchangers cleaning (fouling removal).

This onion diagram for the energy efficiency optimisation of existing industrial systems follows a **bottom-up approach**. In this thesis, modifications on the process technology itself are left out of the propositions for energy saving opportunities. The analysis starts with the actual production route and process configuration.

These layers define guidelines for the identification of EnSO's, guarantying that the optimisation starts at the right point, that is from the process characteristics and its real energy requirements, rather than from the optimisation of the utility system. In reality, strong interactions are found between layers. While the more efficient system can be designed based on thermodynamic targets, it is not necessary the one which will be selected for implementation. Several alternatives for energy saving opportunities should then be identified and evaluated, even if they are in competition. This is the case for example between different direct or indirect heat recovery scenarios, heat pumping configurations, or energy conversion systems.

Each opportunity has to be evaluated economically but also issues linked to its implementation, which can be of safety, technological or topological nature, need to be estimated as key for final decision making. Keeping in mind the minimum energy consumption targets and the energy profile of the system, the best combinations of energy saving opportunities can be selected while still keeping track of the others.

4.2 Example on a case study

This section shows an example of energy saving opportunities that can be identified on a case study, from the system already presented in Chapter 3. The total site profile and grand composite curve of the case study can be respectively seen on Figure 4.2 (a) and (b), with minimum energy requirements (MER) detailed in Table 4.1. It is based on the optimum list of streams introduced at the beginning of the last chapter and available in Table A.4 in the Appendix.

Table 4.1 – Pinch analysis results (T_{pinch} = 89.5°C).

	Hot utility [MW]	**Cold utility** [MW]	**Heat recovery** [MW]
Actual system	31.4	36.2	14.2
MER	25.5	30.3	20
Difference	5.9	5.9	5.9

In the actual system, cooling is carried out by cooling water and heating is provided by steam at two pressure levels: middle pressure (T_{sat} = 207°C) and low pressure (T_{sat} = 142°C) steam. A simplified scheme of the steam network is depicted in Figure 4.3.

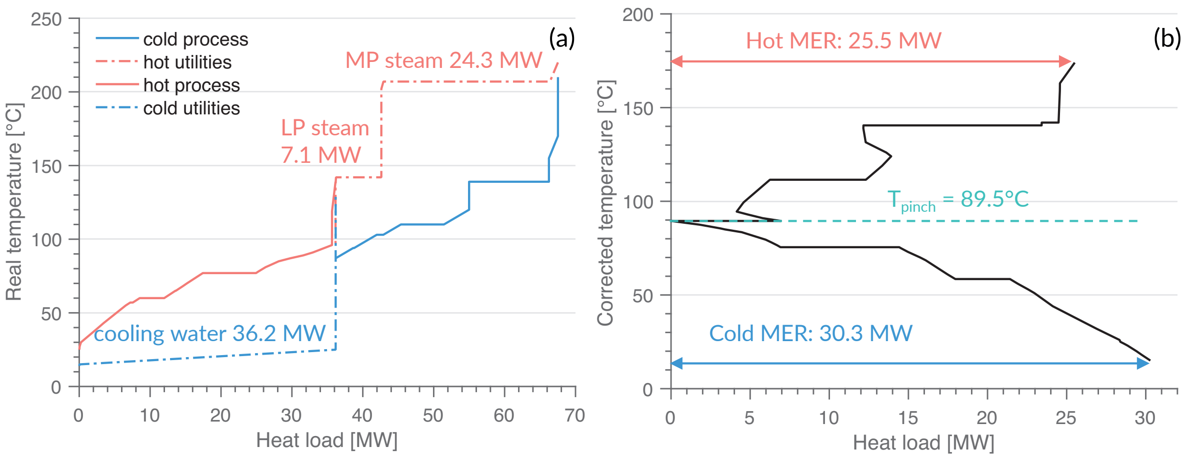


Figure 4.2 – (a) Total site profile and (b) grand composite curve of the case study.

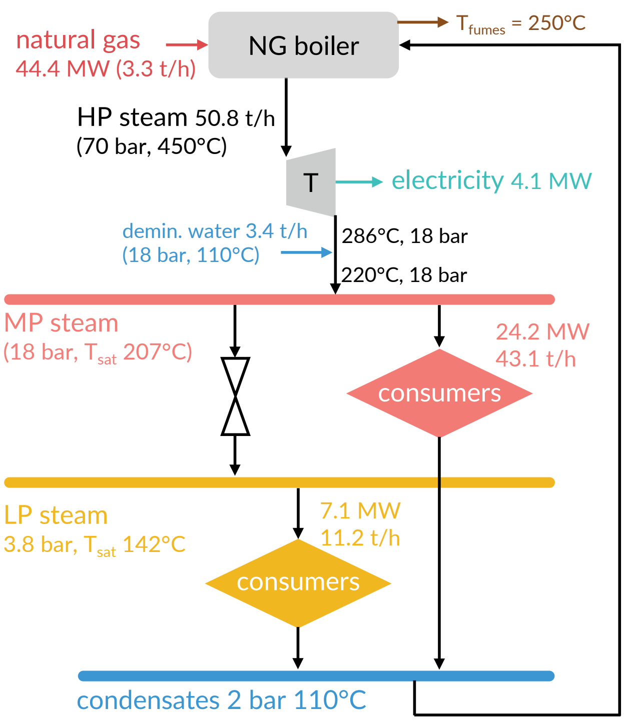


Figure 4.3 – Utility system in place in the case study.

Superheated high pressure steam is first produced in a natural gas boiler and expanded in a back pressure steam turbine down to 18 bar. Middle pressure steam is desuperheated with demineralised water injection. Low pressure steam is obtained via valve expansion from the middle pressure steam header. The electricity production of the turbine is of 4.1 MW under nominal operating conditions. Considering the useful heat and electricity production compared to the natural gas consumption, the system has an efficiency of 80%. Energy prices[1] for natural gas and cooling water consumption, as well as the selling price for electricity are summarised in Table 4.2.

Table 4.2 – Energy prices and economic parameters

Natural gas	Cooling water	Electricity selling	Interest rate	Lifetime
22 €/MWh	0.02 €/m^3	50 €/MWh	8%	20 years

The pinch analysis results show a potential for energy consumption reduction of approximately 6 MW, which is explained by the penalising heat exchanges listed in Table 4.3. Two heat penalties are linked to the use of a cold utility to cool down process streams above the pinch point, and the three others correspond to badly designed process integration, causing heat to be transferred across the pinch. Among the five penalising heat exchanges, two explain 85% of the total penalty. After investigation, the three other penalising streams were removed from the list since the heat penalty was judged to be infeasible to be removed, due to safety issues and location of streams.

These streams were transformed to black box, in order to account for their energy requirement but remove their potential for heat recovery. The new hot and cold minimum energy requirements are respectively 26.2 MW and 31.0 MW.

Table 4.3 – Penalising heat exchangers, total = 6 MW.

	T_{in} [°C]	**T_{out} [°C]**	**Load [kW]**	**T_{in}* [°C]**	**T_{out}* [°C]**	**Q_{pen} [kW]**	**Share [% tot.]**	**penalty type**
RECYCLING	139	119	495	135	115	495	8	cold utility above pinch
COND2_1	**96**	**91**	**2693**	**94.5**	**89.5**	**2693**	**45**	**cold utility above pinch**
EXTRACT1 (with FEED1)	99	27	2225	95	23	170	3	cross pinch
EXTRACT2 (with FEED2)	103	28	878	99	28	111	2	cross pinch
PROD_COND_2 (with HEAT1)	**101**	**89**	**3059**	**99.5**	**87.5**	**2549**	**42**	**cross pinch**

4.2.1 Process operating parameters

The first layer of optimisation focuses on modifications of the process operating conditions which would result in an increase of the energy efficiency. For the case study, such opportunity is located at the level of the first distillation column.

[1] Energy prices observed for case study location in France, in 2014.

The feed stream enters the distillation column at 30°C, while the saturation temperature of the column measured at the feed tray is about 100°C. From the grand composite curve it can be seen that the feed could be preheated until the pinch temperature (T_{pinch}(89.5°C) - $\Delta T_{min}/2$) using excess process heat, which would reduce the load of the reboiler.

Figure 4.4 shows schematically the initial process configuration and the required system modifications to realise the feed preheating. For the latter, the overhead condensation stream of the same column is integrated with the feed to be heated up, since it is the hot stream below the pinch with the highest temperature and the closest in term of geographical location.

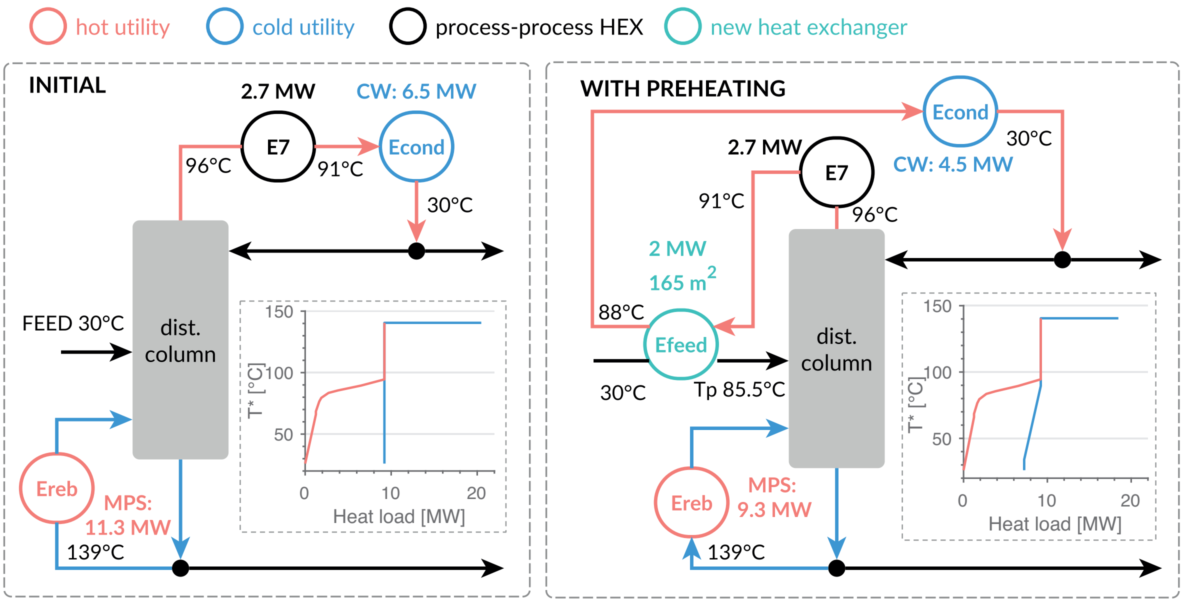


Figure 4.4 – Distillation column without (initial) and with feed preheating.

The start and final temperatures of the hot stream are respectively 91°C (corresponding to the pinch point in real temperature) and 88°C. The new heat exchanger to install is then pinched at the hot end. The implementation of feed preheating would result in a reduction of 2 MW of middle pressure steam (MPS) consumption in the reboiler.

The composite curves displayed on the figure show the heat recovery from the overheads and the decrease in steam requirements for the case with preheating.

Table 4.4 – Thermo-economic analysis of the feed preheating

OC savings [k€/y]	IC [k€]	NPV [k€]	PBT [y]
313	207	3’000	0.66

A summary of the results of the thermo-economic analysis is provided in Table 4.4, showing the expected operating cost savings (OC savings), investment cost (IC), net present value (NPV) and payback time (PBT) of the feed preheating opportunity. Details on calculations related to the heat exchanger cost are available in Appendix C (Table C.3).

This configuration makes use of the excess heat below the pinch. The overhead condensation straight at the outlet of the column occurs above the pinch point with 2.7 of MW of heat to evacuate (heat exchanger E7), and corresponds to the penalising stream COND2_1 being cooled down by a cold utility. The use of this heat to preheat the feed would reduce the reboiler heat load by the same amount for a smaller heat exchanger to install, but it would still be a penalising heat exchange. This option should be considered only if the integration of COND2_1 with other process stream to reach the heat recovery target is judged infeasible.

From this first opportunity, the list of streams has to be updated for the rest of the analysis. A cold stream corresponding to the feed preheating from 30°C to 85.5°C (T_{pinch}-$\Delta T_{min}/2$) is added and the reboiler heat load is decreased. The hot and cold energy requirements are reduced by the 2 MW of heat integration identified in this section.

More generally, distillation columns are major energy consumers in any chemical processes including a separation step. When thermodynamic models of columns are available, modifications of their configuration (i.e. different feed conditions, addition of a side reboiler and/or condenser, reflux ratio modification) can be studied in detail, and the integration of the columns with the rest of the process can be further optimised. A good demonstration can be found in [124], where the temperature-enthalpy profiles of columns are generated and operating conditions and/or columns layout are changed to improve the overall system heat integration.

*NB: It is important to mention here that costing methods for heat exchangers available in the literature turn out to poorly estimate the real investment cost. When presenting cost estimates to industrial partners, it was always pointed out that the values were notably **underestimated**, compared to installation costs they observe. The principal reasons probably being the additional costs linked to piping modification and installation and plant rearrangement. An additional factor should then be introduced to account for these supplementary costs. This observation is valid in this section for all the investment cost estimates related to pieces of equipment.*

4.2.2 Process direct heat integration

The second optimisation layer targets the removal of the heat penalty caused by a non-optimal heat exchanger network configuration. The two penalising streams to remove are COND2_1 and PROD_COND_2 (see Table 4.3). The actual heat exchanger network configuration can be seen on Figure 4.5. The two penalising heat exchangers are displayed in yellow. PROD_COND_2 is cooled down via cooling water above the pinch and 80% of heat exchanger E1 load crosses the pinch point. In order to remove the total heat penalty, the heat exchanger connections and streams temperatures need to be rearranged with respect to the process pinch point and streams definition. To do so, the actual heat integration represented by the black circles on the figure needs to be modified.

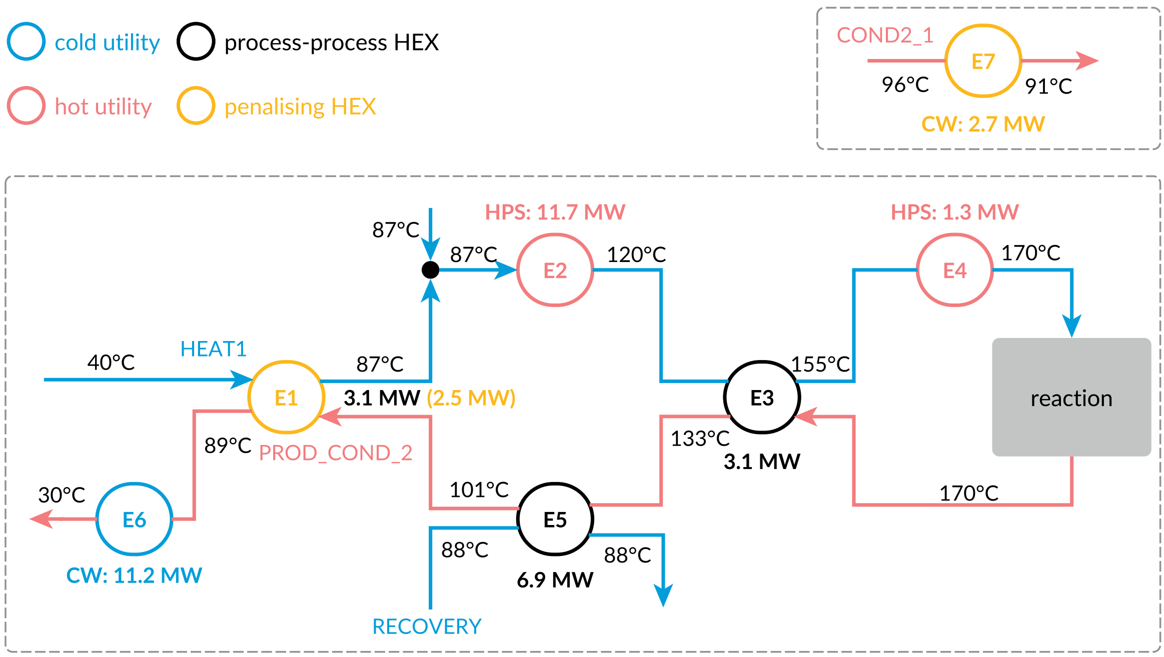


Figure 4.5 – Initial heat exchangers configuration.

A new system configuration, depicted in Figure 4.6, has been identified and proposed. In this new configuration, the evaporating stream RECOVERY is not anymore integrated with the hot process stream exiting the reaction section at the level of E5. Instead, part of the heating is now supplied by the penalising hot stream COND2_1, removing entirely its penalty.

This new heat exchange implies two things. First, an increase in heat exchange area of E7 is required since for the same heat load the temperature gradient is now much smaller, and second an additional heat exchanger needs to be installed to supply the remaining heat load required for stream RECOVERY. Considering its temperature level (88°C), low pressure steam can be used. To be noted that this heating requirement is visible on Figure 4.2 (b), with the plateau at 89.5°C.

The other penalty is removed through a better integration of the hot and cold process streams entering and leaving the reaction section. E4 is required to adjust the temperature level of the stream entering the reaction section, however its heat load can be reduced. The cold stream inlet and outlet temperatures of E3 are then both increased by 4°C. While the heat load is still the same, the temperature gradient is slightly reduced.

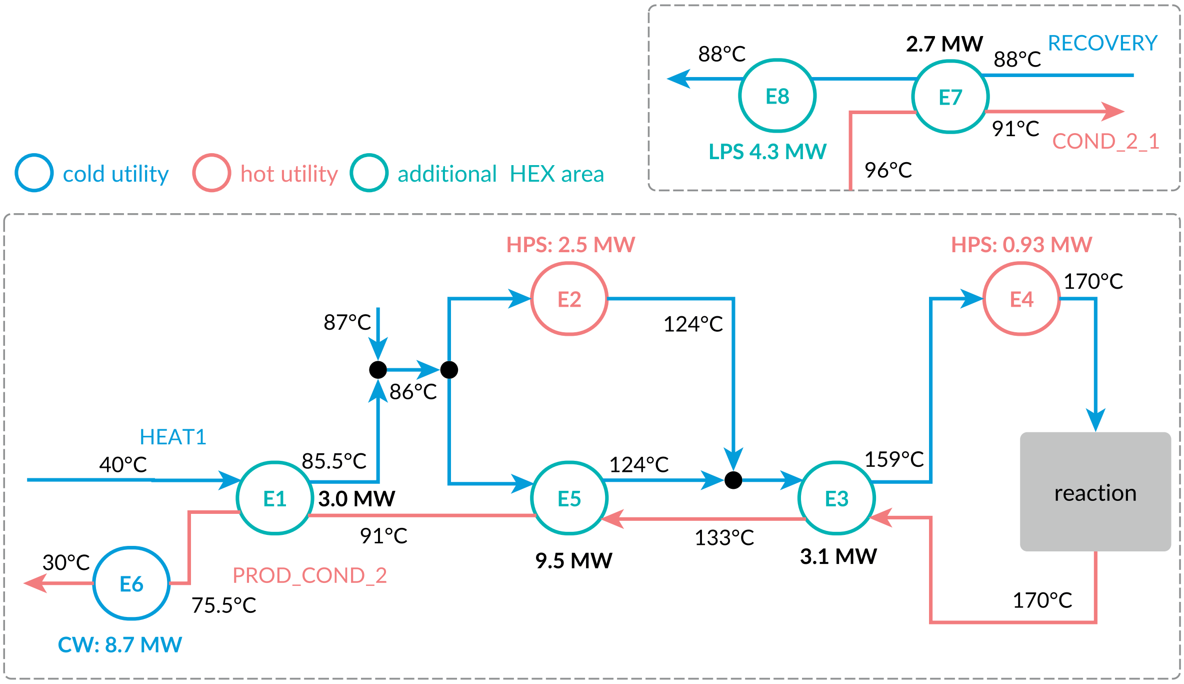


Figure 4.6 – Redesign of the heat exchangers configuration.

The MP steam consumption in E2 is decreased through the cold stream splitting and its integration with the hot stream exiting the reaction section at the level of E5. Finally, PROD_COND_2 inlet and outlet temperatures at the level of E1 are modified in such a way that it becomes a pinch heat exchanger located below the pinch point.

As for stream COND2_1 integration with RECOVERY, these modifications imply additional heat exchange areas to be installed due to the smaller temperature gradients and the increased heat recovery. The thermo-economic analysis results of the proposed heat exchanger redesign can be seen in Table 4.5, with the details on the additional heat exchange area provided in Appendix C.

Table 4.5 – Thermo-economic analysis of the heat exchanger network redesign.

OC savings [k€/y]	IC [k€]	NPV [k€]	PBT [y]
867	2'504	6'005	2.89

4.2.3 Heat pumping

Once direct and indirect heat recovery schemes are investigated, the next layer of optimisation is to check for heat pumping opportunities. Studying the grand composite curve, it can be seen that the process requires 4.3 MW of heat at the level of the pinch point, corresponding to the RECOVERY stream which is involved in the heat exchanger redesign.

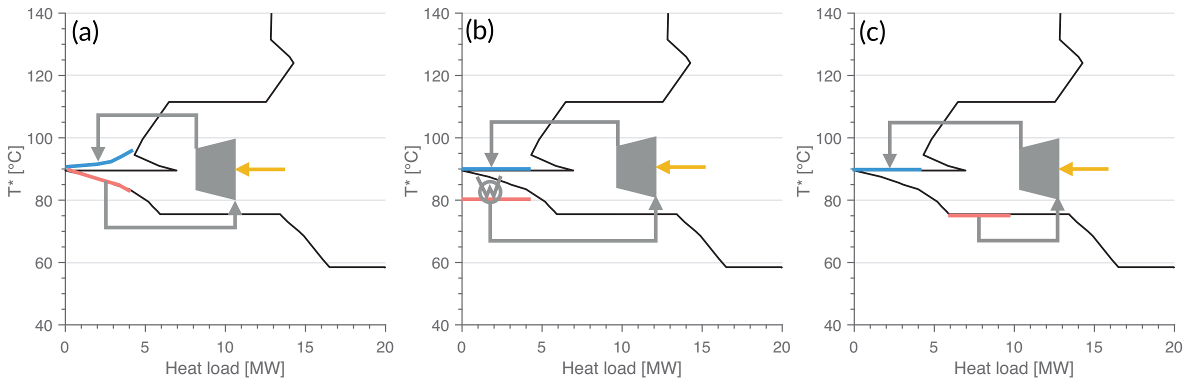


Figure 4.7 – Zoom on the process GCC with heat pumping integration possibilities: (a) MVR or (b) close HP cycle with multi-products stream and (c) MVR with single product condensing stream.

Instead of consuming low pressure steam, heat pumping can be used to lift waste heat from below to above the pinch point. Figure 4.7 shows several possible configurations to do so. The first option (a) is to directly compress a column overhead stream composed of several chemical compounds. The second option (b) uses an external cycle with a working fluid to recover the heat and pump it above the pinch. Finally, the last option (c) involves mechanical vapour recompression of another column overhead stream to heat up the RECOVERY stream, which in reality corresponds to the reboiler of the same column.

After studying each possibility, the last option was selected. While the first one is the most promising in terms of coefficient of performance, the varying composition and multi-product characteristic of the stream were not suitable for direct recompression. This is avoided with the second option but at the expense of an external system, implying the addition of another heat exchanger. The last option is the most promising and convenient due to the proximity of the hot and cold stream and the absence of operational or safety constraints.

The proposed mechanical vapour recompression is depicted on Figure 4.8. The initial temperature of the condensing and evaporating streams being close (respectively 82°C and 88°C) and the overall heat transfer coefficient being rather high since the heat exchange involves two streams changing phase (allowing a small temperature difference), the required pressure increase is only of 0.7 bar. The associated mechanical power to drive the compressor is of 235 kW ($\eta_c = 0.8$).

Table 4.6 – Thermo-economic analysis of the mechanical vapour recompression.

OC savings [k€/y]	IC [k€]	NPV [k€]	PBT [y]
683	1'572	5'138	2.3

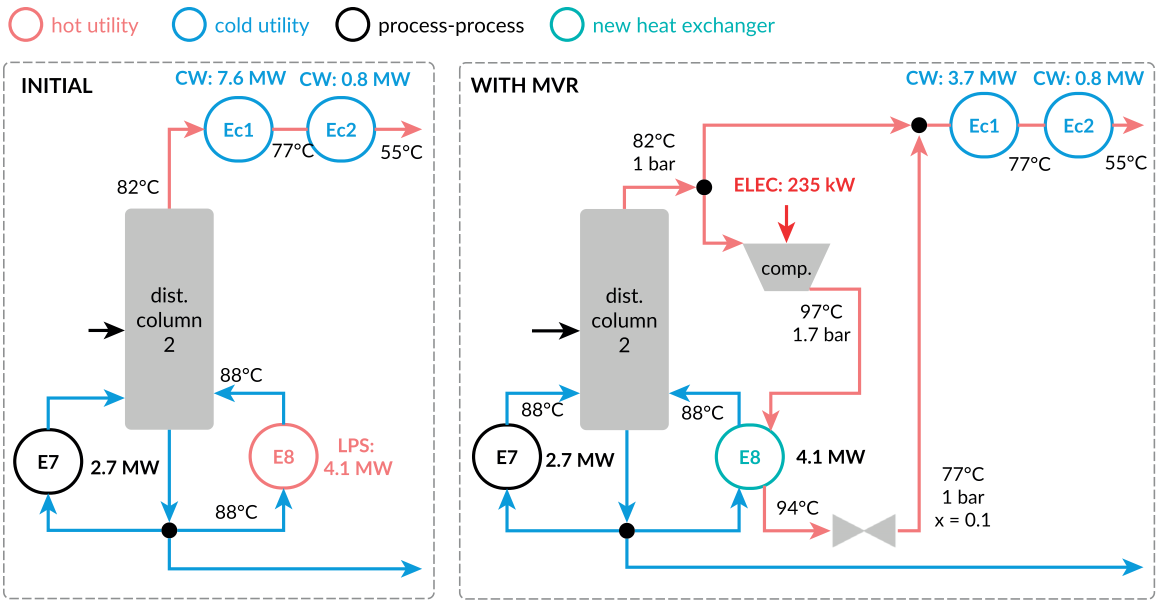


Figure 4.8 – Implementation of mechanical vapour recompression on a distillation column.

One reboiler of the distillation column 2 (E7) is already integrated with another process stream from the heat exchanger network redesign step. The installation of E8 to supply the remaining heat of the reboiling stream also resulted from this redesign. The implementation of the MVR removes the need of steam consumption of the distillation column. Heat exchanger E8 still needs to be installed but its design is changed due to the lower temperature gradient of the process-process heat exchange. Table 4.6 summarises the thermo-economic analysis results of the proposed MVR, with calculation details available in Appendix C.

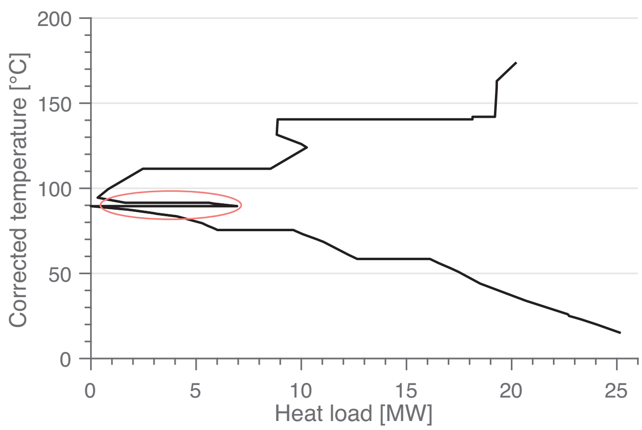


Figure 4.9 – Updated GCC including the mechanical vapour recompression.

The grand composite curve of the process including the mechanical vapour recompression can be seen on Figure 4.9. The new minimum energy requirements are now 20.3 MW of hot utility and 25.2 MW of cold utility.

4.2.4 Energy conversion

The actual energy conversion system is composed of a natural gas boiler producing saturated high-pressure steam which is first expanded in a turbine to cogenerate electricity, before being distributed across the site to heat the process. Cogeneration is then already taking place in the steam network.

However, the actual steam pressure levels could be lowered, thereby generating more electricity thanks to a higher pressure difference. Another turbine (or a new two-stages turbine) could also be added between the high and low pressure steam levels, increasing the electricity production. The temperature of the fumes at the outlet of the boiler, which is of 250°C, can be lowered through a better integration with the steam generation and air preheating below the pinch. Such modifications of the actual utility system configuration would lead to an additional electricity generation of 1.5 MW (with the updated MER after the MVR) and a higher combustion efficiency.

When looking at the temperature-enthalpy profile of the process requirements, with or without the implementation of the energy saving opportunities previously identified, the maximum temperature of the cold streams is 170 °C. Instead of a natural gas boiler, a gas turbine could be installed coupled to the steam network, to supply the heat requirements while cogenerating electricity. In this case, the conversion unit would become at the same time a power production unit.

The integrated composite curves for both situations can be seen on Figure 4.10, in corrected temperatures as well as using the Carnot factor ($1\text{-}T_a/T$) for the y-axis.

When working in the Carnot factor domain, the area between the process and the utility curve represents the exergy destroyed in the system. Here, it is shown how the energy conversion units (i.ie boiler and gas turbine) are integrated with the steam network, the latter delivering heat to the process streams.

With the natural gas boiler, the temperature difference between the combustion gases and the intermediate steam production shows an important exergy loss, represented by the area between the boiler curve ($T_{adiabatic}$ to T_{fumes}) and the superheated steam production (70 bar 450°C). This area is much smaller in the case of the gas turbine integration.

Supplying the heating demand of the process via the cooling down of the combustion gases of the gas turbine implies consuming more natural gas for the same thermal power production. On the other side more than a third of natural gas energy content is converted to electricity. Figure 4.11 shows on the same Sankey diagram, the natural gas conversion to thermal power and electricity for a fixed final heating demand, for the gas turbine and the boiler. It can be seen that the natural gas

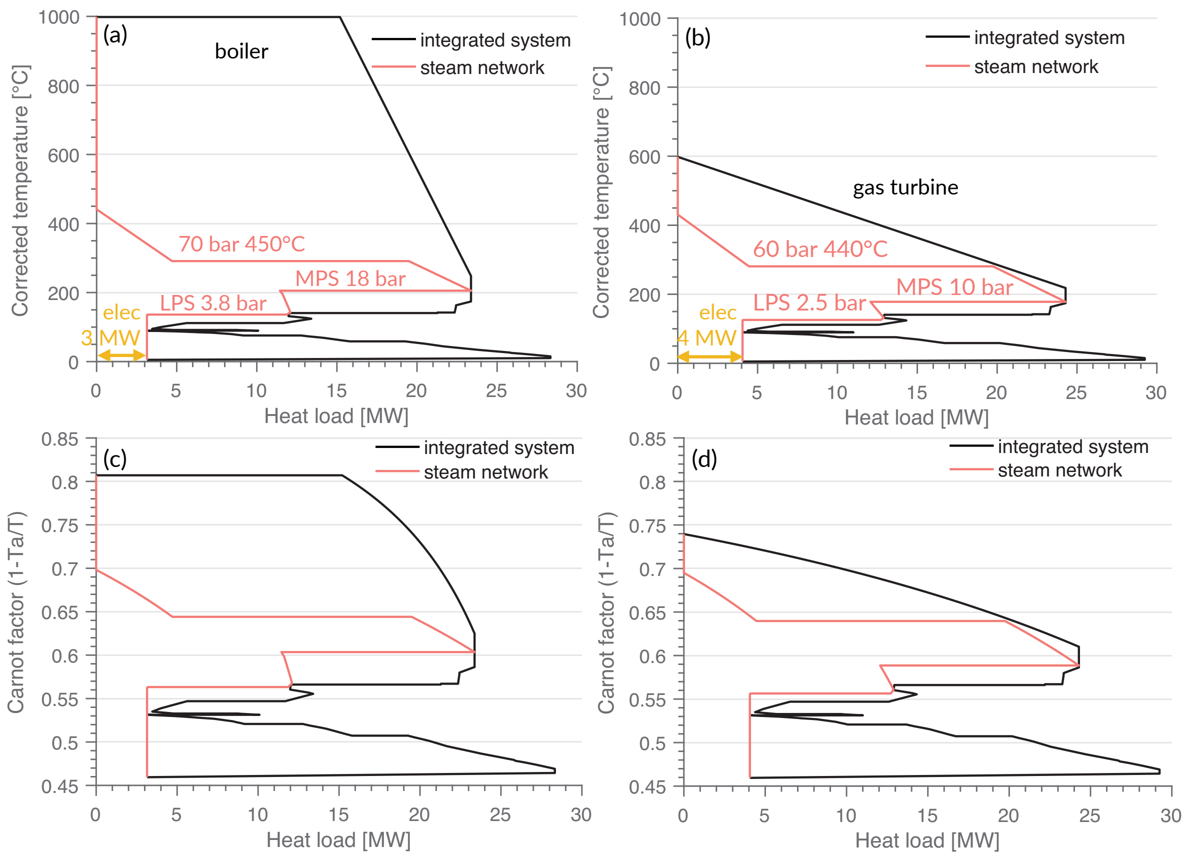


Figure 4.10 – Corrected temperature and Carnot integrated composite curve of the system with (a&c) the initial natural gas boiler and (b&d) a gas turbine with lower steam pressure levels.

consumption is increased by 75% in the case of the gas turbine, corresponding to 21.3 MW. At the same time 17.4 MW of additional electricity is generated.

To be noted that the gas turbine losses at the level of the steam generation (SPgt_L) are higher than what could be achieved with this type of technology. These losses are coming from the flue gases which are exiting at 230°C, since there is no need for additional heat below this temperature level from what is already being delivered to the process.

Depending on the price of these two energy vectors and the electrical demand of the site/cluster as well as neighbouring industrial sites, the installation of a gas turbine can be very interesting. With the energy prices of natural gas and electricity (see Table 4.2), the net yearly operating cost for the gas turbine and the boiler are respectively 150 k€/y and 3044 k€/y, which would correspond to an annual energy bill decrease of 95% thanks to the selling price of electricity. Although it is hard to find detailed cost data for gas turbine, the capital cost was estimated to 16.2 million euros (1101 $/kW [125]).

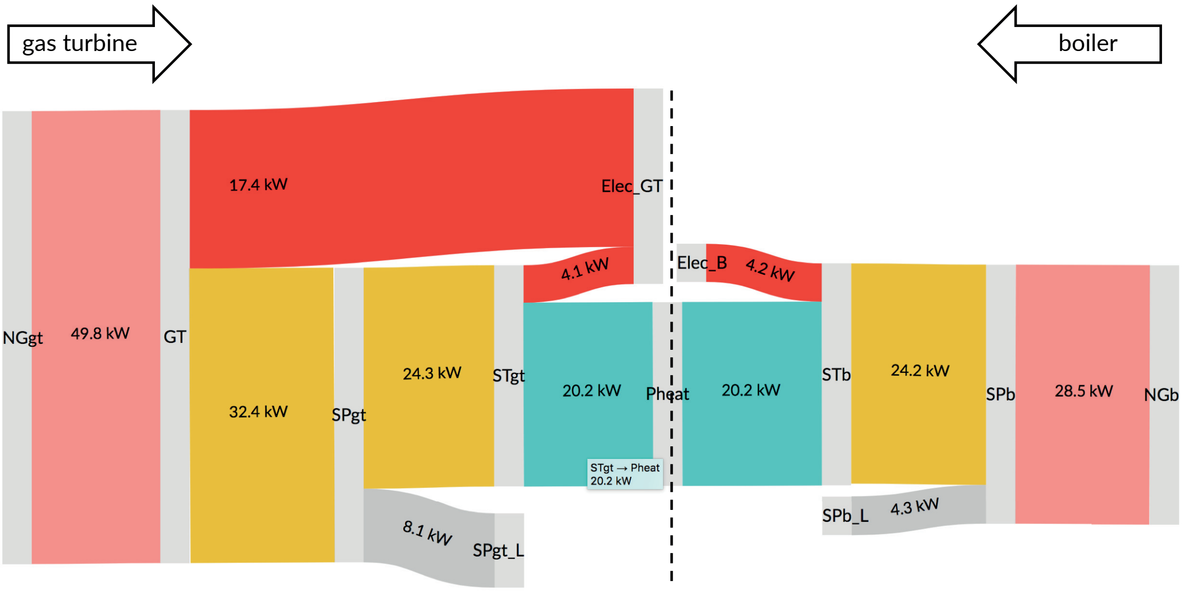


Figure 4.11 – Sankey diagram in the case of gas turbine integration (left to center) and boiler (right to center) to supply the process heating demand.[2]

4.2.5 Summary

Table 4.7 summarises the energy saving opportunities previously described together with the corresponding impact on the hot utility consumption (HU). The bottom-up approach, starting from the process operating parameters and energy requirements, allowed to identify three opportunities which would have been missed if the focus of the analysis were put at the utility optimisation level. The combination of these opportunities leads to an expected 35% decrease in the thermal power consumption of the site (11.1 MW).

Table 4.7 – Summary of the energy saving opportunities.

	OC savings [k€/y]	IC [k€]	NPV [k€]	PBT [y]	HU [MW]
Actual consumption	-	-	-	-	31.4
Option 1: feed preheating	313	207	3'000	0.7	29.5
Option 2: HEX redesign	867	2'504	6'005	2.9	24.3
Option 3: MVR	683	1'572	5'138	2.3	20.3
Option 4: gas turbine	2'894	16'200(?)	12'124	5.6	20.3

While this summary is useful to get a first overview of the different possibilities to increase the energy efficiency of the site and decide on the energy strategy, the values for the economic indicators must be taken with care. Uncertainty on both sides of the thermo-economic analysis has to be kept in

[2] gt/GT = gas turbine, b/B = boiler, SP = steam production, ST = steam turbine, Pheat = process heat, L = losses, Elec = electricity

mind, as well as the other engineering constraints (e.g. safety, topological, technical) which might prevent implementation or increase the investment cost.

4.2.6 Sensivity analysis

This section presents the effect of the uncertainty or variation of costing parameters on the economic indicators used for decision making. The three first options identified in the case study are used as examples. Table 4.8 shows which parameters were selected in the sensitivity analysis.

Table 4.8 – Summary of the energy saving opportunities.

Parameter	Variation
Investment cost	+/- 25%
Steam price (NG cost)	+/- 25%
CO_2 tax	0 - 30 €/t of CO_2
Interest rate	5 - 10 %

The variation range associated with the investment cost of the equipment corresponds to the typical accuracy of preliminary cost estimates [108]. The steam price, which is intrinsically linked to natural gas price, is set to vary around its actual price +/- 25% (+/- 5 €/MWh). The interest rate is allowed to be located anywhere between 5% and 10%. Another parameter is introduced in this section, which is a CO_2 tax for each ton of CO_2 emitted. A reduction in energy consumption automatically leads to a reduction of CO_2 emissions. Depending on the carbon price, additional benefits will come from the implementation of energy saving opportunities.

NB: When electricity consumption or production is involved in the energy saving opportunity, the electricity price variation should also be taken into account in the sensitivity analysis.

Results of the sensitivity analysis are displayed on Figure 4.12 for the three different options. The maximum and minimum payback time can be read in the legend on the right, while the net present value variation is seen on the left vertical axis. The value range of the interest rate for each point can be known thanks to its shape.

As expected, the trend is similar for each opportunity. High PBT and low NPV are linked to high interest rates and low steam price and carbon tax. On the contrary, when energy costs and carbon tax are high, the profitability of the energy saving opportunities is at the highest. While these results seem straightforward they highlight the need to consider the uncertainty on both sides of the thermo-economic analysis, to understand how the economic indicators vary according to the financial conditions of the system.

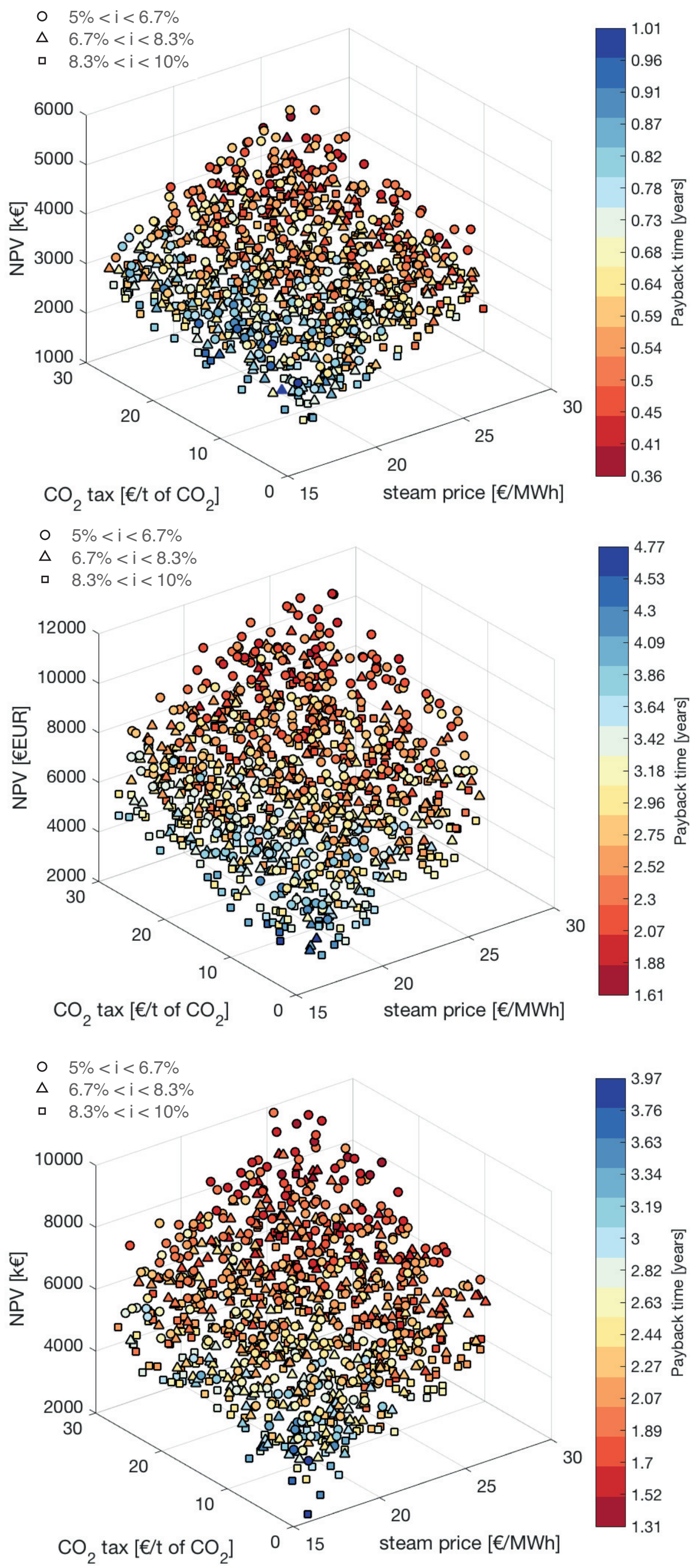


Figure 4.12 – Sensitivity analysis results for the feed preheating (top), heat exchanger network redesign (middle) and mechanical vapour recompression (bottom). Results for 1000 evaluations.

4.3 Study of a new heat transformer

During this thesis, the production of High Density Polyethylene (HDPE) via the slurry process has been investigated, among other polymerisation processes. The study of the composite curves of the system lead to the observation that a significant amount of heat is released by the exothermic reaction below the pinch point, currently being evacuated through a cooling water loop itself cooled down by the cooling water network (see Figure 4.13). This heat load is defined as residual waste heat since it is an unavoidable release by the production process and is in excess below the pinch point [126].

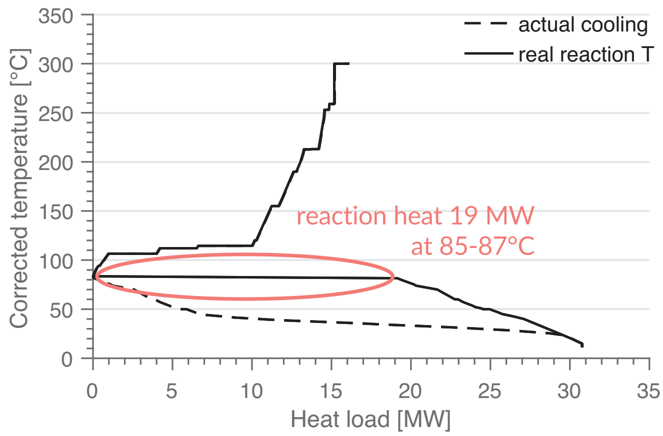


Figure 4.13 – Grand composite curves of the HPDE slurry process when the initial cooling water and real reaction temperatures are considered.

When the current equipment layout is put aside and the real temperature of the reaction medium is considered, the exothermicity of the polymerisation reaction offers a very interesting potential for waste heat valorisation via heat pumping.

In the HDPE slurry process, the reaction heat is released at around 80°C-90°C and low-pressure steam is injected in the stripping section located near the reactors to remove the solvent. The minimum steam pressure for the stripper is 1.6 bar, corresponding to a saturation temperature of 113°C. Low-pressure steam is also consumed at other locations in the plant. The temperature lift of the heat pump has then to be around 40-50°C, depending on the reaction temperature and the temperature difference between the working fluid and the process streams.

The total heat of reaction removed by cooling water is around twice the heat that has to be delivered to the process by low-pressure steam. Instead of using only around half of the heat of the reaction to produce low pressure steam, the rest of the heat could be used to produce directly the mechanical work driving the cycle compressor. This system, which is called a heat transformer, has been investigated in this thesis and applied to the HDPE slurry process in particular.

This section is organised as follows. A literature review on existing waste heat valorisation systems is first carried out, identifying which alternative technologies are related to and competing with the proposed heat transformer. This new technology is then described in a general way before detailing its special features when it is integrated with the HDPE slurry process. The last section investigates the use of other working fluids for the heat transformer and discusses the actual technical limitations of the system and its possible application to other similar processes.

4.3.1 Heat pumping technologies overview

When industrial waste heat is identified, several technologies can be used to valorise this heat, as heat itself at a higher temperature, as electricity or as cold. Main waste heat to heat and waste heat to electricity technologies are depicted on Figure 4.14. Three main technologies are used as active waste heat valorisation to generate useful heat: absorption heat pumps (AHP), absorption heat transformers (AHT) and mechanical vapor compression heat pumps (MVC). The first two technologies rely on the heat of absorption/desorption and are almost entirely thermally driven, since electrical input is only required at the level of the pumps. On the contrary, electricity is required to drive the compressor in mechanical vapour compression cycles. A MVC cycle can be coupled with an organic Rankine cycle (ORC) in order to eliminate the external input of electricity [127, 128]. This system, also referred to as ORC-HP, is called a thermally driven heat pump.

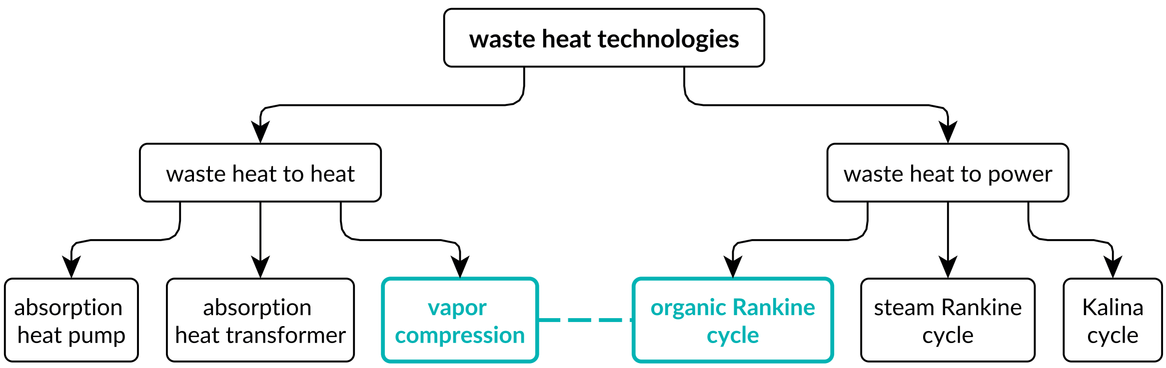


Figure 4.14 – Overview of active waste heat recovery technologies for heat and electricity production (from [3]). The two highlighted technologies are the ones involved in the proposed heat transformer.

The pressure-temperature diagram for each cycle (AHP, AHT, ORC-HP) is depicted in Figure 4.15. In addition to these systems, the P-T cycle of the new heat transformer proposed in this thesis is also represented (d). While all these cycles are waste heat to heat technologies, they differ on several aspects: (1) on the working fluid type, (2) on the number of pressure levels and (3) on the temperature and pressure levels of the heat sources and sinks.

AHP and AHT both use a working fluid pair composed of a refrigerant and an absorbent. The absorption releases heat ($\dot{Q}_{AB}$) as well as the refrigerant condensation ($\dot{Q}_{CO}$). Inversely, desorption ($\dot{Q}_{GE}$) and refrigerant evaporation ($\dot{Q}_{EV}$) require a heat input. The most widely used refrigerant/absorbent pairs are water-lithium bromide (H_2O-LiBr) and ammonia-water (NH_3-H_2O) [129]. The ORC-HP and proposed heat transformer use only a refrigerant as working fluid, which can be a pure fluid or a mix of fluids. The core of the two systems is the turbo-compressor, where the heat pump compressor is driven by the mechanical work generated in the turbine.

The second difference concerns the number of pressure levels. Absorption cycles usually operates between two pressure levels, while the other cycles require three pressure levels.

The last difference is the temperature levels at which waste heat is recovered and the useful heat is produced. AHP and ORC-HP cycles both have a heat input at high and low temperatures (T_H and T_L), while useful heat is delivered at the medium temperature level (T_M). AHT and the proposed HT cycle receive heat at medium temperature, lift a fraction of this heat to a higher temperature level while the remaining heat is evacuated at a lower temperature level.

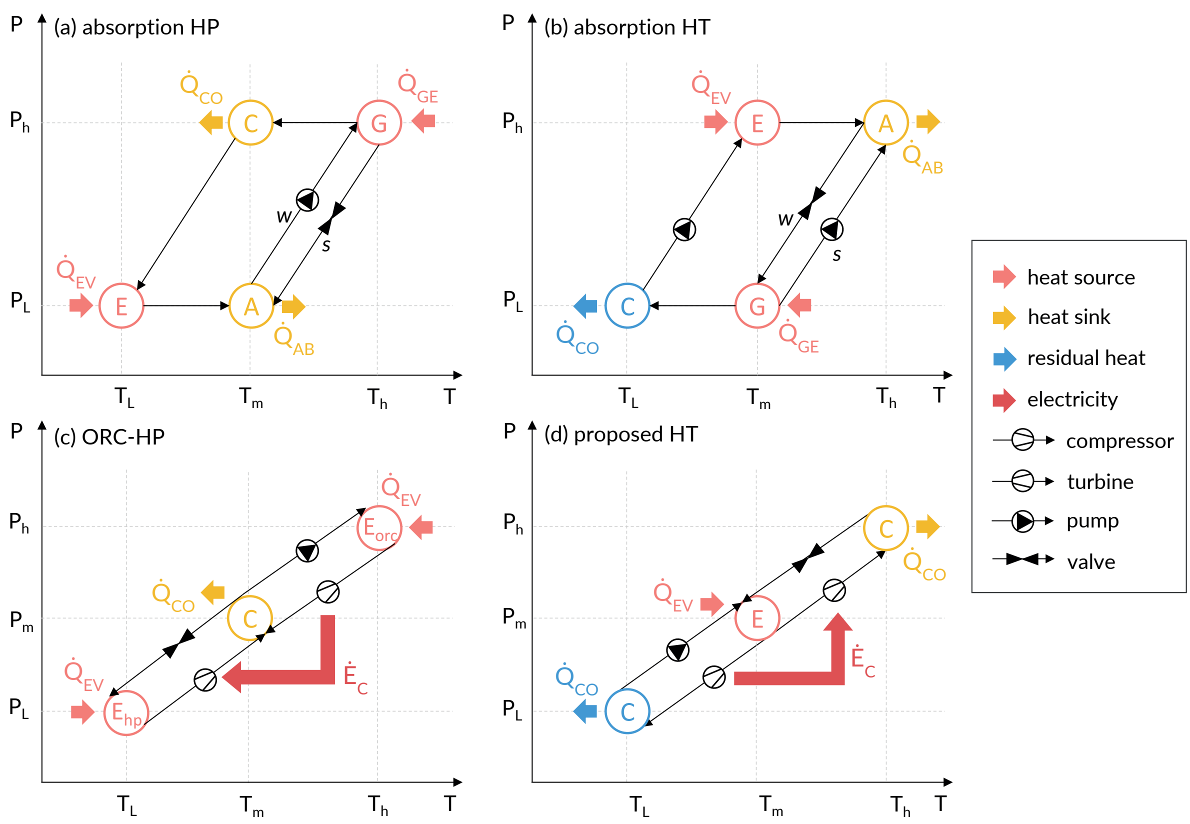


Figure 4.15 – P-T representations of an (a) absorption heat pump, (b) absorption heat transformer, (c) ORC-HP and (d) of the proposed heat transformer (reversed ORC-HP).

Based on this last observation AHP (a) and ORC-HP (c) are referred to as thermally driven heat pumps (TDHP), whereas AHT (b) and the proposed heat transformer (d) are thermally driven heat transformers (TDHT). A heat transformer is then a system which can deliver heat at a higher temperature than the temperature of the heat source, without an external import of electricity [130]. The proposed heat transformer is the reverse operation of the original ORC-HP cycle. Figure 4.16 represents both cycles in a T-s diagram where this can clearly be seen.

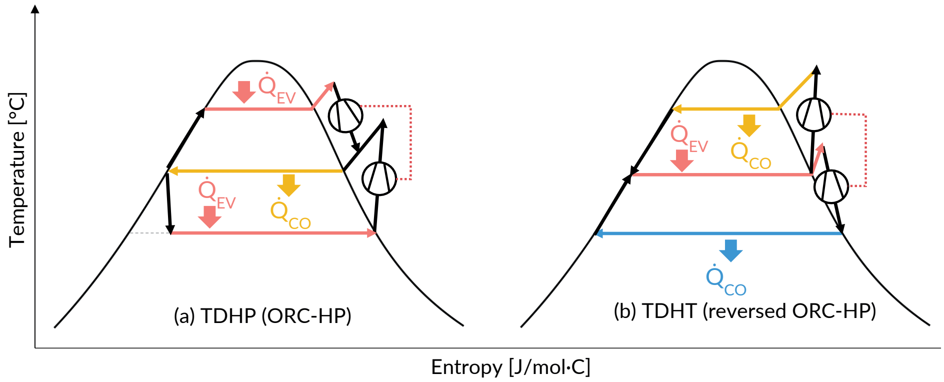


Figure 4.16 – T-s diagrams of (a) the ORC-HP cycle, (b) proposed heat transformer

The temperature levels of thermally driven heat pumps make them more suitable for domestic heating application, coupled with solar energy or boilers. In the petrochemical industry, the excess heat at medium temperature and the need of heat above the pinch point make thermally driven heat transformers and traditional heat pump cycles the technologies of choice.

4.3.2 System description

The proposed thermally driven heat transformer evaporates a working fluid at medium temperature and pressure and compresses part of it to a higher pressure, using the mechanical power produced by the expansion of the other part of the fluid into a turbine. The general layout of the HT is depicted on Figure 4.17.

Working fluids are classified in three categories: wet, dry and isentropic fluids [131]. This classification is based on the slope of the saturation curve on a T-s diagram. If it is positive, the fluid is defined as dry, if it is negative, the fluid is wet. For isentropic fluid the slope is infinite. A wet fluid in saturated vapour state will start to condense with isentropic expansion, whereas a dry fluid at the same state will start to condense with isentropic compression, as it can be seen on Figure 4.18. Only isentropic fluids will remain in the vapor state for both pressure changes.

Depending on the fluid characteristics and cycle temperature and pressure levels, a superheater can be added before the turbine or the compressor and a preheater before the evaporator. The superheater has to be supplied by the heat released from the high-pressure condenser since the superheating temperature is above the waste heat temperature.

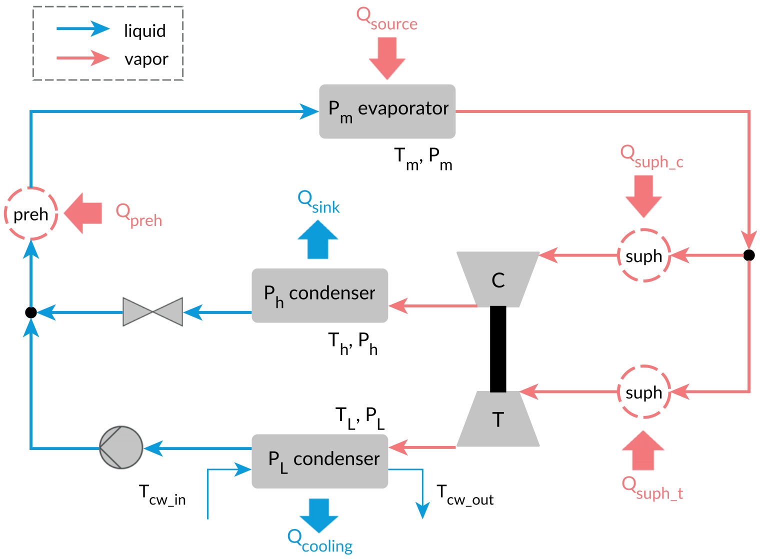


Figure 4.17 – Schematic representation the heat transformer.

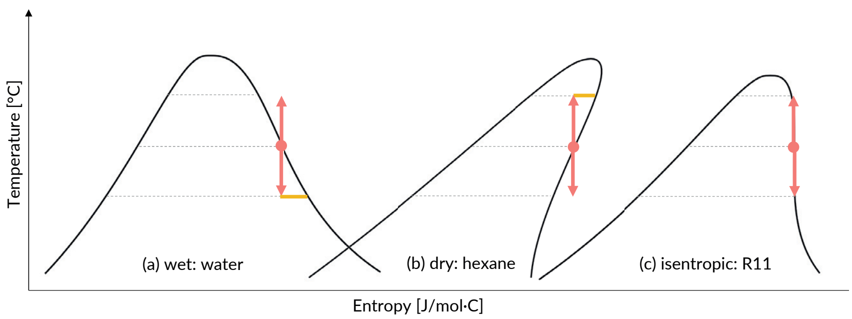


Figure 4.18 – T-s diagrams of a (a) wet fluid, (b) dry fluid and (c) isentropic fluid, and the effect of isentropic expansion or compression from the saturated vapour state.

4.3.3 Integration with polymer production

The integration of the proposed heat transformer on the HDPE slurry process defines the temperature levels for the evaporator and the two condensers of the cycle.

With a reaction heat available around 85-87°C, the fluid evaporation temperature is set to 80°C. The goal of the heat transformer is to produce low pressure steam with a minimum pressure of 1.6 bar, corresponding to a saturation temperature of 113°C. The condensation temperature of the high-pressure condenser is set to 120°C. Finally, the condenser temperature is limited by the use of water cooling with an outlet temperature of 20°C. The condensation temperature of the low-pressure condenser is set to 25°C. In summer, depending on the location and climate, cooling water temperature can increase up to 30°C. The lower temperature level of the cycle will then also be increased, implying a higher split fraction of the fluid towards the turbine side.

The choice of the working fluid is made based on the actual solvent used for the polymerisation reaction. The polymer being in suspension in hexane, this fluid was selected for the heat transformer. In this way, there are no safety issues related to potential leakage and the product is readily handled and available on the site.

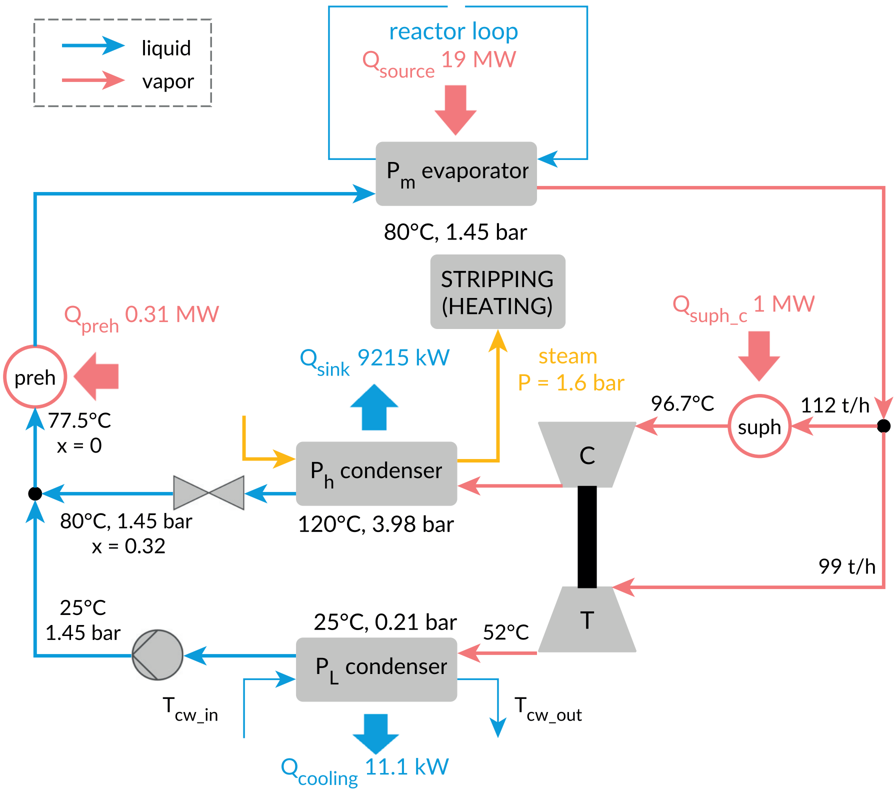


Figure 4.19 – Schematic representation the heat transformer integrated with the HDPE slurry process, using hexane as working fluid.

With hexane as working fluid, the low, medium and high pressure levels are respectively 0.21 bar, 1.45 bar and 3.98 bar. The turbine and compressor pressure ratios are then 6.9 and 2.7. Since it is a dry fluid, a superheater is required before the compressor. The superheated temperature is defined as the minimum temperature required to be able to stay in the vapour state at the outlet of the compressor. With a compressor isentropic efficiency of 80%, the fluid temperature before entering the compressor is of 96.7°C. Pressure drops in heat exchangers are neglected. A schematic representation of the integrated heat transformer using hexane is shown on Figure 4.19 and a screenshot of the Belsim Vali model is available in Appendix D.

System performance

The integrated composite curves of the proposed heat transformer using hexane can be seen on Figure 4.20. The three plateaus from the highest to the lowest temperature correspond to the fluid condensation to produce low pressure steam, the fluid evaporation receiving the reaction heat and the fluid condensation at low pressure, cooled down by cooling water. The small segment between the pinch point and 100°C corresponds to the superheating, and the other one starting at 50°C is the desuperheating after the turbine.

The integration of the heat transformer to the polymerisation process would decrease the low-pressure steam consumption by 8.1 MW, which corresponds to a **50% decrease** in hot utility consumption.

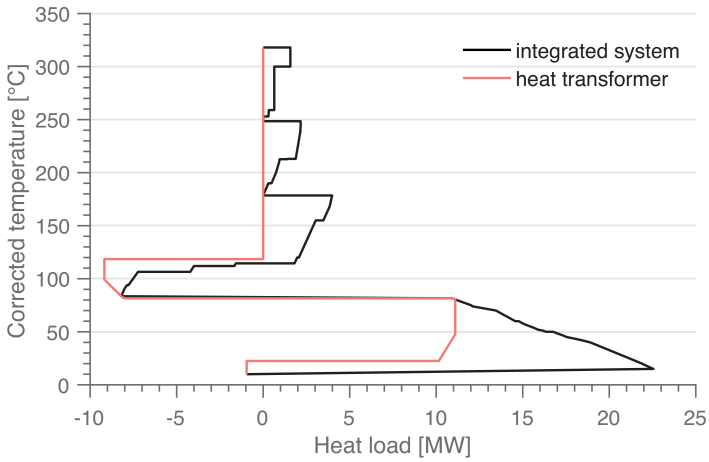


Figure 4.20 – Integrated composite curves of the hexane heat transformer with the rest of the system

The efficiency of a heat pump is denoted by its coefficient of performance (COP). The maximum COP of a heat pump is given by Equation 4.1, where T_{sink} and T_{source} are respectively the temperatures of the heat sink (113°C) and the heat source (85°C) in degree Kelvin.

$$COP_{HP,th} = \frac{T_{sink}}{T_{sink} - T_{source}} \tag{4.1}$$

$$COP_{HP,real} = \frac{\dot{Q}_{sink}}{\dot{E}_{in}} = COP_{th} \cdot \eta \tag{4.2}$$

The observed COP is determined thanks to Equation 4.2, by calculating the ratio between the heat load delivered at high temperature ($\dot{Q}_{sink}$) and the electrical input ($\dot{E}_{in}$). For the proposed heat transformer the electrical input corresponds to the turbocompressor shaft power, which is of 1320 kW. The theoretical and real COP are then respectively of 13.8 and 6.9, giving a system efficiency of the heat pump part of $\eta = 0.5$.

The overall heat transformer efficiency (COP_{HT}) has been defined as the ratio of the useful heat produced ($\dot{Q}_{sink}$) over the heat entering the cycle, which corresponds to the evaporator ($\dot{Q}_{source}$), superheater ($\dot{Q}_{suph_c}$) and preheater ($\dot{Q}_{preh}$) heat loads. It is expressed by Equation 4.3. Based on values from Figure 4.19, the COP of the hexane HT is equal to 0.45.

$$COP_{HT} = \frac{\dot{Q}_{sink}}{\dot{Q}_{source} + \dot{Q}_{suph_c} + \dot{Q}_{preh}} \tag{4.3}$$

This efficiency can be compared with the direct competing technology which are absorption heat transformers, for which the COP is determined by Equation 4.4.

$$COP_{AHT} = \frac{\dot{Q}_{AB}}{\dot{Q}_{GE} + \dot{Q}_{EV}} \tag{4.4}$$

Table 4.9 presents the comparison of the performance of the hexane heat transformer with two recent studies involving AHT with similar temperature levels for the three main heat exchangers (i.e. condenser, evaporator and absorber, which is the high pressure condenser in the proposed HT). The results show that the COP of the hexane HT is slightly lower than the one of AHTs for the temperature levels considered in this study. For a higher temperature lift, the efficiency seems to be lower. Care has to be taken with these literature values since only a few systems with the required temperatures were available for comparison.

Improvement of the HT performance while keeping the same temperatures levels can only be realised by changing the fluid type. Otherwise, the temperatures of the heat sink and source should respectively be decreased and increased. A comprehensive review on absorption heat transformers with different configurations, temperature levels and working fluids can be found in [130].

Table 4.9 – Comparison of system COP with AHT examples.

	T_{evap} [°C]	T_{cond} [°C]	$T_{abs} = T_{cond,hp}$ [°C]	working pair	COP [-]
AHT Guo et al. [132]	74	25	123	H_2O-LiBr	0.45
HT	80	25	120	-	0.45
AHT Horuz Kurt [133]	80	25	130	H_2O-LiBr	0.48
HT	80	25	130	-	0.40

Open cycle configuration

Another option which was identified to recover the polymerisation heat of reaction would be an open cycle heat transformer, using water as working fluid. In this system, water below atmospheric pressure is evaporated thanks to the heat of reaction. Around half of the saturated steam produced is expanded in a condensation turbine coupled with a compressor to produce 1.6 bar steam, which can be directly injected into the process. A water make-up has then to be preheated to be mixed with the water coming back from the turbine side, before entering again the evaporator.

This open heat transformer is represented in Figure 4.21, with the Vali model available in Appendix D. Such configuration has the advantage of directly using the steam from the compressor in the system, which removes the temperature difference between the working fluid and the steam to be produced. As a result, the system is much more efficient for the same final purpose, with a coefficient of performance of 0.55.

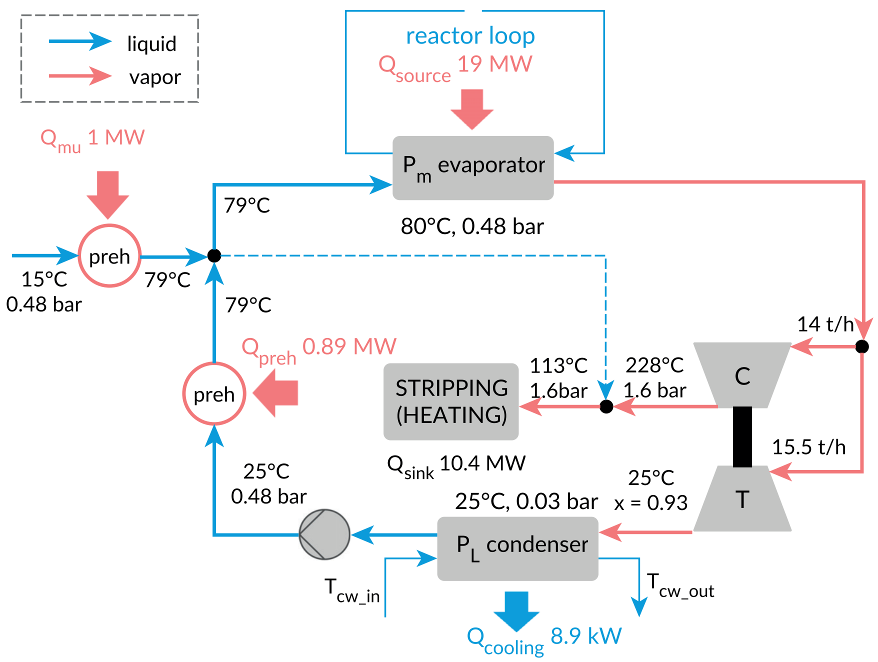


Figure 4.21 – Schematic representation of the integrated open cycle heat transformer using water.

The major disadvantage and technical difficulty is the medium pressure level of 0.48 bar of the evaporator, which requires to operate the reactor cooling below the atmospheric pressure. The integrated composite curves of the open heat transformer can be seen on Figure 4.22. Compared to Figure 4.20 with the closed HT using hexane, the integration of the open heat transformer with the rest of the process eliminates entirely the need for low pressure steam, which is of 10.1 MW. The total hot utility consumption would be **decreased by 63%**.

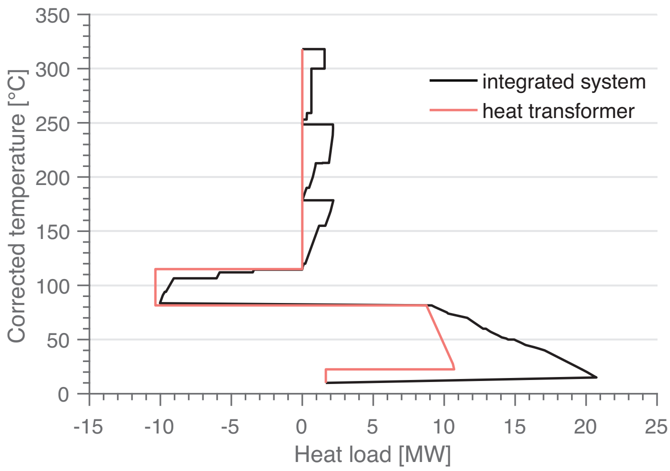


Figure 4.22 – Integrated composite curves of the open heat transformer.

4.3.4 Perspectives

Working fluid selection

For fixed cycle temperatures, the coefficient of performance of the closed HT can be improved by changing the working fluid type. A significant body of work can be found in the literature on the optimal fluid selection for organic Rankine cycles [134, 135, 136].

Table 4.10 – Heat transformer COP and pressure levels for different working fluids.

Fluid	$\dot{Q}_{in}$ [kW]	$\dot{Q}_{sink}$ [kW]	COP [-]	P_h [bar]	P_m [bar]	P_l [bar]	$P_{ratio,T}$	$P_{ratio,C}$
water	1022	484	0.47	2	0.47	0.03	15	4.2
ebenzene	1039	484	0.47	0.64	0.17	0.01	13	3.8
benzene	1025	471	0.46	3	1	0.13	8	3
toluene	1024	469	0.46	1.3	0.39	0.04	10	3.4
R141b	1022	461	0.45	10	4.2	0.78	5.4	2.5
hexane	1069	477	0.45	4	1.45	0.21	7.1	2.8
R113	1054	468	0.44	6.8	2.6	0.45	5.9	2.6
R11	1026	453	0.44	12	5.2	1.1	4.9	2.4
R123	1028	450	0.44	12	4.9	0.91	5.4	2.5
pentane	1055	461	0.44	9	3.7	0.68	5.4	2.5
isopentane	1055	456	0.43	11	4.6	0.91	5	2.4
R245ca	1040	444	0.43	14	5.7	1	5.7	2.5
ammonia	1071	451	0.42	91	41	10	4.1	2.2
R245fa	1010	417	0.41	19	7.9	1.5	5.3	2.4
butane	1005	412	0.41	22	10	2.4	4.2	2.2

The proposed heat transformer being at its early theoretical development stage, only a few common working fluids were investigated in this study. The best fluid for the proposed heat transformer should maximise the electricity production from the ORC cycle (turbine side) while also being suitable for the heat pump cycle (compressor side). The maximum pressure ratios for the turbine and compressor sides were respectively set at 7 and 4.

Results for 15 working fluids can be seen in Table 4.10, including hexane. For the four best fluids in terms of COP, the pressure ratio on the turbine side is considered too high for the turbocompressor to work effectively. Hexane is then one of the best working fluids from this specific list, together with R141B, with a COP of 0.45 and turbine and compressor pressure ratios respectively of 7.1 and 2.8.

Technical limitations

The major limitation for the development and implementation of the proposed heat transformer is of technical nature. Changing the heat removal of the reactor, currently realised with a cooling water loop (30-40°C) itself cooled down by cooling water, and replacing it by the evaporation of a fluid at 80°C implies several considerations.

Temperature control is of major importance in polymerisation processes since it influences the molecular structure and composition of the polymer. Also, the temperature of the reaction medium might not be constant inside the reactor. The use of cooling water eases the cooling of the reactor since the flow can quickly be changed and adjusted and no phase change is involved. Heat removal via the evaporation of a fluid is more technical than water cooling, and the proposed system also implies a much smaller temperature difference between the reaction medium and the cooling fluid.

These two aspects directly impact the design of the reactor itself currently being a loop reactor made of long vertical jacketed sections. Further investigation is required to estimate the technical feasibility of the proposed closed (and open) heat transformer.

Application to other processes

The heat transformer was initially developed based on the temperature-enthalpy profile of the HDPE slurry process. It can however be applied to other processes. Any chemical production process releasing a significant amount of heat below the pinch point (70-100°C) and having steam requirements above (with a maximum temperature lift of 40°C) could theoretically integrate the proposed heat transformer for heat pumping.

4.4 Conclusion

This last chapter corresponds to the last step of the methodology. It aims at answering the following research questions:

How to generate energy savings opportunities in a systematic way from the production process to the integration of utilities and how to properly evaluate their profitability?

What are the available technologies to recover waste heat?

The two first steps of the methodology provide information on the energy efficiency and the maximum heat recovery potential of the system. Based on the shape of the grand composite curve and the identification of penalising heat exchangers, this last step aims at generating a list of energy saving opportunities to improve the energy efficiency of the site, thereby decreasing its energy consumption and CO_2 emissions.

A bottom-up approach is introduced, derived from the onion diagram for chemical process design, which defines optimisation layers for the **generation of EnSO's in a systematic way**. It starts from the modification of process operating parameters towards the last layers which consist of the optimisation of the energy conversion and utility system and the development of maintenance and operation strategies. A case study is used to illustrate the identification of EnSO's.

A **thermo-economic analysis** is carried out for each opportunity, estimating on the one hand the investment cost and on the other hand the expected savings associated to the energy consumption reduction. The uncertainty on the capital costs and the main parameters influencing the operating cost savings is briefly studied, showing how the economic indicators used for decision criteria and risk evaluation are varying according to different sets of economic parameters.

Finally, this chapter highlights the potential for heat pumping in chemical processes, especially when exothermic reactions are taking place. It introduces a **new heat transformer** system made of a mechanical vapour compression cycle coupled with an organic Rankine cycle to generate the mechanical work which drives the compressor. This system has the characteristic of producing both higher temperature heat and mechanical work from the waste reaction heat, rather than importing electricity from the grid. It is shown how its integration to a polymerisation process can reduce the steam consumption by 50 to 63%.

Conclusion

Overview

- Summary of the results and main contributions of the thesis
- Future perspectives

Results summary

The increase of energy efficiency at existing industrial sites has been recognised by the International Energy Agency as one of the key elements to mitigate greenhouse gas emissions of the industry sector [12]. Since 2012, the European Union pushes into this direction through the Energy Efficiency Directive (EED) [4]. This directive regulates the entire energy chain and is part of Europe's strategy to reach its ambitious energy targets for 2030 (35% of energy efficiency increase, endorsed by the European Parliament in plenary sitting on January 17th, 2018 [10]).

The EED requires regular energy audits to be carried out for large industrial companies and promotes the implementation of energy measures and energy management systems. In both cases, it means that the energy consumption should be understood, the energy performance evaluated and energy saving opportunities generated and quantified.

The focus of the thesis is on the chemical and petrochemical industry. This sector is responsible for 19% of Europe's industry final energy consumption [17]. The analysis of the literature revealed a lack of detailed and appropriate methods to carry out energy review on (petro)chemical sites, which adds up to two other important issues that are the availability and reliability of data and the lack of time for a proper analysis.

Chapter 1: Methodology for energy reviews

The first contribution of this thesis corresponds to the development of a systematic methodology for detailed energy reviews in the chemical and petrochemical sector, bringing an answer to the following research question:

How to carry out an energy review covering the whole energy chain and enabling the identification of energy savings opportunities at an adequate level of detail?

The proposed methodology comprises three main steps: 1) the energy consumption analysis 2) the energy consumption reduction targeting and 3) and the achievement of the energy consumption reduction. It makes use of state-of-the-art tools and techniques (e.g. statistical analysis, data reconciliation, pinch analysis) applied in a logical and ordered way, and enables the realisation of detailed energy reviews in compliance with existing regulations and standards in the field. Figure 4.23 extends Figure 2 presented in the introduction, showing which step(s) of the proposed methodology addresses the ISO 50001 energy review requirements.

Although the external context for the thesis relates to the European regulatory context, this methodology for energy reviews in the framework of energy audits and energy management systems is valid worldwide. Energy efficiency is a key element to reduce the environmental impact of industrial activities and reduce the consumption of energy resources.

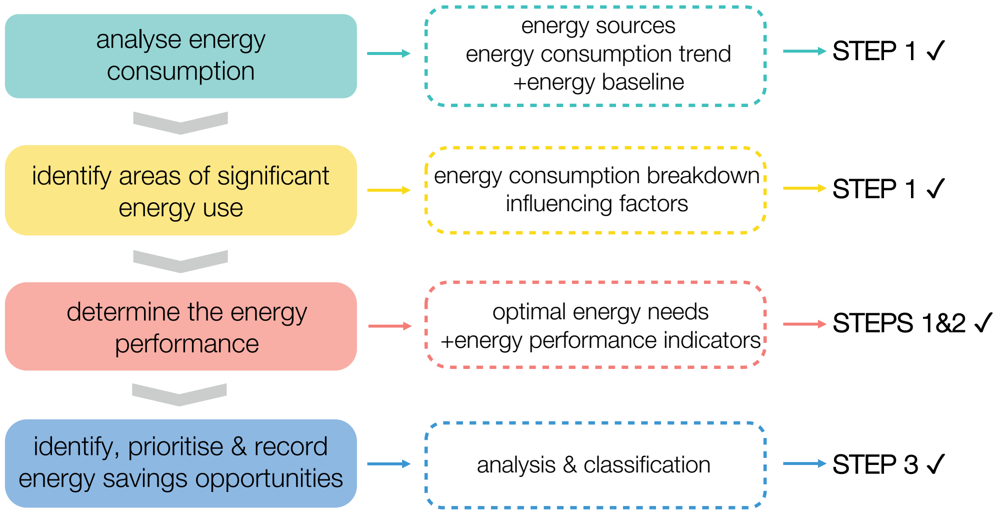


Figure 4.23 – Key requirements of an energy review as defined in ISO 50001 and link to the steps of the methodology.

At each substep of the methodology, open questions and limitations of the existing tools are raised and investigated in the other chapters of the thesis. They are summarised on Figure 4.24 next to the substep to which they belong, together with the different contributions of this thesis to answer to these questions.

The proposed methodology combines a top-down approach at the level of the energy consumption analysis, to characterise the system down to the process and equipment level, and a bottom-up approach to generate the energy savings opportunities starting from this level to the energy conversion system. It includes all the requirements for a proper energy review and can be briefly summarised

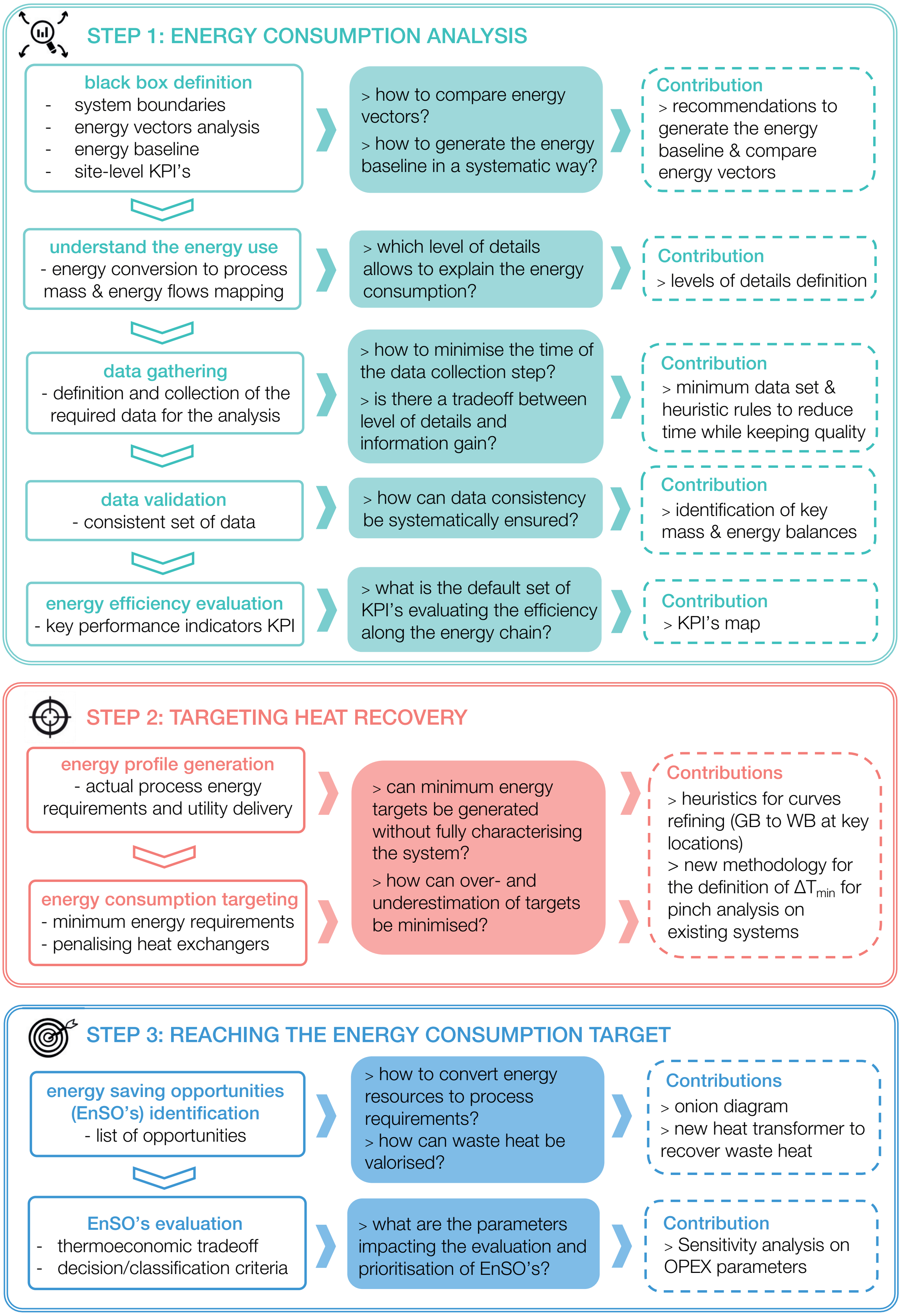


Figure 4.24 – Overview of methodology and thesis contributions

as follows.

In the first step, the energy flows entering the system boundaries are identified and quantified and the energy baseline is generated. From the characterisation of the black box level, the energy consumption is then mapped by gradually entering into the site and processes details in order to spot where and why energy is consumed. The required data to be able to analyse and evaluate the energy efficiency of the system, as well as to carry out pinch analysis in the second step, is collected.

Raw data is then checked and validated to ensure that the results of the analysis can be trusted. Data reconciliation and/or mass and energy balances can then be used to check the consistency of data. Finally, key performance indicators are developed to characterise the energy efficiency of the system, which can also be used for monitoring purposes.

From the data acquisition, leading to a consistent list of streams, pinch analysis in carried out. This second step determines the potential for heat recovery via heat integration and defines minimum energy consumption targets. Based on these results, a list of energy saving opportunities is generated in the third step, aiming at getting as close as possible to the heat integration targets and improving the overall energy efficiency of the system. The level of detail of the energy review allows to identify options covering the entire energy chain, from the process operation to the energy conversion system optimisation. Each opportunity is then evaluated by a thermo-economic analysis.

Chapter 2: Energy consumption analysis

The major issues which were identified at the level of the energy consumption analysis of large industrial sites are the lack of time, the availability and reliability of data and the need for a systematic approach. This lead to the formulation of the following research question:

How to analyse and characterise the efficiency of the energy chain down to the end-use consumers, in a suitable and reliable manner, while keeping the required time for data collection and complexity of the analysis at an acceptable level?

To characterise and evaluate the energy efficiency from the site raw energy consumption down to the final use of energy, a top-down approach is followed with well-defined intermediate level of details (i.e. black box, site map, process block flow diagram and process flowsheet). This approach allows to gradually enter into the site details, track mass and energy flows, to ultimately understand where and why energy is consumed and how efficiently it is done.

At the level of the system boundaries (black box), recommendations for energy vectors characterisation and comparison are provided, as well as guidelines to properly establish the energy baseline. This is important since the energy baseline serves as reference for the evaluation of the energy saving opportunities.

In order to reduce the time required for data collection, this chapter introduces strategies and heuristics (i.e. minimum data set, Pareto principle, hot streams targeting) to answer to the three key questions preparing the input for the pinch analysis: who are the energy consumers? what is the energy used for? and how much each end-usage is consuming? While these guidelines were proven to be very useful in application, it is not bulletproof in all situations. If significant data is missing or when the measurement system is in poor condition, data gathering remains a difficult step.

The reliability of data in energy reviews is of major importance. In order to ensure the validity of data when data reconciliation cannot be applied, key mass and energy balances have been developed at the site-level but also for each main entity of the site map (i.e. energy conversion units, steam network, process units). This consistency check allows to quantify energy flows and determines the order of magnitude for losses. A set of key performance indicators was proposed at the same levels as for the consistency check in order to evaluate the energy efficiency of the system. The balances and KPI's defined in this chapter can be applied in the majority of cases. For sites or production processes with specific characteristics having an impact on the energy consumption, complementary ones could also be developed.

This chapter does not present novel scientific contributions but rather concentrates on providing guidelines, recommendations and best practices to analyse the energy consumption of an industrial site, based on the needs identified in the literature and observed empirically.

Chapter 3: Targeting heat recovery

The research question of the third chapter was expressed as follows:

How to generate economically feasible minimum energy consumption targets in pinch analysis, with the minimum level of detail for streams definition?

The grey-box default level for pinch analysis allows to quickly obtain the temperature-enthalpy profile of the process energy requirements, without spending too much time on data collection. The first energy targets obtained from the heat cascade can however be investigated further to identify additional potential for heat recovery. This chapter provides additional heuristic rules to refine the initial list of process hot and cold streams, targeting "white box" process streams in the area of the pinch point.

The main research contribution of the third chapter concerns the novel methodology for the definition of the minimum approach temperature in pinch analysis when it is carried out on existing systems. Current methods to determine the ΔT_{min}, such as the area efficiency or the use of typical values, show several limitations and often lead to an over- or underestimation of the heat recovery target.

Instead of generating a single optimum ΔT_{min} for the system, the thermo-economic trade-off for heat recovery is carried out for each stream individually along its temperature-enthalpy profile. This approach enables the use of several equipment cost laws, depending on the heat exchanger to be installed, and utility costs depending the temperature levels of the streams. It has the advantage of refining the targeting step and providing more reliable energy integration targets at the early stage, prior to the generation of the heat exchanger network.

Further work needs to be carried out to refine and validate the proposed methodology. The definition of the slope of the fictive stream in the generation of the corrected profiles might be adapted depending on the characteristics of the system. The use of a flat stream will increase the temperature gradient and lead to lower ΔT_{min} compared to parallel streams. A method to generate an intermediate slope can be an option.

A recurring observation made during this thesis is the difficulty to obtain good cost estimates for equipment. Available costing methods in the literature show very different results for the same heat exchanger, and most of them are limited regarding the heat exchanger type, material and pressure factors. Moreover, when capital cost estimations are presented to site managers and engineers, they are often judged insufficient to cover all the indirect costs linked to the installation, although factors to account for these additional expenses are included in literature cost estimates. More accurate and up-to-date costing methods should therefore be developed as this has a major impact on the energy targeting step, but also on the energy saving opportunities economic evaluation.

Chapter 4: Reaching the energy consumption target

The last chapter provides guidelines to generate and evaluate energy saving opportunities and thereby answers the following research question:

How to generate energy savings opportunities in a systematic way from the production process to the integration of utilities and how to properly evaluate their profitability?

It is shown how a bottom-up approach following ordered optimisation layers can generate opportunities for energy efficiency improvement, starting from the modification of the process operating parameters towards the optimisation of the energy conversion and utility distribution system. The best combination of options was presented for a case study. Although the proposed list of opportunities was considered as the optimal one with respect to energy and exergy efficiencies, other sub-optimal alternatives should also be studied and evaluated, in the case where the optimum scenario is not implemented due to diverse reasons (e.g. safety, technical, incorrect estimations, process modifications). In this way, a complete portfolio is available for decision making, based on the thermodynamic and economic characteristics of the system.

Heat pumping opportunities to recover waste heat below the pinch point were often identified in the industrial sites studied in the framework of this thesis. More specifically, polymerisation reactions such as the HDPE slurry process releases a significant amount of heat in the temperature range of 80-90°C, below the pinch point of the global process. A new heat transformer was proposed and described in this chapter, together with its integration with the HDPE slurry process. The proposed system is made of a mechanical vapour compression cycle, coupled with an organic Rankine cycle which generates the mechanical power for the compressor. The same working fluid is evaporated, split and a fraction is compressed to a higher temperature level thanks to the expansion of the rest of the fluid. This system has the advantage of producing the required mechanical power directly from the waste heat rather than importing electricity from the grid. Its potential for thermal energy consumption reduction of the site was evaluated from 50% to 63% depending of the configuration of the heat transformer.

Further research on the technical and economic aspects related to the development and implementation of this heat transformer is required to evaluate its feasibility and relevance, since heat removal in polymerisation reaction is critical to ensure the product quality.

Methodology application

The proposed methodology was developed, tested and refined on 10 different petrochemical sites, enabling a comprehensive analysis of their energy efficiency and leading to the identification of promising energy saving opportunities to increase the energy efficiency and reduce the environmental impact of their production.

Results for 7 of the 10 industrial sites studied in this thesis are presented in Figure 4.25. Considering the three other industrial sites, two featured batch processes. For these specific case studies, significant potential for heat recovery through better scheduling of batches and optimisation of thermal storage was found, but not investigated further due to the lack of time. The main objective for these two sites was to generate the required results and data for ISO 50001 certification. The last industrial site showed no potential for heat recovery, although additional operational cost benefits were found through the maximisation of low-pressure steam and hot water generation to export to the neighbouring sites.

In the upper graph of Figure 4.25, the total height of each bar corresponds to the maximum yearly operating cost savings determined from the pinch analysis outcomes. The lower graph shows how these operating cost savings translate into relative savings in the energy bill related to the thermal power consumption. The contributions of energy saving opportunities to reaching this target can be seen for each site. The size of the circles represents the order of magnitude for CO_2 emissions reduction.

Apart from site A, for which the pinch analysis was carried out at the white box level, the default grey box level was applied to all the other sites. The lower operating cost savings obtained for sites D and E can be explained on one side by the low heat recovery potential typically found with this type of processes (combined with a lower share of thermal power consumption in the total end-use consumption) and the use of coal to produce steam, which is cheaper than natural gas.

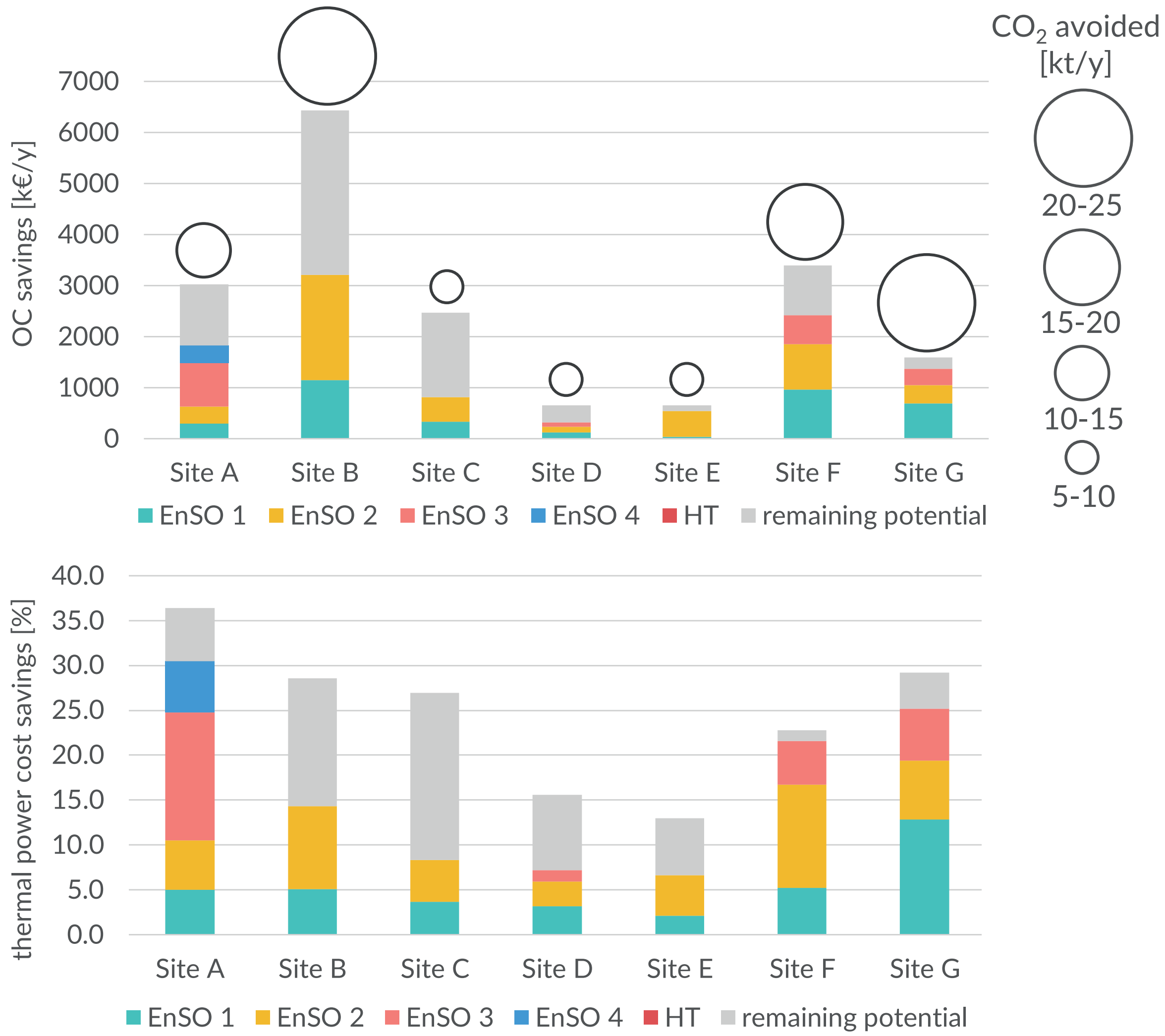


Figure 4.25 – Results of the application of the methodology on different industrial sites.

Perspectives

In addition to the previously mentioned recommendations for further research work related to the thesis contributions, two main complementary lines of research have been identified bringing exciting challenges.

The first one relates to energy consumption monitoring. The energy review covers mostly the energy consumption analysis and the energy efficiency improvement through the identification of energy saving opportunities. The link with energy consumption monitoring is made at the level of the key performance indicators (2.5) and the specific energy consumption models (2.1.4). These two elements can be implemented online for a follow-up and control of the plant operation, as it was investigated in the framework of the MORE European project [48]. However, a recurring observation from the numerous case studies of this thesis is that production solely do not explain energy consumption variation. In several cases, the utility consumption was highly varying for the same production output. In this case, other factors influence the energy consumption, such as the catalyst condition, the reflux ratio, reactants and products composition, etc.

Monitoring strategies could be developed based on the generation of specific energy consumption models including the impact of all influencing factors at different levels (e.g. units, process blocks or major consumers). A powerful combination of modelling, data reconciliation and statistical analysis can be used to generate such surrogate models of production processes from archived data. These models could then be tested and refined by implementing them in real time and be finally used for monitoring and detecting of deviations from normal/expected behaviour. The CoPro European project [57], started in November 2016, includes partly this research by providing tools for site optimisation which should be based on process operation models, thereby including units energy consumption and production models.

The second line of research adds the resource efficiency to the energy efficiency. Production sites are often embedded in larger industrial clusters, either with companies active in the same industrial sector or a different one. By looking at resources efficiency (e.g. reduction of water consumption and waste production, waste valorisation), additional opportunities can be identified across sectors to reduce the environmental impact and energy consumption at a larger scale. This is one of the objectives of the EPOS European project [137], which explores cross-sectorial symbiosis between five different industry sectors, including the petrochemical one.

A List of streams depending on the level of details

Table A.1 – Streams definition for the grey box level.

name	T_{in} [°C]	T_{out} [°C]	Q [kW]	$\Delta T_{min}/2$ [°C]	type
HEAT2_1	87	120	11711	4	cold
HEAT2_3	155	170	1274	4	cold
REBOILER1	139	139	11259	1.5	cold
REBOILER2	110	110	6064	1.5	cold
REBOILER3	103	103	928	1.5	cold
REBOILER4	94	94	131	1.5	cold
REBOILER5	88	88	5	1.5	cold
RECYCLING	139	119	495	4	hot
PROD_COND_3	89	30	11218	4	hot
INTERCOOL	110	38	39	7	hot
COND5	65	65	60	1.5	hot
COND2_1	96	91	2693	1.5	hot
COND2_2	91	87	2714	1.5	hot
COND2_3	87	85	1091	1.5	hot
COND2_4	85	81	838	1.5	hot
COND2_5	81	78	241	1.5	hot
COND2_6	78	70	388	1.5	hot
SUBCOOL	70	30	1249	4	hot
EXTRACT1	99	27	2225	4	hot
COND3_1	68	60	108	7	hot
COND3_2	60	60	3457	1	hot
COND3_3	60	24	664	4	hot
EXTRACT2	103	28	878	4	hot
COND4	57	57	362	1.5	hot
COND6_1	82	77	138	7	hot
COND6_2	77	77	7503	2	hot
COND6_3	77	55	804	4	hot
COOLING	39	27	84	4	hot

Table A.2 – Streams definition for thegrey box Pareto level.

name	T_{in} [°C]	T_{out} [°C]	Q [kW]	$\Delta T_{min}/2$ [°C]	type
HEAT2_1	87	120	11711	4	cold
HEAT2_3	207	207	1274	0	cold
REBOILER1	139	139	11259	1.5	cold
REBOILER2	110	110	6064	1.5	cold
REBOILER3	142	142	928	0	cold
REBOILER4	142	142	131	0	cold
REBOILER5	142	142	5	0	cold
RECYCLING	25	15	495	0	hot
PROD_COND_3	89	30	11218	4	hot
INTERCOOL	25	15	39	0	hot
COND5	25	15	60	0	hot
COND2_1	96	91	2693	1.5	hot
COND2_2	91	87	2714	1.5	hot
COND2_3	87	85	1091	1.5	hot
COND2_4	85	81	838	1.5	hot
COND2_5	81	78	241	1.5	hot
COND2_6	78	70	388	1.5	hot
SUBCOOL	25	15	1249	0	hot
EXTRACT1	25	15	2225	0	hot
COND3_1	68	60	108	7	hot
COND3_2	60	60	3457	1	hot
COND3_3	60	24	664	4	hot
EXTRACT2	25	15	878	0	hot
COND4	25	15	362	0	hot
COND6_1	82	77	138	7	hot
COND6_2	77	77	7503	2	hot
COND6_3	77	55	804	4	hot
COOLING	25	15	84	0	hot

Table A.3 – Streams definition for the white box level.

name	T_{in} [°C]	T_{out} [°C]	Q [kW]	$\Delta T_{min}/2$ [°C]	type
HEAT1	40	87	3059	4	cold
HEAT2_1	87	120	11711	4	cold
HEAT2_2	120	155	3092	4	cold
HEAT2_3	155	170	1274	4	cold
FEED1	14	71	537	4	cold
FEED2	28	74	560	4	cold
RECOVERY	88	88	6947	1.5	cold
REBOILER1	139	139	11259	1.5	cold
REBOILER2	110	110	6064	1.5	cold
REBOILER3	103	103	928	1.5	cold
REBOILER4	94	94	131	1.5	cold
REBOILER5	88	88	5	1.5	cold
RECYCLING	139	119	495	4	hot
GAS_COOL	170	133	3092	7	hot
PROD_COND_1	133	101	6947	1.5	hot
PROD_COND_2	101	89	3059	1.5	hot
PROD_COND_3	89	30	11218	4	hot
INTERCOOL	110	38	39	7	hot
COND5	65	65	60	1.5	hot
COND2_1	96	91	2693	1.5	hot
COND2_2	91	87	2714	1.5	hot
COND2_3	87	85	1091	1.5	hot
COND2_4	85	81	838	1.5	hot
COND2_5	81	78	241	1.5	hot
COND2_6	78	70	388	1.5	hot
SUBCOOL	70	30	1249	4	hot
EXTRACT1	99	27	2225	4	hot
COND3_1	68	60	108	7	hot
COND3_2	60	60	3457	1	hot
COND3_3	60	24	664	4	hot
EXTRACT2	103	28	878	4	hot
COND4	57	57	362	1.5	hot
COND6_1	82	77	138	7	hot
COND6_2	77	77	7503	2	hot
COND6_3	77	55	804	4	hot
COOLING	39	27	84	1.5	hot

Table A.4 – Streams definition for the optimum box level.

name	T_{in} [°C]	T_{out} [°C]	Q [kW]	$\Delta T_{min}/2$ [°C]	type
HEAT1	40	87	3059	4	cold
HEAT2_1	87	120	11711	4	cold
HEAT2_2	120	155	3092	4	cold
HEAT2_3	155	170	1274	4	cold
FEED1	14	71	537	4	cold
FEED2	28	74	560	4	cold
RECOVERY	88	88	6947	1.5	cold
REBOILER1	139	139	11259	1.5	cold
REBOILER2	110	110	6064	1.5	cold
REBOILER3	142	142	928	0	cold
REBOILER4	142	142	131	0	cold
REBOILER5	142	142	5	0	cold
RECYCLING	139	119	495	4	hot
GAS_COOL	170	133	3092	7	hot
PROD_COND_1	133	101	6947	1.5	hot
PROD_COND_2	101	89	3059	1.5	hot
PROD_COND_3	89	30	11218	4	hot
INTERCOOL	25	15	39	0	hot
COND5	25	15	60	0.0	hot
COND2_1	96	91	2693	1.5	hot
COND2_2	91	87	2714	1.5	hot
COND2_3	87	85	1091	1.5	hot
COND2_4	85	81	838	1.5	hot
COND2_5	81	78	241	1.5	hot
COND2_6	78	70	388	1.5	hot
SUBCOOL	25	15	1249	0	hot
EXTRACT1	99	27	2225	4	hot
COND3_1	68	60	108	7	hot
COND3_2	60	60	3457	1	hot
COND3_3	60	24	664	4	hot
EXTRACT2	103	28	878	4	hot
COND4	25	15	362	0.0	hot
COND6_1	82	77	138	7	hot
COND6_2	77	77	7503	2	hot
COND6_3	77	55	804	4	hot
COOLING	25	15	84	0.0	hot

B Scenarios 1 & 2 list of streams

Table B.1 – Scenario 1 - hot streams

Stream	T_{in} [°C]	T_{out} [°C]	Load [kW]	U [W/m^2°C]	Corr. stream
H1	103	40	540	350	CW
H2	96	81	1670	200	CW
H3(a)	118	113	915	600	C11
H3(b)	113	99	2785	600	CW
H4	99	82	1125	610	CW
H5	55	35	1965	200	CW
H6	70	70	1930	1000	CW
H7	60	35	880	300	CW
H8	67	67	550	1100	CW
H9	140	140	2400	900	C8
H10(a)	87	87	875	1200	C1
H10(b)	87	87	3875	1200	CW
H11	77	55	701	400	CW
H12	165	118	2590	200	CW
H13	82	30	985	250	CW
H14	112	30	1113	270	CW
H15	70	30	825	250	CW
H16	102	102	2250	500	CW
H17	55	40	3650	300	CW

Table B.2 – Scenario 1 - cold streams

Stream	T_{in} [°C]	T_{out} [°C]	Load [kW]	U [W/m^2°C]	Corr. stream
C1	35	75	875	250	H10(a)
C2	35	70	900	300	LPS
C3	61	120	3935	350	MPS
C4	145	145	4960	800	MPS
C5	108	108	3030	900	LPS
C6	100	100	585	910	LPS
C7	96	96	4750	600	LPS
C8(a)	127	127	2400	1000	H9
C8(b)	127	127	1650	1000	MPS
C9	130	170	430	450	MPS
C10	62	170	3905	300	MPS
C11	40	75	915	200	H3(a)

Table B.3 – Scenario 2 - hot streams

Stream	T_{in} [°C]	T_{out} [°C]	Load [kW]	U [W/m^2°C]	Corr. stream	HEX type	HEX material	HEX P [bar]
H1	120	70	850	350	CW	FT	CS/CS	8
H2	96	88	1470	400	CW	FH	CS/CS	2
H3	113	100	450	280	CW	FH	CS/CS	1
H4	118	115	460	200	CW	FH	SS/SS	5
H5	55	35	1765	450	CW	FT	CS/CS	1.5
H6	70	70	1730	950	CW	FT	SS/SS	3
H7	60	35	680	600	CW	FH	SS/SS	3.5
H8	101	101	621	730	CW	FT	CS/CS	3
H9	140	140	2200	850	C8(a)	FT	SS/SS	8
H10(a)	87	87	400	600	C1	FT	CS/CS	2
H10(b)	87	87	2150	600	CW	FT	CS/CS	2
H11	77	55	500	600	CW	FH	CS/CS	2
H12	165	120	781	180	CW	FH	CS/CS	3
H13	82	30	485	350	CW	FT	CS/SS	3
H14	120	70	530	270	CW	FH	SS/SS	3
H15	70	30	625	200	CW	FT	CS/CS	3
H16	110	95	1390	210	CW	FH	CS/CS	2.5
H17	110	105	290	300	CW	FH	SS/SS	2.5

Table B.4 – Scenario 2 - cold streams

Stream	**T_{in} [°C]**	**T_{out} [°C]**	**Load [kW]**	**U [$W/m^2 °C$]**	**Corr. stream**	**HEX type**	**HEX material**	**HEX P [bar]**
C1	30	75	400	300	H10(a)	FT	SS/SS	3
C2	30	85	390	300	LPS	FT	CS/CS	2
C3	61	101	962	300	MPS	FT	CS/CS	8
C4	69	117	670	260	MPS	FH	CS/SS	3
C5	120	120	1830	850	MPS	FH	CS/SS	1.5
C6	102	102	415	860	LPS	FH	CS/CS	1.5
C7	91	98	350	200	LPS	FH	CS/SS	2
C8(a)	127	127	2200	950	H9	FT	CS/SS	2.5
C8(b)	127	127	650	950	MPS	FT	CS/SS	2.5
C9	130	170	250	415	MPS	FH	CS/CS	3
C10	62	170	2964	350	MPS	FH	CS/CS	1.5
C11	40	75	415	435	LPS	FT	CS/CS	8

C Calculation details for EnSO's evaluation

Table C.1 – Feed preheating new heat exchanger.

$T_{hot,in}$ [°C]	91
$T_{hot,out}$ [°C]	88
$T_{cold,in}$ [°C]	30
$T_{cold,in}$ [°C]	85.5
LMTD [°C]	22.3
U [kW/m^2°C]	0.53
Area [m^2]	165
HEX type [-]	FH
HEX material [-]	CS/SS
Pressure [bar]	3

Table C.2 – Heat exchanger network redesign.

	E1	E3	E5	E7	E8 (new)
Initial area [m^2]	244	528	382	77	-
Initial LMTD [°C]	28	14	16	73	54
U [kW/m^2°C]	0.46	0.42	0.7	0.65	0.82
New LMTD [°C]	16	10	6.8	5	-
Total area [m^2]	410	741	1994	820	92
Additional area [m^2]	166	212	1612	743	-
HEX type [-]	FH	FH	FH	FH	FH
HEX material [-]	CS/CS	CS/CS	CS/CS	SS/SS	CS/SS
Pressure [bar]	2	2	2	3	3

Table C.3 – Mechanical vapour recompression

Heat exchanger	
LMTD [°C]	6
U [kW/m^2°C]	0.65
Area [m^2]	1058
HEX type [-]	FH
HEX material [-]	CS/SS
Pressure [bar]	3
Compressor	
Material [-]	CS

D Vali models of the heat transformer

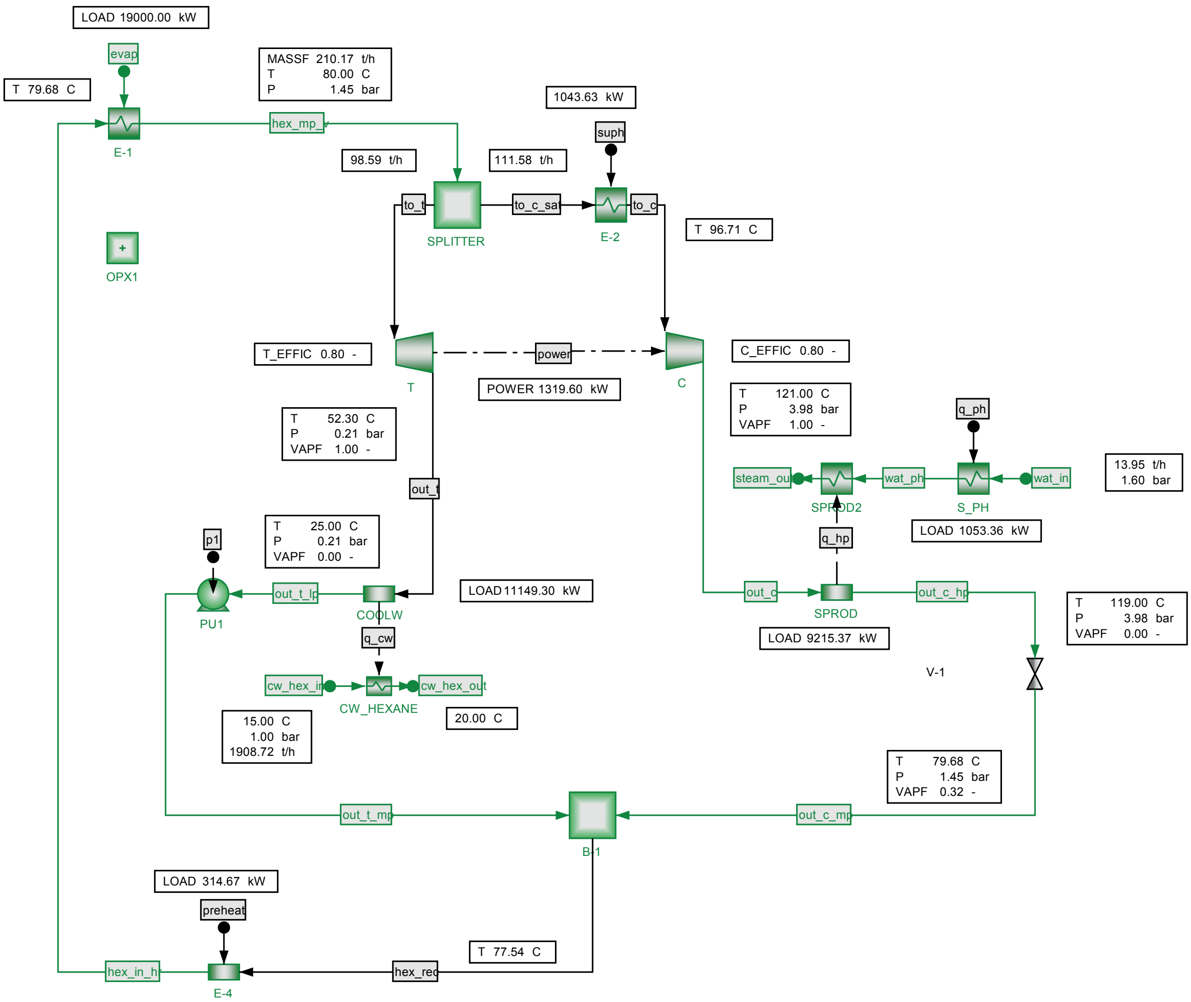


Figure D.1 – Vali model of the integrated heat transformer with hexane as working fluid.

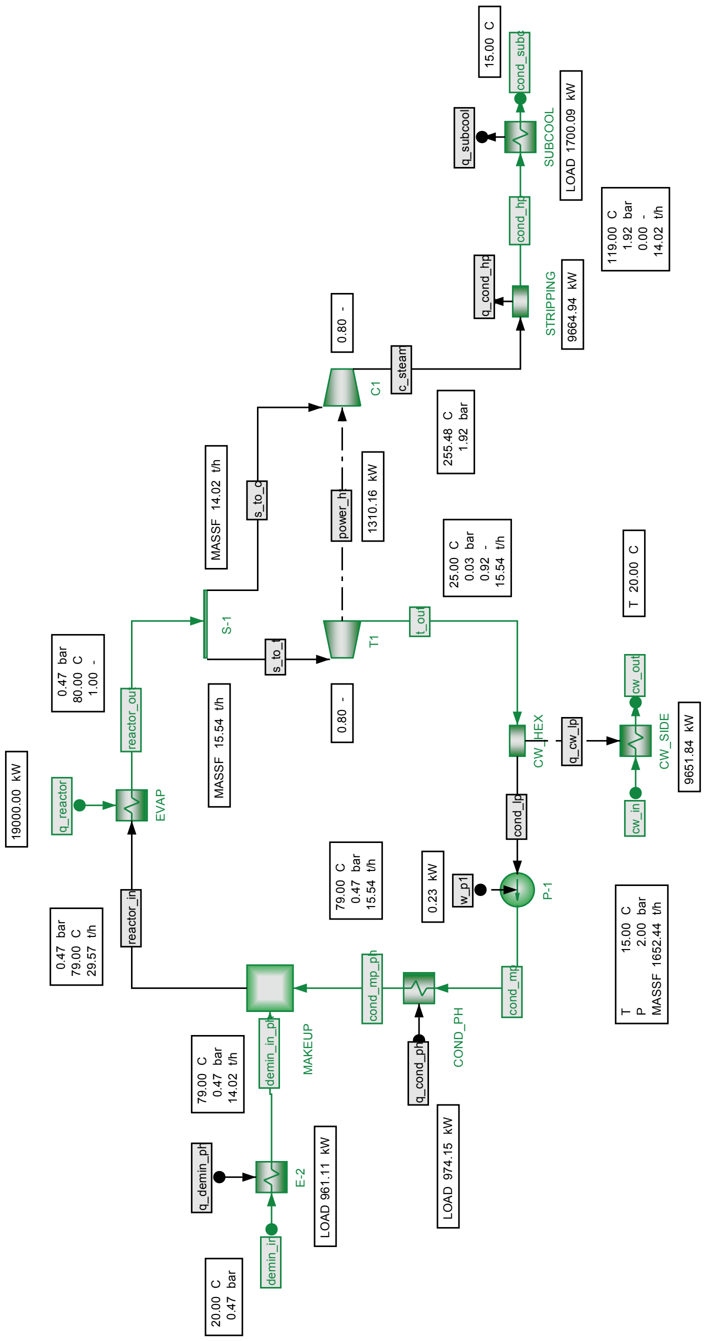


Figure D.2 – Vali model of the open version of heat transformer with water as working fluid.

Bibliography

[1] International Energy Agency. Energy Prices and Taxes online data service. URL https://www.iea.org/statistics/relateddatabases/energypricesandtaxes/.

[2] B. Linnhoff, D. W. Townsend, D. Boland, G. F. Hewitt, B. E. A. Thomas, A. R. Guy, and R. H. Marshall. *A User Guide on Process Integration for the Efficient Use of Energy*. IChemE,Rugby,UK., 1982.

[3] Sarah Brückner, Selina Liu, Laia Miró, Michael Radspieler, Luisa F. Cabeza, and Eberhard Lävemann. Industrial waste heat recovery technologies: An economic analysis of heat transformation technologies. *Applied Energy*, 151:157–167, August 2015.

[4] European Commission. Directive 2012/27/EU on energy efficiency, amending directives 2009/125/EC and 2010/30/EU and repealing directives 2004/8/EC and 2006/32/EC, November 2012.

[5] International Organisation for Standardisation. ISO 50001:2011 Energy management systems — Requirements with guidance for use, 2011.

[6] European Commission. 2020 climate & energy package, . URL https://ec.europa.eu/clima/policies/strategies/2020_en.

[7] European Commission. 2030 climate & energy framework, . URL https://ec.europa.eu/clima/policies/strategies/2030_en.

[8] European Commission. EU leads in implementing Paris climate commitments, January 2017. URL https://ec.europa.eu/environment/efe/themes/climate-action/eu-leads-implementing-paris-climate-commitments_en.

[9] European Commission. Commission proposes 30% energy efficiency target, February 2016. URL https://ec.europa.eu/energy/en/news/commission-proposes-30-energy-efficiency-target.

[10] MEPs set ambitious targets for cleaner, more efficient energy use., January 2018. URL http://www.europarl.europa.eu/news/en/press-room/20180112IPR91629/meps-set-ambitious-targets-for-cleaner-more-efficient-energy-use.

[11] European Commission. 2050 Energy strategy, . URL https://ec.europa.eu/energy/en/topics/energy-strategy-and-energy-union/2050-energy-strategy.

[12] OECD/IEA. 25 Energy Efficiency Policy Recommendations, 2011.

[13] Cross-border guide to energy audits, January 2017. URL /en/insights/thought-leadership/cross-border-guide-energy-audits/cross-border-guide-to-energy-audits.

[14] European Commission. Energy Efficiency Directive, . URL https://ec.europa.eu/energy/en/topics/energy-efficiency/energy-efficiency-directive.

[15] Kit Oung, Steven Fawkes, and John Mulholland. *Energy Audits - The Key to Delivering Real Energy Reductions*. British Standards Institution, 2014.

[16] International Organisation for Standardisation. ISO 50002:2014 Energy audits – Requirements with guidance for use, 2014.

[17] ODYSSEE MURE. Energy Efficiency Trends and Policies In Industry, An Analysis Based on the ODYSSEE and MURE Databases, September 2015.

[18] Petrochemicals Europe. Cost of regulation, July 2016. URL http://www.petrochemistry.eu/policy/cost-of-regulation.html.

[19] Sylvie Cornot-Gandolphe. The Impact of the Development of Shale Gas in the United States on Europe's Petrochemical Industries, IFRI, November 2013.

[20] D. Saygin, M. K. Patel, E. Worrell, C. Tam, and D. J. Gielen. Potential of best practice technology to improve energy efficiency in the global chemical and petrochemical sector. *Energy*, 36(9): 5779–5790, September 2011.

[21] Katharina Bunse, Matthias Vodicka, Paul Schönsleben, Marc Brülhart, and Frank O. Ernst. Integrating energy efficiency performance in production management – gap analysis between industrial needs and scientific literature. *Journal of Cleaner Production*, 19(6):667–679, April 2011.

[22] Patrik Thollander and Mikael Ottosson. An energy efficient Swedish pulp and paper industry – exploring barriers to and driving forces for cost-effective energy efficiency investments. *Energy Efficiency*, 1(1):21–34, February 2008.

[23] Patrik Rohdin, Patrik Thollander, and Petter Solding. Barriers to and drivers for energy efficiency in the Swedish foundry industry. *Energy Policy*, 35(1):672–677, January 2007.

[24] Gökan May, Marco Taisch, Bojan Stahl, and Vahid Sadr. Toward Energy Efficient Manufacturing: A Study on Practices and Viewpoint of the Industry. In *Advances in Production Management Systems. Competitive Manufacturing for Innovative Products and Services*, IFIP Advances in Information and Communication Technology, pages 1–8. Springer, Berlin, Heidelberg, September 2012.

[25] Laurent Gabriel Stéphane Bungener. *Energy Efficiency and Integration in the Refining and Petrochemical Industries.* PhD thesis, Ecole Polytechnique Fédérale de Lausanne, 2016.

[26] Eurelectric. Electrification of European energy demand. URL http://www.eurelectric.org/the-european-power-sector-in-transition/electrification-of-european-energy-demand/.

[27] IPIECA, OGP. Guidelines for implementing ISO 50001 energy management systems in the oil and gas industry, January 2013.

[28] Cefic. Energy Efficiency Best Practices. CARE + Energy Efficiency Handbook for Chemical SMEs, 2009. URL http://www.cefic.org/Policy-Centre/Energy--Climate-Change/Energy-Efficiency/CARE-/Care-Tools/.

[29] Walter Kahlenborn, Sibylle Kabisch, Johanna Klein, Ina Richter, and Silas Schürmann. DIN EN 16001: Energy Management Systems in Practice, A Guide for Companies and Organisations, June 2010.

[30] AFNOR. Mises en oeuvre d'un système de management de l'énergie selon l'ISO 50001, September 2014.

[31] OECD/IEA. Energy Management Programmes for Industry - Gaining through saving, 2012.

[32] Ali Hasanbeigi and Lynn Price. Industrial Energy Audit Guidebook: Guidelines for Conducting an Energy Audit in Industrial Facilities,Ernest Orlando Lawrence Berkeley National Laboratory, October 2010.

[33] Ruzena Kralikova, Miriam Andrejiova, and Emil Wessely. Energy Saving Techniques and Strategies for Illumination in Industry. *Procedia Engineering*, 100:187–195, January 2015.

[34] Matteo Dongellini, Cosimo Marinosci, and Gian Luca Morini. Energy Audit of an Industrial Site: A Case Study. *Energy Procedia*, 45:424–433, January 2014.

[35] Janez Petek, Peter Glavič, and Anja Kostevšek. Comprehensive approach to increase energy efficiency based on versatile industrial practices. *Journal of Cleaner Production*, 112:2813–2821, January 2016.

[36] C. Drumm, J. Busch, W. Dietrich, J. Eickmans, and A. Jupke. STRUCTese® – Energy efficiency management for the process industry. *Chemical Engineering and Processing: Process Intensification*, 67:99–110, May 2013.

[37] François Maréchal and Boris Kalitventzeff. Process integration: Selection of the optimal utility system. *Computers & Chemical Engineering*, 22:S149–S156, March 1998.

[38] Kevin C. Furman and Nikolaos V. Sahinidis. A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century. *Industrial & Engineering Chemistry Research*, 41(10):2335–2370, May 2002.

[39] M. Bojić and S. Dragičević. MILP optimization of energy supply by using a boiler, a condensing turbine and a heat pump. *Energy Conversion and Management*, 43(4):591–608, March 2002.

[40] Liga Zogla, Gatis Zogla, Anna Beloborodko, and Marika Rosa. Process Benchmark for Evaluation Energy Performance in Breweries. *Energy Procedia*, 72:202–208, June 2015.

[41] Gunter Festel and Martin Würmseher. Benchmarking of energy and utility infrastructures in industrial parks. *Journal of Cleaner Production*, 70:15–26, May 2014.

[42] Maarten Neelis, Andrea Ramirez-Ramirez, Martin Patel, Jacco Farla, Piet Boonekamp, and Kornelis Blok. Energy efficiency developments in the Dutch energy-intensive manufacturing industry, 1980–2003. *Energy Policy*, 35(12):6112–6131, December 2007.

[43] E. Giacone and S. Mancò. Energy efficiency measurement in industrial processes. *Energy*, 38 (1):331–345, February 2012.

[44] Jing Ke, Lynn Price, Michael McNeil, Nina Zheng Khanna, and Nan Zhou. Analysis and practices of energy benchmarking for industry from the perspective of systems engineering. *Energy*, 54:32–44, June 2013.

[45] G. J. M. Phylipsen, K. Blok, and E. Worrell. International comparisons of energy efficiency-Methodologies for the manufacturing industry. *Energy Policy*, 25(7):715–725, June 1997.

[46] Sari Siitonen, Mari Tuomaala, and Pekka Ahtila. Variables affecting energy efficiency and CO2 emissions in the steel industry. *Energy Policy*, 38(5):2477–2485, May 2010.

[47] Murray G Patterson. What is energy efficiency?: Concepts, indicators and methodological issues. *Energy Policy*, 24(5):377–390, May 1996.

[48] MORE. Real-time Monitoring and Optimisation of Resource Efficiency in Integrated Processing Plants. URL http://www.more-nmp.eu/.

[49] Gökan May, Ilaria Barletta, Bojan Stahl, and Marco Taisch. Energy management in production: A novel method to develop key performance indicators for improving energy efficiency. *Applied Energy*, 149:46–61, July 2015.

[50] European Commission. Reference Document on Best Available Techniques for Energy Efficiency, February 2009.

[51] Pascal Barthe, Michel Chaugny, Serge Roudier, and Luis Delgado Sancho. Best Available Techniques (BAT)Reference Document for the Refining of Mineral Oil and Gas, 2015.

[52] European Commission. Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry, February 2003.

[53] European Commission. Reference Document on Best Available Techniques in the Production of Polymers, 2007. URL http://eippcb.jrc.ec.europa.eu/reference/pol.html.

[54] Nasibeh Pouransari, Gerald Bocquenet, and Francois Maréchal. Site-scale process integration and utility optimization with multi-level energy requirement definition. *Energy Conversion and Management*, 85:774–783, September 2014.

[55] Flavio Manenti, Maria Grazia Grottoli, and Sauro Pierucci. Online Data Reconciliation with Poor Redundancy Systems. *Industrial & Engineering Chemistry Research*, 50(24):14105–14114, December 2011.

[56] Matthias Bendig. *Integration of Organic Rankine Cycles for Waste Heat Recovery in Industrial Processes*. PhD thesis, Ecole Polytechnique Fédérale de Lausanne, 2015.

[57] CoPro. Improved energy and resource efficiency by better coordination of production in the process industries. URL https://www.spire2030.eu/copro.

[58] Bodo Linnhoff and John R. Flower. Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks. *AIChE Journal*, 24(4):633–642, July 1978.

[59] Jiri Jaromir Klemes and Zdravko Kravanja. Forty years of Heat Integration: Pinch Analysis (PA) and Mathematical Programming (MP). *Current Opinion in Chemical Engineering*, 2(4): 461–474, November 2013.

[60] Maarten Neelis, Martin Patel, Kornelis Blok, Wim Haije, and Pieter Bach. Approximation of theoretical energy-saving potentials for the petrochemical industry using energy balances for 68 key processes. *Energy*, 32(7):1104–1123, July 2007.

[61] Chamil Abeykoon, Adrian L. Kelly, Elaine C. Brown, Javier Vera-Sorroche, Phil D. Coates, Eileen Harkin-Jones, Ken B. Howell, Jing Deng, Kang Li, and Mark Price. Investigation of the process energy demand in polymer extrusion: A brief review and an experimental study. *Applied Energy*, 136:726–737, December 2014.

[62] Yaşar Demirel. *Energy Production, Conversion, Storage, Conservation, and Coupling*. Springer, 2012. ISBN 978-1-4471-2372-9.

[63] R. K. Rajput. *Thermal Engineering*. Laxmi Publications, April 2010. ISBN 978-81-318-0804-7. Google-Books-ID: 65gxCX2dC84C.

[64] Sou Hosokai, Koichi Matsuoka, Koji Kuramoto, and Yoshizo Suzuki. Modification of Dulong's formula to estimate heating value of gas, liquid and solid fuels. *Fuel Processing Technology*, 152:399–405, November 2016.

[65] Emanuela Peduzzi, Guillaume Boissonnet, and François Maréchal. Biomass modelling: Estimating thermodynamic properties from the elemental composition. *Fuel*, 181:207–217, October 2016.

[66] Schyns. Towards a simple, robust and predictable EU Emissions Trading Scheme, 2006.

[67] *Thermodynamique*. 2nd edition.

[68] Stéphane Laurent Bungener, Greet Van Eetvelde, and Francois Marechal. A methodology for creating sequential multi-period base-case scenarios for large data sets. *16th International conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES 2013)*, 35:1231–1236, 2013.

[69] Stephane Bungener, Roman Hackl, Greet Van Eetvelde, Simon Harvey, and Francois Marechal. Multi-period analysis of heat integration measures in industrial clusters. *Energy*, 93:220–234, 2015.

[70] Hélène Cervo, Stéphane Bungener, Elfie Méchaussie, Ivan Kantor, Brecht Zwaenepoel, François Maréchal, and Greet Van Eetvelde. Virtual Sector Profiles for Innovation Sharing in Process Industry – Sector 01: Chemicals. *Sustainable Design and Manufacturing 2017*, pages 569–578, 2017.

[71] Linnhoff March. The methodology and benefits of total site pinch analysis., 2000. URL http://www.environmental-expert.com/articles/the-methodologyand-benefits-of-total-site-pinch-analysis-2957.

[72] Tao Ren. Barriers and drivers for process innovation in the petrochemical industry: A case study. *Journal of Engineering and Technology Management*, 26(4):285–304, December 2009.

[73] Elfie Méchaussie, Stephane Bungener, Greet Van Eetvelde, and Francois Marechal. Methodology for streams definition and graphical representation in Total Site Analysis. In *Proceedings of the 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems*, Portorož, 2016.

[74] NIST. NIST Chemistry WebBook. URL http://webbook.nist.gov/chemistry/.

[75] Aspen Plus, . URL https://www.aspentech.com/.

[76] Belsim Vali, . URL http://www.belsim.com/.

[77] Bruce E. Poling, John M. Prausnitz, and John P. O'Connell. *Properties of Gases and Liquids*. McGraw-Hill, 5th edition, 2000.

[78] Jan F. Kreider, Peter Curtiss, and Ari Rabl. *Heating and Cooling of Buildings: Design for Efficiency*. McGraw-Hill, 2002. ISBN 978-0-07-237341-7. Google-Books-ID: q1ZSAAAAMAAJ.

[79] Damien Muller. *Web-based tools for energy management in large companies applied to food industry*. PhD thesis, Ecole Polytechnique Fédérale de Lausanne, 2007.

[80] Shankar Narasimhan and Cornelius Jordache. *Data Reconciliation and Gross Error Detection: An Intelligent Use of Process Data*. Gulf Professional Publishing, November 1999. ISBN 978-0-08-050371-4.

[81] Miguel J. Bagajewicz and Enmanuel Cabrera. Data Reconciliation in Gas Pipeline Systems. *Industrial & Engineering Chemistry Research*, 42(22):5596–5606, October 2003.

[82] Sisi Guo, Pei Liu, and Zheng Li. Data reconciliation for the overall thermal system of a steam turbine power plant. *Applied Energy*, 165:1037–1051, March 2016.

[83] Timo Korpela, Olli Suominen, Yrjö Majanne, Ville Laukkanen, and Pentti Lautala. Robust data reconciliation of combustion variables in multi-fuel fired industrial boilers. *Control Engineering Practice*, 55:101–115, October 2016.

[84] Stéphane Laurent Bungener. Data reconciliation of steam networks in refineries and petrochemical sites. Technical report available here https://infoscience.epfl.ch/record/215087?ln=fr, 2015.

[85] Heng Wen Zhang, Shuo Dong, Fang Yang, and Liang Ping Shi. The Research and Application of Industrial Boiler Energy Efficiency Test System. *Applied Mechanics and Materials*, 288: 296–302, 2013.

[86] Tjaan N. Tjoe and Bodo Linnhoff. Using Pinch Technology for Process Retrofit. *Chemical Engineering*, 93(8):47–60, 1986.

[87] Roman Hackl, Eva Andersson, and Simon Harvey. Targeting for energy efficiency and improved energy collaboration between different companies using total site analysis (TSA). *Energy*, 36 (8):4609–4615, August 2011.

[88] Vikas R Dhole and Bodo Linnhoff. Total site targets for fuel, co-generation, emissions, and cooling. *Computers & Chemical Engineering*, 17:S101–S109, January 1993.

[89] K. Raissi. *Total site integration*. Ph.D., The University of Manchester, 1994.

[90] J. Klemeš, V. R. Dhole, K. Raissi, S. J. Perry, and L. Puigjaner. Targeting and design methodology for reduction of fuel, power and CO2 on total sites. *Applied Thermal Engineering*, 17(8): 993–1003, August 1997.

[91] Helen Becker and François Maréchal. Energy integration of industrial sites with heat exchange restrictions. *Computers & Chemical Engineering*, 37:104–118, February 2012.

[92] Nasibeh Pouransari and Francois Marechal. Energy Integration of Large-Scale Industrial Sites with Target-Compatible Sub-System Division Strategy. *Pres 2014, 17Th Conference On Process Integration, Modelling And Optimisation For Energy Saving And Pollution Reduction, Pts 1-3*, 39:43–48, 2014.

[93] François Marechal and Boris Kalitventzeff. Targeting the integration of multi-period utility systems for site scale process integration. *Applied Thermal Engineering*, 23(14):1763–1784, October 2003.

[94] Bhargava Krishna Sreepathi and G. P. Rangaiah. Review of Heat Exchanger Network Retrofitting Methodologies and Their Applications. *Industrial & Engineering Chemistry Research*, 53(28): 11205–11220, July 2014.

[95] Hür Bütün, Ivan Kantor, and Francois Maréchal. A process integration method with multiple heat exchange interfaces. In *Proceedings of ECOS 2017 - The 30th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, San Diego, California, USA*, 2017.

[96] Truls Gundersen. Analysis and Design of Heat Recovery Systems for Grassroots and Retrofit Situations. In *Handbook of Process Integration (PI). Minimisation of Energy and Water Use, Waste and Emissions*. Woodhead Publishing, 2013.

[97] Linnhoff March. Introduction to Pinch Technology, 1998. URL http://www.ou.edu/class/che-design/a-design/Introduction%20to%20Pinch%20Technology-LinhoffMarch.pdf.

[98] Sung-Geun Yoon, Jeongseok Lee, and Sunwon Park. Heat integration analysis for an industrial ethylbenzene plant using pinch analysis. *Applied Thermal Engineering*, 27(5):886–893, April 2007.

[99] J. H. Miah, A. Griffiths, R. McNeill, I. Poonaji, R. Martin, A. Yang, and S. Morse. Heat integration in processes with diverse production lines: A comprehensive framework and an application in food industry. *Applied Energy*, 132:452–464, November 2014.

[100] Rickard Fornell and Thore Berntsson. Process integration study of a kraft pulp mill converted to an ethanol production plant – Part A: Potential for heat integration of thermal separation units. *Applied Thermal Engineering*, 35:81–90, March 2012.

[101] Trent Harkin, Andrew Hoadley, and Barry Hooper. Reducing the energy penalty of CO2 capture and compression using pinch analysis. *Journal of Cleaner Production*, 18(9):857–866, June 2010.

[102] Petar Sabev Varbanov, Zsófia Fodor, and Jiří Jaromír Klemeš. Total Site targeting with process specific minimum temperature difference (\Delta Tmin}). *Energy*, 44(1):20–28, August 2012.

[103] Sennai Mesfun and Andrea Toffolo. Optimization of process integration in a Kraft pulp and paper mill – Evaporation train and CHP system. *Applied Energy*, 107:98–110, July 2013.

[104] V. Briones and A. Kokossis. A new approach for the optimal retrofit of heat exchanger networks. *Computers & Chemical Engineering*, 20:S43–S48, January 1996.

[105] Badr Abdullah Al-Riyami, Jiri Klemes, and Simon Perry. Heat integration retrofit analysis of a heat exchanger network of a fluid catalytic cracking plant. *Applied Thermal Engineering*, 21 (13):1449–1487, October 2001.

[106] Chonlada Doungprasertsuk, Kitipat Siemanond, Vivan Thammongkol, and Supareak Susangeim. Heat Exchanger Network Retrofit by Pinch Technology on Reformer Area of Aromatics Plant. *Asian Pacific Confederation of Chemical Engineering congress program and abstracts*, 2004:284–284, 2004.

[107] Ian C. Kemp. *Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy*. Butterworth-Heinemann, 2nd edition, 2006. ISBN 978-0-7506-8260-2.

[108] Richard Turton, Richard C. Bailie, Wallace B. Whiting, Joseph A. Shaeiwitz, and Debangsu Bhattacharyya. *Analysis, Synthesis, and Design of Chemical Processes*. Prentice Hall, 4th edition, June 2012. ISBN 978-0-13-261812-0.

[109] J.M. Kay and R.M. Nedderman. *Fluid mechanics and transfer processes*. Cambridge University Press, 1985. ISBN 978-0-521-31624-8.

[110] Warren D. Seider, J. D. Seader, and Daniel R. Lewin. *Product & Process Design Principles: Synthesis, Analysis and Evaluation*. Wiley, 2nd edition, 2003.

[111] Max S. Peters and Klaus D. Timmerhaus. *Plant Design and Economics for Chemical Engineers*. Number McGraw-Hill. 4th edition, 1991.

[112] Andreja Nemet, Jiří Jaromír Klemeš, and Zdravko Kravanja. Minimisation of a heat exchanger networks' cost over its lifetime. *Energy*, 45(1):264–276, September 2012. ISSN 0360-5442. doi: 10.1016/j.energy.2012.02.049. URL http://www.sciencedirect.com/science/article/pii/S0360544212001636.

[113] Omar Joel Symister. *An Analysis of Capital Cost Estimation Techniques for Chemical Processing*. Thesis, May 2016.

[114] Marcel Taal, Igor Bulatov, Jiri Klemes, and Petr Stehlik. Cost estimation and energy price forecasts for economic evaluation of retrofit projects. *Applied Thermal Engineering*, 23(14): 1819–1835, October 2003.

[115] Antonio C. Caputo, Pacifico M. Pelagagge, and Paolo Salini. Manufacturing cost model for heat exchangers optimization. *Applied Thermal Engineering*, 94:513–533, February 2016.

[116] Ray Sinnot and Gavin Towler. *Chemical Engineering Design*. 5th edition, 2009. ISBN 978-0-7506-8551-1.

[117] Robin Smith. *Chemical Process Design and Integration*. John Wiley & Sons, 2005. ISBN 0-471-48680-9.

[118] Armando B. Corripio, Katherine S. Chrien, and Lawrence B. Evans. Estimate cost of heat exchangers and storage tanks via correlations. *Chemical Engineering*, 89(2):125–127, 1982.

[119] R.S. Hall, J. Matley, and K.J. McNaughton. Current Costs of Process Equipment. *Chemical Engineering*, 89:80–116, 1982.

[120] K.M. Guthrie. Capital Cost Estimating. *Chemical Engineering*, 76(6):114–142, 1969.

[121] Gael D. Ulrich and Palligarnai T. Vasudevan. *Chemical Engineering Process Design and Economics: A Practical Guide*. Process Publishing, 2nd edition, 2004.

[122] Ying Feng and Gade P. Rangaiah. Evaluating Capital Cost Estimation Programs. *Chemical Engineering*, August 2011.

[123] Audun Aspelund, David Olsson Berstad, and Truls Gundersen. An Extended Pinch Analysis and Design procedure utilizing pressure based exergy for subambient cooling. *Applied Thermal Engineering*, 27(16):2633–2649, November 2007.

[124] Nasibeh Pouransari. *Towards practical solutions for energy efficiency of large-scale industrial sites*. PhD thesis, Ecole Polytechnique Fédérale de Lausanne, 2015.

[125] Chris Namovicz and Jim Diefenderfer. Review of Power Plant Cost and Performance Assumptions for NEMS - Technology Documentation Report. Technical report, U.S. Energy Information Administration, April 2016.

[126] Matthias Bendig, François Maréchal, and Daniel Favrat. Defining "Waste Heat" for industrial processes. *Applied Thermal Engineering*, 61(1):134–142, October 2013.

[127] J. Demierre, S. Henchoz, and D. Favrat. Prototype of a thermally driven heat pump based on integrated Organic Rankine Cycles (ORC). *Energy*, 41(1):10–17, May 2012.

[128] Jonathan Demierre, Daniel Favrat, Jürg Schiffmann, and Johannes Wegele. Experimental investigation of a Thermally Driven Heat Pump based on a double Organic Rankine Cycle and an oil-free Compressor-Turbine Unit. *International Journal of Refrigeration*, 44:91–100, August 2014.

[129] Philip Donnellan, Kevin Cronin, and Edmond Byrne. Recycling waste heat energy using vapour absorption heat transformers: A review. *Renewable and Sustainable Energy Reviews*, 42:1290–1304, February 2015.

[130] Kiyan Parham, Mehrdad Khamooshi, Daniel Boris Kenfack Tematio, Mortaza Yari, and Uğur Atikol. Absorption heat transformers – A comprehensive review. *Renewable and Sustainable Energy Reviews*, 34:430–452, June 2014.

[131] Huijuan Chen, D Goswami, and Elias K. Stefanakos. A review of thermodynamic cycles and working fluids for the conversion of low-grade heat. *Renewable and Sustainable Energy Reviews*, 14:3059–3067, 2010.

[132] Peijun Guo, Jun Sui, Wei Han, Jianjiao Zheng, and Hongguang Jin. Energy and exergy analyses on the off-design performance of an absorption heat transformer. *Applied Thermal Engineering*, 48:506–514, December 2012.

[133] Ilhami Horuz and Bener Kurt. Absorption heat transformers and an industrial application. *Renewable Energy*, 35(10):2175–2181, October 2010.

[134] Junjiang Bao and Li Zhao. A review of working fluid and expander selections for organic Rankine cycle. *Renewable and Sustainable Energy Reviews*, 24:325–342, August 2013.

[135] E. H. Wang, H. G. Zhang, B. Y. Fan, M. G. Ouyang, Y. Zhao, and Q. H. Mu. Study of working fluid selection of organic Rankine cycle (ORC) for engine waste heat recovery. *Energy*, 36(5): 3406–3418, May 2011.

[136] R. Rayegan and Y. X. Tao. A procedure to select working fluids for Solar Organic Rankine Cycles (ORCs). *Renewable Energy*, 36(2):659–670, February 2011.

[137] EPOS. Enhanced energy and resource Efficiency and Performance in process industry Operations via onsite and cross-sectorial Symbiosis. URL https://www.spire2030.eu/epos/#.

Elfie Méchaussie

Place du Tunnel 18
1005 Lausanne
+41(0)76 227 64 47
elfie.mechaussie@gmail.com
French, 18.12.1990 (27 yo)

STRENGTHS:

- specialist in **industrial energy efficiency** and energy management
- **energy auditing** skills with good knowledge of **ISO 50001** standard
- **pinch analysis:** all phases

EDUCATION

03-2018 Swiss Federal Institute of Technology (EPFL), **PhD in Energy Systems**
Laboratory for industrial processes and energy systems engineering (IPESE)

2013 **Master of Science in Chemical Engineering** - EPFL
Minor in Energy

2010 **Bachelor** in Chemistry and Chemical Engineering - EPFL

2007 French Baccalaureate in Sciences with high honours
Lycée international de Ferney-Voltaire - France

WORK EXPERIENCE & INTERNSHIPS

09.12-04.13 **INEOS**: Master's thesis in industry (grade 6/6)

- energy efficiency study on a large petrochemical cluster in Köln (DE)

Immersed during 6 months on site, I analysed the steam network of the entire cluster, from steam production to end use consumption, calculating key performance indicators and proposing several modifications to increase its efficiency.

09.11-06.12 **QGel S.A**: Part time employment
Being responsible of the logistics and orders management, I was organising, shipping and tracking all purchase requests for the start-up in its first expansion stage.

01.11-06-11 **EPFL:** Teaching assistant for bachelor courses in chemical engineering.

PROJECTS

INEOS: PhD thesis

- development of a general methodology for energy efficiency applicable on medium to large industrial (petro)chemical sites consuming significant thermal power.

During my thesis I realised and/or supervised around 10 indicative energy audits on existing industrial sites, complying with actual European regulation and aligned with the ISO 50001 standard for energy management. The developed methodology ranges from data validation to the generation of engineering solutions and energy consumption monitoring strategies. Results showed significant plant insight gain, analysis time and complexity reduction and energy savings potential of 5 to 15%.

- Distance teaching for numerous master students for the industrial projects supervision.
- Projects in France, UK, Germany, Italy, Netherlands and Belgium.

SKILLS

Technical skills

- *Pinch analysis:* from traditional to Total Site Analysis, heat pumping & cogeneration potential identification.
- *Process modelling and simulation:* Belsim Vali, Aspen
- *Programming:* Matlab, Lua, Ampl
- MS Office suite (Mac & PC)
- Proficient in communicating complex scientific concepts effectively (concise + clear presentations)

ISO 50001 training (January 2015)

- 2 days of training carried out by a consultant from **DNV GL** to go through the entirety of the energy management standard and master all the key concepts.
- Practice with real-life examples and case studies as well as quizzes.

LANGUAGES

French	Mother tongue
English	Advanced (C1)
German	Elementary, written (B1) and spoken (A2)

EXTRACURRICULAR ACTIVITIES

Track & field 400m/400mH

- practiced for 15 years
- up to 6 training sessions/week during the last 3 years
- numerous French regional and inter-regional titles (400m, 400mH, 200m, long jump, 100mH)
- 5th at the indoor (2017) and outdoor (2015) Swiss Championships on the 400m

Athletissima

Track & field meeting part of the international world-class circuit (Diamond League)

Swiss Olympic Volunteer as member of the call room, which is one of the key teams for the smooth proceedings of competition.

Associative work

From 2009 to 2011, member of several student associations: Forum EPFL (major recruiting event for Switzerland), Baramine (chemisty section), Coaching EPFL (tutoring).

PERSONAL INFORMATION

- Work permit B
- single