Integration of Waste Heat Recovery in Process Sites

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

2015

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Nomenclature

Symbols

A	Heat transfer area (m^2)
cp	Specific heat capacity flowrate (kW/kgK)
LMTD	Log mean temperature difference (°C)
m	Mass flow (kg/s)
P	Pressure (bar)
Q	Heat duty (kW)
T	Temperature (°C)
U	Overall heat transfer coefficient (kW/m^2K)
W	Electrical power (kW)
x	Concentration (weight percent)

Abbreviations

ABS	Absorber
AbC	Absorption chiller
AHP	Absorption heat pump
AHT	Absorption heat transformer
COMP	Compressor
COND	Condenser
COP	Coefficient of performance
DHR	Direct heat recovery
EVAP	Evaporator
EXP	Expander
GCC	Grand composite curve
GEN	Generator
MHP	Mechanical heat pump
MILP	Mixed integer linear programme
MINLP	Mixed integer non-linear programme
Mtoe	Million tonnes of oil equivalent
ORC	Organic Rankine cycle
SHX	Solution heat exchanger
TSA	Total site analysis
WF	Working fluid
WHR	Waste heat recovery
WHRS	Waste heat recovery system
WHS	Waste heat sources

Abstract

Integration of waste heat recovery in process sites
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The University of Manchester
2015
PhD Thesis

Exploitation of waste heat could achieve economic and environmental benefits, while at the same time increase energy efficiency in process sites. Diverse commercialised technologies exist to recover useful energy from waste heat. In addition, there are multiple on-site and off-site end-uses of recovered energy. The challenge is to find the optimal mix of technologies and end-uses of recovered energy taking into account the quantity and quality of waste heat sources, interactions with interconnected systems and constraints on capital investment.

Explicit models for waste heat recovery technologies that are easily embedded within appropriate process synthesis frameworks are proposed in this work. A novel screening tool is also proposed to guide selection of technology options. The screening tool considers the deviation of the actual performance from the ideal performance of technologies, where the actual performance takes into account irreversibilities due to finite temperature heat transfer. Results from applying the screening tool show that better temperature matching between heat sources and technologies reduces the energy quality degradation during the conversion process. A ranking criterion is also proposed to evaluate end-uses of recovered energy. Applying the ranking criterion shows the use to which energy recovered from waste heat is put determines the economics and potential to reduce CO_2 emissions when waste heat recovery is integrated in process sites.

This thesis also proposes a novel methodological framework based on graphical and optimization techniques to integrate waste heat recovery into existing process sites. The graphical techniques are shown to provide useful insights into the features of a good solution and assess the potential in industrial waste heat prior to detailed design. The optimization model allows systematic selection and combination of waste heat source streams, selection of technology options, technology working fluids, and exploitation of interactions with interconnected systems. The optimization problem is formulated as a Mixed Integer Linear Program, solved using the branch-and-bound algorithm. The objective is to maximize the economic potential considering capital investment, maintenance costs and operating costs of the selected waste heat recovery technologies.

The methodology is applied to industrial case studies. Results indicate that combining waste heat recovery options yield additional increases in efficiency, reductions in CO_2 emissions and costs. The case study also demonstrates that significant benefits from waste heat utilization can be achieved when interactions with interconnected systems are considered simultaneously.

The thesis shows that the methodology has potential to identify, screen, select and combine waste heat recovery options for process sites. Results suggest that recovery of waste heat can improve the energy security of process sites and global energy security through the conservation of fuel and reduction in CO_2 emissions and costs. The methodological framework can inform integration of waste heat recovery in the process industries and formulation of public policies on industrial waste heat utilization.

Declaration

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

Oluwagbemisola Oluleye

Copyright statement

Acknowledgement

I would like to express my deepest gratitude to everyone who contributed to the completion of this thesis. First and foremost I am extremely grateful to my supervisors Dr Megan Jobson and Professor Robin Smith. Their constant support, inspiring views, wisdom and feedback made this thesis a reality. I would also like to thank Simon Perry, Steve Doyle, Dr Igor Bulatov, Dr Li Sun and Dr Nan Zhang for their kind support from the onset and sharing their experiences.

Very special thanks to members of Process Integration Research Consortium for providing the financial support for the development of this research. Thank you for sharing your industrial experiences during the consortium which shaped and enriched this research.

Thanks also to all the staff and colleagues from the Centre for Process Integration for their friendship and the good times. A big massive shout out to every remarkable and exceptional researcher in B14!

Finally I would love to appreciate my family for their understanding, support and prayers. Especially to my parents who taught me to always make excellence my lifestyle.

Dedication

To all women who dream dreams that are bigger than their current reality

To all those who struggle to fit in

To my parents, Olufemi and Biodun

To my siblings, Ajibola, Oluwatobi and Opeyemi

To all my teachers and lecturers

To the future!

To God

The Author

As a young child, I had an opportunity to visit an Oil Rig (special thanks to my mum who made sure our personal protective equipment's were colourful and stylish). In the control room I saw the most beautiful yet complicated image that captivated me for the entire trip; it was the process platforms process flow diagram. I was fascinated with the colour schemes used to represent all the processing units, and that I could trace every feed and product stream. This was the beginning of my interest in and passion for Chemical Engineering.

Gbemi received a Bachelor of Science in Chemical Engineering from the Obafemi Awolowo University, Nigeria, for which she obtained a Second Class Upper degree. During her undergraduate studies she undertook an internship with Schlumberger and Atlas polygenics where she developed an interest in energy systems. For her Bachelors dissertation, she developed a mathematical model for measuring the rate of remediation of crude oil spill in water. This earned her an eight month knowledge transfer scheme with the National Oil Spill Detection and Response Agency in Nigeria, where the results were applied on a national scale. After the scheme, she worked as a process engineer in the National Engineering and Technical Company Nigeria, where she participated in front end engineering design and detailed engineering design for various projects.

She then read for the degree of Master of Science in Advanced Chemical Process Design at the Centre for Process Integration (CPI), University of Manchester (UoM), for which she obtained a distinction. During her Masters dissertation she developed a graphical framework for integrating renewable and energy from waste into small scale chemical processes focusing on the food and drinks industrial sector. Afterwards, she worked in Process Integration Limited (UK) where she participated in the development of methodologies for optimizing existing and new industries with an objective to reduce energy consumption, reduce cost and increase the yield of products and application of these methodologies to industrial cases. The methodologies were implemented in software tools (e.g. Heat-int and Dist-int).

She also worked as a research assistant on the Energy Technologies Institute (ETI) Macro Distributed Energy (DE) project where she contributed to the development of a methodology for design of distributed energy systems (including fossil fuel, renewable and biomass based technologies) for the domestic and commercial sectors. She developed a software tool on the design methodology that is currently been used for teaching and research. Outputs from the analysis were scaled up to the UK economy to quantify the opportunity for DE and inform government energy policies. The technologies modelled in the tool are applied in the UK Smart Systems and Heat programs.

She returned to UoM to do a PhD in Chemical Engineering where she developed a graphical and optimization framework to integrate waste heat recovery in process sites. During this period she provided specialist advice on waste heat recovery to an EU project, Efficient Energy Integrated Solutions for Manufacturing Industries (EFENIS). She also collaborated with industries within EFENIS to apply the modelling framework. She has written three peer-reviewed conference papers, five peer-reviewed full length published articles and two full length articles currently under review. She also participated in national and international conferences. She is a widening participation fellow in the school of Chemical Engineering and Analytical Science UoM where she communicates 'Chemical Engineering' to non-specialist and specialist audiences. She is also part of the pastoral care team in the hall of residences.

Chapter 1: Introduction

World demand for energy has increased by 15% over the last ten years, with fossil fuels dominating the energy supply mix (International Energy Agency, 2012). Global population growth increases by approximately 0.2% per annum; therefore, demand for energy is expected to continue to increase (International Energy Agency, 2012). However, reserves of conventional fossil fuel sources are becoming increasingly difficult to exploit. One of the major downsides of increasing demand for fossil fuels is increased emissions of greenhouse gases from fossil fuel combustion. Carbon dioxide (CO_2) emissions from fossil fuel combustion are responsible for over 70% of total emissions (International Energy Agency, 2012). High concentrations of greenhouse gases in the atmosphere result in global warming.

As energy is an important determinant of a nation's growth, the availability, affordability and acceptability of energy is important. Availability of energy refers to having sufficient supplies (Winzer, 2012). Affordability refers to producing energy services at the lowest cost (Winzer, 2012). Acceptability refers to minimizing emissions from fossil fuel combustion (Winzer, 2012). These terms are associated with energy security.

The concept of energy security is context dependent; globally, energy security is defined as the availability of a regular supply of energy at an affordable price while respecting environmental concerns (European Commission, 2012). Therefore, policies and schemes relating to increasing efficiency in the use of fuel to improve global availability, reducing cost of energy, and reducing emissions are related to energy security.

The minimum concentration of greenhouse gases in the atmosphere required to ensure less than 2°C increase in temperature was set by the Intergovernmental Panel on Climate Change (1997). In other schemes, such as the Kyoto Protocol and the European Union Emissions Trading Scheme (EU ETS) started in 2005; binding obligations are set for industrialized countries to reduce greenhouse gas emissions especially carbon dioxide (CO_2). However, even with these schemes, demand for energy (Figure 1.1) and carbon dioxide emissions (Figure 1.2) have continued to increase. Improving global energy security could be possible if a radical change in energy production and consumption is encouraged.

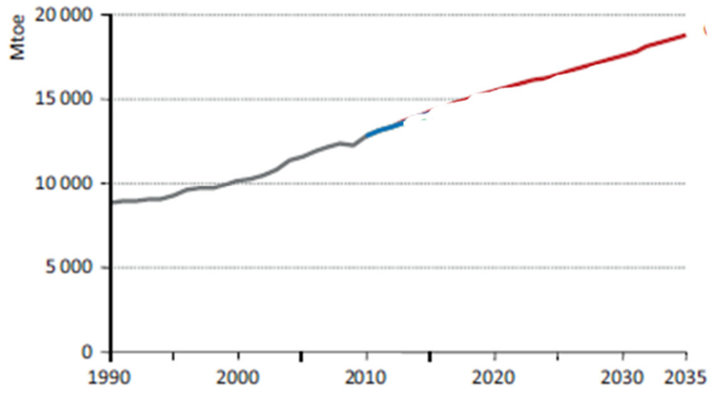


Figure 1. 1 Global energy demand trend (International Energy Agency, 2012)

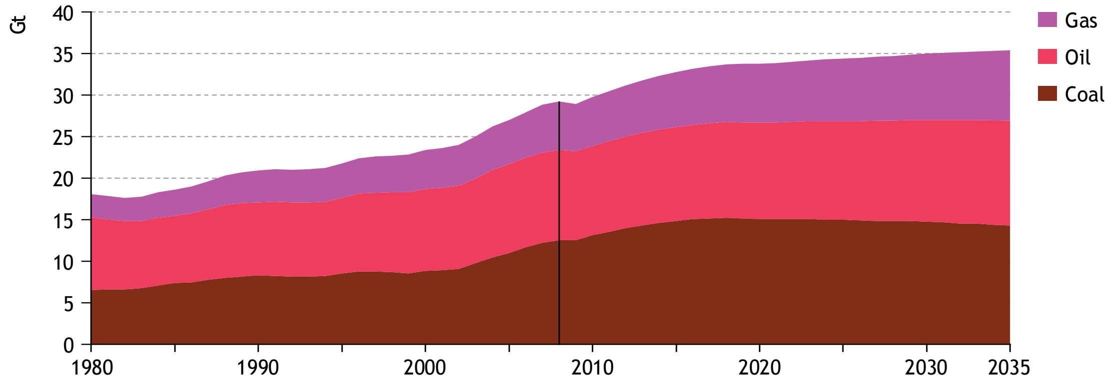


Figure 1. 2 Global trends in carbon dioxide emissions (International Energy Agency, 2012)

The industrial sector comprising agriculture, iron and steel, refining and petrochemicals, non-metals is responsible for over 35% of the world's energy consumption (International Energy Agency, 2012), generating over 30% of world greenhouse gases in the form of CO_2 released from combustion of fossil fuels. Concerns have been raised about the energy consumption patterns of energy intensive industries in the UK (Houses of Parliament, 2012) and worldwide (International Energy Agency, 2014). Globally, only 67% of energy inputs (from fossil fuels, nuclear and renewables) are transformed into a form for final consumption in all sectors including industry, transport and buildings (International Energy Agency, 2012). In the United States, about 50% of the energy input is lost as thermal energy from power generation and industrial manufacturing (Cook, 1971). As of 2008, 20 – 50% of the energy input in the US is still lost as thermal energy (USDOE, 2008). In the UK, about 40% of the energy content of fuel is lost as thermal energy (Ammar et al., 2012). In China, 10 – 50% of the energy content of fuel is lost as thermal energy (Lu et al., 2016). This lost thermal energy has been referred to as waste heat. However, it is necessary to define what industrial waste heat means, taking into account existing energy recovery measures in the process industry.

Waste heat produced in industries worldwide is shown in Figure 1.3. This is compared with total energy consumed by country in Figure 1.4, and compared with industrial energy consumed by country in Figure 1.5. The data in Figures 1.3 – 1.5 are based on energy data published by national and international agencies, company reports and scientific articles (Miro et al., 2015). Even though the quantity of waste thermal energy produced is large, the quality may be low.

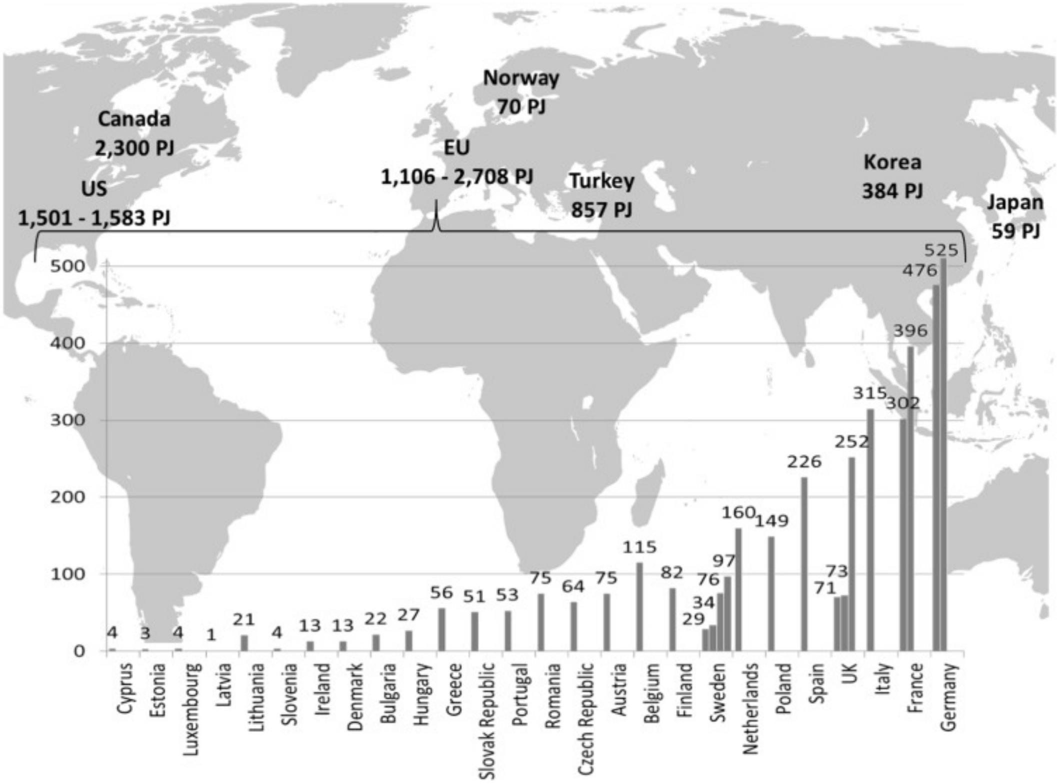


Figure 1. 3 Yearly industrial waste heat produced worldwide (Miro et al., 2015)

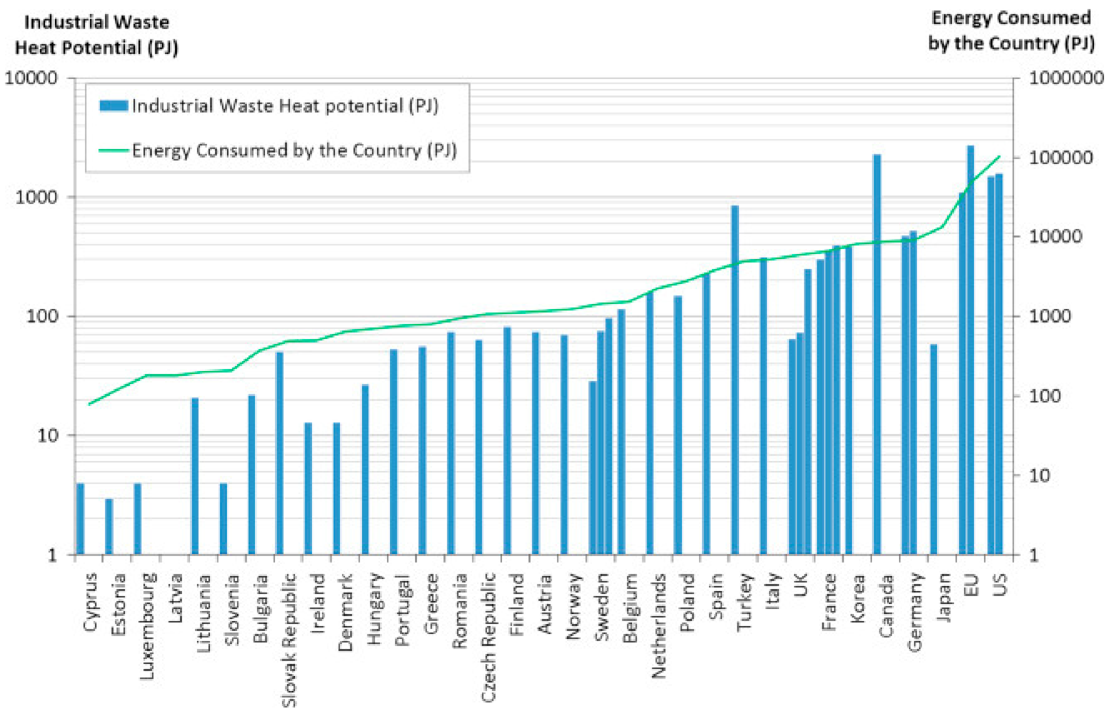


Figure 1. 4 Industrial waste heat produced and energy consumed by country (Miro et al., 2015)

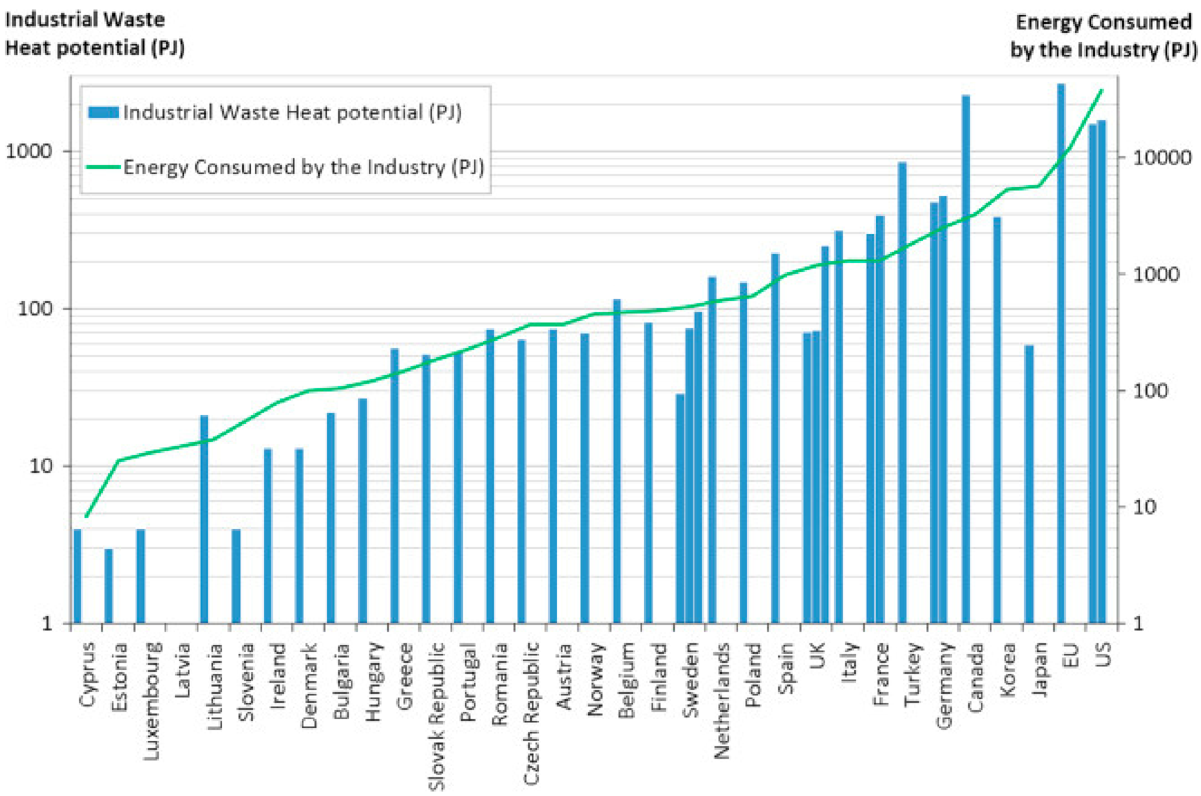


Figure 1. 5 Industrial waste heat produced and industrial energy consumption (Miro et al., 2015)

Exploitation of industrial waste heat could improve global energy security (i.e. availability, affordability and acceptability of energy globally). Improving availability is related to increasing efficiency in the use of primary fuel. One of the European Union (EU) targets is to reduce the use of primary energy with 20% coming through energy efficiency measures (EU, 2010). The Energy Efficiency Directive (EED) raises the importance of using industrial waste heat as a way to reach the EU target (EU, 2012).

1. 1. Process site energy security

The notion of energy security is context-dependent. For process sites comprising several processing units and utility systems designed to satisfy the heat and power demands, the concept of energy security needs to be defined.

Adapting the global definition, process site energy security is defined in this work as satisfying energy demands at high efficiencies, low costs to the process site, and minimal impacts on the environment. Focusing on energy security issues in process sites may be stronger motivations of change.

Concepts based on a system-oriented approach to process design; with an objective to improve efficiency in the use of fuel thereby reducing CO_2 emissions have been introduced. These concepts can be categorized into two; graphical techniques and mathematical optimization techniques. Examples of graphical techniques include Pinch Analysis and Total Site Analysis.

Pinch Analysis is a tool for analysing and developing efficient chemical processes through process integration (Linnhoff and Hindmarsh, 1983). Thermodynamically feasible targets for utility consumption based on maximum energy recovery within a processing unit are set prior to design. There are streams within a processing unit releasing large quantities of thermal energy (i.e. heat sources). There are also streams requiring heating (i.e. heat sinks). Energy recovery via heat exchange is encouraged between the heat sinks and heat sources provided a temperature driving force exists, thereby reducing the external utility requirements. Pinch Analysis has been applied to the process industry with huge success (Smith, 2005). However, the residual heat after maximizing heat recovery within a processing unit is usually rejected to cooling water or air.

Total Site Analysis (TSA) has also been introduced to extend Pinch Analysis to multiple processing units on a site (Dhole and Linnhoff, 1993). Heat recovery between several processing units is achieved through the utility system. However, the residual heat after heat recovery between several processing units is rejected to cooling water. Furthermore, a problem in industrial utility systems is the production of heat at temperatures unsuitable for process heating or power generation using conventional steam based systems, thereby reducing the efficiency in the conversion of primary fuel to heat and power.

Mathematical optimization frameworks have been developed for synthesis, operational optimization and retrofit of processing units and the site utility system. Synthesis of processing units and utility systems can be tackled using Mixed Integer Programming (MIP) techniques (Santibanez and Grossmann, 1980). Such techniques allow for specification of a vector of continuous variables to determine the operation strategies of units, and a vector of integer variables for selection of processing schemes, technologies in the utility system, distribution pressure levels etc. In the MIP approach a superstructure is created to embed all possible design configurations. The superstructure is reduced subject to an objective function and a set of inequality and equality constraints.

There are two forms of MIP problems: Mixed Integer Non Linear Programming (MINLP) problems and Mixed Integer Linear Programming (MILP) problems. Even though many equations in chemical processes are non-linear, discrete variables can be introduced to handle non-linearity, and assumptions on linearity are regarded as reasonable in the conceptual design stage (Santibanez and Grossmann, 1980).

A MILP model was developed in Grossmann and Papoulias (1983) for synthesis of site utility systems. In addition to structural choices, discrete variables were also attached to operating conditions such as pressures and temperatures to create a linear representation of the problem. The use of thermal energy at temperatures too low for conventional steam-based technologies like boilers, steam turbines was not addressed. Even though global optimum is guaranteed when MILP models are solved, the optimum solution only reflects the current situation and is an approximation of the real-world solution (Voll et al., 2015). Hence it is necessary to develop graphical techniques to provide near-optimal solutions to give the designer multiple choices to evaluate with regards practical constraints.

Other works on mathematical optimization techniques relating to processing units and utility systems include the following:

- Shang and Kokossis (2004) developed a multi-period MILP model to identify optimal steam levels for grass root synthesis of site utility systems.
- Varbanov et al. (2004) developed a MINLP model for synthesis of site utility systems. A successive MILP approach was used to solve the MINLP problem.
- Zhao et al. (2015) developed a MINLP model for simultaneous optimization of existing refinery production processes, and the utility system. The MINLP model was decomposed into MILP and NLP problems.
- Luo et al. (2011) developed an LP model for optimizing the operating cost of an existing utility system.
- Micheletto et al. (2008) developed a multi-period MILP model for operational planning of an existing refinery utility system.

However, in the aforementioned works, the use of residual heat when a process (and site) has reached its maximum potential for heat recovery, and use of heat at temperatures too low for conventional steam-based technologies are not addressed.

Industrial waste heat utilization could improve the energy security of process sites and global energy security, as fuel could be used more efficiently. A system perspective (i.e. considering interactions between the processing units and site utility system) is required to predict the benefits of waste heat utilization.

Apart from utilizing waste heat from industrial process sites, a process site energy security can be improved through carbon capture and sequestration (related to improving acceptability of energy), use of renewables and biomass, fuel switching to less carbon-intensive options; however, in all these schemes a significant amount of waste heat could still be present.

1. 2. Challenges related to waste heat utilization in process sites

Industrial waste heat utilization has received global attention in recent years (Ammar et al., 2012). There are several challenges associated with waste heat utilization.

Sources of waste heat on process sites could be from the site processing units and the utility system. The heat sources are dispersed geographically at the site level, supply and reliability fluctuate over time, and temperature of waste heat source streams varies (Lu et al., 2016). A challenge is accounting for the quantity and temperature of all the heat sources, and representing them in a systematic way that allows for selection of one or more waste heat sources. This way, the true potential in industrial waste heat can be realised. Previous research works focus on the quantity of waste heat (Miro et al., 2015). Some works that consider the quantity and temperature simplify the problem by considering only one heat source (Costa et al., 2009; Garimella, 2012; Zhang et al., 2015). Some other works assume the heat sources are available at a single temperature (Kapil et al., 2011; Kwak et al, 2014). The heat sources have also been selected in an unsystematic way (Miah et al., 2015).

Diverse technologies exist to recover useful energy in different forms from waste heat. Examples include Kalina cycles, transcritical power cycles and organic Rankine cycles for power generation; absorption chillers for chilling provision; absorption heat pumps, absorption heat transformers and mechanical heat pumps for upgrading low temperature waste heat to a higher temperature. The choice of technology options may depend on the heat source temperature. A challenge is selecting the best technology option and quality of heat to use, considering thermodynamic limitations and cost (including capital and operating cost) implications. Previous researchers focused on the use of one technology to exploit all the available waste heat (Popli et al., 2013; Chen et al., 2014; Qu et al., 2014). Some other works neglect the financial implications (Chen et al., 2014; Desai and Bandyopadhyay, 2009). Another challenge is modelling these technologies. Some authors focused on using simple models based on an assumed performance which are highly inaccurate (Viklund and Karlsson, 2015; Zhang et al., 2015), or detailed models suitable only for single heat source applications (Grossmann and Zaltash, 2001; Yin et al., 2010).

There are diverse opportunities to use the recovered energy from industrial waste heat within the process site and "over the fence" through heat and power export (Law et al., 2013; Hammond and Norman, 2014). For example if electrical power is recovered using Organic Rankine cycles, end-uses include exporting power to the grid, displacing import of power, supplementing power produced in the existing utility system. Also, heat produced, whether directly via heat exchange or from heat upgrade technologies, can be used for boiler feed water preheating, space heating, steam generation and hot utility reduction. A challenge is selecting the best end-use of recovered energy, taking into account economics and potential to reduce CO_2 emissions. Previous research works focus on use of recovered energy off-site (Fang et al., 2015; Eriksson et al., 2015). Some other authors focus on a single end-use of recovered energy (Le Lostec et al., 2008; Wang and Lior, 2011; Wu et al., 2014).

Waste heat has been referred to as heat for which recovery is not viable economically (Ammar et al. 2012). The operating hours needed to make heat recovery economic were investigated in Bruckner et al. (2015). However, the potential to improve the economics by selecting the end-uses of recovered energy has not been addressed. In the process industry, a technology needs to have a high discount rate (10 – 15%) and a low payback period (less than 5 years) for increased uptake (Bruckner et al., 2015). Therefore, even though there could be potential to increase the operational efficiency of process sites through waste heat utilization, a balance needs to be made between the efficiency increase and capital cost. Also, whilst it is possible to evaluate the operational costs (such as costs of fuel and electrical power tariffs) with a high degree of certainty, there is very little data available to accurately predict the installed capital of waste heat recovery technologies (Tchanche et al., 2014). A challenge is developing a novel design approach to improve the economic viability of waste heat utilization, and to perform sensitivities to show the impact of uncertainties in capital cost estimation.

Addressing these challenges is crucial to increasing uptake of waste heat recovery technologies by industry.

1. 3. Research hypothesis

The research hypothesis of this work is:

"There is potential to increase efficiency in the use of energy (availability) and reduce CO_2 emissions (acceptability) through waste heat recovery and utilization. Improving the affordability of the scheme is possible through a holistic approach to design, where interactions with the site utility system and wise selection of end-uses of recovered energy (and associated technologies) are considered".

Thus, in the context of improving a process site's energy security, the proving of this hypothesis could result in novel thermodynamic insights, analysis and design frameworks. The proving of this hypothesis could also offer a new methodology for integrating different technologies recovering useful forms of energy (power, chilling and heat) from waste heat in process sites. The method may help to determine the true potential in industrial waste heat in industrial sites which can be scaled up to national, and international levels to quantify the possible impact of industrial waste heat utilization under different scenarios.

1. 4. Research problem

This research is developed because the current frameworks for improving a process site energy security neglect the available waste heat. On the other hand, previous works on waste heat recovery technology development, focus on their performance and assume waste heat recovery is homogeneous i.e. the heat is available at a single temperature, can be assumed to be from a single source, and only one end-use of recovered energy is possible. The research is also developed to address the challenges in Section 1.2. These challenges address important details of the problem.

Previous research on integration of waste heat recovery technologies into process sites also assume the problem is homogeneous and neglect waste heat from the site utility system. The possibility of combining different technologies to maximise production of useful energy from waste heat has also been neglected. Thus a new methodological framework is necessary for exploring the heterogeneous nature of waste heat utilization i.e. taking into account the varying quantity and temperature of heat sources from the site processing units and the utility system, multiple end-uses of recovered energy, and choice of technology options.

The heterogeneous nature is explored in this work through the design of waste heat utilization systems. A waste heat utilization system allows the combination of one or more concepts (technologies and end-uses of recovered energy) to exploit industrial waste heat. Combination of concepts to recover multiple forms of energy could result in higher reductions in CO_2 emissions and higher increases in energy efficiency.

A number of processing units are linked to a central utility system in process sites (Smith, 2005). It may be possible to reduce the quantity of waste heat produced through modifications, and changes to the operation of the utility system. Furthermore, energy recovered from waste heat may be used within the site utility system. The benefits of end-uses of recovered energy within the site utility system can only be determined by considering the utility system configuration (Smith, 2005). Hence, considering interactions between the waste heat utilization system and the site utility system is necessary; a system-oriented approach to integrating waste heat recovery in process sites could have significant benefits.

In previous research works where the heterogeneous nature of waste heat utilization is considered, interactions between the waste heat utilization system, the site utility system and processing units are not considered. This can be defined as a stand-alone design, as illustrated in Figure 1.6. Even though waste heat from the utility system and site processing units may be considered, the use of recovered energy within the site utility system and processing units is neglected.

A combined systems design could be more beneficial. This means recovered energy is used in the site utility system and in the site processing units as shown in Figure 1.7, and opportunities to reduce the waste heat produced from the site utility system are explored simultaneously.

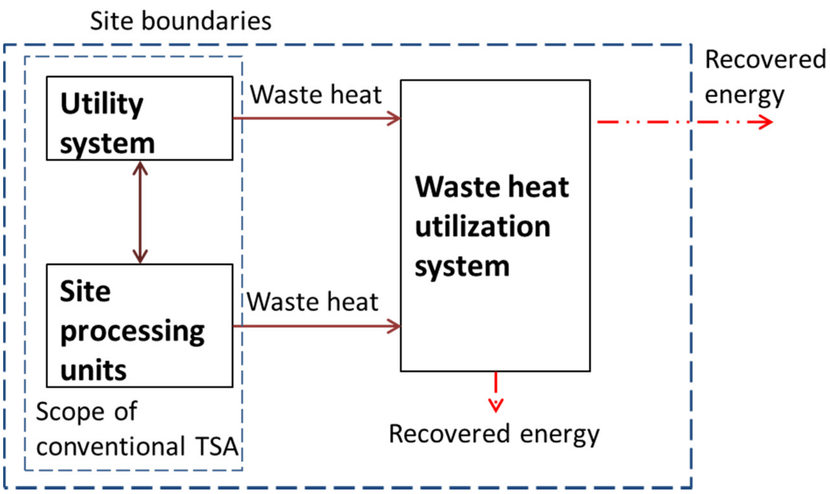


Figure 1. 6 Stand-alone design

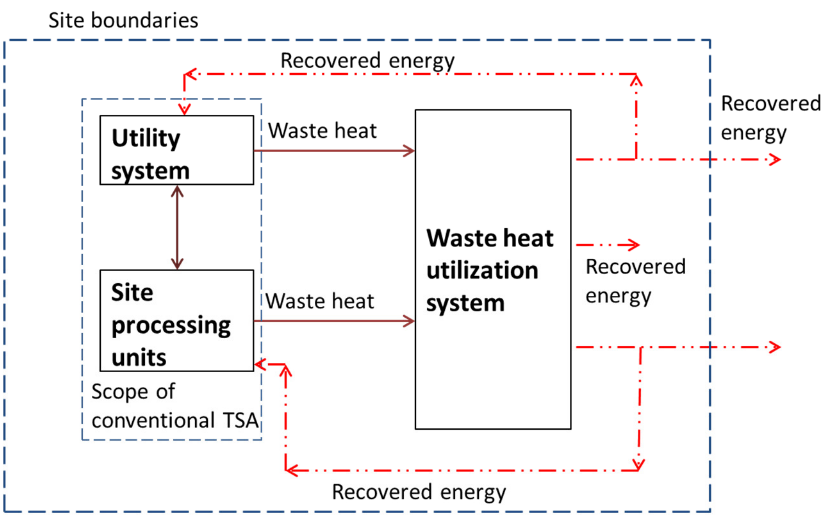


Figure 1. 7 Combined systems design

This research aims to develop a combined systems framework to integrate waste heat recovery into process sites as shown in Figure 1.7. To address this problem, both graphical tools and optimization frameworks will be developed. The graphical tools will provide thermodynamic and physical insights into the design problem, which helps in reducing the size and complexity of the optimization problem. Optimization techniques provide a common framework to solve the problem in a systematic way and capture trade-offs. Development of algorithms for solving the optimization framework is not within the scope of this work. Results from the methodological framework proposed in this work can be used to guide public policies on industrial waste heat utilization.

1. 5. Research objectives

The overall objective of this work is to develop a holistic approach for integrating waste heat recovery in existing process sites in order to prove the stated hypothesis. The approach exploits only thermal energy rejected to cooling water and air from the site processing units and the site utility system. This holistic approach aims to establish the assumptions required to improve availability, affordability and acceptability in industrial sites through waste heat utilization. The methodology proposed in this PhD project specifically aims to:

1. Develop explicit models for waste heat recovery technologies. These models would be easy to integrate with a variety of energy systems. The following issues will be addressed:
    a. Determination of the physical design parameters to include in the model. Such parameters include the operating temperatures of the technology components. For example for the organic Rankine cycle, possible parameters are: the condenser temperature, evaporator temperature, work required by the pump, work produced by the expanders, condenser and evaporator duties.
    b. Predicting the ideal performance and actual (real) performance of technology options. The actual performance takes into account inefficiencies in the technology component and working fluid non-ideal behaviour. The ideal performance is defined in terms of the thermodynamically reversible process.
    c. Consideration of the impact of working fluids on the performance of the technologies, and selection of working fluids.
    d. Validation of the models against rigorous simulation or thermodynamic design data available in literature.

2. Perform a comparative analysis of technology options. A comparative analysis is necessary to determine the best technology to use, form of energy to recover and quality of heat to use. The following issues will be addressed:
    a. Development of a screening criterion to account for the true capabilities of technology options and for irreversibilities due to finite temperature heat transfer.
    b. Development of a screening tool to visualize the results. The screening tool shows the impact of heat source temperatures and guides technology selection. Better matching between heat source temperatures and technology options could reduce irreversibilities due to heat transfer.
    c. Application of the screening tool to rank technology options for waste heat utilization taking into account the quality of heat sources.
3. Rank and evaluate on-site and off-site end-uses of recovered energy. The use to which recovered energy from waste heat is put could affect the economics (i.e. costs and benefits) of the system, and potential to reduce CO_2 emissions. The following issues will be addressed:
    a. Identification of opportunities to use recovered energy within the site and ‘over the fence’.
    b. Development of a ranking criterion to account for both the economic potential and potential to reduce CO_2 emissions.
    c. Application of the ranking criterion to introduce a hierarchy to end-uses of recovered energy i.e. waste heat utilization opportunities.
    d. Perform sensitivity analyses to show the impact of changes in capital cost, fuel prices, electrical power prices, discount rates and technology performance to explore future outlook of waste heat utilization and the impact of uncertainties in the design inputs.
4. Develop graphical techniques for process integration of waste heat recovery technologies. Graphical techniques could provide physical insights into the problem and could be useful for preliminary analysis. The following issues will be addressed:
    a. Development of temperature-enthalpy plots representing heat sources from site processing units and the site utility system.
    b. Assignment of technology options against the temperature-enthalpy plots to determine the best heat source temperature (and associated duty) to exploit.

   c. Assessment of the benefits of integrating more than one technology, and determination for each technology the best temperature at which to use waste heat and the associated heat flows.
   d. Application of the graphical techniques to an industrially relevant case study and evaluation of different scenarios. Such scenarios include infinite demand and finite demand for recovered energy, and on-site, off-site or both on-site and off-site end-uses of recovered energy.
5. Develop a mathematical optimization framework for process integration of waste heat recovery technologies. The optimization framework captures capital–energy trade-offs. The choice of algorithm to solve the framework will depend on the nature of the problem. The following issues will be addressed:
   a. Systematic representation of the waste heat source streams to allow selection of a stream or a combination of multiple streams.
   b. Specification of the system variables (degrees of freedom), considering both operational (continuous) and structural (binary) variables. The structural variables represent the existence of a technology; once a technology exists its operation is represented by continuous variables.
   c. Development of a predictive model describing the system behaviour including technology performance models, and equality and inequality constraints.
   d. Accounting for variability of utilization opportunities through the year, varying operating conditions and energy prices.
   e. Definition of a general configuration (superstructure) that embeds possible design alternatives and allows simultaneous optimization with the site utility system.
   f. Specification of an objective function that considers the benefits associated with end-use of recovered energy and the total annualised cost (including capital, operating and maintenance costs) of the associated technologies.
   g. Application of the framework to industrially relevant case studies.

1. 6. Thesis outline

This thesis contains seven chapters with sections and subsections providing a consistent narrative to understand waste heat utilization in process sites. The “Alternative format” of the University of Manchester is used, incorporating papers published. A list of appended papers is provided in Section 1.7. The outline is summarized in Table 1.1.

Table 1. 1 Thesis outline

Chapter	Description
Chapter 2: Literature review	Previous work related to waste heat utilization in process sites is reviewed. The literature review provided in chapter 2 supplements reviews provided in the appended papers.
Chapter 3: Modelling and integrating waste heat recovery technologies	Chapter 3 contains two publications. In publication 1 models of technology options, such as organic Rankine cycles, absorption chillers and absorption heat pumps, together with graphical approaches for integrating these technologies are provided. Models of heat upgrade technologies, such as absorption heat transformers and mechanical heat pumps, together with a graphical integration strategy are provided in Publication 2. The publications in chapter 3 satisfy objectives 1 and 4.
Chapter 4: Comparing technology options for waste heat utilization	Chapter 4 contains one publication in which a novel screening criterion and tool are developed for comparing technologies for waste heat utilization. Publication 3 satisfies objective 2.
Chapter 5: Waste heat utilization opportunities	Chapter 5 contains one publication. A hierarchical framework for evaluating end-uses of recovered energy from waste heat is provided in publication 4; this satisfies objective 3.
Chapter 6: Design of waste heat utilization systems	Chapter 6 contains three publications. A multi-period optimization framework for integration of waste heat recovery technologies, for use of recovered energy on-site and off-site is presented in Publication 5. Publication 6 contains an optimization framework for integrating heat upgrade technologies. Publication 7 contains a conceptual design methodology for site waste heat utilization systems focusing on utilizing waste heat within a process site. All three publications satisfy objective 5.
Chapter 7: Conclusions and future work	Chapter 7 presents key findings, limitations of the present work and recommendations for future work

1. 7. Appended papers

This thesis is based on the work contained in the following papers (all the papers have been submitted or accepted for publication in peer-reviewed journals):

Publication 1. Oluleye G., Jobson M., Smith R., Perry S.J., Evaluating the potential of process sites for waste heat recovery. Applied Energy (2016); 161: 627–646 doi.org/10.1016/j.apenergy.2015.07.011

Publication 2. Oluleye G., Smith R., Jobson M., Modelling and screening heat pump options for the exploitation of low grade waste heat in process sites. Applied Energy 2016; 169: 267 – 286. doi.org/10.1016/j.apenergy.2016.02.015

Publication 3. Oluleye G., Jiang N., Smith R., Jobson M., A Novel Screening Tool for Waste Heat Utilization Technologies, Energy (under review)

Publication 4. Oluleye G., Jobson M., Smith R. A hierarchical approach for evaluating and selecting waste heat utilization opportunities. Energy 2015; 90: 5–23. doi: 10.1016/j.energy.2015.05.086.

Publication 5. Oluleye G., Jobson M., Smith R. Optimization-based Design of Waste Heat Recovery Systems, conference proceeding for the 28th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, 2015 (lecture number 50219).

Publication 6. Oluleye G., Jobson M., Smith R., Process integration of waste heat upgrading technologies, Process Safety and Environmental Protection (2016), http:/dx.doi.org/10.1016/j.psep.2016.02.003.

Publication 7. Oluleye G., Smith R., Conceptual design of site waste heat utilization systems, Energy (under review)

Co-authorship statement

Gbemi Oluleye is the main author of all the papers. Dr Megan Jobson and Professor Robin Smith supervised the work in all papers. Simon Perry provided technical advice on rigorous simulation of the absorption chillers in Publication 1. Ning Jiang provided technical advice on the comparative analysis carried out in Publication 3.

Chapter 2: Literature Review

Increasing energy efficiency has potential to reduce global carbon dioxide (CO_2) emissions by 44% in 2035 (International Energy Agency, 2012). Waste heat recovery and utilization can increase efficiency in the use of fuel in the process industry. This chapter contains a review of pertinent literature relating to improving energy efficiency and waste heat utilization in process sites. The literature review in this section supplements the reviews provided in the publications presented in Chapter 3, 4, 5 and 6.

2.1 Defining industrial waste heat

Industrial waste heat is defined as heat for which recovery is not viable economically in Ammar et al. (2012). However, the economics of waste heat recovery depends on the choice of technologies, the quantity and quality of the heat sources, the end-use of recovered energy and the design approach. Viklund and Johansson (2014) defined waste heat as a by-product of industrial processes. This definition neglects the potential to recover this heat for use within a single process or between several processing units on a site.

Bendig et al. (2013) defines industrial waste heat as the heat available in a process after heat recovery. Even though their definition takes into account the potential for heat recovery, by limiting it to a single process, it neglects the potential for heat recovery between several processes, and also the waste heat available from a site utility system designed to satisfy the energy demand (heat, power and cooling) of site processes. Morandin et al. (2014) defines industrial waste heat as heat at 'medium to low temperature not used in industrial processes'. This definition neglects heat available from the site utility system, and any high temperature heat not used. Waste heat has also been referred to as excess heat exchanged to a medium such as water, air and flue gas (Viklund and Karlsson, 2015); the same definition is used in Bruckner et al. (2015). However, it is unclear whether this excess heat is available before or after maximizing heat recovery within a process or between several processing units on a site.

Pinch Analysis and Total Site Analysis have been introduced to maximize heat recovery within a single processing unit and between processing units on a site in order to minimize fuel consumption in the process industries. Implementation of techniques based on these concepts has resulted in efficient use of energy and reduction in emissions from process sites

(Coker, 2015). This form of heat recovery is cheap, easy to implement and indicates minimum demand for external utilities (Smith, 2005 and Little and Garimella, 2011).

As part of Pinch Analysis, composite curves were introduced by Linnhoff and Hindmarsh (1983) to represent the aggregate of possible heat transfer within process streams in a single processing unit. Composite curves represent, in temperature–enthalpy diagrams, the heat available in a process (hot composite curve), and heat required by a process (cold composite curve). Construction of the composite curves requires that the mass and energy balances for a process are established. A simple schematic is shown in Figure 2.1. The region of overlap between the hot and cold composite curves shows the potential for heat recovery within a process. The heat recovery potential is maximized when the two curves are separated by the minimum approach temperature (ΔT_{MIN}). Maximizing heat recovery within a process minimizes demand for external hot and cold utility. Steam is the most common hot utility, available at several pressure levels. Cold utility could be cooling water, air or refrigeration. The composite curve is not a suitable tool for utility determination in terms of quantity and temperature. Hence the Grand Composite Curve (GCC) was developed as a tool for utility selection (Linnhoff et al., 1982).

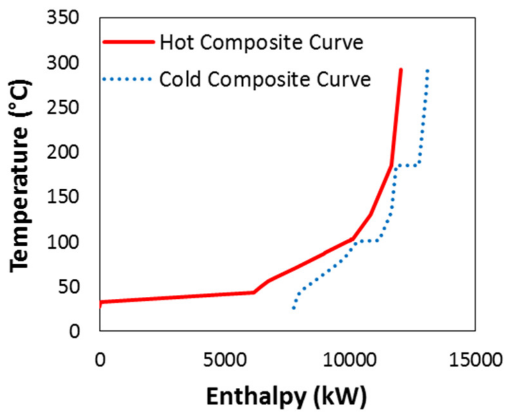


Figure 2. 1 Composite curves illustration

The GCC is a graphical representation of the variation of heat supply and demand within a process. The process streams are divided into two regions: those above and those below the pinch. A simple schematic of a GCC is shown in Figure 2.2. The temperatures are shifted by half the minimum temperature approach.

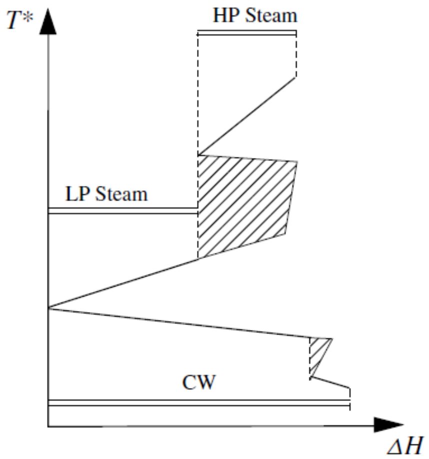


Figure 2.2 Grand Composite curve (Smith, 2005)

There are typically multiple processing units in energy intensive industries such as petrochemicals, refineries and chemicals. Therefore the residual heat available from single processing units may be recovered for use in another processing unit through the site utility systems via Total Site Analysis (Dhole and Linnhoff, 1993). There is more potential for heat recovery in a total site context (Smith, 2005).

Several processing units are incorporated in Total Site Analysis and connected through a central utility system (Dhole and Linnhoff, 1993). This implies heat recovery between several processing units is achieved through the utility system. Total Site Profiles (TSP) are constructed using the residual heat sinks and sources from individual processing units. The Site Sink Profile is plotted from the residual heat sinks above the pinch in the grand composite curve, while the Site Source Profile is from residual heat sources below the pinch in the grand composite curve. The temperatures in TSP are shifted by a minimum temperature approach. The total site profile provides an overall view of heat surplus and deficit for all processing units. It also shows the scope for heat recovery between several processing units, and the amount of residual heat rejected to cooling water and air. A simple schematic of a total site profile is shown in Figure 2.3.

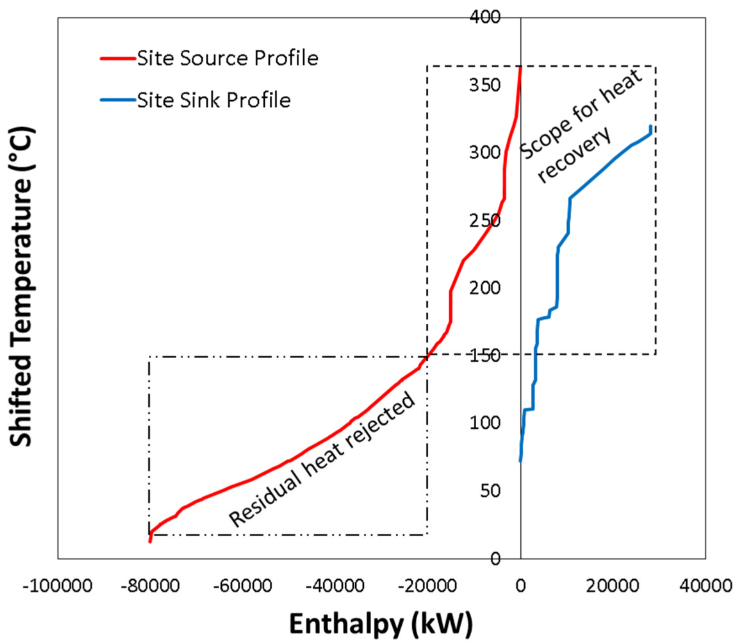


Figure 2.3 Total site profile

In this work the residual heat rejected to cooling water and air when a single process or a site has reached its limit for heat recovery (i.e. when a process or site is pinched) is defined as waste heat. The definition also includes the residual heat rejected from a site utility system designed to satisfy the energy demand of sites processes. Waste heat from site processing units and utility system is discarded by the evaporation of water in cooling towers, forced air cooling or through the stack. The definition of waste heat in this work implies that heat from the by-product of chemical reactions is only considered as waste heat after the potential for heat recovery is maximized. A robust definition of industrial waste heat helps to establish the scope for integrating unconventional technologies such Organic Rankine cycles, absorption heat transformers and absorption chillers for waste heat utilization in process sites. However, it is necessary to compare these unconventional technologies with heat recovery via heat exchange. Such comparisons will provide confidence in the recovery of heat via heat exchange first.

Sometimes it may be impossible to maximize heat recovery based on practical limitations; in this case, the residual heat can be considered as waste. Furthermore, not all existing process sites are designed based on the principles of TSA; therefore, in addition to the unconventional recovery technologies, heat recovery via heat exchange will also be considered in this work.

Industrial waste heat may exist over a wide range in quantity and temperature. However, previous researchers simplified the design by assuming the heat to be from a single source and at a single temperature level (Kapil et al., 2011 and Kwak et al., 2014). Some other authors focus on a single heat source; for example Bruno et al. (1999); Costa et al. (2009); Garimella (2012); Zhang et al. (2015).

2.2 Overview of site utility systems

Combustion of fuel to generate heat and power in site utility systems is responsible for majority of the CO_2 emissions in energy intensive process industries (International Energy Agency, 2014). The fuel consumed in site utility systems also represents one of the major operating costs (Berntsson et al. 2013). The utility system creates interactions between site processes (Coker, 2015). These interactions could be exploited to maximize waste heat utilization in process sites.

Utility system components are technologies for combustion of fuel (boilers, gas turbines), expansion of steam to generate power (back pressure steam turbines and condensing turbines), and expansion of steam to lower pressure levels (expansion valves). Steam (a hot utility) is delivered to the process in pipes know as steam headers or distribution mains. Higher temperature heating is achieved using fired heaters. Figure 2.4 is a simple schematic of a site utility system. A utility system may generate both heat and power from the same fuel source, and sale of power to the central grid to generate revenue. A utility system may also generate only heat; in this case any power demand is imported from the grid (Smith, 2005).

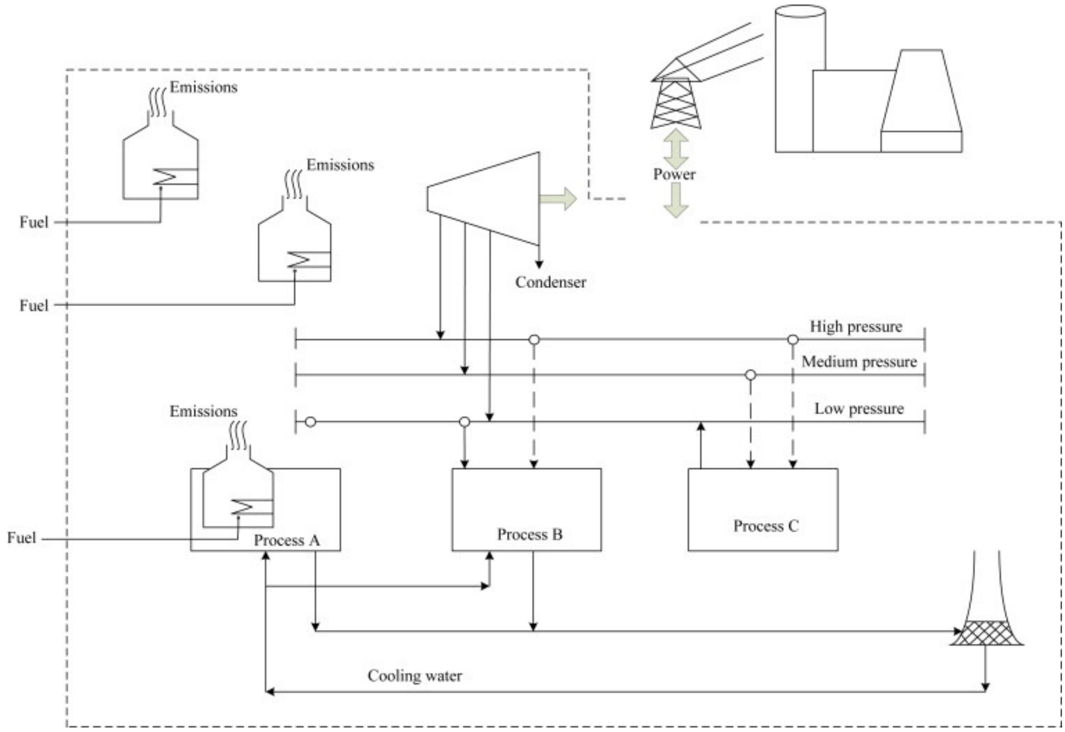


Figure 2.4 Site utility system schematic (Klemes et al., 1997)

Accurate modelling of utility system components is necessary to estimate the residual heat rejected to cooling water and air. Models of steam turbines, boilers and gas turbines that account for the variability of equipment efficiency with load, size and operating conditions were developed by Varbanov et al. (2004). Even though the models show a good description of the part load performance, they are non-linear. Use of non-linear expressions could result in complex optimization routines.

Simple explicit linear models for utility system components such as steam turbines, gas turbines and boilers as functions of operating temperature, saturation temperature and steam flow rate at full load and part load were developed by Aguilar et al. (2007). These models are adopted in this research as the equipment performance depends on both unit size and load.

Previous studies of waste heat available from utility systems only considered heat in the exhaust flue gas (Chen et al., 2012; Lu et al., 2016), which is usually extracted above the acid dew point to avoid corrosion and ensure flue gas buoyancy (Chen et al., 2012). However in these studies, the flow of fuel, heat and power in the main utility system has been left unchanged, resulting in a stand-alone design. Furthermore, the heat recovered is limited to its use for hot water generation. Bade and Bandyopadhyay (2015) also developed a methodology based on pinch analysis to integrate heat in gas turbine exhaust with the process plant to minimize fuel consumption. Graphical approaches for utility system analysis (including for grassroots design, operational improvement and retrofit) are reviewed in Section 2.2.1. In Section 2.2.2 approaches based on mathematical optimization techniques are reviewed.

2.2.1 Graphical approaches for utility system analysis

It is possible to set targets prior to design of site utility systems for boiler steam demand and fuel consumption, steam generation from site processing units, and power generation from steam expansion.

In Dhole and Linnhoff (1993), targets for fuel consumption, steam generation and use are determined using Total Site Profiles. The potential for steam generation from site processing units is determined using the saturation temperature of distribution mains. The steam is generated into the utility system and used for process heating. Figure 2.5 shows the total site profile with steam generation and use, and the boiler fuel demand. Using only the saturation temperatures neglects any superheating and boiler feed water preheating. This could result in inaccurate targets for boiler fuel demand. Furthermore, the possibility of reducing fuel consumption through the use of residual heat after heat recovery is not addressed.

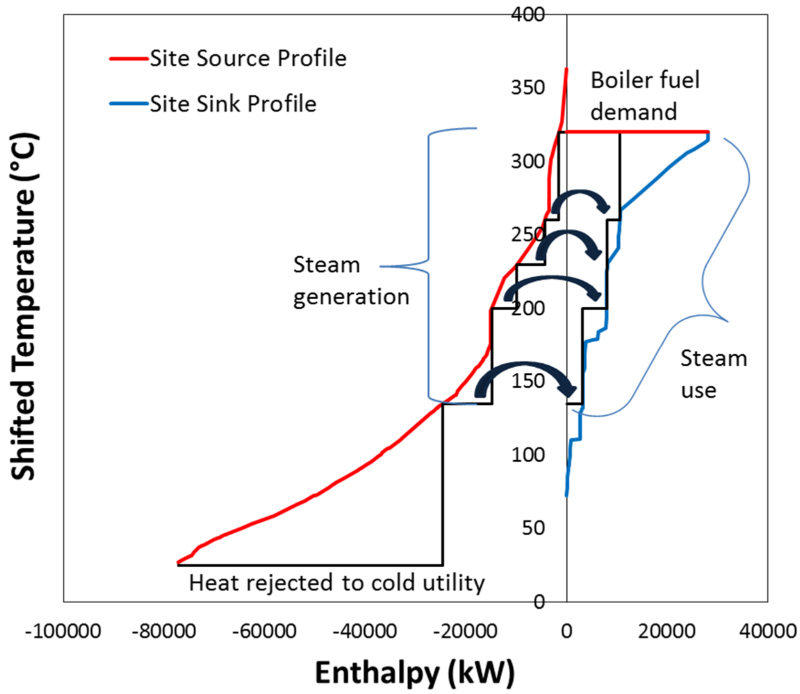


Figure 2.5 Total site profile showing targets before design

Recently, Sun et al. (2015) developed a more realistic targeting procedure taking into account boiler feed water preheating, steam superheating for steam generation and steam desuperheating for process heating. Again the potential to utilize the residual waste heat (i.e. heat rejected to the cold utility) was neglected.

A process site's power demand could be met by importing electricity from the central grid and/or by cogeneration. Different methodologies have been developed for estimating power produced from steam expansion in a site. A simple approach using the Site Utility Grand Composite Curve (SUGCC) to represent the overall picture of expansion zones for power production was developed by Dhole and Linnhoff (1993). The SUGCC is a plot of the difference between the total site source and sink profiles. An illustration is shown in Figure 2.6.

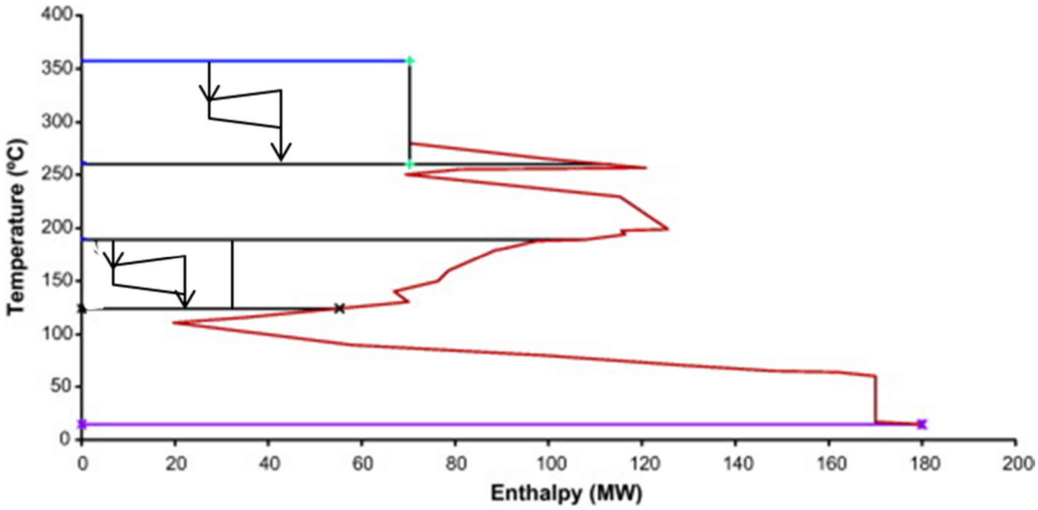


Figure 2.6 Site utility grand composite curve showing steam expansion levels (Kapil et al. 2012)

Dhole and Linnhoff (1993) estimate the ideal shaft power using the Carnot factor, assuming a turbine is installed between the expansion zones (Figure 2.6). A constant efficiency factor was multiplied by the ideal power generation to estimate the actual shaft power generation. Using a constant efficiency factor neglects the inlet and outlet conditions of the turbines, making the estimation inaccurate. Furthermore, power generation at temperatures too low for steam based technologies was not addressed. The large quantities of heat available at such temperatures warrant recovery (Kapil et al., 2012).

Due to the inaccuracy in the model used for shaft power estimation in Dhole and Linnhoff (1993), Mavromatis and Kokossis (1998) developed a turbine hardware model (THM). The

THM model represents the variation of isentropic efficiency with turbine size and part load. However, it does not estimate shaft work accurately as the effect of back pressure is not taken into account (Raissi, 1994). Raissi (1994) used a temperature-enthalpy model for power estimation based on assumption of saturated steam at the outlet and inlet of turbines. Both works of Mavromatis and Kokossis (1998) and Raissi (1994) neglect the potential for power generation from heat when temperatures are too low for conventional steam-based systems.

Some other researchers focus on improving the accuracy of the turbine model, but neglect the utilization of waste heat. For example, Bandyopadhyay et al. (2010) propose simple linear models utilizing a rigorous energy balance at the steam header; however, the degree of superheat in the mains is not accounted for. The degree of superheat is accounted for in Ghannadzadeh et al. (2012), where an iterative bottom-to-top model (IBTM) was developed to estimate the shaft work using a constant isentropic efficiency steam turbine model. The power generated is calculated from the lowest steam expansion level (at 120-130°C) to the highest level, allowing the degree of superheat to be estimated. However, power generation from heat below 120-130°C is not addressed. Even though boilers and gas turbines are highly efficient, putting them together in a system results in lower overall efficiencies compared to the individual technology efficiency, due to waste heat available in large quantities.

More recently, Sun et al. (2014) proposed a graphical approach based on the Site Grand Composite Curve. The SGCC is obtained from the site sink and source profiles. It provides greater clarity for interactions between site processes and the utility system. Again, use of waste thermal energy at the lowest temperature level after expansion i.e. exhaust steam, is not addressed.

Exhaust steam can be expanded to vacuum conditions using a condensing turbine. However, to ensure the exhaust has an acceptable dryness fraction, the degree of superheat needs to be adjusted. Adjusting the degree of superheat changes the cogeneration potential and increases primary fuel consumption; in this case, the exhaust temperature of the lowest expansion level is usually increased to ensure the condition of steam after expansion is dry. This means that large quantities of heat are rejected from ambient conditions to 90°C (Bruckner et al. 2015).

Another option is to use the exhaust steam to drive waste heat recovery technologies generating power using organic fluids. Examples include organic Rankine cycles and Kalina cycles. A challenge is the lack of hardware models for waste heat recovery technologies that are easily adaptable for use in existing graphical methodological frameworks for utility system analysis.

For synthesis of site utility systems, Shang and Kokossis (2005) proposed the use of thermodynamic efficiency curves (TEC). The TEC gives an overview of the maximum useful energy produced (both heat and power) per unit of fuel input for all possible design cycles, such as combined steam and gas turbine cycles, steam turbine cycles, condensing turbine cycles and simple gas turbine cycles. The TEC curve is useful for screening and ranking design alternatives and reduces the size and complexity of the optimization problem. However, generating the curve is based on conservation of energy quantity which assumes heat and power are equal entities. Since multiple energy flows occur in energy systems, a choice of technology option should consider both conservation of energy quantity and degradation of energy quality. The case study presented by Shang and Kokossis (2005) shows that increasing the power produced by cogeneration does not always improve the thermodynamic efficiency of the utility system. This inefficiency can be attributed to the large quantities of waste heat at temperatures too low for conventional steam-based systems.

For existing utility systems, targeting tools such as the grand composite curve that shows the placement of existing utilities in a single process and the site profile that shows utility placement for multiple processes are useful tools for operational improvement and retrofit (Smith, 2005). Generating total site profiles for an existing site can also show the available waste heat in quantity and temperature. The R-curve concept developed by Kenney (1984) for simple systems and applied to complex utility systems by Kimura and Zhu (2000) suggests the operation of an existing utility system is improved without capital investment. The R-curve is a plot of the site cogeneration efficiency and the power to heat ratio (R-ratio). The concept involves development of steam marginal prices to reflect the most valuable steam worth saving. The case study presented in Kimura and Zhu (2000) shows that increasing the R-ratio reduces the site cogeneration efficiency. Again, this inefficiency could be attributed to waste heat which cannot be used for power generation using conventional steam-based systems.

Karimkashi and Amidpour (2012) extended the R-curve concept to include R-value for emissions reduction and costs savings. However, reduction in emissions, costs and increase in efficiency by utilizing waste heat was not addressed. Makwana et al. (1998) introduced the concept of power generation efficiency curves showing the potential for steam saving in existing process sites. The power generation efficiency curves are based on the concept of heat flow paths through the utility system, distinguishing between 'current' and 'optional' paths. Current paths were analysed to find scope for steam saving through reduction in process consumption and optional paths were identified to utilize any steam surplus provided by the current paths. The concept of using power generation efficiency curves was further improved by Varbanov et al. (2004) to allow for efficient automation and for use with more complex configurations. From the analysis in Varbanov et al. (2004) at high R values, the cogeneration efficiency was low. The potential to improve the cogeneration efficiency by utilizing waste heat was not explored. A novel thermodynamically-based diagram was developed by Bade and Bandyopadhyay (2015) to integrate gas turbine exhaust for process heating. The diagram shows the gas turbine pressure ratio as a plot of the power-to-heat ratio. However, use of waste heat from the process plant is not addressed.

Graphical tools can provide useful physical insights for understanding the problem and potential solutions. The outputs of graphical based tools can reduce the size and complexity of mathematical optimization approaches (Smith, 2005). Waste heat recovery and utilization could improve efficiency in the use of fuel; hence there is a need to develop graphically-based thermodynamic tools for exploring opportunities for recovery and re-use of waste heat in process sites, considering also the site utility system.

2.2.2 Mathematical optimization techniques for utility system analysis

Graphical tools support understanding of a problem. However, they do not provide a common framework for solving problems in a systematic way; neither do they guarantee optimality (Grossmann and Papoulias, 1983). Optimization strategies, on the other hand, provide a systematic decision-making approach enabling design of utility systems to be improved, while ensuring capital-energy trade-offs are captured (Smith, 2005). Site utility systems can be optimized subject to diverse objective functions such as minimum total cost (both capital and operating), minimum operating costs, minimum emissions or using multiple objectives (Varbanov et al., 2004). The formulation for an optimization problem could be linear or non-linear, and integer programs consider structural variables. Finding the global optimum is guaranteed when linear programs are used (Smith, 2005).

Mathematical programming frameworks exist to tackle rigorous synthesis of site utility systems. Shang and Kokossis (2004) developed a multi-period Mixed Integer Linear Programming (MILP) model to identify optimal steam levels for a utility system. The framework accounts for interactions between the utility system and processing units by developing a 'transhipment' network to represent the heat flows of a total site. The transhipment model introduces temperature intervals in the total site profiles; the kinks on the profile represent turning points. Major decision variables include temperature of steam levels, overall fuel requirement, the cogeneration potential and cooling utility demand. The use of residual heat at temperatures too low for conventional steam-based systems is not addressed.

To determine the best structure to produce heat and power (i.e. best combination of technology options) that minimizes total costs, Shang and Kokossis (2005) developed a multi-period MILP model, applying the transhipment model for steam levels of Shang and Kokossis (2004). The framework combines benefits from Total Site Analysis, thermodynamic analysis and mathematical optimization techniques. Integration of thermodynamic concepts reduces the complexity of the optimization model, since it is able to screen alternative designs based on efficiency (i.e. sum of useful heat and power output to fuel input). However, the thermodynamic analysis is based on conservation of energy quantity, which assumes that heat and power are similar entities. Furthermore, degrees of freedom were limited to selection of steam levels and the utility system layout, neglecting the utilization of residual heat rejected to cooling water.

Taking into account environmental objectives, Papandreou and Shang (2008) developed a multi-objective MILP model addressing both environmental impact and cost. The synthesis problem focused on developing a superstructure for possible combinations of technologies and fuel; the use of waste heat is not addressed.

Mathematical optimization techniques also exist for operational optimization of site utility systems. This involves changing the current operation without need for capital investment. A robust optimization procedure for existing utility systems is proposed by Varbanov et al. (2004). The procedure uses a successive MILP approach to solve a Mixed Integer Non Linear Problem (MINLP) to minimise operating cost. In their work, improved models of utility system components, accounting for part loads are developed; degrees of freedom include choice of firing machines, flowrate of steam distributed in steam networks, and use of condensing turbines. The procedure is applied to a case study, resulting in a 14% reduction in operating cost. The quantity and temperature of waste heat reduced as a result of the operational optimization is not determined. In some scenarios, a decrease in operating costs does not always mean an increase in efficiency. This is especially true when additional electrical power is generated for export thereby providing an income stream for the site, and resulting in considerable amount of heat at temperatures too low for conventional steam systems.

Micheletto et al. (2008) developed a multi-period MILP model for operational planning of an existing refinery utility system. The objective was to minimize the utility cost. Potential savings of up to 11% are identified, implying that existing utility systems are not always optimal. In energy-intensive chemical processes, the industry standard is to satisfy heat requirements first and then power (Shang and Kokossis, 2005); therefore in operational optimization of existing systems, the benefits are usually gained from exporting power, but usually produce large quantities of residual heat at temperatures too low for steam-based systems.

Luo et al. (2011) developed a linear optimization model to minimise operating cost of an existing utility system. This was applied to a case study, where a 5% reduction in cost is achieved. The cost savings achieved through optimizing an existing system could be due to production of additional power for export (thereby generating waste heat) or to reduced fuel consumption. In both instances there could be reduction in CO_2 emissions but not waste heat. From thermodynamic analysis in the works of Kimura and Zhu (2000) and Shang and Kokossis (2005), increasing the power-to-heat ratio reduces the cogeneration efficiency. Therefore, an operational optimization framework needs to be developed to allow for reducing the quantity of waste heat produced whilst improving economics and the potential to reduce CO_2 emissions.

Chae et al. (2010) developed an optimization framework for designing waste heat recovery networks, taking into account waste heat exchanged between several process sites. Even though 82–88% reductions in energy cost were obtained in the case study presented, the utility system in each process site is unchanged. This could mean two things: (1) potential opportunities to reduce energy costs are neglected and (2) less savings in energy costs since optimizing the utility system simultaneously will predict the true value of utility savings (taking into account the steam distribution pressure levels), compared to using a fixed value for all steam pressure levels. Furthermore, capital cost implications are unknown.

Much more recently, Zhao et al. (2015) developed a MINLP model for simultaneous optimization of refinery production processes and the utility system. In order to reduce the model complexity, the MINLP model was decomposed into MILP and NLP models which were solved iteratively. Their work shows that better economic benefits are obtained by simultaneous optimization of these interconnected systems. However, the potential to reduce fuel consumption, CO_2 emissions and cost by exploiting the available waste heat was neglected.

Zhang et al. (2015) also developed an MINLP model for simultaneous optimization of processing units and the site utility system. Even though the framework accounts for balance of utility streams in total sites, production planning of raw materials, energy requirements of process units based on pinch analysis and operational planning of utility system, the utilization of waste heat is not addressed. In the case study presented in Zhang et al. (2015), the heat rejected to cooling water from the processing units i.e. heat below the process pinch is available in temperatures from 40 to 280°C. Their analysis also shows that significant economic benefits are possible by simultaneous optimization of the processes and the utility system together.

Optimization techniques identify solutions that can be implemented to reduce and utilize the available waste heat in existing process sites. It may be possible to reduce the quantity of waste heat through operational optimization of existing utility systems. Waste heat utilization is also possible through integrating technologies to recover useful energy from waste heat. The optimization framework for integrating waste heat recovery in process sites can be formulated as a mixed integer program allowing the optimization of structural and operational variables. Since optimization techniques are complex, it may be necessary to explore graphically if there are any benefits derived from process integration of waste heat recovery technologies. Furthermore, the optimization framework needs to be developed to address cases where heat recovery between several processing units is maximized using TSA and cases where heat recovery is not maximized.

Technologies for recovering useful energy (in the form of electrical power, chilling and heat) from waste heat are introduced and reviewed in Section 2.3; several of these are described in more detail in Sections 2.3.1 to 2.3.6.

2.3 Overview of waste heat recovery technologies

There is a wide range of technologies recovering useful energy in the form of power, chilling and heat from waste heat. Integration of waste heat recovery technologies introduces complications, and new opportunities to maximize waste heat exploitation in process sites in order to improve a site's energy security. Table 2.1 is a summary of technologies available for waste heat utilization.

Table 2. 1 Review of thermodynamic cycles for exploiting industrial waste heat

Technology	Description	Advantages	Demerits
1. Kalina cycle	Uses a mixture of water and ammonia as working fluid to produce electrical power from waste heat	• Better temperature matching between heat carrier and mixed working fluid compared to pure fluids	• Complex system architecture • High cycle pressure, results in high capital costs • Not achieved wide adoption • Not been commercially tested compared to the organic Rankine cycle
2. Phase change materials	Electricity is produced from heat through volume expansion of a paraffin mixture	• Works with low temperature heat sources 25 – 95°C	• Low efficiency • Still under demonstration
3. Transcritical power cycles	Power production from waste heat using CO_2 as working medium	• Working fluid is non-toxic and inert in the temperature	• Low efficiency • Still under development

			range considered • Working fluid is abundant in nature and cheap	
4.	Thermoelectric power generation	Temperature gradient in the material causes a voltage difference in a conductor thereby generating electricity	• Little maintenance (no moving parts)	• Low efficiency • Small-scale systems commercially available • Not industrially tested
5.	Organic Rankine cycles	Uses low boiling point organic fluids for electrical power generation from waste heat	• Simple start-up procedure • Good part load performance • Uses relatively low driving temperature • Designed for unmanned operation with little maintenance	• Performance highly dependent on working medium
6.	Absorption chillers	Waste heat provides energy to drive the cooling processes.	• Noise free • Driven by thermal energy compared to high quality power required by vapour compression systems	• Corrosion and crystallization problems from refrigerant/ absorbent working fluid pair

7.	Adsorption chillers	The cycle operates by cycling adsorbate between the condenser, adsorber and evaporator. Solvent is generated using waste heat.	• Quiet operation, low maintenance due to no moving parts, and no vibration • No corrosion and crystallization problems	• Low coefficient of performance • Large footprint and mass • Lack of continuity of operation
8.	Adsorption heat pumps	Upgrades waste heat to a higher temperature. The cycle operates by cycling adsorbate between the condenser, adsorber and evaporator. Solvent is generated using waste heat.	• Operates with low temperature (60 – 150°C) driving energy sources • No moving parts required for working fluid circulation • Can be employed as thermal storage device	• Non-continuous working principle • Low coefficient of performance • Large volume and weight relative to traditional mechanical heat pumps
9.	Absorption heat pumps	Thermally activated heat upgrade technology. Waste heat provides the driving energy to separate the working fluid pair in the generator.	• Operates with thermal energy • Low maintenance required	• Corrosion and crystallization problems due to working fluid pair • Possible large equipment
10.	Absorption heat	Upgrades low temperature heat to	• Requires almost no electrical	• High capital costs • Possible large

transformers	higher temperature. The temperature of thermal energy required to drive the AHT is lower than that of the upgraded heat.	energy, low maintenance required • Recycles up to 50% waste heat energy	equipment
11. Mechanical heat pumps	Upgrades low temperature waste heat using mechanical energy	• High coefficient of performance	• High quality electrical power required • Some refrigerants are ozone depleting

In this work, mature and commercialized technologies (up to industrial scale) namely Organic Rankine cycles, absorption chillers, absorption heat pumps, absorption heat transformers and mechanical heat pumps are selected for further investigation. The wide range of selected technologies can produce electrical power (Organic Rankine cycles), chilling (absorption chillers) and heat (absorption heat pumps, heat transformers and mechanical heat pumps) from industrial waste heat. Heat recovery via heat exchange is also included in the technology mix. The methodological framework can be extended to integrate other waste heat recovery technologies not covered in this research.

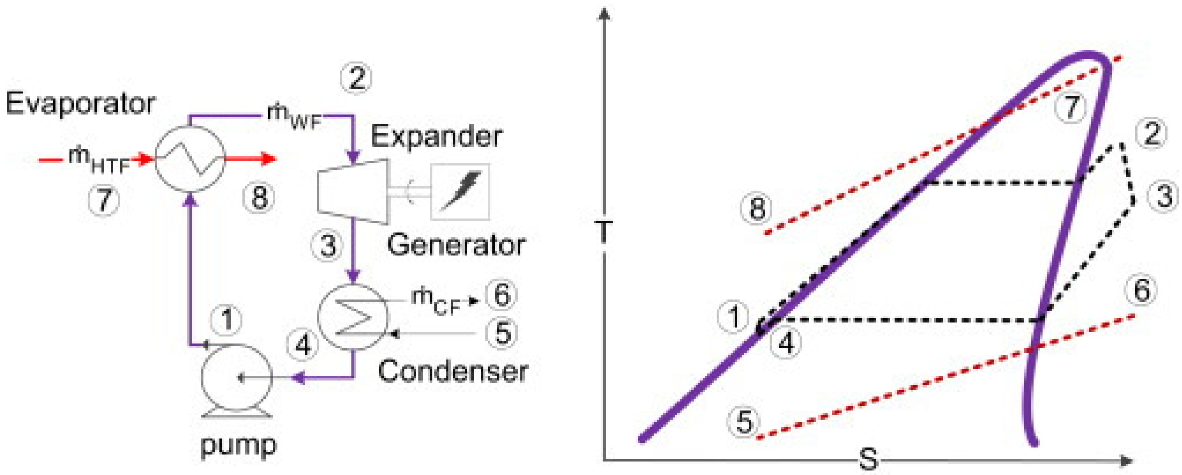
2.3.1 Organic Rankine Cycles (ORC)

Organic Rankine cycles generate electrical power from waste heat using organic fluids. At such temperatures using steam in a Rankine cycle may be economically and thermodynamically inadequate, due to significant condensation during expansion in the turbines. Furthermore, there is a risk of erosion of liquid. Although this risk can be improved by superheating the steam, additional energy is required for superheating and may not be available from the waste heat source. In addition, using organics for medium to low temperature waste heat has a significant reduction in the work of expansion compared to steam (Invernizzi, 2013). This is because the specific vaporization heat of organic fluids is generally much lower than that of water. Using organic fluids for low temperature heat sources also results in smaller volume ratio of the working fluid at the turbine inlet and outlet, compared to water, thus allowing for the use of simpler and cheaper turbines (Saleh et al., 2007).

Typical sizes of organic Rankine cycles for industrial applications range from 0.5 – 20 MW (Invernizzi, 2013). Sources of thermal energy for the ORC include geothermal energy, solar energy, energy from biomass and industrial waste heat. The biggest margin for growth has been forecast in the field of industrial waste heat recovery (Invernizzi, 2013).

Challenges associated with ORC are the economics, poor thermal exchange properties, potential risks to safety (flammability) and health (toxicity), depending on the choice of working fluids. The greatest challenge is not the thermodynamic efficiency but the reduction of costs. Reducing these costs may be possible through the development of a holistic approach to integrating ORC in process sites.

A simple schematic of an ORC is shown in Figure 2.7(a). Waste heat provides the thermal energy to vaporize the working fluid in the evaporator (state 1 and 2), which expands to produce electrical power (state 2 and 3). The working fluid is condensed (state 3 and 4) and pumped to a higher pressure (state 4 and 1), and the cycle repeats. The ORC has four major components; the expander, condenser, pump and evaporator. Shaft power is converted into electricity by an electric generator coupled with the expander, and enclosed in the same housing. Typical generator efficiencies range from 90 to 100% (Lee et al., 2014).



(a) (b)

Figure 2.7 (a) Basic ORC cycle layout. (b) Basic ORC T-s diagram (Yari and Mahmoudi, 2011)

The expanders in ORC systems have special characteristics to handle large differences in the thermo-physical properties of organic fluids (Invernizzin, 2013). They are turbo machines or scroll expanders and require fewer expansion stages compared to steam for a given pressure ratio. Therefore single-stage expanders can be employed for ORC systems (Quoilin et al., 2013).

Both shell-and-tube and plate heat exchangers can be used as the evaporator (Lee et al., 2014). However, shell-and-tube heat exchangers are mostly used since they have a more stable oscillation when the exit superheat is reduced, preventing liquid entrainment into the expander (Lee et al., 2014). The overall heat transfer coefficient for the evaporators and condensers range from 0.3 – 1.2 kW/m^{2}K (Invernizzi, 2013). Condensers are shell and tube heat exchangers with working fluid in the shell and water pumped inside the tube. The refrigerant pump (state 4 and 1 in Figure 2.7(a)) is usually a vertical multi-stage centrifugal pump. The temperature-entropy diagram for the expansion process is shown in Figure 2.7(b).

The basic ORC cycle has been modified to maximize the temperature difference between heat addition (state 7 and 8, in Figure 2.7(b)) and heat rejection (state 5 and 6, in Figure 2.7(b)). Some modifications include addition of a recuperator as shown in Figure 2.8 and regenerative cycles with turbine bleeding as illustrated in Figure 2.9 (Lecompte et al., 2015).

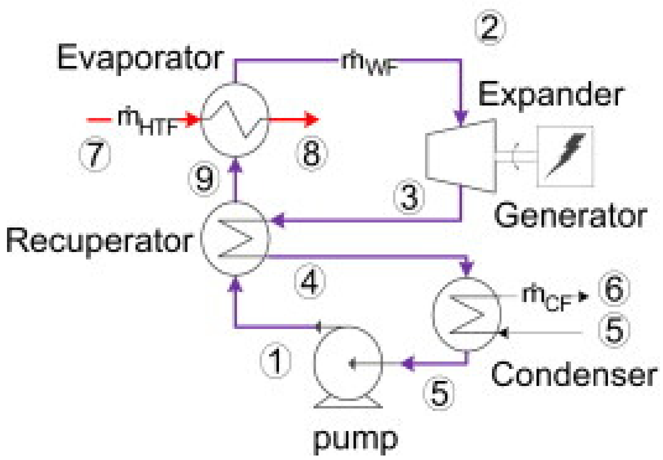


Figure 2.8 ORC cycle with recuperator layout (Yari and Mahmoudi, 2011)

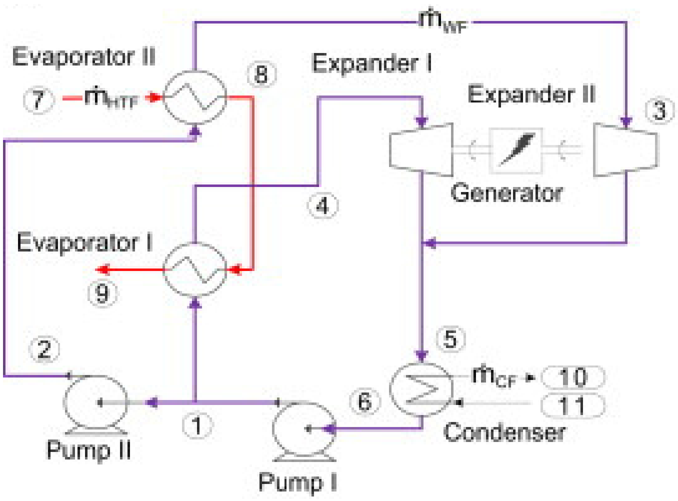


Figure 2.9 ORC with turbine bleeding cycle layout (Yari and Mahmoudi, 2011)

A recuperator reuses the heat after the expander to preheat the working fluids. Even though the efficiency increases, the quantity of waste heat exploited reduces. Furthermore there is increased pressure drop and extra recuperator cost. Regenerative cycles with turbine bleeding require two expanders, two pumps and three heat exchangers (Figure 2.9). A small portion of the working fluid is extracted from the turbine, and mixed with the working fluid before entering the evaporator. This has potential to increase the thermodynamic efficiency of the cycle; however, the net shaft-work reduces due to extraction of the working fluids from the turbine (Desai and Bandyopadhyay, 2009). Furthermore, less heat is transferred to the cycle from a waste heat source.

The modification to the ORC mentioned above increases the efficiency by decreasing the heat input into the cycle, keeping the power output the same (Desai and Bandyopadhyay, 2009). The ultimate aim in the design of ORC for waste heat recovery applications is a maximum power output from any given heat source (Saleh et al., 2007). Thus implying that for waste heat utilization, maximization of the net power output by exploiting the available heat is crucial. Furthermore, the additional complexity may not justify the increase in efficiency.

Supercritical ORC has also been introduced using CO_2 as working fluid, due to low critical temperature resulting in an easily achievable supercritical state. However, due to the high critical pressure, component costs are high and safety regulations severe (Lecompte et al., 2015). Furthermore, the high pumping power required to manage the large pressure degrades the cycle's power output (Lecompte et al., 2015). Finally, there is limited knowledge about heat exchange and pressure drop correlations for supercritical fluids. Moreover, uncertainties in working fluids are highest close to the critical point (Andreasen et al., 2014).

Therefore, in this work, the basic ORC is selected, since it is the best cycle design from both economic and thermodynamic perspective for waste heat recovery applications.

There are several approaches to model the ORC and determine the useful power generated from a given heat source. Detailed models based on enthalpy balances for each component in the cycle have been used (Kwak et al., 2014). The models are represented in Eq. 1 – 4 for each cycle component. The thermal efficiency is defined as the useful net power output, calculated by subtracting the electrical power (W) required by the pump (Equation 1) from the power produced (Equation 3) to the heat input (Equation 2).

For the pump:

$$W_{PUMP} = \frac{m_{WF} \times (h_4 - h_{1s})}{\eta_{is,PUMP}} \qquad \text{Equation 1}$$

For the evaporator (EVAP):

$$Q_{EVAP} = m_{WF} \times (h_2 - h_1) \qquad \text{Equation 2}$$

For the expander (EXP):

$$W_{EXP} = m_{WF} \times (h_2 - h_{3s}) \times \eta_{is,EXP} \qquad \text{Equation 3}$$

For the condenser (COND):

$$Q_{COND} = m_{WF} \times (h_4 - h_3) \qquad \text{Equation 4}$$

Where h is the specific enthalpies in the respective state points, m_{wf} is the working fluid mass flow rate and η_{is} is the isentropic efficiency.

Even though applying detailed enthalpy balances are accurate, it is difficult to analyse multiple heat source streams or systematically select streams without the need for multiple iterations.

The ideal Carnot engine concept has also been used in ORC models. For an ideal ORC, the isentropic efficiency of the pump and expander is 1, heat exchanger areas are assumed infinite and the cycle receives and rejects heat reversibly. In Lu et al. (2016), the ideal ORC model is used to evaluate the potential for power generation from industrial waste heat. However, the model neglects the inefficiencies in the cycle's components and the working fluid's non-ideal behaviour. This non-ideal behaviour is due to high densities, phase changes and dissociation of the fluid. The Peng Robinson equation of state predicts this non-ideal behaviour (Peng and Robinson, 1976).

Some other authors have used a constant efficiency for a particular temperature range, for example, Viklund and Karlsson (2015); however, this neglects the influence of working fluid. A more rigorous approach, based on simulation models in Aspen HYSYS was used in Kapil et al. (2012). Even though the non-ideal behaviour of working fluids and component inefficiencies can be predicted with high accuracy, it is difficult to analyse multiple heat sources systematically, or to set up an optimization framework for ORC integration applying commercial simulation software.

Therefore in this work, novel simple explicit thermodynamic models are developed for ORC, taking into account the relationship between the enthalpy-based performance and the ideal performance. The models proposed aim to be easily applicable in existing tools for optimizing site utility systems and processing units, and to be adaptable to varying heat sources and working fluids.

2.3.1.1 Working fluid selection for organic Rankine cycles

The amount of power generated from waste heat using ORCs depends on the choice of working fluids (Invernizzi, 2013). Working fluids affect the efficiency of the system, sizes of system components, design of the expansion machine and system stability (Bao and Zhao, 2013). Working fluids for ORC should be non-toxic, non-carcinogenic, non-explosive, have zero ozone depletion potential, low global warming potential and short atmospheric lifetimes. The critical temperature and molecular complexity play a fundamental role in determining the choice of working fluids. The critical temperature determines the position of the limiting curve in the thermodynamic plane, and establishes the region in which the cycle will operate (Invernizzi, 2013). The molecular complexity determines both the shape of the limiting curve and the behaviour of the thermodynamic cycle inverted in the limiting curve (Invernizzi, 2013).

Organic fluids are desirable working fluids due to their low boiling point temperatures, medium vapour pressures at moderate temperatures, low specific volume and low isentropic turbine enthalpy drop (Hipolito-Valencia et al., 2013). Thousands of substances can be used: hydrocarbons, aromatic hydrocarbons, perfluorocarbons, alcohols and siloxanes. Zeotropic mixtures can also be used as working fluids.

Working fluids are categorized according to the shape of the saturation vapour curve and the state of the working fluid after expansion at the turbine outlet. ‘Dry’ fluids have a positive slope i.e. the working fluid enters the turbine inlet as saturated vapour and leaves as superheated vapour. ‘Wet’ fluids have a negative slope i.e. working fluid enters the turbine inlet as saturated vapour and leaves a two phase liquid. Isentropic fluids have a nearly infinite slope. Figure 2.10 shows the shape of the temperature-entropy (T–S) curve for dry, wet and isentropic fluids.

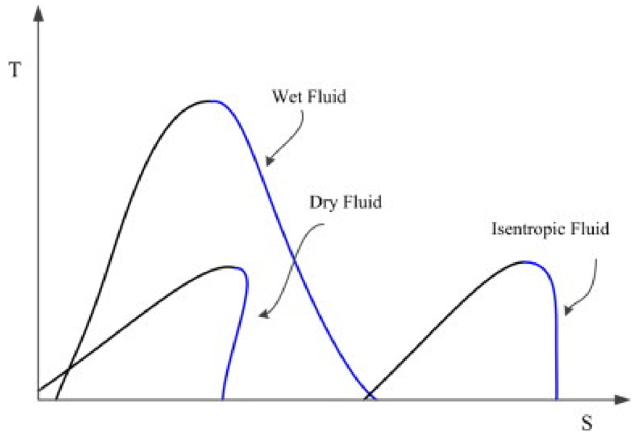


Figure 2.10 T–S diagram of different categories of working fluids (Yu et al., 2015)

A review of working fluids with low environmental impact and adequate chemical stability in the desired temperature range is performed in Chen et al. (2010). In the analysis, isentropic and dry fluids are shown to be better suited to ORCs to avoid liquid droplet impingent on the turbine blades during expansion. Bao and Zhao (2013) also identified dry and isentropic fluids as more suitable for ORC applications.

Mixed organics may perform better than pure organics, since pure organic fluids boil and condense at constant temperature potentially leading to large temperature differences in the evaporator and condenser. Victor et al. (2013) developed an optimization model for determining the composition of mixed working fluids for the ORC and Kalina cycle. Their results show that pure component organic fluids are more energy efficient than some mixed organic fluids. A novel methanol/water mixture more efficient than the ammonia/water Kalina cycles, and steam Rankine cycles was proposed. However, this analysis assumed sub-cooling conditions in the condenser, the wetness of the mixture after expansion was not accounted for, and only heat sources between 100 – 250°C were analysed. Furthermore, even though binary properties of mixtures provide non-isothermal evaporation and condensation in the cycle which could result in high efficiency, the cycle efficiency using a mixture lies between the efficiency of the individual pure components. Therefore, in this work, screening of pure fluids and the methanol/water mixture will be performed over a wider heat source temperature range, and will assume saturated conditions in the evaporator and condenser.

Andreasen et al. (2014) developed a systematic methodology using genetic algorithm optimization to find promising pure fluids for mixtures to maximize the net electrical power output. It was discovered that any mixed fluid is only more efficient than one of the pure fluids in the mixture. Again the maximum temperature of heat sources examined was 120°C.

Saleh et al. (2007) screened 31 pure component working fluids using the BACKONE Equation of State (EOS) for heat source temperatures between 30 – 100°C, with evaporation pressure limited to 20 bar. Again, the highest thermal efficiency was obtained for high boiling substances that are dry. The BACKONE EOS is a family of physically based EOS able to describe thermodynamic properties of non-polar, dipolar and quadrupolar fluids with good degree of accuracy (Saleh et al., 2007).

Desai and Bandyopadhyay (2009) analysed 16 different working fluids (including n-pentane, n-hexane, isobutene, isopentane, benzene and R113). Again, dry and isentropic fluids are most preferred (since there is no liquid after expansion to damage the blades and reduce the turbine isentropic efficiency).

Long et al. (2014) used genetic algorithm optimization to obtain the maximum overall efficiency and relative evaporator temperature for different working fluids. Their results show that working fluids performance depends on the evaporation temperature and that superheating in the ORC will not increase the exergy efficiency. Working fluids explored include n-pentane over a low temperature range from 50°C – 130°C. Therefore the heat source temperature (which determines the evaporator temperature) and working fluid selection play significant roles in improving the ORC performance.

Yu et al. (2015) determined optimum working fluids and corresponding operating conditions simultaneously based on Pinch Analysis. The system performance was evaluated using the amount of heat recovered. The pinch point was measured between the working fluids and the waste heat carrier; there are two possible influences on the pinch point: (1) the waste heat source temperature, (2) the heat capacity flowrate of the waste heat. It was discovered that the heat capacity flowrate of the waste heat source exerts no effect on the pinch point. This means that the evaporator temperature can be determined from the heat source temperature.

Li et al. (2015) used the thermal efficiency as a parameter to screen two wet fluids and six dry fluids. Again, dry fluids showed the highest thermal efficiency with saturated vapour conditions in the turbine inlet. However, the influence of working fluids under different heat source temperatures was not taken into account.

Sarkar and Bhattacharyya (2015) screened commercially used fluids including n-pentane, R245fa, R134a, toluene, benzene and ammonia using the net power output, thermal efficiency, turbine expansion ratio and total heat transfer requirement. Using different criteria to screen working fluids yields different results but dry fluids are generally found to be the best in terms of the ORC performance and heat exchanger compactness (Sarkar and Bhattacharyya, 2015).They found that the best choice of working fluid depends on the heat source temperature and noted that even though using ammonia is promising, the high working pressure required could result in expensive capital outlay.

The literature review showed that there is no single “winner” amongst working fluids. In this work, pure fluids with high latent heat of vaporization, high density vapours, low liquid specific heat and high boiling points are screened and compared with methanol/water mixture. Fluids that are cheap, non-toxic, non-flammable, have high auto-ignition temperature compared to the heat source temperature and have zero ozone depletion potential will be explored. The working fluids will be screened taking into account the heat source temperature. Table 2.2 contains some working fluids for ORC applications.

Table 2. 2 Possible working fluids for ORC applications (Desai and Bandyopadhyay, 2009)

Working fluid	Chemical formula	$T_{critical}$ (°C)	$P_{critical}$ (MPa)	Boiling point (°C)	Global warming potential
n-pentane	C_5H_{12}	196.6	3.370	36.1	Very low
Benzene	C_6H_6	288.9	4.894	80.1	Very low
n-butane	C_4H_{10}	152.0	3.796	−0.6	Very low
n-hexane	C_6H_{14}	234.7	3.034	68.7	Very low
Isobutane	C_4H_{10}	134.7	3.640	−11.7	Very low

Isohexane	C_6H_{14}	224.6	3.040	60.2	Very low
Isopentane	C_5H_{12}	187.2	3.396	27.8	Very low
n-perfluro-pentane	C_5F_{12}	147.4	2.045	29.8	8900
Trichloro-1,1,2-Trifluoro-1,2,2-ethane	$C_2Cl_3F_3$	214.1	3.392	47.6	6000
2,2-Dichloro-1,1,1-trifluoroethane	$C_2HCl_2F_3$	183.7	3.662	27.8	120
1,1-Dichloro-1-fluoroethane	$C_2H_3Cl_2F$	204.4	4.212	32.1	700
1,1,1,2,3,3-hexafluoropropane	$C_3H_2F_6$	139.3	3.502	6.2	1200
1,1,2,2,3-pentafluoropropane	$C_3H_3F_5$	174.4	3.925	25.1	640
1,1,1,3,3-pentafluoropropane	$C_3H_3F_5$	154.0	3.651	15.1	950
1,1,1,3,3-pentafluorobutane	$C_4H_5F_5$	186.9	3.271	40.3	890
Toluene	C_7H_8	318.6	4.126	110.6	Very low

2.3.1.2 Process integration of organic Rankine cycles

Integration of the ORC into process sites has potential to reduce cold utility demand and generate shaft power (Desai and Bandyopadhyay, 2009). Process integration techniques (such as Pinch Analysis, Total Site Analysis and system-oriented optimization frameworks) can be applied to identify opportunities to improve the thermodynamic efficiency and economics of the ORC.

Desai and Bandyopadhyay (2009) presented a methodology for appropriate integration and optimization of an ORC with the background process using the Grand Composite Curve (GCC). However, the variations in quantity and temperature of heat available were accounted for in a non-systematic manner. Heat below the pinch can be utilized at the lowest temperature (corresponding to the highest duty, Q) or a higher temperature (corresponding to the lower duty, Q) as illustrated in Figure 2.11. Also, at any temperature below the pinch, the cumulative heat or actual heat available can be utilized. Furthermore in energy intensive processes, there could be competition to use the heat available from a single process for recovery using TSA.

The GCC is made up of several streams; for retrofit analysis the integrity of each stream needs to be maintained. Desai and Bandyopadhyay (2009) also considered integrating the condenser with the background process, as heat transfer from the ORC to the process may produce high efficient designs; however, the benefits depends on the value (price) of the hot utility being displaced. In addition, their study neglects interactions with the utility system. There could be more benefits when the process, utility system and the ORC are optimized simultaneously compared to the sequential approach of Desai and Banyopadhyay (2009).

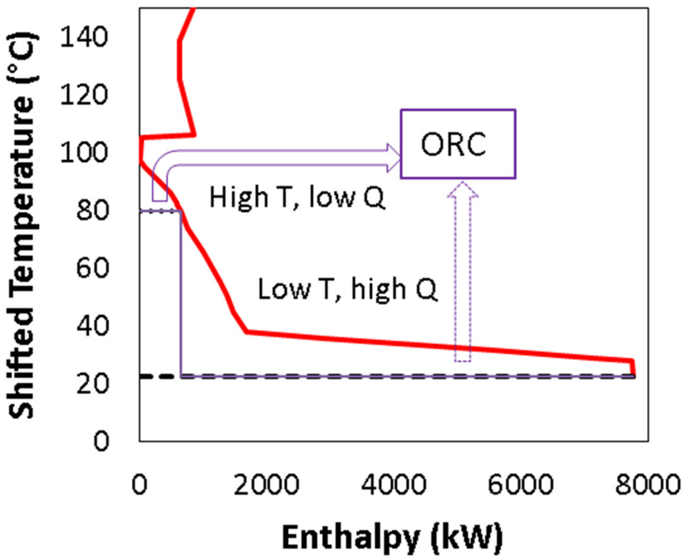


Figure 2.11 ORC integration using the GCC

Hipolito-Valencia et al. (2013) developed an integrated stage wise superstructure for representing the interconnections and integration between the heat exchanger network (HEN) and the ORC using a MINLP model. Even though the methodological framework explicitly accounts for economic trade-offs and interactions between the HEN (taking into account the heat sources on a stream basis) and the ORC, using the same price for steam provided at different pressure levels could lead to misleading results. Furthermore, possible benefits from allowing quantity and temperature of heat to vary within a stream are neglected, since all the heat is extracted at the target temperature of a stream. The ORC was allowed to accept and reject heat to process streams. This resulted in an increase in the hot utility required by the process per additional unit of electrical power produced. Since interactions with the site utility system are not considered, predicting the cost associated with extra hot utility required may not be accurate. Furthermore, only one end-use of electrical power is considered i.e. export of electricity to the grid; other end-uses such as using the power within the site or reducing any import of power may be more economic.

Chen et al. (2014) also presented a MINLP mathematical model for recovery of waste heat from the heat surplus zone of a processing unit using the ORC. The ORC was integrated to maximize the work produced from waste heat without increasing hot utility required by the process. However, only one end-use of recovered energy was considered and interactions with the utility system were neglected. Even though analysis is done on a stream level, possible benefits from varying the quantity and temperature of waste heat sources were not considered. The economics (costs and benefits) of the design was not also considered.

In previous studies on integrating ORC into process sites, the pressure levels and the expansion ratios have been chosen without considering the temperature levels of the heat sources (Invernizzi, 2013). There is lack of extensive data to accurately predict the installed capital of the ORC. Typical costs range from 1000 – 3000 £/kWe (Tchanche et al., 2014). A retrofit factor of 1.5 – 3 is usually used as the installation factor for retrofit (Tchanche et al., 2014).

In this research, a novel systematic hybrid methodology incorporating graphical techniques and mathematical optimization framework is developed for integrating the ORC in process sites. The graphical techniques allow preliminary evaluation of the potential benefits from ORC integration prior to detailed design. It also allows determination of the key degrees of freedom and development of physical insights into the problem. The optimization framework takes into account possible benefits from varying the quantity and temperature of heat sources, multiple end-uses of recovered electrical power, and possible benefits from exploiting a holistic approach to design, by simultaneous optimization with the existing site utility system.

2.3.2 Absorption Chillers (AbC)

Absorption chillers are closed-loop cycles providing chilling from waste heat. They are driven by low temperature waste heat (< 100°C) compared to conventional vapour compression cycles that require high quality power (Somers et al., 2011). A refrigerant–

absorbent pair is used as working fluid in the AbC. A single effect cycle is represented in Figure 2.12.

In the cycle, waste heat vaporizes the refrigerant in the evaporator; the refrigerant is then absorbed by the absorbent (states 1 and 2) and pumped to a high temperature (states 3 and 4). The separation of the refrigerant–absorbent pair occurs in the generator, which is driven by waste heat (state 5, 8 and 9). The absorbent flows back to the absorber (state 6, 7 and 8), while the refrigerant is condensed (states 9 and 10), expanded in a valve (states 10 and 1), flows to the evaporator and the cycle repeats. A solution heat exchanger is added to recover heat from the rich absorbent stream flowing out of the generator (states 8 and 7), to heat up the lean absorbent stream into the generator (states 4 and 5). This solution heat exchanger reduces the temperature of heat into the generator, thereby increasing the coefficient of performance (Somers et al., 2011).

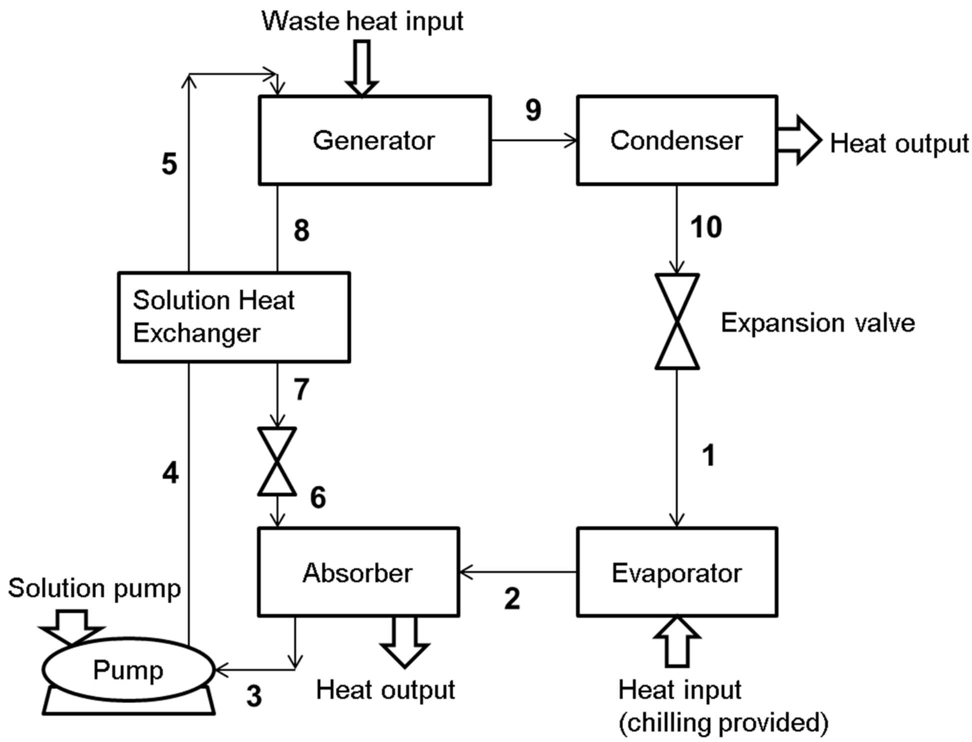


Figure 2.12 Single effect absorption chiller schematic

The ABC has seven components: the evaporator, absorber, pump, expansion valves, generator, solution heat exchanger and the condenser. The generator can be designed as a conventional industrial evaporator (Li et al., 2011). The absorber is typically a falling film-type heat exchanger with internal tubes placed vertically (Li et al., 2011). The waste heat stream is coupled to the generator directly (Garimella, 2012). The condensers and evaporators are shell and tube heat exchangers.

Absorption chillers have different cycle architectures from single effect to triple effect. Even though multi-effect cycles have higher coefficient of performance (COP), they require more components (Somers et al., 2011). Furthermore, the complexity and cost of multi-effect systems may not be justified unless multiple cooling requirements exist within the plant (Popli et al., 2013). Therefore, in this work single effect cycles are considered.

There are two major approaches to modelling absorption chillers: physical or thermodynamic models and empirically-based models. Thermodynamic models can be derived from detailed mass and energy balances for every component in the cycle. These models predict the useful chilling provided from waste heat required to drive the generator and vice versa. The mass and energy balances based on the individual components are outlined below.

For the evaporator:

$$m_1 = m_2 \qquad \text{Equation 5}$$

$$Q_{EVAP} = m_2 \times (h_2 - h_1) \qquad \text{Equation 6}$$

For the absorber:

$$m_3 = m_2 + m_6 \qquad \text{Equation 7}$$

$$m_3 x_3 = m_6 x_6 \qquad \text{Equation 8}$$

$$Q_{ABS} = m_2 h_2 + m_6 h_6 - m_3 h_3 \qquad \text{Equation 9}$$

For the solution heat exchanger (SHX):

$$m_4 + m_8 = m_5 + m_7 \qquad \text{Equation 10}$$

$$Q_{SHX} = m_4 h_4 + m_8 h_8 - m_5 h_5 - m_7 h_7 \qquad \text{Equation 11}$$

For the expansion valve (state 6 and 7):

$$m_6 = m_7 \qquad \text{Equation 12}$$

$$m_6 h_6 = m_7 h_7 \qquad \text{Equation 13}$$

For the generator:

$$m_9 + m_8 = m_5 \qquad \text{Equation 14}$$

$$Q_{GEN} = m_9 h_9 + m_8 h_8 - m_5 h_5 \qquad \text{Equation 15}$$

For the water valve (state 10 and 1):

$$m_1 = m_{10} \qquad \text{Equation 16}$$

$$m_1h_1 = m_{10}h_{10}$$ Equation 17

For the condenser:

$$m_9 = m_{10}$$ Equation 18

$$Q_{COND} = m_9(h_{10} - h_9)$$ Equation 19

For the pump:

$$W_{PUMP} = \frac{m_3 \times (h_3 - h_{4S})}{\eta_{is,PUMP}}$$ Equation 20

Where *h* is the specific enthalpy at the respective state points, η_{is} is the isentropic efficiency, *m* represents the mass flow of the working fluid, *W* is the power produced or consumed and *Q* represents the heat duty.

The enthalpy-based (real) coefficient of performance is the ratio of the chilling duty provided (calculated using Equation 6) to the sum of the waste heat flow input to the generator (calculated using Equation 15) and power required by the pump (calculated using Equation 20), expressed in Equation 21.

$$COP_{AbC,real} = \frac{Q_{EVAP}}{Q_{GEN} + W_{PUMP}}$$ Equation 21

Even though the detailed thermodynamic models in Equation 5 to 20 predict the working states and energy flows to a high degree of accuracy, analysing multiple heat sources systematically may lead to complex iterations. Grossmann and Zaltash (2001) developed a modular simulation tool called ABSIM incorporating all the detailed thermodynamic models. The tool calculates the thermal loads of each components and internal state points for given working fluids specifications and operating conditions within the cycle. However, convergence of the simulation models is not assured when multiple heat sources are analysed (Labus et al., 2013).

Yin et al. (2010) also applied detailed thermodynamic models based on mass and heat transfer relationships for each component, detailed energy and mass balances and working fluid property relations. Even though detailed thermodynamic models are accurate, a lot of input parameters are required which are not always available and comprehensive knowledge of the cycle's internal state point is also required.

A simple empirical model was developed by Gordon and Ng (1995) in which physical principles are fitted to manufacturers' data using regression. The method assumes manufactures' catalogues provide operating conditions of each of the cycle component. However, the assumption is not always the case.

Another empirical model is the characteristic equation model developed by Hellmann and Ziegler (1999). The model predicts the AbC performance using two simple algebraic equations to calculate the waste heat input and the cooling provided. Even though simple linear correlations are convenient, the cooling capacity may deviate from linear behaviour. Furthermore, the model was developed from small datasets.

Artificial neutral networks (ANN) have also been applied to AbC modelling. The ANN model predicts the performance by using only the working temperatures in the four main components as inputs (Manohair et al., 2006). However, the accuracy of an ANN model (regressed) depends on the accuracy of the data set used for model training. Simulation software (Aspen Plus) was used by Somers et al. (2011) to model the AbC. Even though the model shows good agreement with experiments, Aspen Plus is not set up to systematically analyse multiple heat sources and would struggle to model 'heat' flows (with given temperatures) if 'heat' is not attached to a material stream.

In this work simple explicit steady-state models that can be embedded within large process synthesis models are developed. These models are characterized by a low number of input parameters and allow systematic analysis of multiple waste heat sources. The models are developed by combining thermodynamic models with empirical models.

2.3.2.1 Working fluid selection for absorption chillers

A refrigerant–absorbent pair is used as the working fluid in an AbC. The literature lists approximately 40 refrigerants and 200 absorbents compounds (Srikhirin et al., 2001). Pairs of working fluids investigated in the literature include acetone/zinc bromide, water/lithium bromide (LiBr), water/monomethylamine, water/potassium formate, ammonia/lithium nitrate, ammonia/water, ammonia/sodium thiacyanate and methanol/lithium bromide.

The two most common working fluid pairs for absorption chillers are water/LiBr and ammonia/water. Water/LiBr is attractive because of its higher coefficient of performance and low toxicity compared to ammonia/water (Somers et al., 2011). In addition, the low volatility of LiBr means there is no need for a rectifier after the generator. Water/LiBr systems have lower installation, operating and maintenance costs compared to ammonia/water systems (Popli et al., 2013). Therefore in this work water/LiBr systems are adopted. However, the methodology is general, so other pairs could be accommodated.

Challenges associated with water/LiBr systems include crystallization of LiBr (LiBr is a salt) at moderate concentrations and ice formation at very low temperatures. Crystallization can also occur when the absorber temperature rises at fixed evaporating pressure (Wang et al. 2011). Various crystallization control strategies are used, including use of chemical inhibitors, mass and heat transfer enhancement methods, absorption system control strategies and thermodynamic cycle modifications (Wang et al. 2011). However, most control strategies reduce the coefficient of performance (Wang et al. 2011). The best strategy is to operate at low generator temperatures, below the crystallization line identified on the Duhring plot (water/LiBr phase diagram). The Duhring plot is the pressure-temperature-concentration (P-T-x) characteristics of the AbC shown in Figure 2.13. It can be used to determine the concentration of lithium bromide in the cycle.

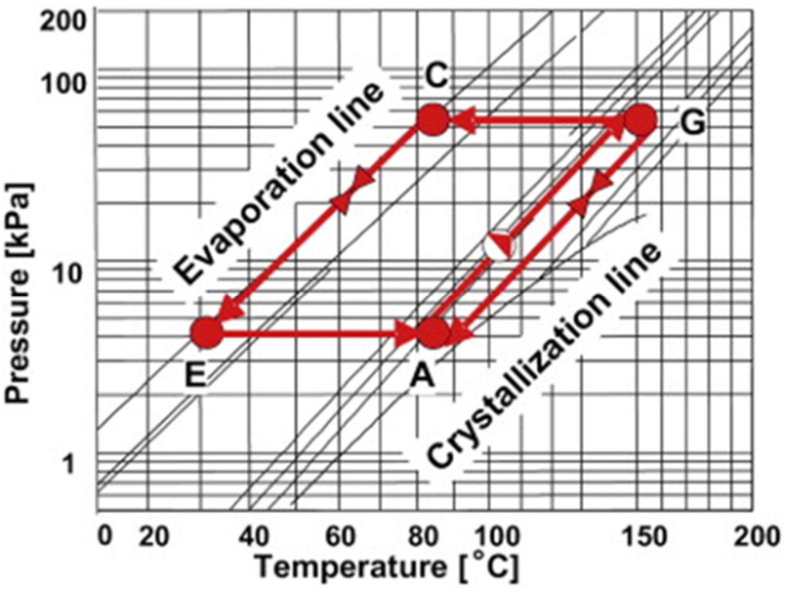


Figure 2.13 Duhring diagram of single-effect absorption chiller (Bakhtiari et al., 2010).

2.3.2.2 Process integration of absorption chillers

Previous studies on absorption chillers focused on modelling the cycle performance, use of solar energy to drive the AbC, but did not consider integration of AbC in process sites. Application with the use of low temperature waste heat is promising (Bruno et al., 1999).

Bruno et al., (1999) studied the integration of an absorption chiller in a process site. Additional steam was produced in the utility system to drive the absorption chiller. The possibility of using waste heat to drive the AbC was not explored.

The performance of gas turbines is affected by ambient temperature and relative humidity. Gas turbines are constant density machines, at high ambient temperature; the air mass flow rate reduces, reducing the power output. Popli et al. (2013) explored waste heat extracted from a gas turbine (in the utility system) exhaust to drive an absorption chiller to chill the gas turbine inlet air. The waste heat was extracted above the acid dew point of the flue gas. This integration resulted in an increase in power produced from the gas turbine. The payback for this integration was between 1.3 – 3.4 years, depending on the amount of cooling provided. However, the study by Popli et al. (2013) only considered a single heat source/ end-use applications.

Garimella (2012) studied the recovery of waste heat from a gas stream at 120°C to drive an absorption chiller and reported benefits, including operational savings from power displaced in the conventional vapour compression systems. Interactions with the site utility system are neglected, as waste heat at this temperature is high enough for low pressure steam generation. This application only considers one end-use of recovered energy and one heat source.

Drawbacks associated with absorption chillers integration in process sites include high capital cost (Bruno et al., 1999). Based on the economic analysis carried out by Bruckner et al. (2015), absorption chillers are profitable when operated for over 2500 hours in a year. Typical investment costs range from 222 – 350 £/kW of chilling capacity (Bruckner et al., 2015).

In this work, an novel integration framework for absorption chillers that considers multiple sources and end-uses of recovered energy, other potential ways of utilizing the heat source (for example power generation using organic Rankine cycles) and possible interactions with the site utility system is developed. Both graphical and optimization techniques are developed for process integration of AbC. The graphical techniques allow preliminary evaluation of the potential benefits from AbC integration prior to detailed design. The optimization framework takes into account possible benefits from varying the quantity and temperature of heat sources, multiple end-use of recovered chilling, and possible benefits from simultaneous optimization with the site utility system.

2.3.3 Absorption heat pumps (AHP)

Absorption heat pumps upgrade waste heat by raising its temperature. They are driven by thermal energy, rather than high quality electrical power, as required to drive mechanical heat pumps. The driving thermal energy is diverse, ranging from waste heat, hydrocarbon fuel combustion to solar and geothermal energy (Wu et al., 2014). The AHP is similar to the AbC (shown in Figure 2.12). However, in the AHP, medium temperature heat is recovered from heat released in the absorber and condenser. A schematic is shown in Figure 2.14. Low temperature heat is upgraded using high temperature heat in the generator. Absorption heat pumps play an important role in renewable energy use and waste heat recovery (Wu et al., 2014).

Absorption heat pumps could be single stage, double lift or triple lift. Complex cycles such as double lift and triple lift are less common (Bruckner et al., 2015). Even though complex cycles reduce the driving heat (generator temperature) and increase the temperature lift (difference between the condenser and evaporator temperature), they have lower coefficient of performance compared to single cycles (Bruckner et al., 2015). Therefore in this work, the single effect AHP is adopted.

The equipment design is simplified by assuming the absorber and condenser operate at the same temperature to ensure useful heat is released to a single carrier fluid (Costa et al., 2009).

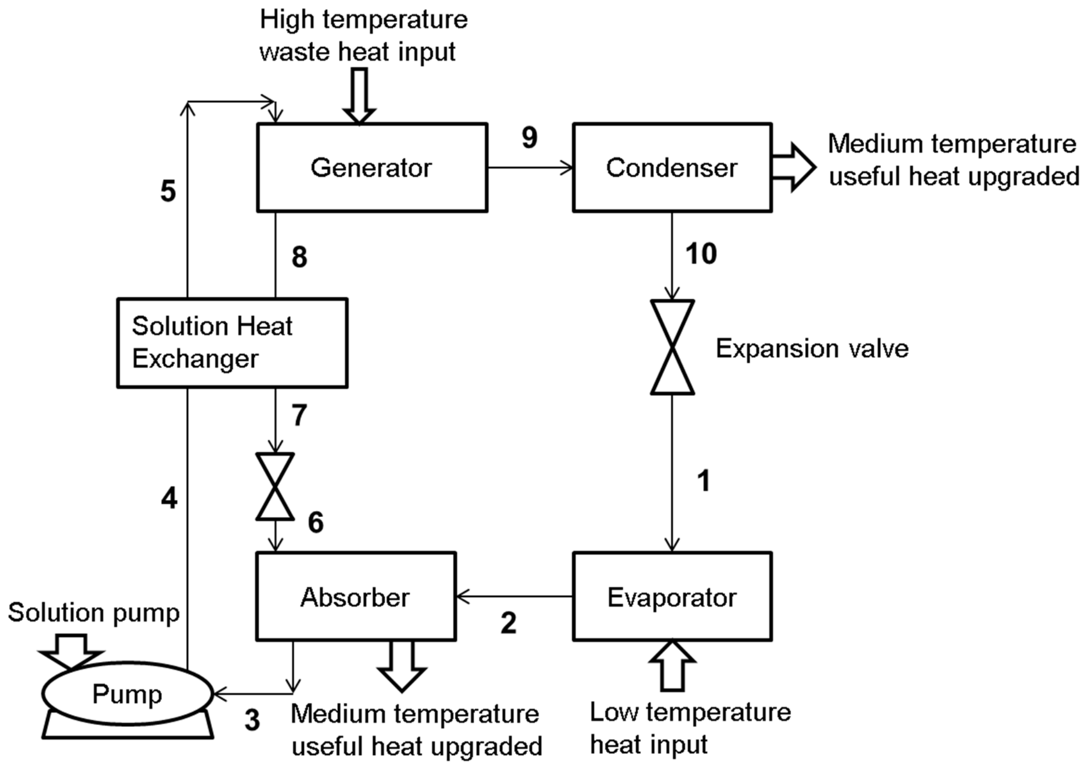


Figure 2.14 Single effect absorption heat pump

Thermodynamic modelling of AHP uses detailed mass and energy balances for each component of the cycle as shown below:

For the evaporator:

$$m_1 = m_2 \qquad \text{Equation 22}$$

$$Q_{EVAP} = m_2 \times (h_2 - h_1) \qquad \text{Equation 23}$$

For the absorber:

$$m_3 = m_2 + m_6 \qquad \text{Equation 24}$$

$$m_3 x_3 = m_6 x_6 \qquad \text{Equation 25}$$

$$Q_{ABS} = m_2 h_2 + m_6 h_6 - m_3 h_3 \qquad \text{Equation 26}$$

For the solution heat exchanger:

$$m_4 + m_8 = m_5 + m_7 \qquad \text{Equation 27}$$

$$Q_{SHX} = m_4 h_4 + m_8 h_8 - m_5 h_5 - m_7 h_7 \qquad \text{Equation 28}$$

For the expansion valve (state 6 and 7):

$$m_6 = m_7 \qquad \text{Equation 29}$$

$$m_6 h_6 = m_7 h_7 \qquad \text{Equation 30}$$

For the generator:

$$m_9 + m_8 = m_5 \qquad \text{Equation 31}$$

$$Q_{GEN} = m_9 h_9 + m_8 h_8 - m_5 h_5 \qquad \text{Equation 32}$$

For the water valve (state 10 and 1):

$$m_1 = m_{10} \qquad \text{Equation 33}$$

$$m_1 h_1 = m_{10} h_{10} \qquad \text{Equation 34}$$

For the condenser:

$$m_9 = m_{10} \qquad \text{Equation 35}$$

$$Q_{COND} = m_9 (h_{10} - h_9) \qquad \text{Equation 36}$$

For the pump:

$$W_{PUMP} = \frac{m_3 \times (h_3 - h_{4S})}{\eta_{is,PUMP}} \qquad \text{Equation 37}$$

Where h is the specific enthalpy in the respective state points and η_{is} is the isentropic efficiency.

The enthalpy based (real) Coefficient of Performance (COP) is defined as the ratio of the heat released in the absorber (calculated from Equation 26) and condenser (calculated from Equation 36) to the sum of the waste heat input to the generator (calculated from Equation 32) and power required by the pump (calculated from Equation 37), expressed in Equation 38.

$$COP_{AHP,real} = \frac{Q_{COND} + Q_{ABS}}{Q_{GEN} + W_{PUMP}} \qquad \text{Equation 38}$$

The mechanical energy required by the pump is negligible compared to the thermal energy required in the generator (Costa et al., 2009). The detailed mass and energy balances have been integrated into ABSIM, an ABsorption SIMulation tool. Qu et al. (2014) applied ABSIM to evaluate working states and system COP. ABSIM contains subroutines for the basic components of the AHP. Even though the model of Qu et al. (2014) agrees with experimental data, it is difficult to integrate with a variety of waste heat sources and systems; also modelling of complex interactions is tedious and susceptible to user errors, making it suitable for single heat source/end-use applications.

Bakhtiari et al. (2011) developed analytical design and dimensioning models for a water/lithium bromide AHP. In the model, each cycle component was treated as a control volume; the cycle performance was described by mass balances on water and LiBr, energy balances for each component, and overall energy balance and heat transfer equation between the external, and internal streams. The model shows good accuracy compared to experimental data, but several non-linear equations need to be solved even for a single heat source. Thus the model is not sufficiently versatile enough to embed in a framework for systematic analysis of multiple heat source streams and end-uses of upgraded heat.

Sun et al. (2010) also developed a mathematical model for the AHP. The model considers local values of heat and mass transfer coefficients, thermal parameter dependent properties of working fluids, and the influence of both the geometry parameters and operational parameters on the thermal performance. The model shows reasonable agreement with experimental data. The model consists of multiple non-linear equations; adapting for AHP in a process site with multiple heat sources streams is likely to require several complex iterations.

Absorption heat pumps have also been modelled in a simple manner based on constant average COP (Zhang et al., 2015). However, this approach is inaccurate since it neglects the influence of system temperatures and the working fluid non-ideal behaviour.

Existing models of AHP are not suitable for analysing multiple heat sources systematically. Therefore in this work, simple explicit steady state models are developed for AHP. The models are embeddable in large process synthesis models to allow for systematic analysis of multiple heat sources.

2.3.3.1 Working fluid selection for absorption heat pumps

Working fluids for AHP are grouped into five categories, depending on the choice of refrigerant: alcohol series, water series, ammonia series, halogenated hydrocarbon series and other refrigerants (Sun et al., 2012). The working fluid should be non-corrosive, chemically stable, environmentally friendly and non-explosive. Performance of an AHP is dependent on working fluid thermodynamic properties (Sun et al., 2012).

Industrial applications of AHP use ammonia/water and water/LiBr as working fluids (Bakhtiari et al., 2010). Water/LiBr is preferred since it has a high enthalpy of vaporization, it is nontoxic, and operates at medium to low temperatures. The boiling point difference between water and LiBr is large; therefore no rectification step is required after the generator compared to ammonia/water systems (Sun et al., 2012). Therefore in this work, water/lithium bromide absorption heat pumps are used.

One of the challenges of using water/ LiBr is the crystallization of the salt at high concentrations. In the work of Bakhtiari et al. (2011), this was overcome by adding an addictive (2-ethyl-1-hexanol). However, this additive reduces the cycle COP. The best strategy is to operate above the crystallization line (Sun et al., 2010). The crystallization line is visible on the Duhring plot, Figure 2.15 shows the representation of AHP on the water/LiBr phase diagram.

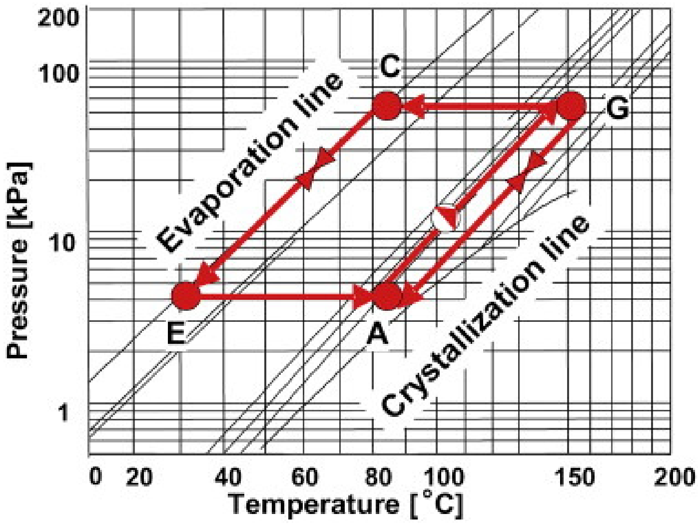


Figure 2.15 AHP representations in water/LiBr phase diagram (Bakhtiari et al., 2010)

2.3.3.2 Process integration of absorption heat pumps

Industrial applications of absorption heat pumps include absorption assisted distillation, drying and low grade waste heat upgrade. The application of an AHP can save about 50% of primary energy required for useful heat provision (Keil et al., 2008).

Heat pump-assisted distillation is attractive due to the potential to reduce energy consumption (Wu et al., 2014). Wang and Lior (2011) and Wu et al. (2014) report up to 45% savings from AHP assisted distillation. The study by Wang and Lior (2011) did not consider multiple heat sources and end-uses of upgraded heat.

Using AHP for drying consumes 60 – 80% less energy than conventional direct heat dryers operating at the same temperature (Wu et al., 2014). Abrahamsson et al. (1997) integrated an AHP to utilize the latent heat of exhaust air from a drier. Le Lostec et al. (2008) also applied an AHP for wood chip drying. Again, the study conducted by Abrahamsson et al. (1997) and

Le Lostec et al. (2008) did not consider multiple heat sources and end-uses of upgraded heat. Furthermore the temperature of heat required to separate the absorbent refrigerant pair in AHP can compete with low pressure steam generation. Since interactions with the site utility system was not considered in the aforementioned works, the trade-offs were not determined.

Keil et al. (2008) applied an AHP to upgrade waste heat from 40 – 50°C to 80°C. This resulted in fuel savings associated with the hot utility that would have been provided. However, the generator for the AHP was coupled with a gas-fired generator, and the fuel associated with the gas-fired generator is not taken into account. In Garimella (2012), the exhaust gas was supplied to an AHP to generate chilled water and hot water. Estimated savings up to $186/h were achieved.

Costa et al. (2009) performed a preliminary feasibility study for integration of AHP in a Kraft pulping process. The heat pump was driven by medium pressure steam extracted from the steam turbine in a cogeneration unit, to upgrade waste heat to produce low pressure steam. The economics of such heat upgrade scheme depend on the price of hot utility (i.e. steam) required by the generator and hot utility displaced. In their work, the same cost was attributed to medium pressure and low pressure steam. The frameworks for integrating AHP in Keil et al. (2008), Garimella (2012) and Costa et al. (2009) are suitable for single heat source/end-use applications.

Taking into account multiple sources of heat, Bakhtiari et al. (2010) presented a method for integrating AHP based on Pinch Analysis and applied it to a Kraft pulping process. Low temperature heat available below the pinch was upgraded to produce hot water. The AHP was driven by a heat source high enough to produce medium pressure steam. Concepts of Pinch Analysis were used to appropriately position the AHP in a process. In this context, the condenser and absorber releases their heat above the pinch point to reduce the hot utility requirement, as illustrated in Figure 2.16. The evaporator accepts heat from below the pinch, reducing the cold utility requirement also shown in Figure 2.16. However, the generator receives heat from above the pinch, increasing the hot utility requirement.

In existing process sites, with already designed heat exchanger networks, reconfiguring to allow heat above the pinch to drive the generator could result in large heat exchange areas. Furthermore, the increase in hot utility requirement might not justify the placement of AHP.

In processes with a high pinch temperature, the integration of AHP might be advantageous; otherwise, there is a need to identify other heat sources, such as the exhaust of fired heaters. In order to assess the potential benefits of AHP integration, interactions with the site utility system need to be considered, to predict the value of steam displaced or required. In Bakhtiari et al. (2010), the heat source analysis was done in a simplistic manner i.e. neglecting the impact of varying quantity and temperature.

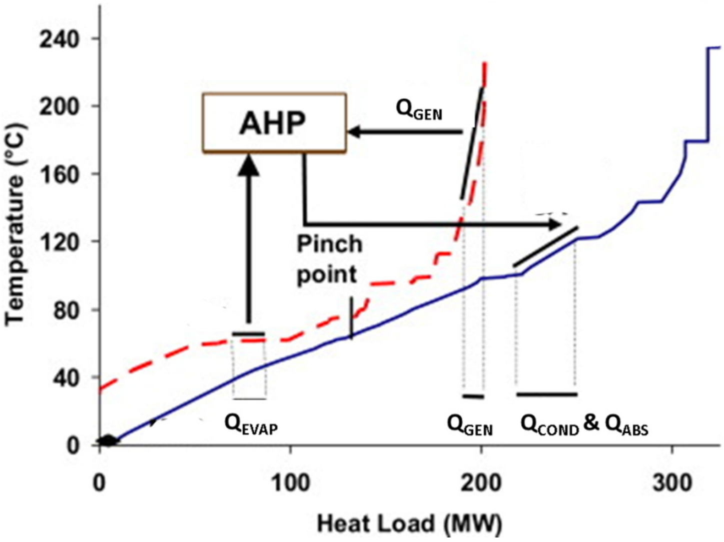


Figure 2.16 Appropriate positioning of an AHP (Bakhtiari et al. 2010).

The exhaust flue gas of a boiler (at 150°C) was used to drive an AHP in the study by Qu et al. (2014) to generate hot water. Interactions with the site utility system were neglected. Even though the boiler efficiency increases by 5–10%, a higher percentage increase could have been obtained by generating low pressure steam directly.

Zhang et al. (2015) integrated an AHP into a combined heat and power utility system. Waste heat recovered from exhausted steam in the steam turbine was used to drive the AHP. The heat upgraded from the absorber and condenser was used for boiler feed water preheating, reducing demand for the high value steam which would have been extracted for heating. The saved steam is used to generate electrical power in a steam turbine. The study did not consider multiple heat sources and end-uses of upgraded heat.

Two of the challenges associated with AHP are economics and the high temperature heat required for operating them, which could compete with low pressure steam generation (Donnellan et al., 2015). AHP were found to be economic when operated over 3000 hours in a year (Bruckner et al., 2015). Such operating hours are possible in the process industry. Typical investment costs range from 240–610 £/kW of heat upgraded (Bruckner et al., 2015).

Previous works on process integration of AHP did not consider multiple heat sources and end-uses of upgraded heat. Therefore in this work, a novel integration framework for AHP taking into account varying quantity of heat sources and end-uses of upgraded heat, interactions with the site utility system to account for trade-offs such as generate low pressure steam or drive an AHP and capital cost limitations is developed. Both graphical and optimization techniques will be developed for process integration of AHP. The graphical techniques aim to allow preliminary evaluation of the potential benefits from AHP integration prior to detailed design, including accounting for the competition with steam generation. The optimization framework aims to take into account possible benefits from varying the quantity and temperature of heat sources, multiple end-uses of upgraded heat (for boiler feed water preheating, possible steam generation and hot utility reduction), and interactions with the site utility system.

2.3.4 Absorption heat transformers (AHT)

Absorption heat transformers are absorption heat pumps operating in reverse. The evaporator and absorber operate at high pressure than the condenser and generator. This implies the temperature of waste heat energy to drive the cycle is lower than the heat rejected from the absorber (Donnellan et al., 2015). A simple schematic is shown in Figure 2.17.

Absorption heat transformers play a fundamental role in waste heat recovery and renewable energy use, for example solar and geothermal sources (Wu et al., 2014). In AHT negligible quantities of electrical energy are required and up to 50% of waste heat can be recovered (Donnellan et al., 2015). They have simple designs, long life, are flexible and have good efficiency at partial load (Horuz and Kurt, 2010).

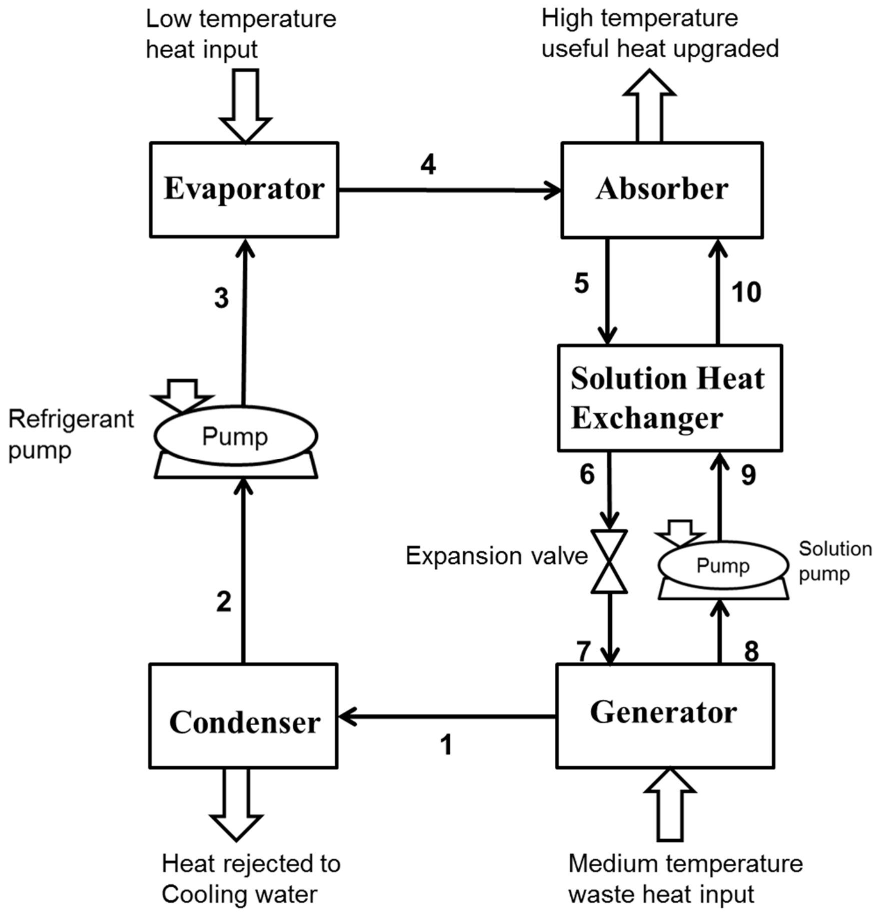


Figure 2.17 Schematic diagram of the AHT (Ibarra-Bahena et al., 2015)

The medium temperature heat source supplied to the generator separates the more volatile component (refrigerant) from the absorbent by evaporation (states 7, 1 and 8). The refrigerant vapour is condensed in the condenser (states 1 and 2), discharging its latent heat to cooling water. The outlet of the condenser is pumped to a higher pressure (states 2 and 3) before entering the evaporator. In the evaporator, an external heat source vaporizes the refrigerant (states 3 and 4). The refrigerant vapour is absorbed into the strong absorbent solution in the absorber (states 4, 5 and 10). Some of the heat given off from the absorption process is recovered at a higher temperature.

The heat released during the absorption process is higher than the heat input in the evaporator and generator due to the exothermic reaction between the refrigerant and absorbent (Parham et al. 2014). The weak absorbent solution exiting the absorber (states 5 and 6) preheats the strong absorbent solution entering the absorber from the generator (states 9 and 10) using a solution heat exchanger. The weak absorbent solution is expanded in a valve (states 6 and 7) before entering the generator. The strong absorbent solution from the generator is pumped before entering the solution heat exchanger (states 8 and 9) and the cycle repeats.

The solution heat exchanger increases the amount of sensible heat transported by the weak solution from the absorber to the generator (Horuz and Kurt, 2010). Whilst some authors believe that including the solution heat exchanger increases the COP by 10%, some other report little benefit (Donnellan et al., 2015).

The Coefficient of Performance (COP) is the ratio of useful heat recovered from the absorber to sum of heat input in the evaporator, generator and work input in the pumps, as shown in Equation 39. A higher COP is possible when the evaporator temperature is equal or greater than the generator temperature (Parham et al., 2014).

$$COP_{AHT,real} = \frac{Q_{ABS}}{Q_{EVAP}+Q_{GEN}+W_{PUMP}} \qquad \text{Equation 39}$$

There are numerous cycle architectures for the AHT. Examples include multi-compartment absorbers and generators and open cycle transformers with multi-compartment absorber and generator. Unfortunately no comparisons have been drawn between these multi-compartment cycles and simple cycles (Donnellan et al. 2015). The double stage AHT gives a higher temperature lift compared to single stage cycles; however, the COP of the single stage AHT is higher (Donnellan et al., 2015). Furthermore, the capital cost of complex systems hinder application. Therefore in this work, single stage absorption heat pumps are adopted. The modelling approach can be extended to complex architectures.

AHT can be modelled based on detailed mass and energy balances for each component, as shown in Equations 40 – 48.

For the evaporator:

$$Q_{EVAP} = m_4 \times (h_4 - h_3) \qquad \text{Equation 40}$$

For the absorber:

$$m_5 = m_4 + m_{10} \qquad \text{Equation 41}$$

$$Q_{ABS} = m_4 h_4 + m_{10} h_{10} - m_5 h_5 \qquad \text{Equation 42}$$

For the condenser:

$$Q_{COND} = m_2 \times (h_2 - h_1) \qquad \text{Equation 43}$$

For the generator:

$$m_7 = m_1 + m_8 \qquad \text{Equation 44}$$

$$Q_{GEN} = m_1 h_1 + m_8 h_8 - m_7 h_7 \qquad \text{Equation 45}$$

Assuming no mass accumulation in the condenser and evaporator:

$$m_1 = m_2 = m_3 = m_4 \qquad \text{Equation 46}$$

For the water pump (states 2 and 3):

$$W_{PUMP} = \frac{m_2 \times (h_2 - h_{3S})}{\eta_{is,PUMP}} \qquad \text{Equation 47}$$

For the solution pump (states 8 and 9)

$$W_{PUMP} = \frac{m_8 \times (h_8 - h_{9S})}{\eta_{is,PUMP}} \qquad \text{Equation 48}$$

Where h is the specific enthalpy in the respective state points and η_{is} is the isentropic efficiency.

These equations are applied by Horuz and Kurt (2010) and are shown to have good accuracy compared to experimental results. However, model applicability is expected to be less robust when the problem size increases, for example, when multiple heat sources need to be considered.

In Hernandez et al. (2009), a thermodynamic model and a neural network model are developed for the AHT. Since the thermodynamic model can only be used in steady state applications, a neural network model was developed for both steady and transitory states. The neural network model shows better correlations; however, its range of operating conditions is small. Other methods developed for modelling the AHT include pace regression, sequential minimal optimization, and decision table (Parham et al., 2014). However, these models require high computation time and are suitable for single heat source/end-use applications.

In this work, models for the AHT that allow systematic analysis of multiple waste heat sources, prediction of the performance to a reasonable degree of accuracy, and are easily embedded in large process synthesis frameworks are developed.

2.3.4.1 Working fluid selection for absorption heat transformers

Absorption heat transformer systems using water/lithium bromide perform better than systems using ammonia/water (Parham et al., 2014). However water/lithium bromide systems require a practical upper temperature limit to prevent crystallization. Reducing the risk of crystallization is possible through thermodynamic cycle modification, mass and heat transfer enhancement, using chemical inhibitors and changing working fluids.

Parham et al. (2013) compared the performance of water/lithium chloride and water/lithium bromide AHT. Even though using water/lithium chloride reduces the risk of crystallization, the coefficient of performance (COP) of water/lithium bromide systems is 1.5 – 2% higher than water/lithium chloride systems.

Zhuo and Machielsen (1996) compared the use of water/lithium bromide to that of Alkitrate. Even though the COPs are similar under the same operating conditions, and Alkitrate reduces the risk of crystallization, Alkitrate is limited at low temperatures due to solubility problems.

Also in Yin et al. (2000), a comparative study between water/lithium bromide, 2,2,2-triuoroethanol/N-methyl 1-2-pyrrolidone, 2,2,2-triuoroethanol/dimethylethertetraethylene glycol and 2,2,2-triuoroethanol/2-pyrrolidone was performed. Results show that water/lithium bromide had higher COP below 150°C, and the others performed better at higher temperatures (up to 200°C). In practice, most applications use water/lithium bromide (Parham et al., 2014). Therefore in this work, water/lithium bromide systems are adopted. To prevent crystallization of the salt in solution, the AHT will be operated above the crystallization line visible from the P-T-x diagram as shown in Figure 2.18.

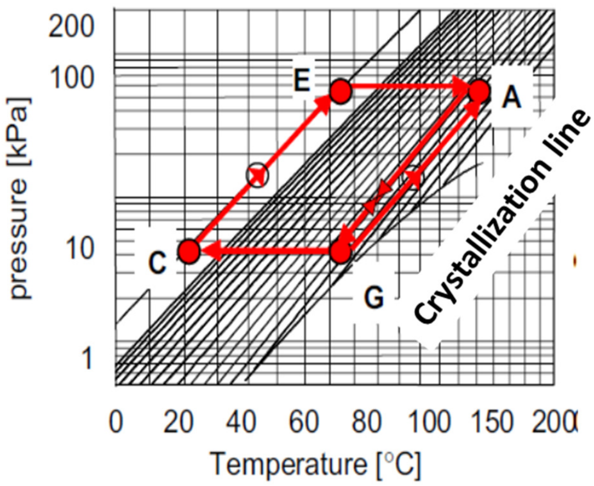


Figure 2.18 AHT representations in water/LiBr phase diagram (Costa et al., 2009)

2.3.4.2 Process integration of absorption heat transformers

Previous research focused on thermodynamic performance of the system; there are few studies on integrating an AHT into process sites (Donnellan et al., 2015).

Scott et al. (1999) integrated an AHT into a sugar mill. Waste heat from the plant's crystallization unit is used to drive the AHT to provide heat to a multi-effect evaporator. Benefits recorded were reduction in the amount of live steam required by the plant. However, the study focused on a single heat source/end-use of upgraded heat. Ma et al. (2003) applied an AHT to heat water from 95 to 100°C using waste heat at 98°C in a rubber plant. Benefits include reduction in steam requirements. Again the study only considered a single heat source/ end-use of upgraded heat. In typical process sites there may be multiple sources of waste heat from the site processing units and the utility system, there may also be multiple end-uses of upgraded heat. There is a need to allow systematic analysis of multiple heat sources and end-uses.

Cortes and Rivera (2010) integrated an AHT in a pulp and paper mill to preheat water before entering a boiler. They reported 25% reduction in the plants steam consumption. However, the study focused on a single heat source/end-use of upgraded heat. Furthermore the economic viability was not documented. The payback for AHT installations depends on the operating time and ranges from 2.1 years for 8600 hours per annum, 2.7 years for 8000 hours per annum to 11.7 years for 2,500 hours per annum (Donnellan et al., 2015).

Horuz and Kurt (2010) integrated an AHT in a cogeneration system to produce hot process water (low pressure steam) at 120°C. The thermal energy required to drive the AHT was hot water (at 90°C) generated by a cogeneration system in a textile company. The study considered a single heat source/ end-use system.

Donnellan et al. (2014) conducted a case study on the potential installation of an AHT in an oil refinery, examining various different natural gas scenarios. Two heat sources were considered from 179 to 87°C and 120 – 40°C. Their analyses show that the quantity of waste heat is important and the economic attractiveness increases with natural gas price. The upgraded heat was used to heat hot oil or used as a heat transfer medium in the heat exchanger network to reduce utility consumption. However, the cost of utility displaced was considered in a simple manner. It is necessary to consider what utility to reduce i.e. low pressure, medium pressure or high pressure steam. The cost can only be estimated by considering the site utility system (Smith, 2005).

In AHT the temperature of heat required to drive the generator is lower than that of the heat upgraded. Therefore conceptually, waste heat available below the pinch can be upgraded using waste heat also available below the pinch to drive the generator as illustrated in Figure 2.19. The upgraded heat can be used to reduce the hot utility required above the pinch. Compared to an AHP in Figure 2.16, integrating AHT would not increase the hot utility requirement. However, the COP of AHT is lower than AHP.

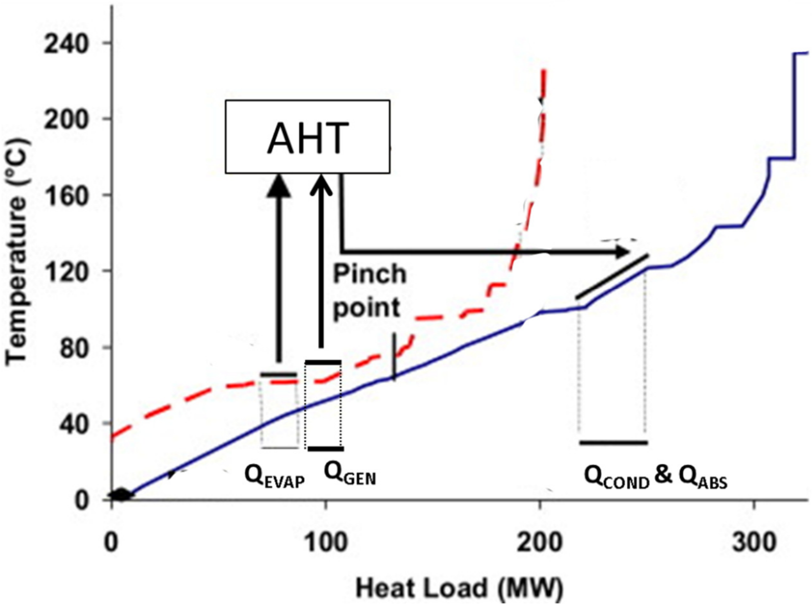


Figure 2.19 Illustration for AHT positioning.

Previous studies on process integration of AHTs focus on a single waste heat source and end-use of upgraded heat. Therefore, in this work, a novel integration framework for AHT taking into account varying quantity of heat sources and end-uses of upgraded heat, interactions with the site utility system to consider the waste heat available, and to predict the true value of steam saved, as well as capital cost implications is developed. Both graphical and optimization techniques are developed for process integration of AHT. The graphical techniques allow preliminary evaluation of the potential benefits from AHT integration. The optimization framework aims to take into account possible benefits from varying the quantity and temperature of heat sources, multiple end-uses of upgraded heat (for boiler feed water preheating, possible steam generation and hot utility reduction), and interactions with the site utility system.

2.3.5 Mechanical heat pumps (MHP)

A MHP can provide cooling and heating by receiving waste heat in the evaporator and rejecting upgraded heat in the condenser. The MHP has been proven at industrial scale, and can reduce both hot utility and cold utility requirements (Becker et al., 2011). Mechanical heat pumps can also achieve higher temperature lifts than absorption heat pumps and heat transformers. However, they require high quality electrical power to operate them.

A mechanical heat pump has four major components: the evaporator, compressor, condenser and expansion valve. A schematic is shown in Figure 2.20. The refrigerant (working fluid) vaporizes by accepting thermal energy from a low temperature waste heat source (state 1 and 2). The vapour is compressed using mechanical energy to a higher temperature and higher pressure (state 2 and 3). Condensation of the compressed vapour releases heat to a high temperature sink (state 3 and 4). The condensed vapour is expanded in a valve, and the cycle repeats (state 4 and 1). A thermostatic expansion valve with external pressure equalizer can be used, and a single cylinder reciprocating hermetic type compressor can also be used as the compressor (Fatouh and Elgendy, 2011). The evaporators and condensers are typically shell and tube heat exchangers with refrigerant flowing through the evaporator tube and condenser shell (Fatouh and Elgendy, 2011).

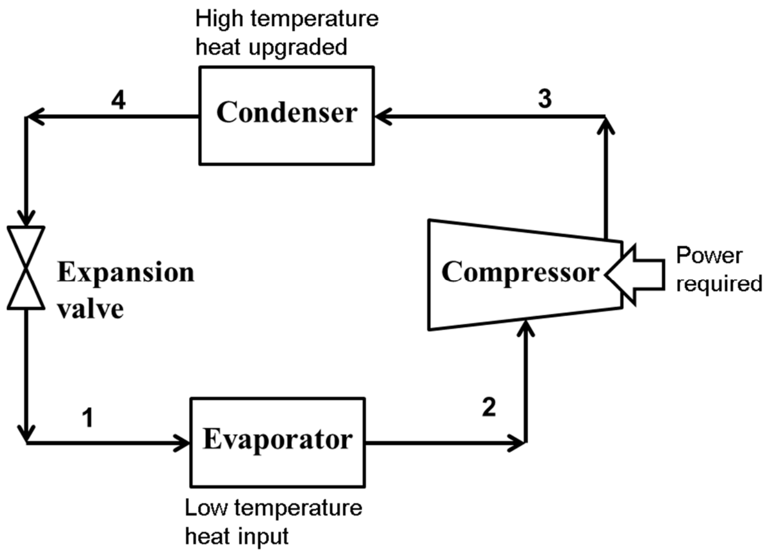


Figure 2.20 Schematic of a simple mechanical heat pump

Modifications have been made to the simple cycle to improve the performance; for example addition of a heat exchanger to recover heat from the condenser to heat up the evaporator inlet (Park et al., 2015). This heat exchange reduces the quantity of heat required in the evaporator, increases the temperature of the compressor inlet stream, and increases the degree of sub cooling; since the expansion process in the valve becomes isentropic. Including an internal heat exchanger also reduces the temperature at condenser outlet. The increased temperature of the compressor inlet decreases the compressor volumetric efficiency, which degrades the cycle performance.

Another modification is to replace the expansion valve with an expander (Park et al., 2015). This expansion provides some additional electrical power which can be used to drive the compressor. However, installation of an expander results in large pressure difference inside the machine which might result in internal leakage.

Two-stage configurations can increase the temperature difference between heat source and heat sink. However, addition of new components increases the cost and complexity of the cycle. Therefore in this work, a single stage mechanical heat pump is considered. The modelling approach can be extended to complex configurations.

The coefficient of performance (COP) for the MHP is defined as the heat upgraded to the power required by the compressor (Equation 49).

$$COP_{MHP,real} = \frac{Q_{COND}}{W_{COMP}} \qquad \text{Equation 49}$$

The modelling of MHP to predict the COP is possible through detailed energy balances for each component in the cycles as shown in Figure 2.18. Modelling equations are shown below in Equations 50 – 52.

Stage 1 to 2: Evaporation

$$Q_{EVAP} = m_{wf} \times (h_2 - h_1) \qquad \text{Equation 50}$$

Stage 2 to 3: Compression

$$W_{COMP} = \eta_{is} \times m_{wf} \times (h_3 - h_2) \qquad \text{Equation 51}$$

Stage 3 to 4: Condensing

$$Q_{COND} = m_{wf} \times (h_3 - h_4) \qquad \text{Equation 52}$$

Where h is the specific enthalpy in the respective state points and η_{is} is the isentropic efficiency.

The Engineering Equation Solver (EES) contains the models shown above and detailed mass and heat transfer correlations for MHPs. This software was used by Park et al. (2015) to predict the performance of the MHP. However, it is difficult to model multiple heat source streams systematically without the need for complex iterations.

Bell and Lemort (2015) used a set of non-linear equations accounting for detailed mass and heat transfer models of compressors, evaporators and condensers to predict the performance of a mechanical heat pump. However, application was limited to a specific heat source/end-use system.

To simplify MHP modelling, some authors multiply the ideal COP by a constant efficiency factor. The ideal COP is for an inverse Carnot cycle. For example an inefficiency factor of 0.6 to 0.7 is used in Bruckner et al. (2015), and 0.8 used in Matsuda et al. (2012). Even though the ideal coefficient of performance accounts for cycle temperatures, a constant efficiency factor does not account for the non-ideal behaviour of working fluids. A constant actual COP has also been used to simplify heat pump modelling in Miah et al. (2015), this is highly inaccurate.

Process simulation software namely Aspen HYSYS is used in Waheed et al. (2014) to model the MHP. Even though simulations results show good agreement with experiments, it is difficult to develop a systematic framework that allows for consideration of multiple heat source streams and end-uses of upgraded heat in Aspen HYSYS.

In this research, explicit models of mechanical heat pumps will be developed by combining thermodynamic models and empirical models.

2.3.5.1 Working fluid selection for mechanical heat pumps

Working fluids for MHP must meet operational, safety and environmental requirements. Working fluids employed in literature for MHP with low global warming potential include ammonia, propane, carbon dioxide and isobutane (Miah et al., 2015). Bell and Lemort (2015) screened 33 environmental friendly working fluids for use in mechanical heat pumps. This screening was done for a particular heat source (at 40°C) and sink (at 90°C) application. Isobutane shows the most promise compared to ammonia and butane (Kim and Perez-Blanco, 2015). In this research, screening of working fluids for MHP is considered as part of the methodological framework. Six working fluids will be screened based on the coefficient of performance, they are: propylene, propane, i-butane, n-butane, ammonia and water. Water can be used as a refrigerant for higher temperature lifts (Chamoun et al., 2014).

2.3.5.2 Process integration of mechanical heat pumps

A heat integration framework incorporating heat pumps was developed in Miah et al. (2015) and applied to a case study. Total energy reduction of about 32% was obtained. In the framework, design was done by selecting waste heat source streams to be upgraded. However, selection of heat source streams was not systematic. Furthermore, the streams heat duty was exploited at their target temperatures and interactions with the utility system were not considered.

Modla and Lang (2013) integrated a mechanical heat pump with a batch distillation column. The MHP was used to upgrade the heat rejected by the condenser to satisfy the heat demand of the reboiler (heat sink). Their analysis showed that the payback for MHP integration depends on the quantity of heat upgraded. The study conducted by Modla and Lang (2013) focused on a single heat source/end-use of upgraded heat.

Becker et al. (2011) integrated a MHP into a brewery using the heat available below the pinch to satisfy the heat required above the pinch. Their optimization framework considered practical constraints of the technology, such as operating temperature range of given refrigerants, but it does not consider the value of hot utility displaced or interactions with the utility system.

Based on the economic analysis in Bruckner et al. (2015), mechanical heat pumps are economic when operated for over 4000 hours in a year. This could make them suitable for industrial applications. Typical investment costs range from 110 – 370 £/kW heat upgraded (Bruckner et al., 2015).

In this work, an integration framework for MHP is proposed to consider different heat sources and sink temperature combinations and interactions with the site utility system. The heat source temperature to the evaporator affects the heat pump COP (Fatouh and Elgendy, 2011). The heat source and sink temperatures affect the limitations of heat pump applicability (Ommen et al., 2015).

2.3.6 Heat recovery via heat exchange

Heat exchangers are used for recycling waste heat to heat or to preheat other processes. Heat exchangers for heat recovery can be stainless steel counter current shell-and-tube exchangers (Chen et al., 2012).

Heat recovered from process waste heat is useful for steam generation, hot utility reduction, boiler feed water preheating and hot water generation. The end-use (sink) depends on the heat source temperature. One of the barriers to direct heat recovery is the lack of availability of suitable heat sinks.

Heat transfer between a waste heat source and a sink is illustrated in Figure 2.21. The heat recovered is calculated based on Equation 53 and heat exchange area (A) by Equation 54.

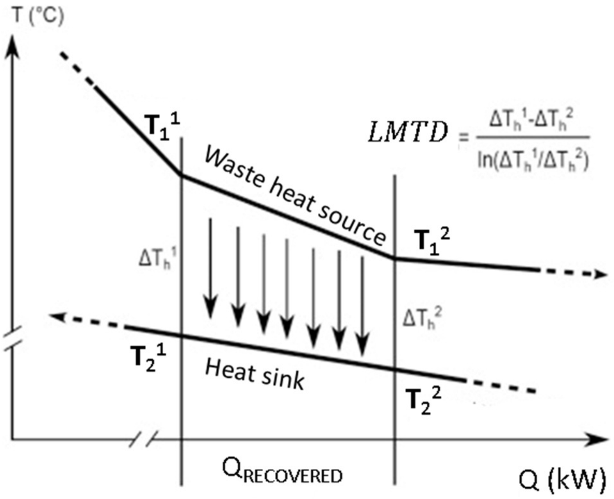


Figure 2.21 Heat transfer from waste heat source to sink (Eriksson et al., 2015)

$$Q_{RECOVERED} = m_{WHS} \times cp_{WHS} \times (T_1^1 - T_1^2) \quad \text{Equation 53}$$

$$A = \frac{Q_{RECOVERED}}{LMTD \times U} \quad \text{Equation 54}$$

In this present work, heat transfer resistances are addressed by specifying values of overall heat transfer coefficients (U), considering a general U-shape shell and tube heat exchanger arrangement with the waste heat sink at the shell side, and waste heat source at the tube-side with stainless steel for the shell and tubes (to handle any corrosiveness).

Luo et al. (2012) conducted a study to recover process surplus heat for boiler feed water (BFW) preheating in the site utility system. They developed a non-linear optimization framework. In their framework, the two decision variables were the terminal temperature and heat load of the process-heated BFW. Luo et al. (2012) discovered that it is better to preheat BFW to the maximum possible temperature. BFW preheating can occur at various points in the site utility system, before the deaerator (state 1 in Figure 2.22), after the deaerator (state 2 in Figure 2.22), and after the feed pump (state 3 in Figure 2.22). The study in Luo et al.

(2012) focused on BFW preheating before and after leaving the deaerator. Focusing on feed water before and after the deaerator restricts the choice of outlet temperature, since the aim will be to prevent a two-phase mixture entering the boiler feed pump. However, after the feed pump the only restriction is the boiler design.

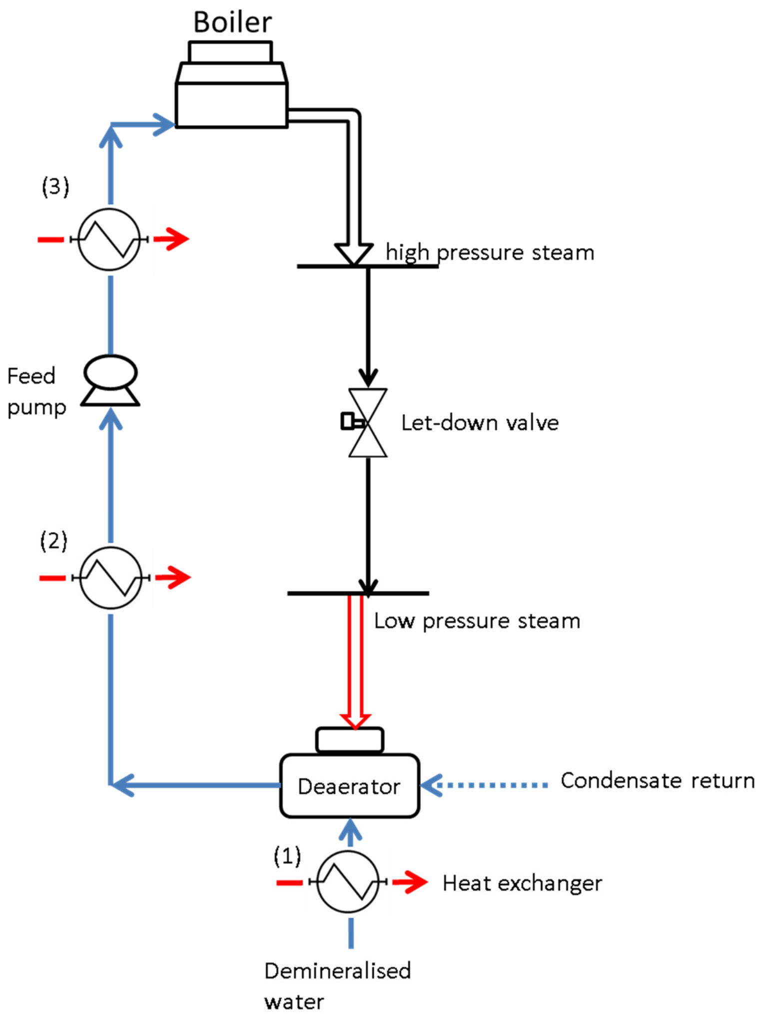


Figure 2.22 Simplified schematic of site utility system showing feed water flow to the boiler (Illustration)

Heat recovery for hot water generation and steam generation is considered in Hackl and Harvey (2015). Different heat recovery systems were generated and screened based on required investments. However they did not account for heat available from the site utility system.

Waste heat (in the form of flue gas) from an industrial utility system is used to dry biomass in Li et al. (2012). Advantages of dried biomass compared to fuel with high moisture are improved boiler performance and lower CO_2 emissions. The flue gas temperature was from

250 – 450 °C; two cases of use were investigated. The first case was to use the flue gas directly and the second case was to generate steam from the flue gas (using hot water available at 90°C in the system) using a heat exchanger. Direct use of flue gas was selected based on the lower capital investment required. However, the benefits of allowing for steam expansion in a turbine to generate power and also provide drying at the same time were not considered.

The recovery of waste heat for use outside the boundaries of process sites has been investigated by numerous researchers. In 2011, waste heat accounted for 7.2% of the heat delivered to district heating networks in Sweden (Viklund and Karlsson, 2015). Fang et al. (2015) developed a simulation framework for waste heat recovery for district heating. Their framework presented a method to find the optimal way of collecting heat from multiple waste heat sources. The case study presented show that benefits from utilizing waste heat in district heating networks are reduction in carbon dioxide emissions and water requirement. A challenge in heat recovery for district heating is that the heat demand for domestic use is always lower than the available waste heat in process sites (Fang et al., 2015). Therefore it is necessary to consider both heat recovery and heat utilization options within the process site and off-site to maximize waste heat exploitation.

Viklund and Karlsson (2015) performed an energy system analysis to recover waste heat for district heating under different market scenarios. Both economics and environmental benefits were recorded. Use of excess heat for district heating was also explored by Eriksson et al. (2015) this methodological framework involved detailed cost targeting for the heat collection system. There is a need to develop a framework that compares multiple end-uses of waste heat within and outside the boundaries of process sites.

Cooper et al. (2015) investigated the feasibility of district heating networks as consumers of industrial waste heat from the UK process industry. District heating systems are used to supply heat from a collective heating system. They found that less than one third of the heat rejected by industry can be utilized by district heating networks. The economics of the network depend on the heat demand density, which is usually low close to industrial sites. Therefore, in addition to considering heat export, there is need to consider options to use waste heat within the process site. In addition, seasonality of demand is a challenge.

Therefore frameworks formulated to consider off-site process integration should be a multi-period one.

Swithenbank et al. (2013) considered the use of industrial waste heat for district heating. Two challenges are identified from their work: (1) installation of a heating network is expensive; (2) most industries are located far away from residential areas. The thermal demand of few residents and farms living close to industries is small compared to the quantity of waste heat produced. Even though direct heat recovery is the most common form of utilizing waste heat, there are restrictions in demand.

2.4 Concluding remarks

Growing global energy shortages and environmental concerns place increasing pressure on the process industries to integrate waste heat recovery. This chapter has reviewed various approaches for evaluating the available waste heat in process sites, graphical and mathematical analysis of site utility systems, modelling waste heat recovery technologies, working fluid selection for recovery technologies and process integration of waste heat recovery technologies.

The available waste heat occurs over a wide range in quantity and temperature. Previous authors simplified the problem by assuming all the heat is available at a single temperature and from a single heat source (for example in Kwak et al., 2014). Some other authors only considered a single heat source (Garimella et al., 2012; Popli et al., 2013; Zhang et al., 2015). There is currently no methodological framework that considers the varying quantity and temperature of waste heat sources and takes into account all the available waste heat from the site processing units and the site utility system. There is also no framework that can systematically select and combine heat sources for exploitation in waste heat recovery technologies.

Technologies such as organic Rankine cycles, absorption chillers, absorption heat pumps, absorption heat transformers, mechanical heat pumps and heat recovery via heat exchange are considered in this work. The literature review shows that these technologies allow utilization and recovery of waste heat. There are currently no models of technologies (except heat recovery via heat exchange) that allow for systematic analysis of multiple heat sources without complex iterations, easily applicable in a variety of energy systems modelling frameworks, allow for non-tedious complex system modelling, and predict the technology performance in a simple yet sufficiently accurate way.

Three different heat upgrade technologies are used in this work, absorption heat pumps and heat transformers, and mechanical heat pumps. Their coefficients of performance are presented in Equations 38, 39 and 49 respectively. The COP has been used to evaluate heat pump systems and choose between heat pumps. However this analysis neglects the missed opportunity for steam generation from the high temperature heat required to drive the generator of absorption heat pumps. Using the COP also neglects the fuel and waste heat associated with the high quality electrical power required by mechanical heat pumps. A new performance criterion apart from the coefficient of performance needs to be developed for heat upgrade technologies.

It is widely believed that direct use of heat is more feasible and effective compared to other waste heat utilization options (Luo et al. 2012). However such decisions have been made solely on economics and the performance of technologies based on conservation of energy quantity (from the first law of thermodynamics). The performance of technologies is calculated using different basis, less than 100% for organic Rankine cycles and absorption chillers, more than 100% for absorption heat pumps, heat transformers and mechanical heat pumps and 100% (neglecting distribution and transmission losses) for heat recovery via heat exchange. The performance calculation is often misleading because it assumes work and heat are equal entities. Currently, comparison of technology options based on conservation of energy quantity and energy quality degradation has not been done. Such comparisons may provide useful thermodynamic insights into the choice and operation of technology options. In Section 2.1, the scope for waste heat utilization was defined after heat recovery between several processing units on a site using TSA. A comparative analysis of all technology options (including heat exchangers) will help to prove this definition, and establish the range of temperatures where other ways of utilizing thermal energy are beneficial.

In previous works, numerous researchers neglect the heterogeneous nature of industrial waste heat utilization i.e. the varying quantity and temperature of heat sources, multiple end-uses of recovered energy and multiple technology options. A waste heat utilization system considers this heterogeneous nature together with the possibility of combining one or more technology options to exploit the available waste heat and possible interaction with the site utility system.

Viklund and Karlsson (2015) performed an energy systems analysis to determine how waste heat should be used, and the impact on CO_2 emissions. Their MILP framework was used to synthesize the system to minimize costs. The framework only considers off-site use of recovered energy for district heating, district cooling and power export to the grid. Interactions between the existing utility systems producing the waste heat are not considered. Furthermore, modelling of the technologies was done in a simplified manner i.e. constant performance.

Multiple end-uses exist within the site and off-site for energy recovered from waste heat. Poor selection of end-uses could result in uneconomic designs. The evaluation of the different end-uses to determine the most economic option(s) (and the associated environmental benefits) has not been done before.

Applying process integration principles to design of site waste heat utilization systems needs to emphasize the unity of the process and the site utility system which was neglected by previous researchers. It may be possible to improve the economics of waste heat utilization by expanding the framework to allow for simultaneous optimization with the site utility system. Such analysis has not been done before.

The main aim of this work is to propose a new design approach for process integration of waste heat recovery technologies and design of site waste heat utilization systems. The methodology considers: (1) modelling of technology options, (2) comparing between different technology options, (3) ranking of end-uses of recovered energy and (4) waste heat utilization system design. The methodology proposed for system design considers simultaneous optimization with the site utility system.

Chapter 3: Modelling and Integrating Waste Heat Recovery Technologies

Mature and commercialized technologies exist to produce useful energy from industrial waste heat. Technologies considered in this work are organic Rankine cycles for power generation from waste heat (section 2.3.1), absorption chillers for chilling provision (section 2.3.2), absorption heat pumps (section 2.3.3), heat transformers (section 2.3.4) and mechanical heat pump for heat upgrade (section 2.3.5) and heat recovery via heat exchange (section 2.3.6).

Explicit models of waste heat recovery technologies are proposed in this chapter as part of the methodological framework. The modelling framework combines both physical and empirical modelling techniques. Physical models are used to determine the ideal performance for each technology. Empirical techniques are then applied to relate the ideal performance to the actual (real) performance. Data for the correlation are obtained from rigorous simulations in Aspen HYSYS, Aspen Plus and from thermodynamic design data in literature. These models predict the actual performance with high accuracy and can be easily embedded in optimization frameworks.

The performance of organic Rankine cycles and mechanical heat pumps depends on the working fluids applied. Screening of working fluids for these technologies is done in this chapter. Water/lithium bromide is selected as working fluid for the absorption systems (discussed in Section 2.3.2.1, 2.3.3.1 and 2.3.4.1).

Integrating waste heat recovery technologies in process sites could have potential to increase efficiency in the use of fuel, reduce cold utility demand and possible savings in hot utility. The technologies exploit the available waste heat rejected to cooling water and air, from the site processing units and the site utility system.

To address the heterogeneous nature of the waste heat, a temperature-enthalpy diagram is proposed to represent waste heat sources rejected by the site processing units and the site utility system. Graphical techniques for integrating waste heat recovery technologies in process sites are also proposed in this chapter as part of the methodological framework. The tools are also used to explore the impact of demand for recovered energy and benefits from recovering multiple forms of energy.

This chapter includes two papers, referred to as Publication 1 and Publication 2. Both papers describe the models of waste heat recovery technologies and the graphical tools. Publication 1 contains models for the organic Rankine cycles, absorption chillers and absorption heat pumps, together with a graphical tool for integrating single technologies and multiple technologies. Publication 2 contains models of absorption heat pumps, heat transformers and mechanical heat pumps and graphical tools for integrating them. The models are applied in Publication 3, 4, 5, 6 and 7.

3. 1. Introduction to Publication 1

The paper presented in this section contains models of technologies using waste heat as the primary energy source. Section 1 discusses the background and justifies selection of the organic Rankine cycle, absorption chillers and absorption heat pumps to support the review provided in section 2.3 (Table 2.1) and contributions of the paper.

The concept of the energy efficiency of a site is defined in Section 2. The site energy efficiency estimates the quantity of useful heat wasted. In section 3, composite curves and total site profiles are extended to represent the waste heat sources in process sites. The waste heat source profile shows the quantity and temperature of heat sources rejected to cooling water and air.

Models of organic Rankine cycles, absorption chillers and absorption heat pumps are presented in Section 4. Validation of the models against rigorous simulation is also presented. Pure and mixed workings fluids for the organic Rankine cycle is screened in this section.

A methodology based on graphical techniques for process integration of organic Rankine cycles, absorption chillers and absorption heat pumps is presented in section 5. The methodology is applicable for integrating single technology options and multiple technology options.

In section 6, the methodology is applied to a medium scale refinery case study; conclusions and future work are presented in section 7. Results show that there is potential in industrial waste to increase the efficiency of process sites. Higher increase in efficiency is possible when multiple forms of energy are recovered.

3. 2. Publication 1

Oluleye G., Jobson M., Smith R., Perry S.J., Evaluating the potential of process sites for waste heat recovery. Applied Energy (2016); 161: 627–646.
doi.org/10.1016/j.apenergy.2015.07.011

Applied Energy 161 (2016) 627–646

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Evaluating the potential of process sites for waste heat recovery

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HIGHLIGHTS

- Analysis considers the temperature and duties of the available waste heat.
- Models for organic Rankine cycles, absorption heat pumps and chillers proposed.
- Exploitation of waste heat from site processes and utility systems.
- Concept of a site energy efficiency introduced.
- Case study presented to illustrate application of the proposed methodology.

ARTICLE INFO

Article history:
Received 17 January 2015
Received in revised form 7 June 2015
Accepted 4 July 2015
Available online 23 July 2015

Keywords:
Waste heat recovery
Waste heat source profile
Site energy efficiency
Organic Rankine cycle
Absorption chiller
Absorption heat pump

ABSTRACT

As a result of depleting reserves of fossil fuels, conventional energy sources are becoming less available. In spite of this, energy is still being wasted, especially in the form of heat. The energy efficiency of process sites (defined as useful energy output per unit of energy input) may be increased through waste heat utilisation, thereby resulting in primary energy savings.

In this work, waste heat is defined and a methodology developed to identify the potential for waste heat recovery in process sites; considering the temperature and quantity of waste heat sources from the site processes and the site utility system (including fired heaters and, the cogeneration, cooling and refrigeration systems). The concept of the energy efficiency of a site is introduced – the fraction of the energy inputs that is converted into useful energy (heat or power or cooling) to support the methodology. Furthermore, simplified mathematical models of waste heat recovery technologies using heat as primary energy source, including organic Rankine cycles (using both pure and mixed organics as working fluids), absorption chillers and absorption heat pumps are developed to support the methodology. These models are applied to assess the potential for recovery of useful energy from waste heat.

The methodology is illustrated for an existing process site using a case study of a petroleum refinery. The energy efficiency of the site increases by 10% as a result of waste heat recovery. If there is an infinite demand for recovered energy (i.e. all the recoverable waste heat sources are exploited), the site energy efficiency could increase by 33%. The methodology also shows that combining technologies into a system creates greater potential to exploit the available waste heat in process sites.

1. Introduction

The process industries are responsible for 27% of global energy consumption, and annual demand for heat and electricity is expected to grow by 1.9% and 2.4%, respectively [1]. Energy-intensive process industries, such as for the manufacture of iron and steel, cement, petrochemicals, chemicals, oil and gas exploration, and pulp and paper, currently account for 69% of total industrial energy consumption [1]. In spite of the increasing demand, depleting reserves of fossil fuels and increasing energy prices, energy in the form of low-grade heat is still being wasted. Globally, the percentage of energy inputs from coal, natural gas, oil, nuclear and renewables converted into electricity, heat and transformed into another form for use in the various sectors of an economy i.e. industry, transport, building and others is 67% [1], while for the process industries in the UK, at least 40% [2] of the energy content of fuel is wasted. Using energy more efficiently could reduce demand for fuel; thereby conserving resources, reducing operating costs and reducing CO_2 emissions. Improving energy efficiency of the process industries has the potential to reduce global emissions by 44% in 2035 [3]. To this end, concepts have been developed to increase energy efficiencies in the process industries and minimise industrial demand for energy.

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http://dx.doi.org/10.1016/j.apenergy.2015.07.011

Nomenclature

a	regression coefficient for absorption chiller
b	regression coefficient for absorption chiller
c	regression coefficient for absorption heat pump
COP_{AbC}	absorption chiller coefficient of performance
COP_{AHP}	absorption heat pump coefficient of performance
d	regression coefficient for absorption heat pump
ΔH	change in enthalpy (kW)
P	pressure (kPa)
Q	heat load (kW)
T	temperature (°C)
T_s	stream supply temperature (°C)
T_t	stream temperature (°C)
ΔT_{min}	minimum temperature difference (°C)
W	work (kW)

Greek letters

α	regression coefficient for organic Rankine cycles
β	regression coefficient for organic Rankine cycles
γ	regression coefficient for organic Rankine cycles
η_{real}	ORC real efficiency
η_{ideal}	ORC ideal efficiency

The concept of Pinch Analysis was introduced and applied in the process industries to maximise heat recovery in a process plant by heat exchange [4]. This concept is based on estimating thermodynamically feasible energy targets by recovering and reusing the heat energy within a process until the process is constrained or "pinched" i.e. a minimum temperature approach is reached. However, even when heat recovery within a process is maximised, some residual heat is typically rejected to cooling water or to air; depending on the pinch point, the temperature of the heat rejected could be high enough to be a valuable source of heat, or it may be too close to ambient conditions to be worth recovering.

To maximise heat recovery between processes on a site, the concept of total site analysis was developed [5]. This concept takes into account surplus and residual heat from different processes on a site using the site profiles from which the site energy demand for heating, cooling, refrigeration and power can be determined to maximise energy recovery between processes on the site. While residual heat of a suitable temperature can be used to generate steam by heat recovery, that at lower temperatures is typically rejected to ambient heat sinks.

Demand of a process (or site) for utilities, such as, steam, power, high temperature heat and cooling can be determined using Pinch Analysis for a single process or total site analysis for multiple processes on a site. A central utility system is usually designed to satisfy demand for steam and power, high temperature heat demand requires fired heating in a furnace, while cooling demand is met by a cooling water system, air cooling or a refrigeration system [6]. Utility systems are designed to generate heat and power to maximise the utilisation of the energy content of a given amount of fuel [7]. However, a major drawback with cogeneration units is the large amount of residual heat left, especially at temperatures too low for steam generation or in quantities that exceed the demand on site for process heating.

Therefore to address the problem of excessive residual heat, a methodology is introduced in Varbanov et al. [6] to improve energy utilisation by evaluating the true value of steam and saving steam through reduction in process consumption or generation of additional power. The potential to use residual heat at temperatures too low for steam generation, power generation using Rankine cycles and heat in exhaust of combustion devices such as boilers and gas turbines is not considered. Zhang et al. [8] proposed an optimisation procedure for retrofitting existing utility systems by employing heat integration within a process, between processes to recover surplus heat and low temperature heat recovery. However, the low temperature heat recovery is limited to temperatures high enough for steam power generation and boiler feed water preheating. To evaluate the potential to generate useful energy (power, heat and chilling) from the residual heat it is necessary to define the term 'industrial waste heat'.

Various definitions have been attributed to industrial waste heat. Viklund and Johansson [9] define waste heat as heat generated as a by-product of industrial processes. In this definition, the potential for heat recovery within and between processes is omitted. Ammar et al. [2] define waste heat as heat for which recovery is not viable economically, while Bendig et al. [10] defines waste heat as the sum of the exergy available in a process after heat recovery and utility integration. Both Ammar et al. [2] and Bendig et al. [10] recognise the possibility of heat recovery within a process, but neither accounts for the heat rejected from a site utility system which is designed to satisfy the process energy demand.

In this paper, industrial waste heat is defined as the sum of the residual heat rejected from the processes on a site and residual heat rejected from the site utility system designed to satisfy the energy demand, namely heating, cooling, refrigeration and power [11]. With respect to the processes on a site, waste heat is the heat rejected to cooling water and air after heat recovery within a process or heat recovery between processes on a site using Total Site Integration [5]. Therefore the scope for waste heat is defined for when a process and a site has reached their maximum potential for heat recovery. Recovering heat within a process or between processes until the process or site is pinched is relatively inexpensive and easy to implement [9]. With respect to the utility system, waste heat is the heat rejected to cooling water and air from a utility system designed to satisfy the energy demand of a site [11]. Waste heat can occur over a wide temperature range and from multiple sources in process sites, and the use of excess heat could provide a way to reduce primary energy demand.

Diverse technologies exist to recover energy in the form of power, cooling and heat from waste heat using waste heat as the primary energy source. Examples of technologies for work generation include thermoelectric generators, phase change materials, organic Rankine cycles (ORC), Kalina cycles and trilateral flash cycles. In thermoelectric generators, electricity is generated when a voltage difference occurs in a conductor because of a temperature gradient caused by the transfer of thermal energy through the material [12]. Commercially available low-temperature thermoelectric materials are up to 250 °C [13]. The generators have no moving parts, are compact, quiet, highly reliable and environmentally friendly [14]. However, relatively low efficiency has limited its use (typically around 5–10%) but they have high capability for utilising huge amounts of waste heat in an easy and simple manner [14]. Phase change materials use the expansion and contraction of a paraffin mixture as it changes from solid to liquid state to produce electricity from heat. Mechanical energy from expansion and contraction is converted into electricity in a generator [10]. The electrical efficiency is very low; 2.5–9% [15] and the technology are still in demonstration phase [15]. The Organic Rankine cycle uses a circulating organic fluid pumped around the circuit and heated by waste heat in the evaporator to produce a vapour which expands to generate electricity [13]. It has received interests in recent years due to high efficiency and flexibility [16]. Kalina cycles generate electricity from waste heat using a mixture of two fluids with different boiling points [17]. More heat can be extracted from the heat sources compared to some pure working fluids because the mixture evaporates gradually over a range of temperatures [18].

Organic Rankine cycles and Kalina cycles can be evaluated by comparison with steam under the same residual condition. Firstly, the ORC has higher thermal efficiency, smaller system volume and weight [19]. Secondly, the Kalina cycle has a better thermodynamic performance [20]. Trilateral flash cycles deliver power by flash expansion of pressurized boiling water, and have smaller thermal efficiencies than organic Rankine cycles at the same maximum and minimum cycle temperatures, but are still in a state of technical development [21]. Even though the power output for the Kalina cycle is 3% [23] more than the organic Rankine cycle, the Kalina cycle has greater cycle complexity and higher capital outlay [22]. Also this small gain in performance requires a complicated plant scheme, large surface heat exchangers and particular high pressure resistant and no corrosion materials [24]. The organic Rankine cycle is the most mature and tested technology when compared to Kalina cycles and thermoelectric generators [22].

Johansson and Söderström [15] reviewed thermodynamic cycles for converting waste heat into electricity using thermoelectric generators, organic Rankine cycles and phase change materials with respect to temperature range of the heat source, conversion efficiency; the organic Rankine cycles has a higher conversion efficiency and longer technical life. Bianchi and De Pascale [25] also compared the electric efficiency of thermoelectric generators, Organic Rankine cycles, Stirling engines and inverted Brayton cycles, and the ORC has the highest efficiency and is suitable for power generation from 30 kW to 20 MW. Therefore the present work considers Organic Rankine cycles because they are mature and commercially available in sizes from 30 kW – 20 MW, and industrial demonstration projects also exist. The methodology developed can be applied to other thermodynamic cycles producing electricity from waste heat.

Examples of technologies for chilling provision from waste heat are adsorption chillers and absorption chillers (AbC). In adsorption chillers, solids with large superficial area and porosity capable of adsorbing large quantities of refrigerant bring about chilling [26]. Waste heat liberates the adsorbed refrigerant and the most common adsorbent refrigerant pairs are silica gel/water and zeolite/water [26]. Although a promising technology for chilling generation using waste heat, work still needs to be done on possible implementation in commercial and industrial applications [27]. Absorption chillers are thermally activated cooling technologies i.e. a heat source is used to provide chilling. The heat source provides energy to desorb the absorption liquid which is then condensed, flows through an expansion valve to the evaporator, where it is evaporated, producing a refrigeration effect [28]. Absorption chillers have a higher chilling per unit heat input compared to adsorption chillers [26].

Absorption chillers are recommended for use in processes with available low temperature waste heat and cooling requirements, in order to increase the overall efficiency [29]. Compared to adsorption chillers, absorption chillers are more suitable for low temperature waste heat since they can be operated continuously and not intermittently; they are also mature and further developed [30]. Therefore in this work absorption chillers are selected for chilling provision from waste heat. The most common refrigerant–absorbent pairs are water-lithium bromide and ammonia-water. The ammonia-water system has a lower COP [31] and requires a rectifier to remove water vapour from ammonia vapour [30]; however, water-lithium bromide systems are more susceptible to crystallization [32]. Due to the high latent heat of vaporisation of water they perform better than the ammonia-water system but can only operate above 0 °C [28]. Water-lithium bromide systems have been identified as the most successful working fluid for an absorption system [33] and are adopted in this work.

Waste heat can be upgraded to a higher temperature using absorption heat pumps (AHP) where the evaporation, expansion and condensation of the working fluid are similar with a conventional compressor driven system. The difference is the circuit of a liquid absorbent circulating by a pump which replaces the compressor [34]. They have enormous potential for primary energy savings in both domestic and industrial applications, and are commercially available [35]. Water-lithium bromide systems have been identified as the most successful working fluid for an absorption system [33] and are adopted in this work.

There are numerous examples of using absorption heat pumps for waste heat recovery in literature. In Backstrom [36], saturated steam at 150 °C is used to drive four absorption heat pumps using low temperature condensate in the evaporator, Eisa et al. [37] presents' possible combinations of operating temperatures, salt concentration and related thermodynamic data for this technology. Tufano [38], used absorption heat pumps for heat recovery in distillation columns, noticeable energy savings are recorded, but the modelling and operation is not adaptable to changes in both heat loads and temperatures. In Wallin and Berntsson [39] a method is proposed for integration of heat pumps in an industrial process using the energy profile i.e. the grand composite curve, where the heat below the pinch is upgraded and used to satisfy the energy demand above the pinch. This method takes into account the temperature enthalpy profile of the heat sources but neglects the possibility of using that heat in another process or considering waste heat sources from the site utility system.

The potential to upgrade waste heat using an absorption heat pump driven by the exhaust of a natural gas boiler is explored in Qu et al. [40]; results show an increase in the boiler efficiency by 5–10%. In their work Absorption Simulation (ABSIM) [41] was used to evaluate working states and system overall efficiency using Engineering Equation Solver (EES) [42], experiments were also conducted to validate the model. Even though the EES allows computation of thermo physical properties of working fluids with good accuracy when compared to experimental results [40], it is not easy to integrate with a variety of energy sources and systems; also modelling of complex processes is tedious and susceptible to user errors [29]. To this end, Kohlenbach and Ziegler [43] developed a dynamic model based on external and internal steady-state enthalpy balances for each component; however, the modelling lacks adaptability to varying heat input from different sources, and is difficult to integrate with existing models of utility systems. Somers et al. [29] also modelled absorption systems in Aspen Plus [44], which is a more user friendly simulation tool and compared results with the EES property routines as well as experimental data provided in Liao [45]. The results had good agreement with error less than 3%.

Aspen Plus allows for expandability into large process models but may be difficult to integrate with optimisation solvers; therefore it is necessary to develop performance models for absorption chillers and heat pumps that can be integrated with large process models and optimisation models. Various characteristics of absorption cycles can be described by simple explicit equations of physical design parameters [46], the design parameter can be fitted with original numerical data from rigorous simulations in Aspen Plus. In the work of Qu et al. [40] and Somers et al. [29], design for only a single temperature heat source is considered.

The potential for using absorption chillers to provide chilling to improve the power generation efficiency of a gas turbine, by reducing the compressor inlet air temperature is explored in Popli et al. [47], the absorption chiller is modelled using the Engineering Equation Solver. However, the model is applicable for a single heat source and difficult to integrate with existing process simulation and optimisation software's. Kalinowski et al. [48] compared the use of an absorption refrigeration system driven by waste heat to a propane chiller for LNG recovery process, for the case the absorption refrigeration system was more efficient than the propane chiller but modelling was done for a single heat source.

The potential for power generation from available waste heat in a gas turbine exhaust is explored in Pierobon et al. [49] and for a diesel engine exhaust in Hajabdollahi et al. [50], only a single source of heat is considered, and the organic Rankine cycle is modelled based on equation based models tailored for this specific application; solving may require an iterative process which results in complications when applied to multiple heat sources over a wide temperature range. In the work of Quoilin et al. [51] a thermodynamic optimisation model for an organic Rankine cycle is developed to compare the performance of several working fluids by changing the systems evaporating temperature. The possibility of integrating the system into a process site was not considered as the temperature of the available waste heat might determine the operating conditions of the organic Rankine cycle. In Khatita et al. [52], an ORC was integrated into an existing gas treatment plant, working fluid selection is considered as well as the cycle optimum operating conditions based on the net power produced, efficiency, volumetric flow rate and irreversibility; however, analysis is done for a single heat source. Hung et al. [53] also reviewed organic Rankine cycles for waste heat recovery but the work was focused on working fluid selection and not integration into a process site.

To understand the effect of changing heat inputs and sources in an organic Rankine cycle, Auld et al. [54] introduced a method of pinch point analysis to model the ORC over a wide range of operating conditions using different working fluids for multiple heat sources. The heat sources were LP steam from an industrial plant utility system, hot brines from wells and waste heat available from internal combustion engines. Again only one heat source from an industrial plant is considered. He concluded that optimising the cycle for thermal efficiency may not be the best strategy; however, it may be possible to optimise the cycle for both thermal efficiency and waste heat exploitation on process sites. Desai and Bandyopadhyay [55] developed a methodology for integrating an ORC with a background process using the heat rejection profile of the background process. The choice of cycle configuration for appropriate integration depends on the heat rejection profile of the background process. This strategy considers the waste heat available in a single process, but it neglects the possibility of using this heat for another process and the heat available from a site utility system.

There are different configurations of Organic Rankine cycles such as superheated cycles, supercritical cycles, ORC with internal heat exchange, ORC with reheating, ORC with integrated feed liquid heaters, binary fluid ORC. Previously the system architecture has been determined to improve the system efficiency [56], and not to exploit the waste heat available efficiently, therefore in this work simple cycles are considered first and in the future, the choice of system architecture will be determined using the heat source temperature profile. Choice of working fluid will also be considered taking into account the temperature of the available heat sources

Most applications of waste heat recovery technologies such as organic Rankine cycles, absorption chillers and absorption heat pumps are focused on determining the system's operating point, working fluid selection without knowledge of the heat sources, modelling the technologies for a single heat source, and using models that cannot be integrated with a process flow sheet. However, in the context of process sites and considering multiple sources of heat, the potential for work generation is analysed in Bendig et al. [10] using exergy analysis to evaluate the maximum extractable electrical power from waste heat rejected from a process. The potential for work generation is a theoretical maximum that disregards the efficiency of the technologies as well as other useful forms of energy, such as cooling, that can be derived from waste heat. Also, waste heat available from the site utility system was not considered.

In the work of Kapil et al. [57] the potential to generate work, heat and chilling is evaluated using the heat available from processes on a site. In their work, the waste heat sources are collected at a single temperature, and heat rejected from the site utility system is not included, thus interactions between the utility system and the site processes are neglected. Also in the work of Kwak et al. [58], only waste heat available from processes on a site is considered. Furthermore the available waste heat is assumed to be at a single temperature. The potential for power generation using an ORC, thermo electric generator and phase change material was analysed in Johansson and Söderström [15], only waste heat from a single process is considered. A complete analysis for waste heat recovery should consider various sources of waste heat at various temperatures from site processes and the site utility system. In order to consider these diverse sources, a systematic way needs to be developed to represent the sources in quantity and temperature.

The aim of this paper is to evaluate the potential in industrial waste heat by developing a systematic way to represent the waste heat available in existing process sites and evaluate the potential for generation of power, chilling and heat from the available waste heat. Mature and commercialised technologies using waste heat as the primary energy input will be considered. They include Organic Rankine cycles, absorption chillers and absorption heat pumps. Models of these technologies are provided in order to evaluate how much useful energy can be recovered from waste heat in process sites.

2. Site energy efficiency

Energy flows in a site process can be represented using Fig. 1, process demand for steam at different pressure levels is satisfied by the cogeneration system; demand for high temperature heating satisfied by the fired heaters; site refrigeration requirements satisfied by the refrigeration system and site power demand satisfied by the cogeneration system or power can be imported into a site. The residual heat from the site processes and the site utility system is rejected to cooling water and air. The cogeneration efficiency i.e. the fraction of the energy in fuel consumed producing useful heat and power, has been used to evaluate the performance of a cogeneration system [6,7]. When considering waste heat recovery in process sites, this indicator is inadequate as it does not consider energy flows in other systems, such as refrigeration cycles and fired heaters. In this work, the concept of the energy efficiency of a site defined as the fraction of the total energy inputs (from fuel combustion, process steam generation, power imports, etc.) converted into useful energy consumed i.e. heat, power and cooling required by the site processes is introduced.

A mathematical expression shown in Eq. (1). The site energy efficiency captures interactions between the utility systems on a site, as shown in Fig. 1. Even though the site energy efficiency can be used to determine how much of the input energy is wasted it does not show how much is recoverable. The characteristics of the waste heat sources, available heat recovery technologies, and operational

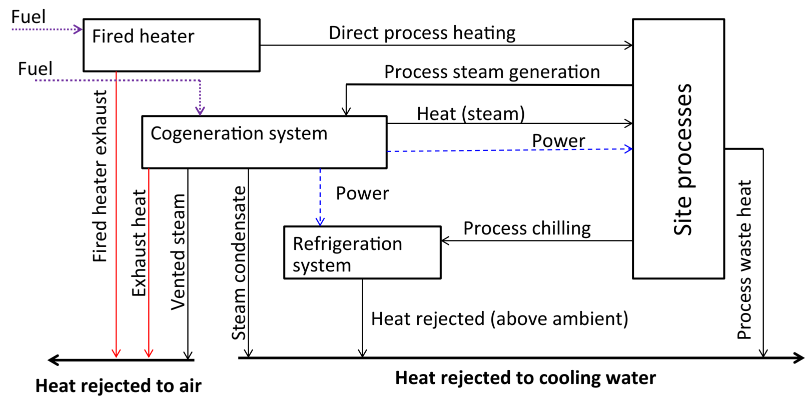

Fig. 1. Energy flows in a process site.

limits of these technologies and physical limitations of a site dictate what waste heat it is feasible to recover. Also, the site energy efficiency does not show the temperature and duties of the sources of recoverable i.e. available waste heat, therefore there is need to develop a temperature-enthalpy plot of the available waste heat sources. In this work the site energy efficiency is used to determine how much heat is wasted and to evaluate the impact of integrating waste heat recovery technologies within process sites.

$$\text{Site Energy Efficiency} = \frac{\text{Total Useful Energy Consumed}}{\text{Total Energy Input}} \quad (1)$$

3. Waste heat source profile

The energy profiles for a process have been represented using composite curves [4]; in Linnhoff and Hindmarsh [5] the total site profile is introduced to represent energy profiles for several processes on a site. The composite curves and the site profiles show the potential for heat recovery within a process and between processes on a site respectively [7]. These concepts can be extended to represent the waste heat sources in process sites.

To create a waste heat source profile, first, data related to the waste heat rejected from the site processes and the site utility systems are extracted. The duties of the sources, as well as the supply and target temperatures are extracted. The target temperature is determined to account for operational limits of waste heat recovery technologies and physical limitations of a site such as the stack temperature for fired heaters to avoid corrosion. The waste heat source profile is generated by plotting the heat source temperature (shifted by an appropriate minimum temperature difference, $\Delta T_{\min}$, to allow for feasible heat transfer) against the net duties of the waste heat sources. For design purposes, two waste heat source profiles can be generated: a profile for waste heat rejected to cooling water and waste heat rejected to air. The waste heat source profile allows evaluation of the potential for waste heat recovery in existing process sites since it shows the temperatures and duties of the waste heat sources.

To evaluate the potential of a process site for waste heat recovery, appropriate waste heat recovery technologies can be identified considering the temperature range at which the technology can exploit the waste heat and assigned against the profile using the heat recovery temperature.

The heat recovery temperature is determined in two stages, first preliminary recovery temperatures are determined corresponding to the kinks on the profile as they represent the beginning or end of a stream, using the kinks as the preliminary heat recovery temperature also ensures high temperature waste heat can be explored before low temperature waste heat i.e. hot streams are kept hot. The final heat recovery temperature is then determined by selecting the preliminary heat recovery temperature where the useful energy recovered is highest for a particular form of energy (heating, cooling or power).

3.1. Illustration for waste heat source profile

The data extracted for heat rejected to cooling water from a site are shown in Table 1; temperatures are shifted by a minimum temperature difference to allow for feasible heat recovery between the heat sources and the recovery technologies. T_s^* and T_t^* represent the shifted supply and target temperatures. For this analysis 10 °C is assumed as the minimum temperature difference.

The generated waste heat source profile is shown in Fig. 2(a). Fig. 2(b) shows the kinks on the profile used as preliminary heat recovery temperatures. The final heat recovery temperatures will be determined to maximise the useful energy recovered.

4. Mathematical modelling of waste heat recovery technologies

Waste heat recovery technologies can be modelled rigorously using process simulation software such as Aspen HYSYS [59], Aspen Plus [29], and equation oriented tools such as the Engineering Equation solver [40]. However, simple models suitable for evaluation of multiple heat sources, and are easy to integrate with optimisation frameworks for utility system need to be developed. Such models show the relationship between key variables to evaluate the useful energy recovered. In this work, established mathematical models and new models are proposed for a basic organic Rankine cycle, absorption chiller and absorption heat pump. Future work will involve complex configurations tailor made to suit the process waste heat conditions.

4.1. Organic Rankine cycle (ORC)

An ORC produces shaft power from low to medium temperature heat sources (50–220 °C, [2]) using pure and mixed organic fluids [9]. A schematic of a basic cycle is shown in Fig. 3, where expansion of a vaporised working fluid using waste heat produces power.

Table 1
Extracted waste heat sources data for illustration.

Stream name	T_s (°C)	T_t (°C)	ΔH (kW)	T_s^* (°C)	T_t^* (°C)
Stream 1	165	150	10,000	155	140
Stream 2	170	99.9	5000	160	89.9
Stream 3	99.9	50	15,000	89.9	40
Stream 4	150	40	7500	140	10

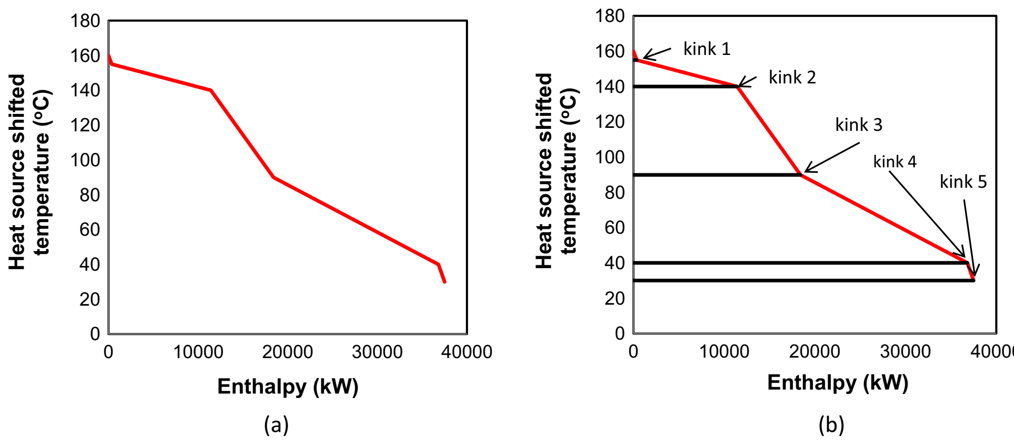

Fig. 2. (a) Waste heat profile for illustration, (b) heat source profile showing preliminary heat recovery temperatures.

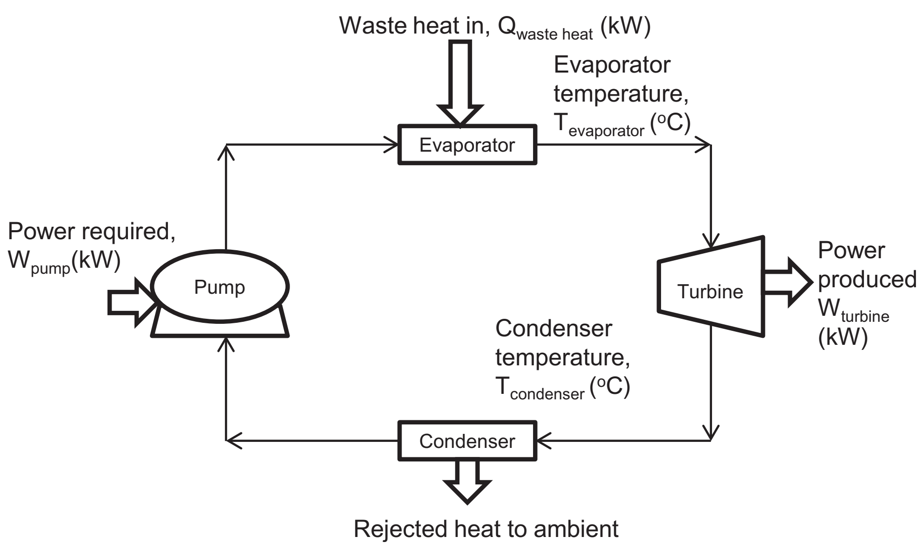

Fig. 3. Organic Rankine Cycle schematic.

Efficiency (η) of an ORC is defined as the fraction of power (W) produced from heat as shown in Eq. (2). The ideal performance is expressed using the Carnot factor in Eq. (3), relating this to the real efficiency in Eq. (4) and a factor accounting for inefficiencies in the system components (the condenser, evaporator, pump and turbine). This factor can be correlated with the ideal efficiency for a pure working fluid Eq. (5) or an organic mixture Eq. (6) by regression against the results of rigorous simulations or manufacturers data. The constants α, β, γ represent the non-ideal behaviour of the working fluid and the cycle's components inefficiencies and are evaluated by regressing the model against rigorous simulation in Aspen HYSYS [59] where the physical properties of the working fluids are calculated using Peng Robinson equation of state.

Analysis was done for steady state condition and model assumptions are outlined below;

1. Saturated vapour in evaporator
2. Saturated liquid in condenser with a condensing temperature of 30 °C
3. The evaporator temperature is between the boiling point and critical temperature of the working fluids
4. Negligible pressure drop in condenser and evaporator
5. Turbine and pump adiabatic efficiency at 75%
6. Minimum temperature difference assumed to be 10 °C

The values of α, β, γ depend on the working fluid (Table 2.). Model validation for a pure working fluid (benzene) is shown in Fig. 4a and a mixed fluid (methanol and water) in Fig. 4b, average errors of 0.46% and 0.12% for the pure and mixed fluids respectively were obtained.

$$\eta_{real} = \frac{W_{turbine} - W_{pump}}{Q_{waste\ heat}} \tag{2}$$

$$\eta_{ideal} = 1 - \frac{T_{condenser}}{T_{evaporator}} \tag{3}$$

$$\eta_{real} = Factor_{ORC}.\eta_{ideal} \tag{4}$$

$$Factor_{ORC} = \alpha.\eta_{ideal} + \beta \tag{5}$$

$$Factor_{ORC} = \alpha.\eta_{ideal}^2 + \beta.\eta_{ideal} + \gamma \tag{6}$$

The performance of organic rankine cycles strongly depends on the working fluid selected [60]. Working fluids should fulfil safety criteria, be environmentally friendly and allow for low cost for the power plant [61].

4.2. Working fluid selection for Organic Rankine cycles

Working fluids for organic Rankine cycles are classified into three groups based on the shape of the saturated vapour line in

Table 2
Selected working fluids for organic Rankine cycle application.

Working fluid	Chemical formula	$T_{critical}$ (°C)	$P_{critical}$ (MPa)	Boiling point (°C)	α	β	$T_{evaporator}$ (°C) range
Cyclopentane	C_5H_{10}	238.4	4.257	48.78	−0.5979	0.7622	48.78–238
n-Pentane	C_5H_{12}	196.6	3.370	36.10	−0.7625	0.7497	36.10–196
n-Hexane	C_6H_{14}	234.7	3.034	68.70	−0.7402	0.7506	70–200
Isobutane	C_4H_{10}	134.7	3.640	−11.70	−0.9648	0.7436	30–134
Isopentane	C_5H_{12}	187.2	3.396	27.80	−0.7965	0.748	31–187
Propane	C_3H_8	96.75	4.257	−42.15	−1.3267	0.7322	31–95
Benzene	C_6H_6	288.9	4.894	80.10	−0.5085	0.7663	81–270
Toluene	C_7H_8	318.6	4.126	110.60	−0.5507	0.775	111–300
R113	$C_2Cl_3F_3$	214.1	3.392	47.60	−0.7006	0.7475	48–195
R114	ClF_2CCF_2Cl	145.9	3.261	3.57	−0.8867	0.7428	50–120
R134a	$C_2H_2F_4$	101	4.055	−26.13	−1.2582	0.7451	31–90

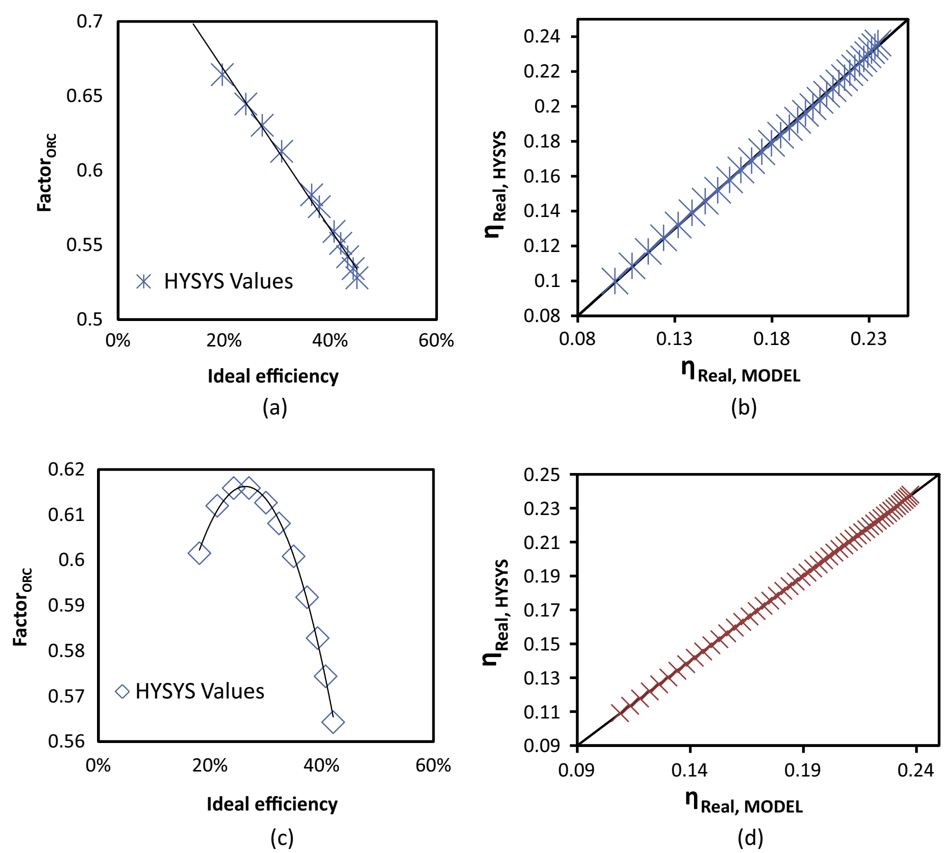

Fig. 4. Validation of ORC model (a–b) single working fluid, (c–d) mixed fluid (methanol/water).

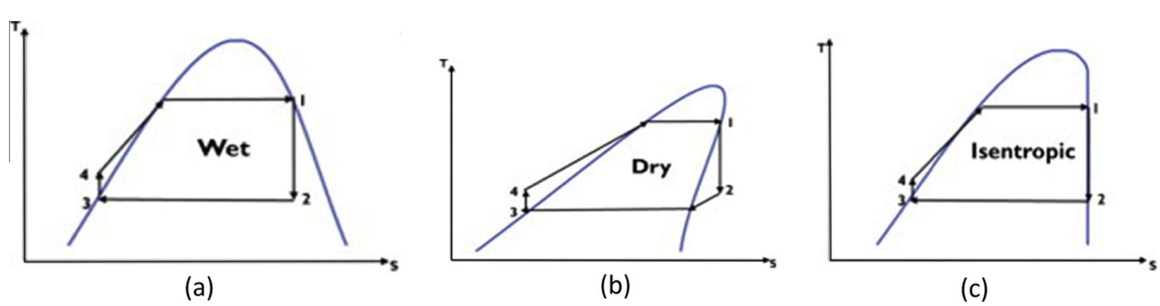

Fig. 5. T-s diagram for ORC working fluids (Kwak et al. [62]) (a) wet fluids, (b) dry fluids and (c) isentropic fluids.

the temperature entropy diagram [61], this affects the condition of steam after expansion in the turbine. There are three different working fluid groups: wet, dry and isentropic fluids. Wet fluids have a negative slope and are wet after expansion (Fig. 5a). In Liu et al. [63] wet fluids were regarded as inappropriate for low temperature organic Rankine cycle applications as mechanical damage from wearing of the turbine blades could occur. Dry fluids are dry after expansion as they have a positive gradient (Fig. 5b).

Achieving superheated vapour at the turbine inlet always gives a higher thermal efficiency. Isentropic fluids have an infinite gradient (Fig. 5c).

The choice of working fluid depends on the temperature of the heat sources, cooling medium temperature and criterion employed to assess ORC performance [60]. The impact of working fluid selection has been highlighted by numerous authors [61,65,64] and [65]. In Saleh et al. [61], 31 potential pure component working fluids are evaluated based on the cycle efficiency for low temperature (below 100 °C) organic rankine cycles. The highest efficiency values are obtained for high boiling substances that are dry. Liu et al. [63] also analysed some wet, isentropic and dry fluid using the heat recovery efficiency. The choice of working fluids depends on the temperature range of heat sources; and the screening criteria are important to working fluid selection [64] hence there is no single winner. In this work potential dry, wet and isentropic fluids investigated from various previous studies are reviewed (Table 2). The screening criteria used is the system's efficiency in Eq. (4) as the objective is to reduce the inefficiencies accompanying the energy conversion process.

The choice of fluids depends on the heat source temperature, the fluids selected to maximise electricity generation from waste heat using an organic Rankine cycle are benzene (above the boiling point of benzene) and cyclopentane (below the boiling point of benzene).

Mixed organics may be more efficient than some pure component fluid due to the non-isothermal evaporation and condensation in the cycle leading to lower temperature differences in the evaporator, higher efficiencies and higher surface areas. In Victor et al. [66] an optimisation model is applied to determine the composition of mixed working fluids for organic Rankine cycles with an objective to maximise thermal efficiency. A novel alcohol –water mixture (methanol/water) is proposed which is more efficient at high temperatures compared to some pure component organic fluids. The steam condition after expansion in the turbine was not taken into account. In this work the methanol/water mixture is compared with Benzene and cyclopentane, taking into account the dryness fraction of the mixture after expansion in the turbine. Different compositions of methanol/water are considered and the cycle efficiency compared with pure fluids selected from Fig. 6. The parameters α, β and γ in Eq. (6) are shown for different methanol compositions in Table 3.

The higher the concentration of methanol the lower the cycle efficiency compared to other pure working fluids (Fig. 7). However, the dryness fraction reduces with efficiency as shown in Fig. 8a below (for methanol mass fraction of 0.1). Prolonged usage could lead to mechanical damage of the turbine blades. Whereas for Benzene the condition after expansion is always dry (Fig. 8b).

To decrease the wetness, the working fluid can be superheated in the evaporator. Analysis of working fluids in superheated

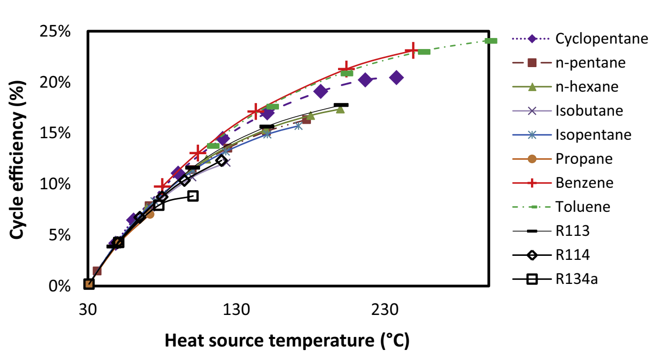

Fig. 6. Screening of pure working fluids using the cycle efficiency.

Table 3
Values of α, β and γ for methanol water mixture.

Methanol composition (mass fraction)	α	β	γ
0.1	−0.4826	−0.0059	0.7130
0.2	−0.7197	0.1883	0.6657
0.3	−1.0523	0.4428	0.6038
0.4	−1.4044	0.7009	0.5448
0.5	−1.7424	0.9291	0.4975
0.6	−1.8624	1.0011	0.4812
0.7	−1.9998	1.0485	0.4787
0.8	−2.1230	1.0412	0.4958
0.9	−2.2887	0.9914	0.5337

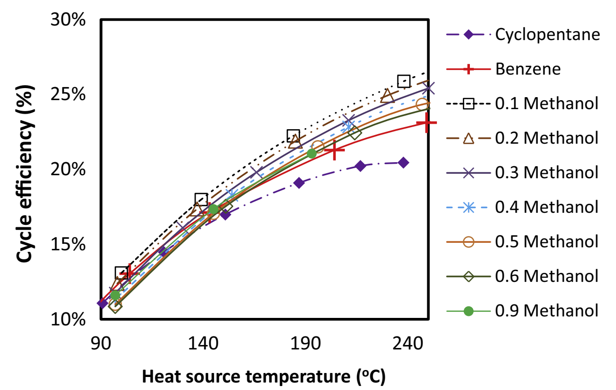

Fig. 7. Screening of methanol/water mixture, benzene and cyclopentane.

methanol/water cycles is shown in Fig. 9. The efficiency reduces compared to Benzene and cyclopentane and increases after 205 °C for cyclopentane and 230 °C for benzene. However, even with 60 °C superheat the condition of steam is still wet (Fig. 10). Therefore in this work, benzene and cyclopentane are selected as working fluids because of their high waste heat to electricity conversion efficiency, dryness of steam after expansion, low global warming and ozone depletion potential.

4.3. Absorption Chillers (AbC)

Chilling is provided by vaporising the refrigerant in the evaporator which is then absorbed in the absorber, and pumped to a higher pressure before separation takes place in the generator using waste heat. The rich absorbent is sent back to the absorber while the pure refrigerant is condensed in the condenser, enters the valve and the cycle repeats. The system has two working fluids: an absorbent and a refrigerant. A single-effect absorption chiller has four main components the generator, absorber, condenser and evaporator [67] (Fig. 11). The ideal coefficient of performance (COP) is the product of the ideal efficiency of a turbine operating between the generator and absorber temperatures and a vapour compression heat pump operating between the sink (evaporator) and source (condensing) temperatures [68] as shown in Eq. (7).

The calculations were performed based on the following assumptions:

1. The refrigerant in the condenser is saturated liquid at 30 °C.
2. At the evaporator outlet, the refrigerant is a saturated vapour.
3. Pressure drops in pipes and other components are negligible.
4. All components are externally adiabatic.

Validation of the model using lithium bromide/water as the fluid pair is shown in Fig. 12. The generator temperature is

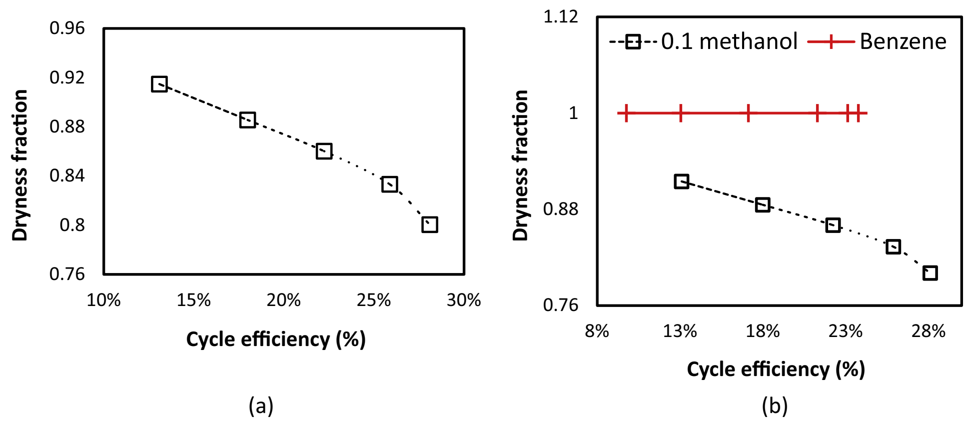

Fig. 8. Dryness fraction versus cycle efficiency (a) Methanol/water mixture and (b) Benzene and methanol/water mixture.

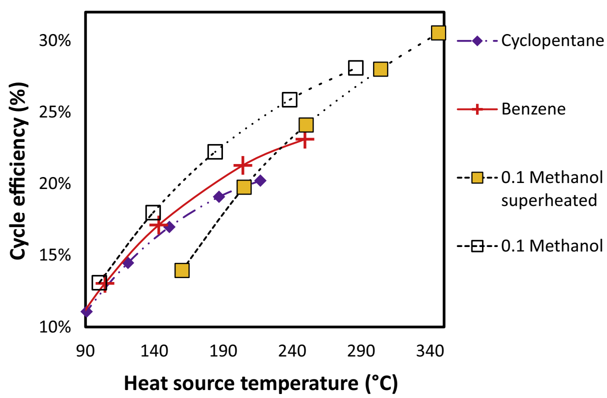

Fig. 9. Cycle efficiency for superheated methanol/ water mixture compared with benzene and cyclopentane.

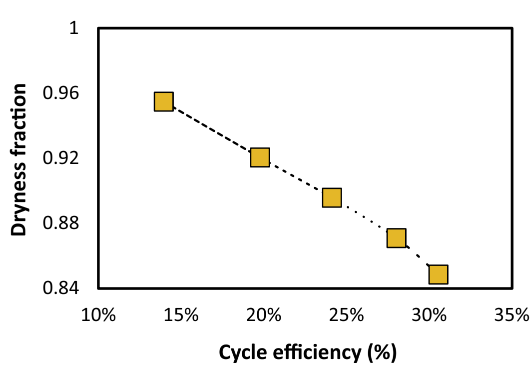

Fig. 10. Dryness fraction for superheated cycle using methanol/water.

determined from the system saturation pressure set to prevent the working fluid from crystallizing [69]. Values of *a* and *b* for lithium bromide absorption chillers are −0.5672 and 1.0049 respectively for producing chilling between 0 and 25 °C driven by 89.9 °C waste heat and rejecting heat at 30 °C in the condenser.

$$\mathrm{COP_{AbC,ideal}} = \left(1 - \frac{\mathrm{T_{condenser}}}{\mathrm{T_{generator}}}\right)\left(\frac{\mathrm{T_{evaporator}}}{\mathrm{T_{condenser}} - \mathrm{T_{evaporator}}}\right) \tag{7}$$

$$\mathrm{COP_{AbC,real}} = \frac{\mathrm{Q_{evaporator}}}{\mathrm{Q_{waste\ heat}} + \mathrm{W_{pump}}} \tag{8}$$

$$\mathrm{COP_{AbC,real}} = \mathrm{factor_{AbC}.COP_{AbC,ideal}} \tag{9}$$

$$\mathrm{COP_{AbC,real}} = \mathrm{a.(factor_{AbC}) + b} \tag{10}$$

4.4. Absorption Heat Pumps (AHP)

Heat pumps can be driven by electrical power or thermally driven, as in absorption heat pumps. Absorption heat pumps are identical to absorption chillers; however, the objective of a heat pump is to recover heat from the absorber and condenser [68] (Fig. 13). The ideal coefficient of performance is estimated using by Eq. (11) [68] and the real COP is expressed in form of energy flows in the condenser, absorber, generator and pump as shown in Eq. (12). To evaluate the real COP in terms of the system temperatures, Eqs. (13) and (14) are solved simultaneously. The factor in Eq. (14) accounts for inefficiencies in the system components the working fluid non-ideal behaviour. Parameters *c* and *d* can be regressed from rigorous simulations or from manufacturer data. In this work the parameters were determined from rigorous simulation of an absorption chiller in Aspen Plus [44]. The cycles operating temperature and pressure were determined using the equilibrium chart for lithium bromide solution shown in Appendix A.

The simulation was performed based on the below assumptions:

1. System is in steady flow.
2. Solutions leaving the generator and absorber are saturated.
3. Refrigerant leaving the evaporator is saturated vapour.
4. Refrigerant leaving the condenser is saturated liquid.
5. The solutions leaving the generator and absorber are both saturated.
6. The throttling in expansion valves are isenthalpic processes.
7. Pressure losses in pipes and components are ignored.

Validation of the model is shown in Fig. 14 using a Lithium Bromide/water mixture. The generator temperature is determined from the system saturation pressure set to prevent the working fluid from crystallizing [69]. Values of *c* and *d* obtained for an absorption heat pump producing hot water below 80 °C using waste heat above 140 °C, and upgrading heat below 60 °C are −0.0351 and 1.7818 respectively (Fig. 14).

$$\mathrm{COP_{AHP,ideal}} = 1 + \left(1 - \frac{\mathrm{T_{condenser}}}{\mathrm{T_{generator}}}\right)\left(\frac{\mathrm{T_{evaporator}}}{\mathrm{T_{condenser}} - \mathrm{T_{evaporator}}}\right) \tag{11}$$

$$\mathrm{COP_{AHP,real}} = \frac{\mathrm{Q_{Absorber}} + \mathrm{Q_{condenser}}}{\mathrm{Q_{waste\ heat}} + \mathrm{W_{pump}}} \tag{12}$$

$$\mathrm{COP_{AHP,real}} = \mathrm{factor_{AHP}.COP_{AHP,ideal}} \tag{13}$$

$$\mathrm{COP_{AHP,real}} = \mathrm{d.(factor_{AHP}) + c} \tag{14}$$

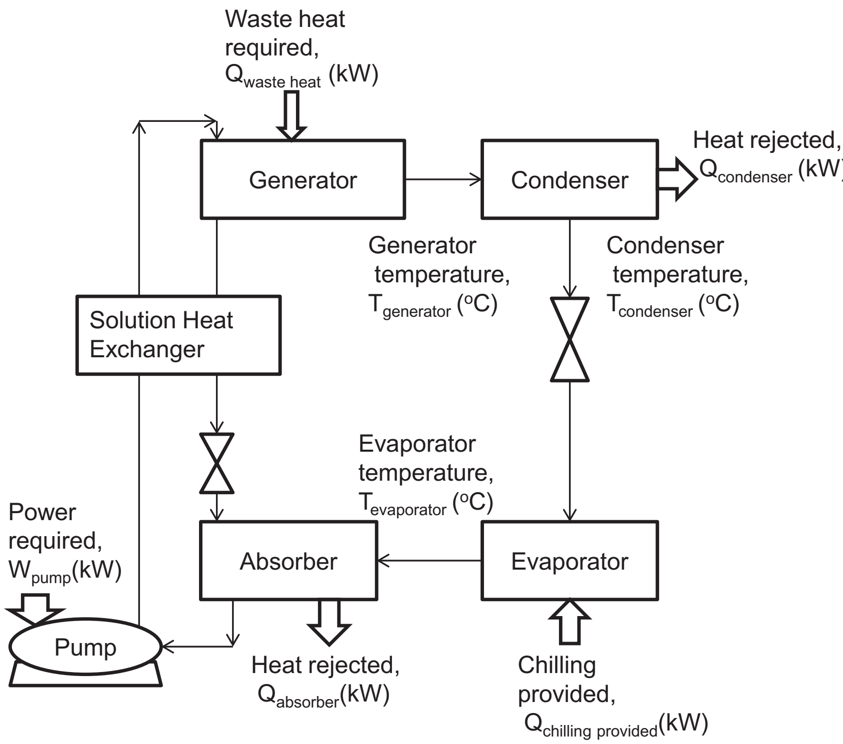

Fig. 11. Absorption chiller schematic.

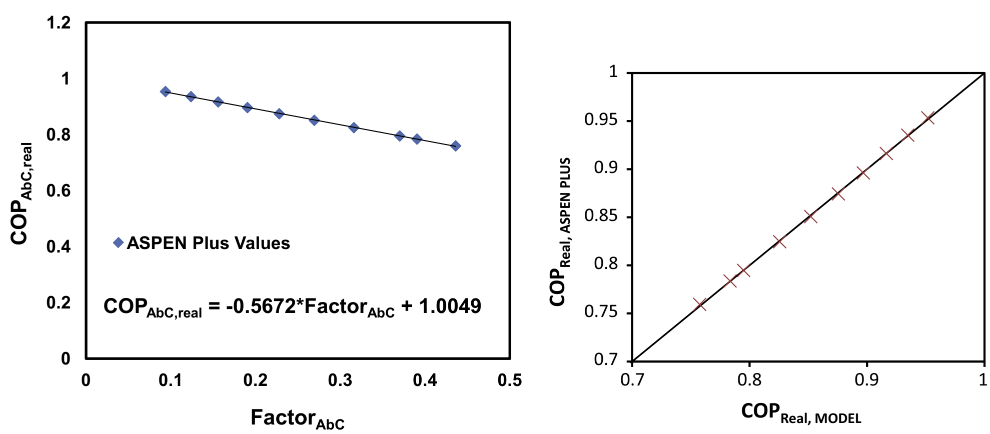

Fig. 12. Validation of absorption chiller model (a) equation of fit and (b) comparison with Aspen Plus model.

5. Methodology

The methodology presented in this paper is focused on

(1) Generating the waste heat source profiles for a site;
(2) Using the kinks on the profiles as the preliminary heat recovery temperature (PHRT);
(3) Assigning recovery technologies against the profile (at the kinks);
(4) Using the simplified models to estimate the quantity of useful energy in the form of power, chilling and heating for every preliminary heat recovery temperature;
(5) Determining the final heat recovery temperatures by selecting the preliminary temperatures corresponding with the highest useful energy recovered, and
(6) Evaluating the waste heat recovery impact on a site by estimating the site energy efficiency before and after generating useful energy from the available waste heat.

A summary of the methodology is shown in Fig. 15.

The methodology is applicable for single forms of recovered energy and multiple forms of recovered energy. In the case where multiple technologies can be used, the final heat recovery temperature for each form of recovered energy is determined to maximise useful energy recovery i.e. the preliminary heat recovery temperature where each technology maximises the useful energy recovered and the site energy efficiency.

5.1. Illustration of methodology for single form of energy (power generation)

The profiles generated in Section 3.1 can be used to illustrate the application of the methodology for a single form of recovered energy. Fig. 2 shows the waste heat source profile. Only heat sources above 58.78 °C can be recovered based on the boiling point of cyclopentane in Table 2 and a minimum temperature difference of 10 °C.

The available waste heat profile is shown again in Fig. 16. Table 4 shows the cumulative heat at the preliminary heat recovery temperatures (used as the kinks on the profile). Using the preliminary heat recovery temperatures, the power generated is also shown in Table 4 and the values compared with Aspen HYSYS [59] results.

The power generated plotted against the preliminary heat recovery temperature is shown in Fig. 17.

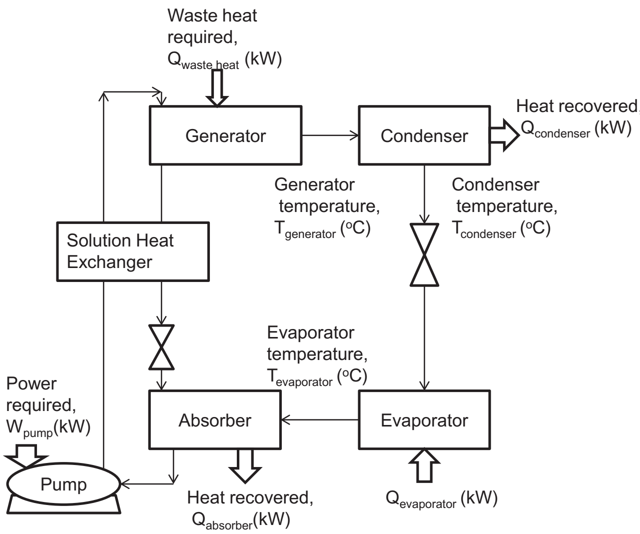

Fig. 13. Absorption heat pump schematic.

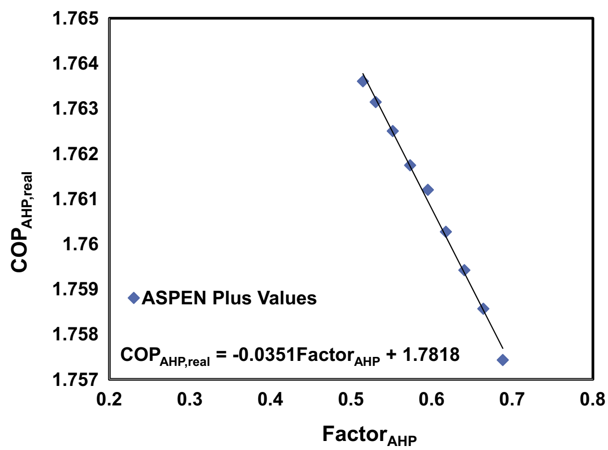

Fig. 14. Validation of absorption heat pump model.

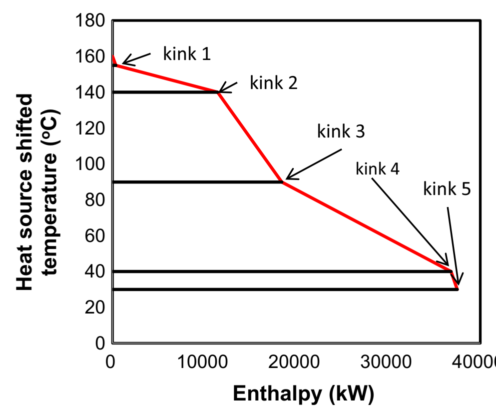

Fig. 16. Recoverable waste heat source profile showing the kinks.

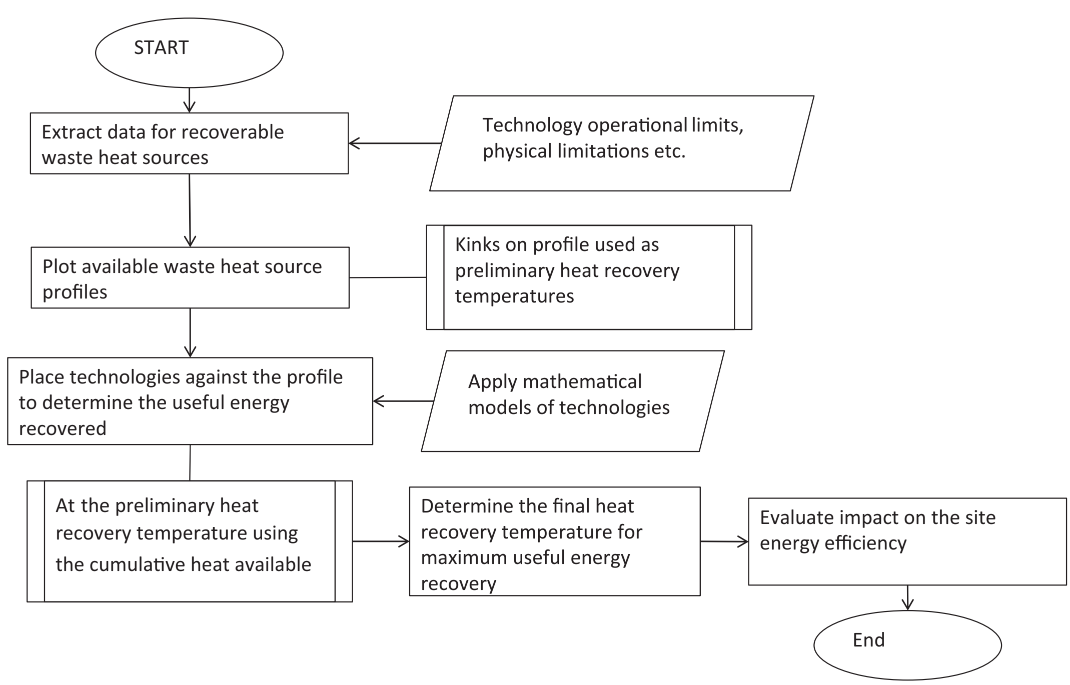

Fig. 15. Methodology flow sheet.

Table 4
Cumulative heat available, working fluid selected and power generated at preliminary heat recovery temperatures.

Preliminary heat recovery temperature (°C)	Cumulative heat available (kW)	Working fluid selected	Power generated (Model)	Power generated (Aspen HYSYS [59])	Error (%)
155	360	Benzene	64.3300	64.6612	0.51
140	11,430	Benzene	1919.41	1921.95	0.13
89.9	18,420	Benzene	2073.45	2065.50	0.39
48.8	33,600	Cyclopentane	1425.82	1413.42	0.88

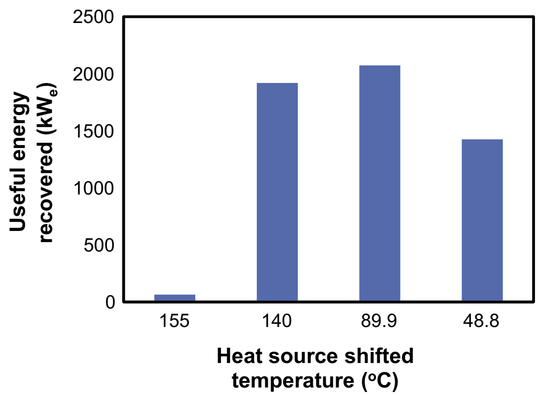

Fig. 17. Power generated at the PHRT.

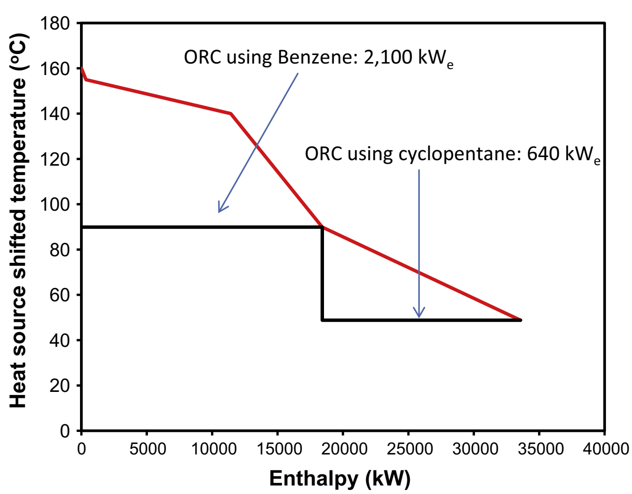

Fig. 18. Placement of an ORC against the heat source profile.

Therefore to maximise the useful energy recovered the final heat recovery temperatures are 89.9 and 48.8 °C. Placements of an organic rankine cycles against the heat source profile using the saturation temperature are shown in Fig. 18.

Two organic rankine cycles are required to maximise the useful energy recovered from the waste heat sources by exploiting both the quality and quantity of the recoverable waste heat.

6. Case study for a refinery

The case study presented is for a medium scale petroleum refinery with seven processing units: crude distillation unit, three hydrotreaters (for naphtha, kerosene and diesel), a platformer, a visbreaker and a fluidised catalytic cracking unit [70]. The site profiles showing the potential for heat recovery between the seven processes, potential for steam generation, steam use, boiler fuel demand, cooling and refrigeration requirements is shown in Fig. 19.

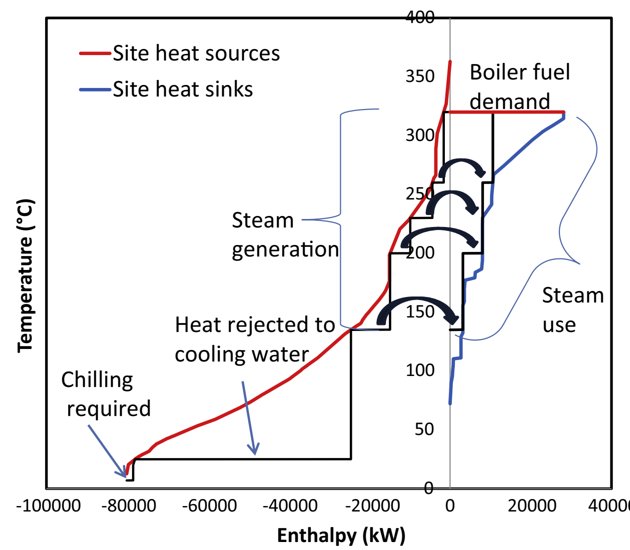

Fig. 19. Refinery total site profile.

Table 5
Steam use, steam generation, cooling and chilling loads.

Steam main	Saturation temperature (°C)	Generated load (kW)	Used load (kW)
VHP	320	1574	17,500
HP	260.07	2800	2530
MP1	230	5500	47
MP	200	5000	4850
LP	135	9700	3170
Cooling water	25.1	55,040	
Refrigeration	7.1	420	

Table 6
Data extracted for heat rejected to air.

Stream	Name	T_{supply} (°C)	T_{target} (°C)	Enthalpy (kW)
1	Crude distillation unit fired heater exhaust	320.1	150	4,440
2	Naphtha hydrotreaters fired heater exhaust	328.4	150	35
3	Platformer fired heater exhaust	320.1	150	1360
4	Coal boiler fired heater exhaust	291.3	150	18,330

Site demand for heating (at different pressure levels), cooling and refrigeration is shown in Table 5. The crude distillation unit, naphtha hydrotreaters and platformer require 62 MW of high temperature heat which is supplied by a fired heater burning coal; site power demand is 50 MW.

Table 7
Data extracted for heat rejected to cooling water.

Stream	Unit	Name	T_{supply} (°C)	T_{target} (°C)	Enthalpy (kW)
1	Crude/vacuum distillation unit	CDUVDU 9	116.8	31.1	5970
2		CDUVDU 5	116.8	50.5	106
3	Diesel hydrotreaters	DHT 3	112.97	26	333
4		DHT 2	112.97	30	1235
5		DHT 1	112.97	34	4540
6	Fluidised catalytic cracking unit	FCCU 3	140.9	37.51	950
7		FCCU 10	140.9	104	220
8		FCCU 10.1	104	51	810
9		FCCU 8	140.9	104	200
10		FCCU 1	140.9	90	1150
11		FCCU 9	104	38	10,700
12		FCCU 4	104	27.61	2783
13	Kerosene hydrotreaters	KHT 2	140.6	30	560
14		KHT 3	136.1	27.2	19.4
15		KHT 4	140.6	33.3	2880
16	Naphtha hydrotreaters	NHT 4	101.7	88.3	331
17		NHT 3	67.2	61.7	560
18		NHT 2	67.2	50	3290
19		NHT 1	67.2	33.9	1914
20	Platformer	PLAT 4	67.2	36.7	1930
21		PLAT 5	73.84	26.7	1160
22		PLAT 7	67.2	32.2	1390
23		PLAT 7.1	73.84	67.2	84.7
24		PLAT 8	67.3	25.7	35.6
25		PLAT 9	67.2	27.2	3020
26		PLAT 10	67.2	32.2	330
27		PLAT 11	43.3	26.3	81.1
28		PLAT 12	73.84	65	16
29		PLAT 13	73.84	32.2	320
30	Visbreaker	VBU 1	134.88	30.01	2050
31		VBU 2	134.88	75	1150
32	Utility system	VHP COND	320	76.32	7900
33		HP COND	260.07	76.32	970
34		MP1 COND	230	76.32	8
35		MP COND	200	76.32	1370
36		COND	90.1	90	131,150

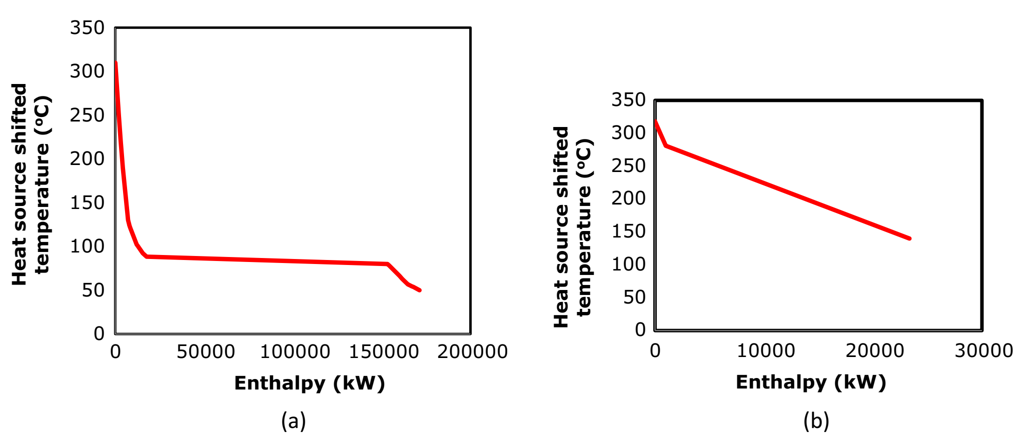

Fig. 20. (a) Profile for heat rejected to cooling water and (b) profile for heat rejected to air.

The site energy (heat and power) demand is satisfied using a cogeneration system comprising of a gas turbine, coal boiler, deaerator, five expansion valves, 4 back pressure turbines and 1 extraction turbine. A vapour compression refrigeration system also exists for chilling, and a cooling water system for above ambient cooling.

Based on the total energy inputs from fuel combustion in the cogeneration system and fired heater, process steam generation, refrigeration and cooling system the site energy efficiency is 50.2%. Of the total energy wasted 11.7% is unrecoverable due to stack restrictions and operational limits of waste heat recovery technologies. Data extracted for recoverable heat from all seven processes and the site utility system is shown in Table 6 (for heat rejected to air) and Table 7 (for heat rejected to cooling water).

The waste heat profiles for heat rejected to cooling water and air are shown in Fig. 20a and b respectively. The kinks on the profile are used as preliminary heat recovery temperatures.

The objective of this case study is to evaluate the potential to generate power, chilling and heat from the available waste heat

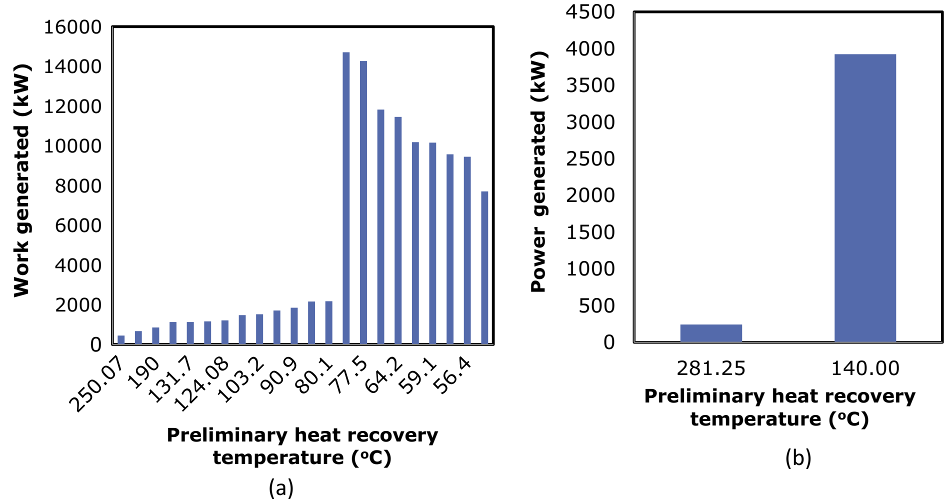

Fig. 21. Power generated at the PHRT's from (a) heat that was rejected to cooling water and (b) heat that was rejected to air.

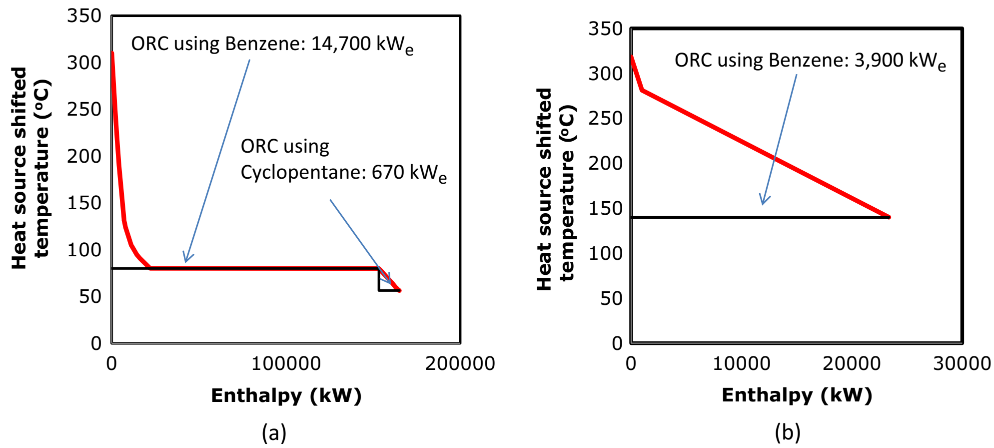

Fig. 22. Placement of ORC against (a) profile for heat that was rejected to cooling water (b) profile for heat that was rejected to air.

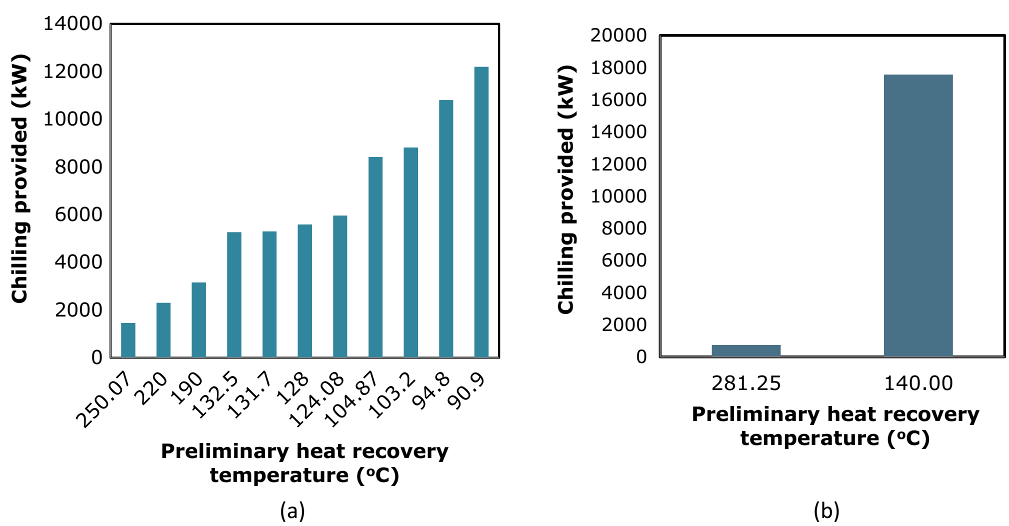

Fig. 23. Chilling provided at every PHRT using (a) profile for heat that was rejected to cooling water and (b) profile for heat that was rejected to air.

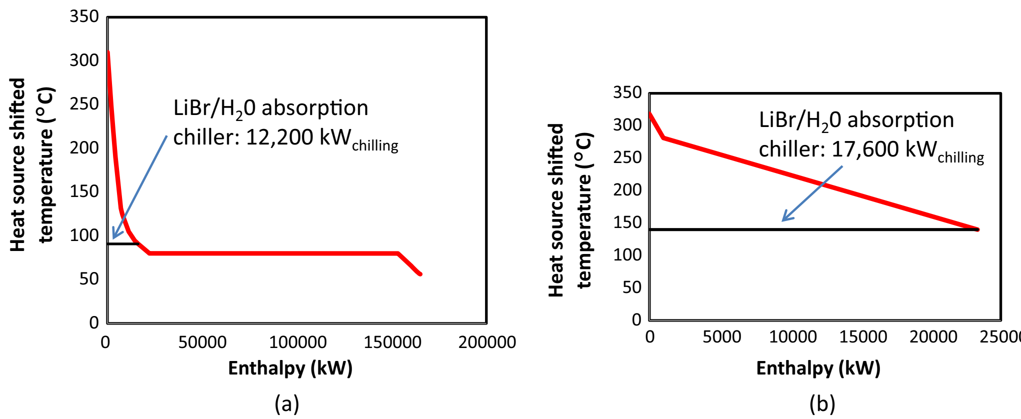

Fig. 24. Placement of absorption chillers against the profiles for (a) heat that was rejected to cooling water and (b) heat that was rejected to air.

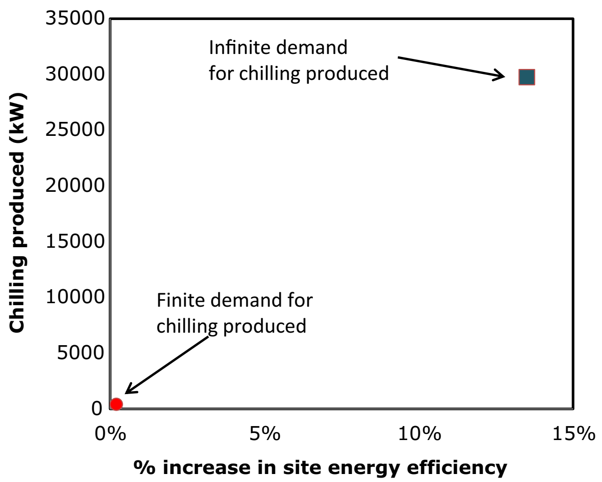

Fig. 25. Chilling produced versus % increase in the site energy efficiency.

(profiles shown in Fig. 20(a) and (b). The site currently exports 25 MW of electricity and has allowance for more; the site also has a neighbourhood requiring 2.4 MW of hot water at 80 °C. For this analysis the minimum permissible temperature difference is 10 °C and 10% distribution loss is assumed for heat export.

6.1. Potential for power generation

Using the cumulative heat available at the preliminary heat recovery temperatures for heat rejected to cooling water and air (kinks on the profiles in Fig. 20(a) and (b) and Eqs. (2)–(6), the power generated can be evaluated at every preliminary heat recovery temperature using benzene as working fluid (above its boiling point) and cyclopentane as working fluid (below benzene's boiling point). Fig. 21(a) and (b) show the power generated at every PHRT for heat that was rejected to cooling water and air respectively.

The temperature at which power generation is highest is 80 °C (using an ORC driven by benzene). Then using the cumulative heat available below 80 °C, the next temperature is 56.4 °C (using an ORC driven by cyclopentane). For the heat rejected to air, maximum power is generated at 140 °C. Placement of the organic Rankine cycle against the profiles for heat that was rejected to cooling water and air are shown in Fig. 22(a) and (b) respectively. If this is implemented the site energy efficiency increases by 9%.

6.2. Potential for chilling provision

The chilling generated at each preliminary heat recovery temperature using a lithium bromide/water absorption chiller (modelled using Eqs. (7)–(10)) are shown in Fig. 23(a) and (b) for heat rejected to cooling water and air respectively. Since the generator temperature is 89.9 °C (Section 4.2), only heat sources above this

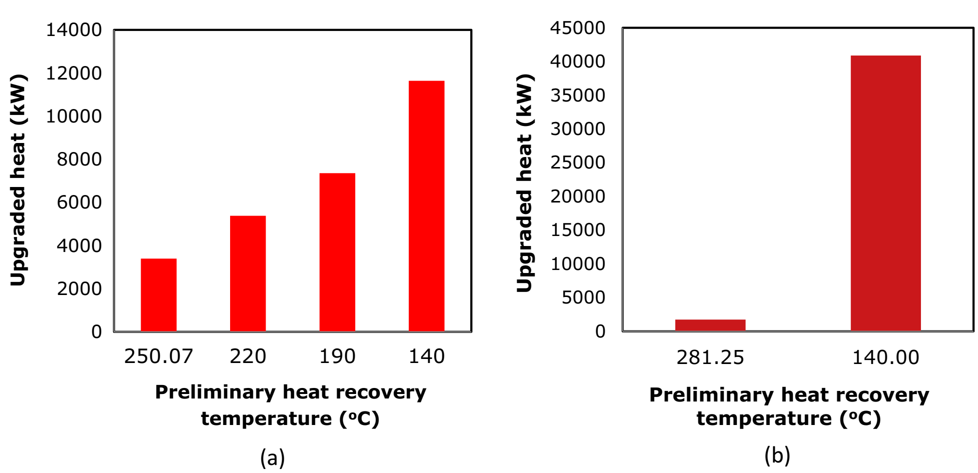

Fig. 26. Heat upgraded at every PHRT using the profiles (a) heat that was rejected to cooling water and (b) heat that was rejected to air.

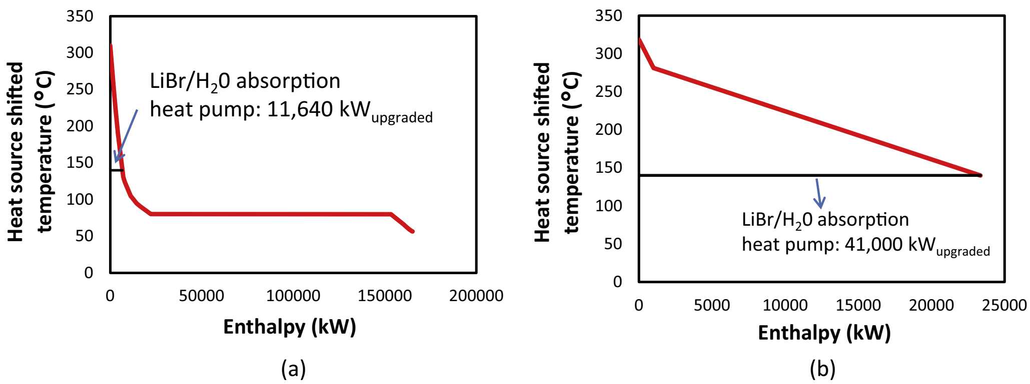

Fig. 27. Placement of absorption heat pump against the profile for (a) heat that was rejected to cooling water and (b) heat that was rejected to air.

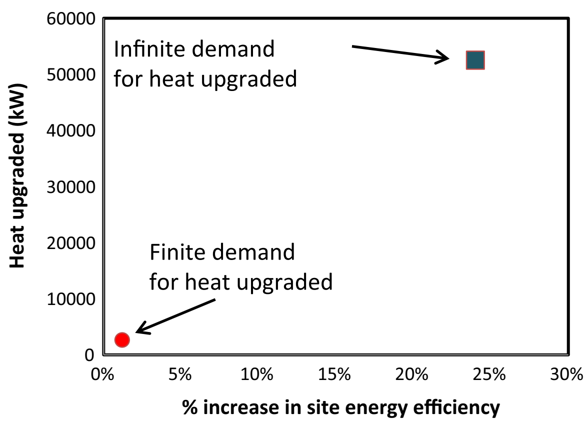

Fig. 28. Heat upgraded versus % increase in the site energy efficiency.

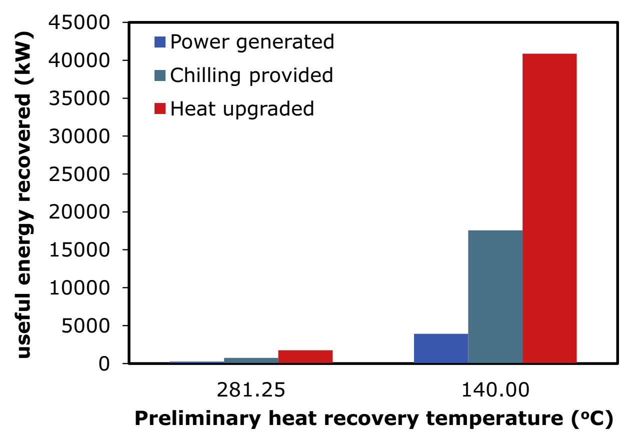

Fig. 30. Useful energy (power, chilling and heat) recovered from heat that was rejected to air at the PHRT's.

temperature can be used to drive an absorption chiller for chilling provision.

From Fig. 23a, the temperature at which chilling provision is highest is 90.9 °C and from Fig. 23b, 140 °C. The total chilling produced can increase the site energy efficiency by 13.5% (Fig. 35). Placements of absorption chillers are shown in Fig. 24(a) and (b) against the profiles for heat that was rejected to cooling water and air respectively. However, the site demand for chilling is 0.42 MW and if this is satisfied, the site energy efficiency increases by 0.2% (Fig. 25).

6.3. Potential for heat upgrade

To evaluate the potential for heat upgrade using a Lithium bromide/water absorption heat pump, Eqs. (11)–(14) were used. Only

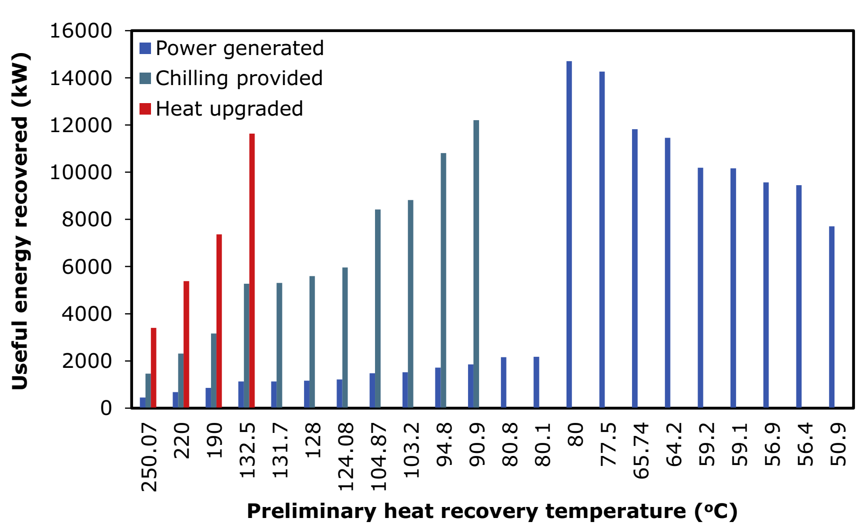

Fig. 29. Useful energy (power, chilling and heat) recovered from heat that was rejected to cooling water at the PHRT's.

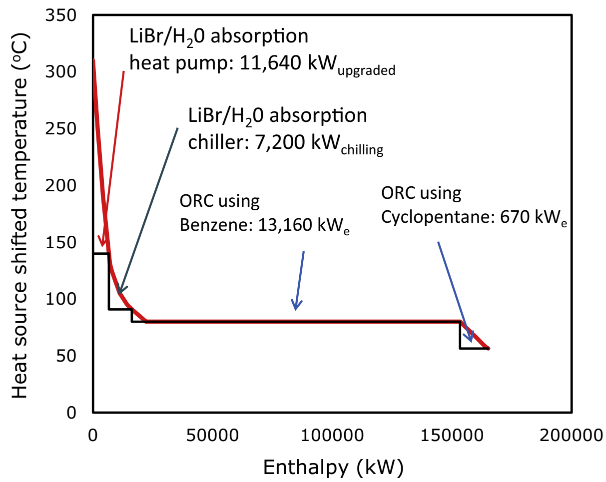

Fig. 31. Placement of technologies against the heat source profile for heat that was rejected to cooling water (infinite demand for recovered energy).

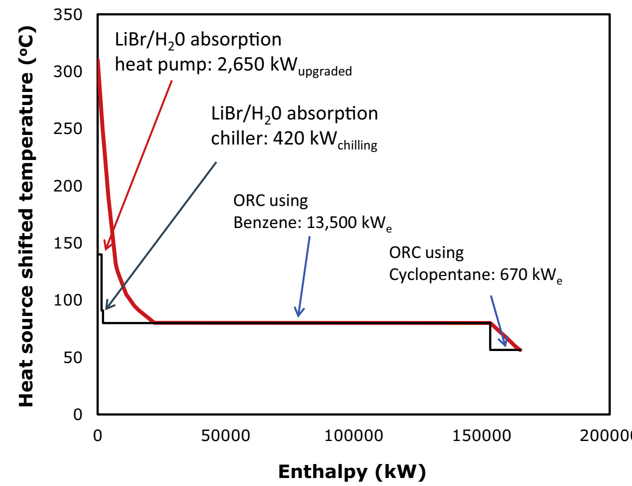

Fig. 33. Placement of technologies against the heat source profile for heat that was rejected to cooling water (finite demand for recovered energy).

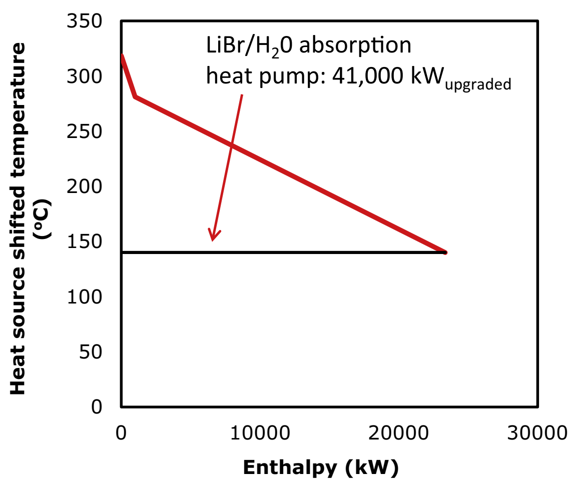

Fig. 32. Placement of technologies against the heat source profile for heat that was rejected to air (infinite demand for recovered energy).

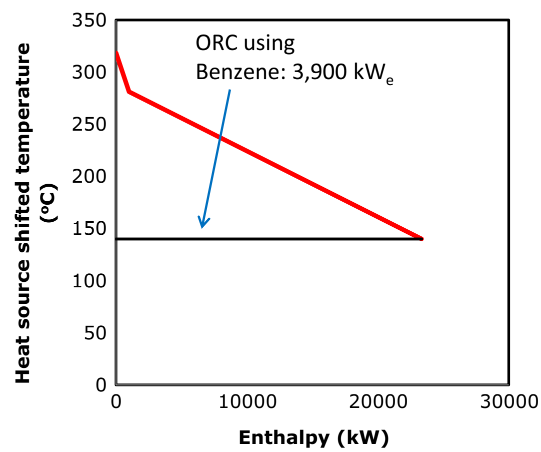

Fig. 34. Placement of technologies against the heat source profile for heat that was rejected to air (finite demand for recovered energy).

heat sources above 140 °C are considered (Section 4.3). The heat will be upgraded to 90 °C for hot water generation at 80 °C. Fig. 26(a) and (b) shows the useful heat recovered from absorption heat pumps for every preliminary heat recovery temperature

The final heat recovery temperature at which upgrading heat is maximised is at 140 °C (for heat rejected to cooling water (Fig. 26a) and heat rejected to air (Fig. 26b). Placement of an absorption heat pump against the profile for heat that was rejected to air and cooling water is shown in Fig. 27(a) and (b) respectively. The site energy efficiency increases by 24% (from using all the heat upgraded) (Fig. 28) and by 1.2% when only demand for recovered energy is satisfied (Fig. 28).

6.4. A system perspective

Combining different waste heat utilisation technologies may improve the site energy efficiency compared to single forms of energy since all the available heat will be exploited. Figs. 29 and 30 shows the useful energy recovered (power, chilling and heat) for heat rejected to cooling water and air for each preliminary heat recovery temperature.

To exploit all the available heat, for heat rejected to cooling water in Fig. 29, heat at 140 °C can be used to drive the generator in an absorption heat pump, residual heat at 90.9 °C for chilling provision, residual heat at 80 °C and 56.9 °C for electricity generation. While for heat rejected to air in Fig. 30, heat at 140 °C can be used to drive an absorption heat pump. Placements of technologies against the heat source profile are shown in Figs. 31 and 32 for heat that was rejected to cooling water and air respectively.

The total useful energy recovered is 73,670 kW increasing the site energy efficiency by 33%. This is possible when exploitation of all the heat sources is possible for an infinite demand for recovered energy. However, this is not always the case, as demand for recovered energy should be taken into account. Placement of technologies against the profile when demand for recovered energy is accounted for is shown in Figs. 33 and 34 for heat that was rejected to cooling water and air. Since the demand for heat and chilling is satisfied from the heat rejected to cooling water, all the heat rejected to air will be used for power generation. The recovered energy (in Figs. 33 and 34) increases the site energy efficiency by 10%.

Fig. 35a shows the increase in the site energy efficiency for all cases (both single forms of energy and a system approach) where an infinite demand for recovered energy is assumed. The site energy efficiency increase is highest when a system approach is used i.e. technologies are combined to exploit the available waste heat.

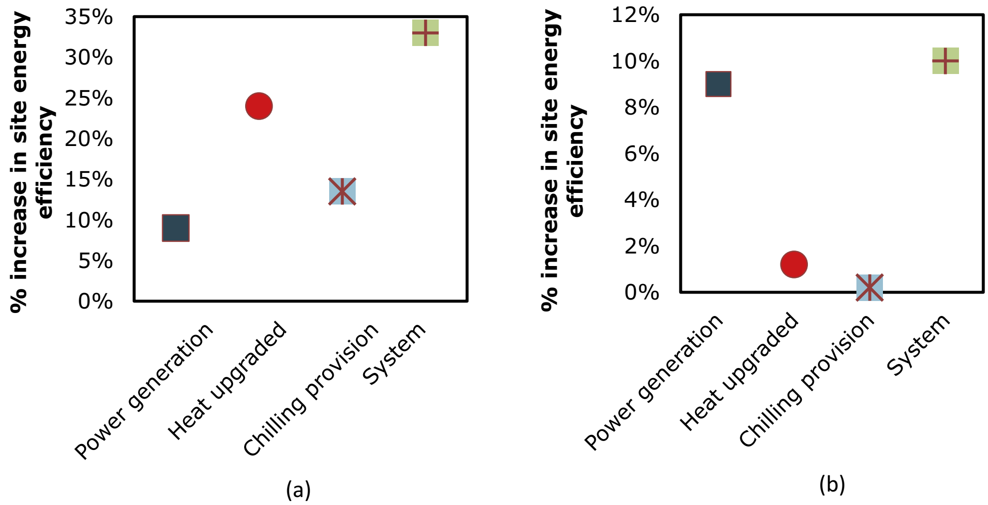

Fig. 35. Increase in site energy efficiency for all options (a) infinite demand and (b) finite demand.

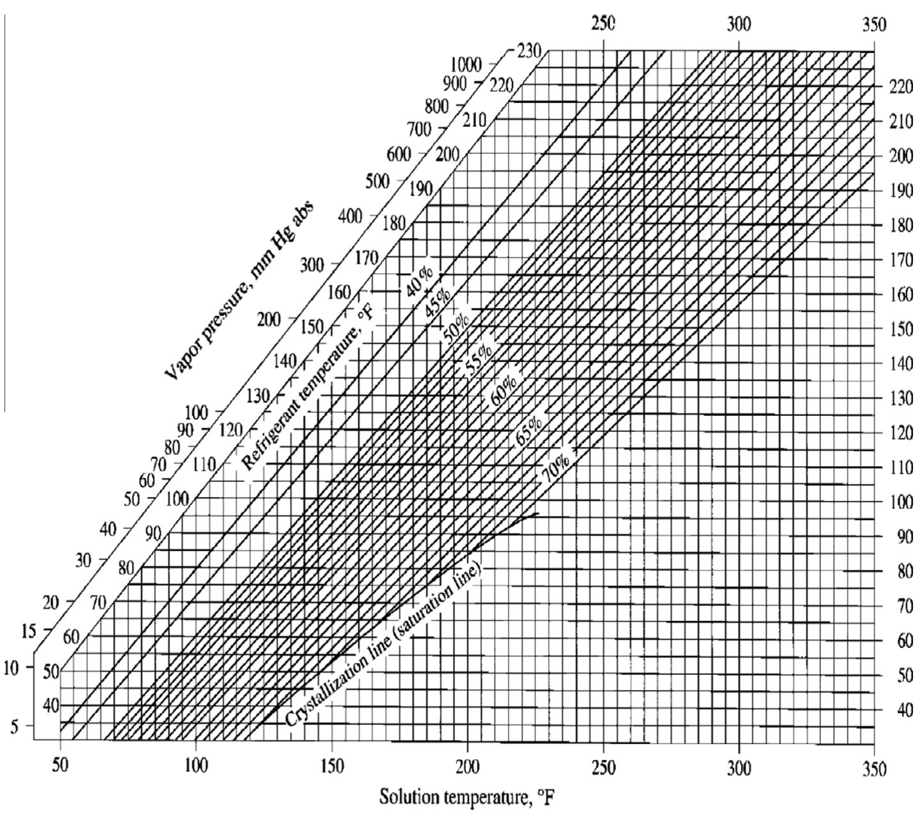

Fig. 36. Equilibrium chart for the water-lithium bromide solution (Brown [34]).

For a finite demand for recovered energy using the site needs, Fig. 35b shows how the site energy efficiency increases. Again a system perspective has the highest increase in site energy efficiency. Since this analysis was to evaluate the impact on the site energy efficiency, a detailed economic analysis is required to make a final decision.

7. Conclusions and future work

Waste heat utilisation has received interest in recent years due to energy sources becoming less available and there is potential in waste heat to improve the energy efficiency of process sites. A methodology is presented to explore the potential to generate electricity, chilling and heating from available waste heat in process sites. This work accounts for waste heat from site processes and the site utility system by formulating a waste heat source profile that captures the temperature and duties of the heat sources. New mathematical models of waste heat recovery technologies are presented and applied to identify and compare feasible technical opportunities to convert the waste heat to useful energy. Analysis was carried out to maximise the site energy efficiency. The methodology was applied to the case study for a medium scale petroleum refinery; the highest increase in the site energy efficiency was obtained when waste heat recovery technologies were combined to exploit all the available waste heat without taking into account the demand for recovered energy. However, when the demand for recovered energy is taken into account; the site energy efficiency increased by 10%. The availability of demands for recovered energy can increase the site energy efficiency. This analysis was done to evaluate the impact on the site energy efficiency; final decisions can be made after a detailed economic analysis.

In this present work, simple cycles of organic Rankine cycles, absorption chillers and absorption heat pumps were considered, future work includes (1) using the waste heat source profile to determine the architecture for complex cycles for waste heat utilisation, (2) providing models of complex configuration for waste heat recovery technologies, (3) extend the model to include part load performance of technologies, and (4) development of a thermo-economic Optimisation framework.

Appendix A

See Fig. 36.

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3. 3. Introduction to Publication 2

Determination of the heat upgrade technology to use and associated temperatures (i.e. low temperature heat to be upgraded, high temperature heat sink required to use the upgraded heat and low to medium temperature heat required by absorption systems) has been determined using the coefficient of performance. However, the COP neglects interactions with interconnected systems. Therefore, the primary fuel recovery ratio is introduced as a criterion for analysing heat pump integration in process sites. Higher savings in primary fuel may be possible using a systems-oriented criterion.

Section 1 of this paper discusses the importance of upgrading low temperature waste heat, even though the thermodynamic availability is low. The literature review presented in section 1 supports the review in Chapter 2 (sections 2.3.3, 2.3.4 and 2.3.5).

Models for the mechanical heat pump, absorption heat pump and absorption heat transformers are presented and validated in Section 2. Screening of working fluids for the mechanical heat pump is also performed in this section.

The primary fuel recovery ratio (PRR) is presented in Section 3 for heat pump analysis in process sites. The PRR measures the reduction in primary fuel consumption as a result of heat upgraded. It accounts for the primary fuel consumed (and associated waste heat) for power generation to drive the mechanical heat pump and missed opportunities for steam generation when absorption systems are used. The graphical methodology for applying the PRR for process integration of heat pumps is presented in section 4. The method is applied to a medium scale refinery case study in section 5. Results show that higher savings in hot utility and primary fuel is possible using the PRR compared to using the COP. Section 6 contains conclusions and future work.

3. 4. Publication 2

Oluleye G., Smith R., Jobson M., Modelling and screening heat pump options for the exploitation of low grade waste heat in process sites. Applied Energy 2016; 169: 267 – 286. doi.org/10.1016/j.apenergy.2016.02.015

Applied Energy 169 (2016) 267–286

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Modelling and screening heat pump options for the exploitation of low grade waste heat in process sites

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HIGHLIGHTS

- Explicit thermodynamic models proposed for heat upgrade technologies.
- Novel system oriented criterion introduced to screen technology options.
- Diverse temperatures and quantity of waste heat sources and sinks accounted for.
- Methodology developed to apply the criterion for heat pump analysis in process sites.
- Case study presented to illustrate application of the proposed methodology.

ARTICLE INFO

Article history:
Received 29 July 2015
Received in revised form 15 January 2016
Accepted 2 February 2016

Keywords:
Waste heat recovery
Low-grade heat upgrade
Mechanical heat pump
Absorption heat pump
Absorption heat transformer
Comparative analysis

ABSTRACT

The need for high efficiency energy systems is of vital importance, due to depleting reserves of fossil fuels and increasing environmental problems. Industrial operations commonly feature the problem of rejecting large quantities of low-grade waste heat to the environment. The aim of this work is to develop methods for the conceptual screening and incorporation of low-temperature heat upgrading technologies in process sites.

The screening process involves determination of the best technology to upgrade waste heat in process sites, and the combination of waste heat source and sink temperatures for a technology. Novel simplified models of mechanical heat pumps, absorption heat pumps and absorption heat transformers are proposed to support this analysis. These models predict the ratio of the real performance to the ideal performance in a more accurate way, than previous simplified models, taking into account the effect of changing operating temperatures, working fluids non-ideal behaviour and the system component inefficiencies.

A novel systems-oriented criterion is also proposed for conceptual screening and selection of heat pumps in process sites. The criterion (i.e. the primary fuel recovery ratio) measures the savings in primary fuel from heat upgraded, taking into account power required to drive mechanical heat pumps and missed opportunities for steam generation when absorption systems are used.

A graphical based methodology is also developed for applying the PRR in process sites and applied to a medium scale petroleum refinery. Results show that applying the PRR yields 9.2% additional savings in primary fuel compared to using the coefficient of performance to screen and incorporate heat pumps.

1. Introduction

1.1. Background

The energy-intensive process industries (especially petrochemicals and refineries) account for 69% of total industrial energy consumption [1], and 45% of global carbon dioxide emissions; the majority of which are from combustion of fuel to produce heat and electricity [2]. In spite of this, around one sixth of overall industrial energy use is wasted at low temperatures (below 120 °C) [3]. Low grade waste heat is often rejected to cooling towers and stacks [3]. Large amounts of low grade heat may justify developing means of recovering it for useful purposes, even though the thermodynamic availability of the heat rejected is low [4].

Adoption of advanced technologies to upgrade low temperature heat to higher temperatures could provide considerable energy savings in industry, along with 7–12% reductions in today's global

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http://dx.doi.org/10.1016/j.apenergy.2016.02.015
0306-2619/

Nomenclature

A, B	regression coefficients for mechanical heat pump (–)
C, D	regression coefficients for absorption heat pump (–)
$COP_{AHP,real}$	absorption heat pump real coefficient of performance (–)
$COP_{AHT,real}$	absorption heat transformer real coefficient of performance (–)
$COP_{MHP,real}$	mechanical heat pump real coefficient of performance (–)
$COP_{AHP,ideal}$	ideal coefficient of performance for an absorption heat pump (–)
$COP_{AHT,ideal}$	ideal coefficient of performance for an absorption heat transformer (–)
$COP_{MHP,ideal}$	ideal coefficient of performance for a mechanical heat pump (–)
COP_{real}	heat upgrading technologies real coefficient of performance (–)
E, F	regression coefficients for absorption heat transformer (–)
HT	high temperature waste heat (°C)
HP	high pressure steam (bar)
i	temperature intervals on waste heat source and sink profile (–)
LP	low pressure steam (bar)
LT	low temperature waste heat (°C)
MP	medium pressure steam (bar)
MT	medium temperature waste heat (°C)
P	pressure (bar)
P_{COMP}	compressor outlet pressure (bar)
P_{EVAP}	evaporator pressure (bar)
PRR	primary fuel recovery ratio (–)
PRR_{AHP}	absorption heat pump primary fuel recovery ratio (–)
PRR_{AHT}	absorption heat transformer primary fuel recovery ratio (–)
PRR_{MHP}	mechanical heat pump primary fuel recovery ratio (–)
P_{sat}	steam main saturation pressure (bar)
Q	heat transfer rate (kW)
Q_{ABS}	heat released in the absorber (kW)
QAC	actual heat available (kW)
QAC_{T_i}	actual heat available in interval i on the waste heat source profile (kW)
$QAC_{T_{ri}}$	actual heat available in region r within interval i on the existing site sink profile (kW)
Q_{COND}	condenser heat duty (kW)
QCUM	cumulative heat available (kW)
$QCUM_{T_{ri}}$	cumulative heat available in region r within interval i on the existing site sink profile (kW)
Q_{EVAP}	evaporator duty (kW)
Q_{fuel}	fuel consumption in the site cogeneration system (kW)
Q_{GEN}	generator duty (kW)
$Q_{upgraded}$	useful heat released from technology options (kW)
Q_{T_i}	heat source required by technology options (kW)
$Q_{T_{ri}}$	heat sink satisfied from upgraded heat (kW)
Q_{steam}	steam produced from the site cogeneration system (kW)
$Q_{WH(1)}$	waste heat rejected to cooling water and air from the site processes and cogeneration system (kW)
$Q_{WH(2)}$	additional waste heat generated from power produced for the mechanical heat pump (kW)
T	temperature (°C)
T_{ABS}	absorber temperature (°C)
T_{COND}	condenser temperature (°C)
T_{EVAP}	evaporator temperature (°C)
T_{GEN}	generator temperature (°C)
T_{op}	steam main operating temperature (°C)
T_{SUPPLY}	waste heat source stream inlet temperature (°C)
T_{sat}	steam main saturation temperature (°C)
T_{TARGET}	waste heat source stream end temperature (°C)
VHP	very high pressure steam (bar)
W_{COMP}	compression power required (kW)
W_{PUMP}	pumping power required (kW)
$W_{produced}$	power produced from the site cogeneration system (kW)

Greek letters

η_{AHP}	efficiency factor for an absorption heat pump (–)
η_{AHT}	efficiency factor for an absorption heat transformer (–)
η_{MHP}	efficiency factor for a mechanical heat pump (–)
$\Delta Q_{fuel(1)}$	change in primary fuel consumed in the site cogeneration system (kW)
$\Delta Q_{fuel(2)}$	additional primary fuel required to provide electrical power for a mechanical heat pump (kW)
η_{cogen}	site cogeneration efficiency (–)
η_{power}	efficiency of electrical power generation for the mechanical heat pump (–)
ΔT_{min}	minimum permissible temperature difference (°C)

CO_2 emissions from fossil fuel displaced [5]. These technologies can also facilitate energy savings when direct heat recovery is infeasible. The benefits of upgrading low temperature heat depend on the temperatures, and quantities of the heat in the waste streams as well as the demand for the recovered energy [6].

Examples of commercialised technologies for low-grade heat upgrade are: mechanical heat pumps, absorption heat pumps and absorption heat transformers. Mechanical heat pumps (MHP) absorb thermal energy from low temperature heat sources in order to increase it for use in a high temperature heat sink using mechanical energy. In absorption heat pumps (AHP), the evaporation, expansion and condensation of the working fluid are similar with a mechanical heat pump. The difference is the circuit of a liquid absorbent circulating by a pump which replaces the compressor [7]. An absorption heat transformer (AHT) is a reversed absorption heat pump. They supply thermal energy at a higher temperature than the waste heat required i.e. the evaporator and absorber operate at a pressure higher than the condenser and generator [8]. Even though these technologies are mature and commercialised, uptake by industry is slow.

There are several challenges associated with incorporating heat pumping technologies in process sites. Firstly, the available waste heat occurs over a wide temperature range and from multiple sources (including the site processing units and the site cogeneration system) [9]. Secondly, there are multiple sinks to exploit the upgraded heat [9]. For example heat upgraded can reduce hot utility required by the processing units at different temperature levels. In incorporating heat pumps, it is necessary to determine the best combination of heat sources and sinks for any heat pump type, and the best heat pump to use. The coefficient of performance (COP) has been previously applied [10]; however, it neglects interactions with interconnected systems. Higher savings in primary fuel may be possible by developing a systems-oriented criterion for heat pump analysis in process sites. The third challenge relates to modelling of heat upgrading technologies. Simple models based on a constant ratio of the real to the ideal performance has been used

[8]. However, they are inaccurate and neglect the effect of different heat source and sink temperatures as well as the impact of working fluids. Even though detailed models exist to improve the accuracy, they are difficult to embed in existing synthesis frameworks for energy systems. Other challenges include economics and practical issues. These challenges are addressed in this paper and contributions of this work presented in Section 1.3.

1.2. Literature review

1.2.1. Mechanical heat pumps for low grade heat upgrade

There are numerous applications of MHPs for heat upgrade in process sites. However, determination of the best combination of heat source, and sink temperatures (and associated duties), taking into account the diverse range of low-grade heat sources and sinks for upgraded heat in process sites has been neglected. For example, Kapil et al. [11] screened and compared different design options for exploiting waste heat including mechanical heat pumps. However, the available waste heat was assumed to be at a single temperature and only heat from the site processes was considered. Furthermore, a single sink was considered for upgraded heat and working fluid selection not addressed. Modla and Lang [12] applied a mechanical heat pump to upgrade heat available in the condenser (heat source), for the reboiler (heat sink) in order to reduce the external energy demand of a batch distillation process. Selection of working fluids is an important degree of freedom in the system but was not considered. Again, their study focused on a single heat source–sink application. One of the drawbacks to being able to screen multiple heat sources and sinks of upgraded heat for MHP is the way in which the technology is modelled.

Scarpa et al. [13] developed a model to predict the energy performance of mechanical heat pumps using existing catalogue data to determine the system's basic parameters. An iteration process is required to solve the model, and solving becomes more complex when multiple heat sources and sinks for upgraded heat need to be screened. Lazzarin [8] applied a simple model that compares the performance of a real MHP with a reference (related to the reversible Carnot cycle). Even though the model is relatively simple; a constant value (0.5) is assumed as the ratio of the real to the ideal performance i.e. the efficiency factor. Using a constant efficiency factor neglects the effect of working fluid selection and the technology components inefficiencies. There is need to develop explicit models of MHPs that can be applied to screen the multiple heat sources and sinks for upgraded heat in process sites.

1.2.2. Absorption heat pumps for low grade heat upgrade

Absorption heat pumps have an enormous potential for primary energy savings in both domestic and industrial applications, and are commercially available [10]. For industrial applications, Bakhtiari et al. [10] considered the diverse range of heat source temperatures for AHP application, but the use of the upgraded heat was limited to a single temperature heat sink. Tufano [14] recorded noticeable energy savings for applying an AHP for heat recovery in a distillation column. Again, the study focused on a single heat source–sink application. This drawback could be attributed to the way in which AHPs are modelled. Kohlenbach and Ziegler [15] developed a dynamic model based on external and internal steady-state enthalpy balances for each component, to predict the system overall performance and working states. However, a lot of input parameters are required for analysing multiple low-grade waste heat sources. Qu et al. [16] applied Absorption Simulation (ABSIM) software to evaluate working states and system overall performance, experiments were also conducted to validate the model. Even though ABSIM computes the physical properties of working fluids with good accuracy compared to experimental results, it is not easy to integrate with a variety of energy systems. In addition, modelling for multiple heat sources and sinks is tedious and susceptible to user errors.

The performance of AHP is also dependent on the working fluid pair. Water/lithium bromide is the only working fluid in current industrial use [17]due to water's high enthalpy of evaporation, higher coefficient of performance compared to other pairs like ammonia/water, good heat and mass transfer capabilities and low toxicity. In addition, compared to water/ammonia systems, they do not require rectifying apparatus since lithium bromide is non-volatile [18]. Disadvantages of using lithium bromide/water as working fluid pair are high corrosivity, risk of crystallisation, especially at high salt concentrations, and requirement of sub-atmospheric working pressures [19].

1.2.3. Absorption heat transformers for low grade heat upgrade

Absorption heat transformers (AHT) can recover about 20–50% of low-temperature waste heat and give an opportunity to reuse it in industrial processes [20]. Scott et al. [21] reported the technical feasibility of incorporating an AHT to increase the efficiency of energy use of an evaporation-crystallization plant in a sugar mill. The simulation demonstrated that the total amount of steam used can be reduced by 11.8–16.4%. Rivera et al. [22] applied a heat transformer in water purification. Modelling was done by providing detailed thermodynamic analysis for every component in the cycle. Even though good accuracy for a single heat source and sink system was recorded, solving the equations when multiple heat sources are involved (like in process sites) become very complex and may suffer intrinsic systematic errors. Ma et al. [23] applied an AHT to recover waste heat in a rubber plant to provide hot water from 95 °C to 110 °C. However, the study focused on a single heat source. There is need to develop explicit models of AHTs suitable for screening multiple heat sources and sinks for upgraded heat available in process sites.

1.2.4. Comparing between multiple heat pumps

Mechanical heat pumps and absorption systems show the most promise for industrial use [24]. Due to constraints on capital investments and space, it is necessary to compare between them to determine which one to apply for a particular low-grade heat upgrade application. The coefficient of performance (COP) has been widely used to evaluate heat upgrade systems. The COP of a MHP is the useful heat upgraded per unit power input, while for AHP and AHT, the COP is the useful heat upgraded per unit heat input. The coefficient of performance for a MHP is higher than both absorption heat pumps and heat transformers [25]. The main disadvantage of using mechanical heat pumps is the high quality electrical power required. Producing this high quality electrical power requires additional primary fuel consumption and waste heat production. Furthermore, the COP does not take into account the impact on interconnected systems.

Absorption heat upgrade systems seem more attractive than MHP because they are driven by waste heat and do not require primary energy for their operation except for small auxiliary equipment [4]. However, high temperature heat energy is required to separate the working fluid pair, resulting in missed opportunities for steam generation. Absorption heat transformers on the other hand require low temperature thermal energy to drive the generator, but the COP (0.1–0.5) is lower than MHP and AHP [17]. In addition, the COP of absorption heat pumps and heat transformers do not decline steeply at higher temperature lift compared to mechanical heat pumps [5].

For a comparative analysis between mechanical and absorption heat pumps, Abrahamsson et al. [25] used the useful energy output per unit of energy input. However, comparison was done for a single heat source/heat sink application and the impact on primary fuel neglected. Furthermore, the additional waste heat generated from fuel converted to power to drive the MHP was neglected in their analysis.

Kew [24] defined the primary energy ratio (PER) for mechanical heat pumps and absorption systems. The PER of a MHP is the product of the efficiency of electricity generation and transmission, the efficiency of conversion of electrical energy to shaft work and the COP. While for absorption systems, the PER is defined as the efficiency of conversion of primary energy into heat supplied to the generator multiplied by the COP. However, the primary energy ratio is only suitable for accessing the technical performance of heat pumps, especially when compared to other technologies, but not suitable to compare between heat pumps for use in low grade heat upgrade applications, since the PER neglects waste heat exploited and additional waste heat created by the heat pumps.

1.3. Contributions of this work

Novel explicit models of low-grade heat upgrading technologies are proposed in this work. These models are suitable for integration with existing energy system optimisation tools. The framework is a general thermodynamic modelling approach based on correlations between the real heat pump and ideal heat pump performance. In previous studies, the ratio of the real heat pump performance to the ideal performance i.e. the efficiency factor was assumed constant. The non-ideal behaviour of the technology working fluids affects the efficiency factor. Therefore, the approach derives equation-fit explicit models for the heat upgrading technologies. The real performance is obtained from rigorous simulations in Aspen HYSYS [26] or from thermodynamic data in literature [7,27]. These simplified models are much better suited for preliminary screening of heat pumping schemes. Development of such models could increase uptake of heat pumps in industry.

In addition to the explicit models proposed for heat upgrading technologies, a novel systems-oriented criterion is also proposed for screening and selecting heat upgrading technologies in process sites. The criterion considers impacts on interconnected energy systems by taking into account the useful energy recovered, primary fuel saved (from heat upgraded), any additional primary energy consumed and available waste heat in existing process sites. The criterion also determines the best combination of heat source temperatures (and duties) and heat sink temperatures (and duties) for any technology. A methodology is also presented for applying the criterion for heat pump analysis and screening in process sites. A systems-oriented criterion for heat pump analysis could yield additional savings in primary fuel compared to using the COP.

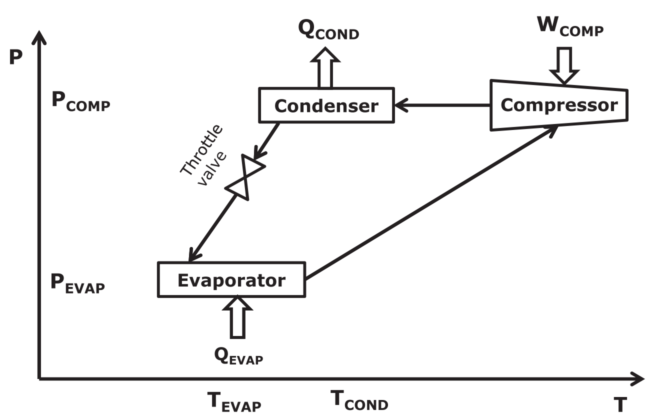

Fig. 1. Mechanical heat pump schematic.

Table 1
Working fluid properties for mechanical heat pumps.

Working fluid	Molecular weight (kg/kmol)	Boiling point (°C)	Critical point (°C)
Propylene	42.08	−47.6	91.85
Propane	44.1	−42	96.75
i-butane	58.12	−1	134.9
n-butane	58.12	−1	152
Ammonia	17.03	−33.34	132.4

2. Modelling low grade heat upgrading technologies

The ideal performance of heat pumps has been used to estimate the heat upgraded for preliminary screening of heat pump options. However, this screening approach neglects the inefficiencies in the cycle's component and working fluid non-ideal behaviour. To this end, some authors have multiplied the ideal coefficient of performance (COP) by an efficiency factor. Different values have been applied literature, for example, US Department of Energy [5] used 0.7, Kew [24] used 0.3, and Matsuda et al. [28] used 0.8. The efficiency factor may be dependent on the non-ideal behaviour of working fluids and the technology operating temperatures. In this section, simplified thermodynamic models for the MHP, AHP and AHT are proposed based on the relationship between the real performance and ideal performance of these thermodynamic cycles. The models allow for extension to large process models, and are easily embedded in large optimisation solvers.

2.1. Mechanical heat pumps (MHP)

Mechanical heat pumps have four main components: the compressor, condenser, evaporator and expansion valve. The components are connected in a closed or open-loop. For closed loop systems, heat flows from the waste heat source to the working fluid in the evaporator, thus vaporising the working fluid. The vapour is compressed to a higher pressure and temperature, and hot vapour enters the condenser, where it is condensed and gives off useful heat that is recovered. Finally, the high-pressure working fluid is expanded to the evaporator pressure, in the expansion valve and the cycle repeats. A schematic of a mechanical heat pump on a pressure temperature diagram is shown in Fig. 1.

The real COP (i.e. enthalpy based) is defined as the useful heat upgraded per unit power required in Eq. (1). The ideal COP is expressed using a reverse Carnot factor in Eq. (2), the ratio of the

Table 2
Validation of MHP simulation in Aspen HYSYS.

T_{COND}	T_{EVAP}	$Q^{COND\ (experiment)}$	$Q_{COND,\ (HYSYS)}$	$W_{COMP\ (experiment)}$	$W_{COMP\ (HYSYS)}$	$COP_{MHP,\ real\ (experiment)}$	$COP_{MHP,\ real\ (HYSYS)}$	% error
120	10	1267.0746	1179.4819	662.0746	635.5857	1.9137	1.85573	3.03
120	30	1100.4961	1028.0377	481.4961	460.263	2.2855	2.2335	2.27
120	50	985.23681	899.7372	340.5026	316.7139	2.8934	2.8408	1.82
120	70	863.67712	784.43845	214.7223	198.3351	4.0222	3.9551	1.67

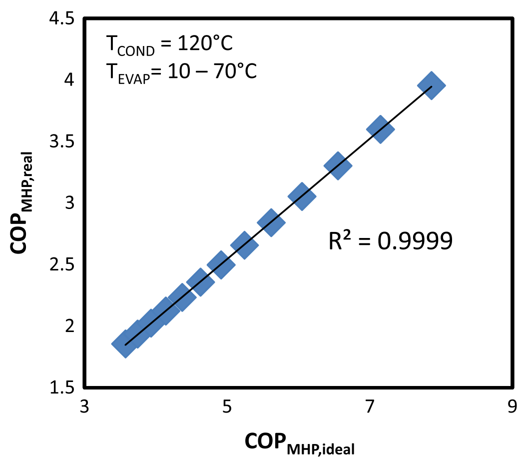

Fig. 2. MHP real and ideal COP relationship.

Table 3
Values of *A* and *B* for propylene.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
Propylene	50	10–40	0.6705	−0.4313
	60	10–50	0.6391	−0.4264
	70	10–60	0.5913	−0.3847
	80	10–70	0.511	−0.2541

Table 4
Values of *A* and *B* for propane.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
Propane	50	10–40	0.6811	−0.5107
	60	10–50	0.655	−0.529
	70	10–60	0.6165	−0.5254
	80	15–70	0.5554	−0.4697

Table 5
Values of *A* and *B* for isobutane.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
Isobutane	50	10–40	0.723	−0.5688
	60	10–50	0.7108	−0.5859
	70	10–60	0.7024	−0.6724
	80	15–70	0.6871	−0.7265
	90	20–80	0.6663	−0.7795
	100	25–90	0.6375	−0.8269
	110	25–100	0.5861	−0.7916

Table 6
Values of *A* and *B* for n-butane.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
n-butane	50	10–40	0.7319	−0.5154
	60	10–50	0.7259	−0.5602
	70	10–60	0.7181	−0.6077
	80	15–70	0.7081	−0.6582
	90	20–80	0.6952	−0.7107
	100	25–90	0.6781	−0.7639
	110	30–100	0.6551	−0.8149
	120	35–110	0.6217	−0.8504
	130	35–110	0.5586	−0.7767

real COP to the ideal is expressed using the efficiency factor η_{MHP} in Eq. (3)

$$COP_{MHP,real} = \frac{Q_{COND}}{W_{COMP}} \quad (1)$$

Table 7
Values of *A* and *B* for ammonia.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
Ammonia	50	10–40	0.7267	−0.4774
	60	10–50	0.7132	−0.4003
	70	15–60	0.7006	−0.3861
	80	25–70	0.6932	−0.4851
	90	25–80	0.6628	−0.3684
	100	25–90	0.6294	−0.282
	110	25–100	0.5732	−0.1195
	120	25–100	0.4971	0.0586

Table 8
Values of *A* and *B* for water.

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	*A*	*B*
Water	125	100–110	0.7484	−0.5518
	135	100–120	0.7482	−0.5363
	145	100–130	0.7476	−0.5177
	155	100–140	0.7468	−0.5014
	165	100–150	0.7448	−0.4729
	175	100–160	0.7448	−0.4746
	185	100–170	0.7435	−0.4639
	195	100–180	0.7418	−0.4547
	205	100–190	0.7399	−0.4474
	215	100–200	0.7376	−0.4410

$$COP_{MHP,ideal} = \frac{T_{COND}}{T_{COND} - T_{EVAP}} \quad (2)$$

$$COP_{MHP,real} = \eta_{MHP} \times COP_{MHP,ideal} \quad (3)$$

Besides the working conditions, the performance of mechanical heat pumps depends on the working fluid. Table 1 contains working fluids that fulfil safety criteria and are environmentally friendly.

A rigorous simulation of a MHP using ammonia as working fluid was done in Aspen HYSYS [26]. The physical properties of the working fluids are calculated using Peng Robinson Equation of State. Validation of HYSYS simulation against experimental thermodynamic design data for ammonia, provided by Milora and Combs [29] is shown in Table 2. The simulation shows good agreement with experiment (less than 3% error). Analysis was done for steady state subcritical conditions.

Model assumptions for rigorous simulation in HYSYS are:

1. Negligible pressure drop in condenser and evaporator.
2. Saturated vapour in evaporator and saturated liquid in condenser.
3. Compressor isentropic efficiency at 75%.
4. Minimum temperature difference assumed to be 10 °C.

A plot of the real COP to the ideal COP is shown in Fig. 2, the efficiency factor depends on the system's operating temperatures.

In order to deduce an explicit model for a MHP, the efficiency factor η_{MHP} is represented as a function of the ideal COP as shown in Eq. (4). A linear representation of the relationship is possible. This implies embedding this model in complex optimisation frameworks to systematically select the working temperatures can guarantee optimality. The temperatures in Eqs. (2)–(4) are in Kelvin (K).

$$\eta_{MHP} = A + \frac{B}{COP_{MHP,ideal}} \quad (4)$$

Values of *A* and *B* in Eq. (4) depend on the working fluid selected and the temperatures as shown in Tables 3–6 for fluids in Table 1, and in Table 8 for water (above atmospheric pressure). Even though water is applicable for higher temperature lifts i.e. above the critical points of fluids in Table 1, the high specific volumes of steam in the corresponding temperature range would require large and expensive compressors [25].

Validation of the models for different working fluids at different condensing temperatures is shown in Fig. 3.

The real COPs shown in Fig. 3 are theoretical values based on mass and energy balances. The real COP can be used to determine the best working fluid taking into account evaporation and condensation temperatures, as shown in Fig. 4. Selection of working fluids depends on the cycle operating temperatures. Working fluids

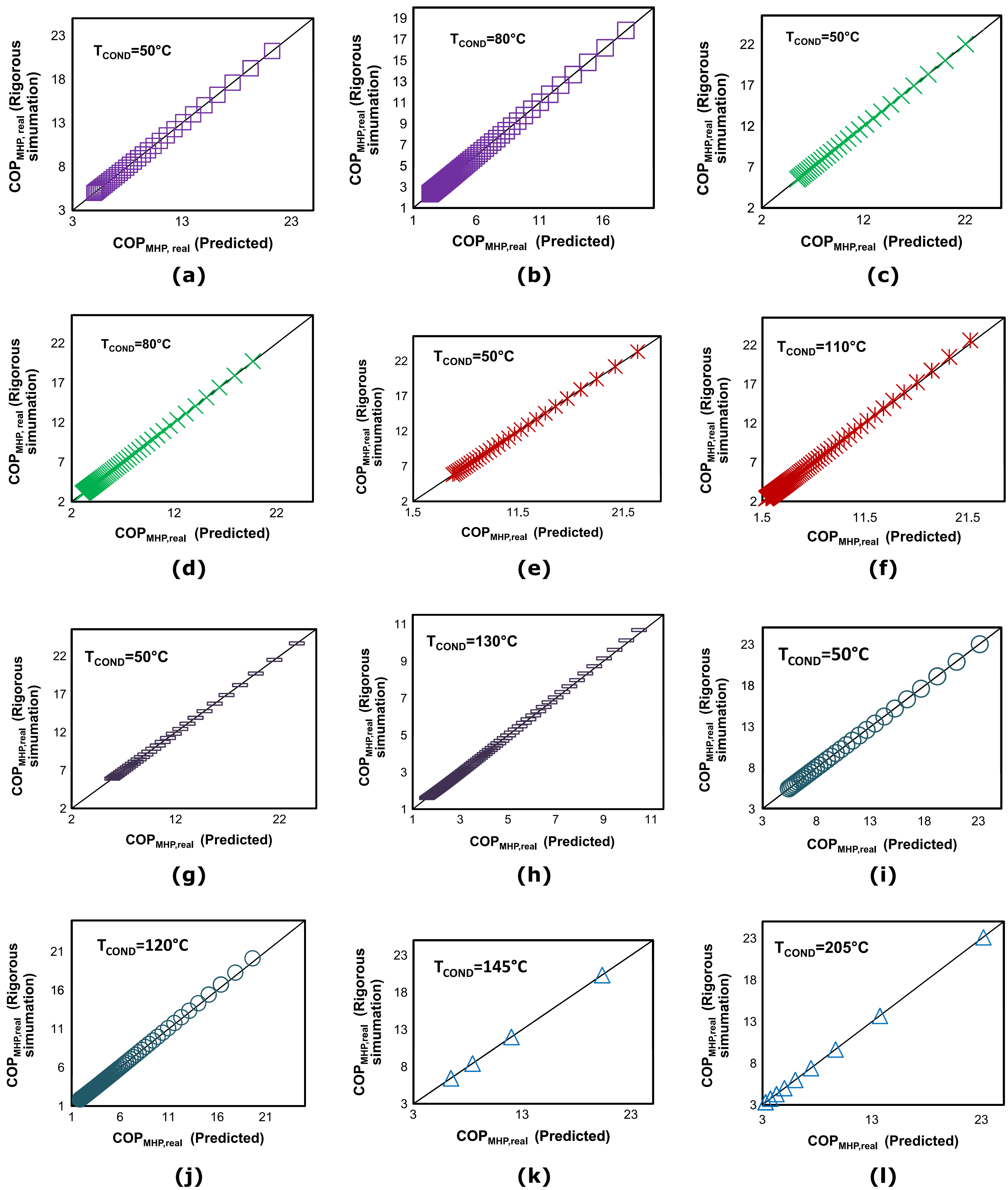

Fig. 3. Model validation using different working fluids: propylene (a and b), propane (c and d), isobutane (e and f), n-butane (g and h), ammonia (i and j), water (k and l).

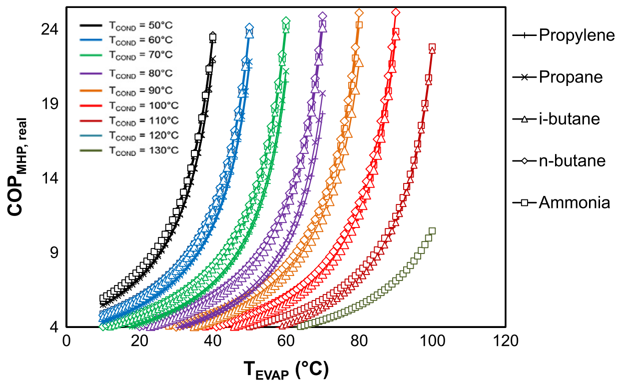

Fig. 4. Working fluid screening for MHP using the real (theoretical) coefficient of performance.

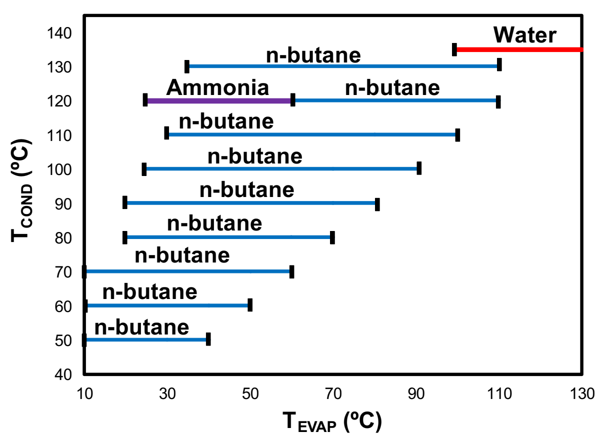

Fig. 5. Selected working fluids based on different combinations of evaporating and condensing temperatures for a MHP.

with the highest real COP and the associated system temperatures are shown in Fig. 5. Note that final selection of working fluids should take into account manufacturing costs and operational safety.

2.2. Absorption heat pumps (AHP)

In the absorption heat pump cycle, the compression of the working fluid is achieved thermally in a solution circuit, consisting of a generator, an absorber, a solution pump, and an expansion valve (Fig. 6(a)). Waste heat at low temperature produces low-pressure vapour in the evaporator, which is absorbed in the absorbent generating heat. The solution is pumped to a higher pressure and enters the generator, where the working fluid is boiled off with external high temperature heat, often provided through waste heat, high-pressure steam or gas-fired processes. The working fluid is condensed and the absorbent returns to the absorber via the expansion valve. Useful heat is recovered at medium temperature in the condenser and absorber. The mechanical energy required to pump the liquid is negligible compared to the high grade energy input in the generator [7]. A pair of liquids or salts absorbs the vapour of the working fluid. The most common working pairs for absorption systems are water (refrigerant) and lithium bromide (absorbent). A thermodynamic equilibrium diagram for water/lithium bromide is shown in Fig. 6(b). Solution concentrations are determined partly by the waste heat temperature and by the heat sink temperature [4]. It is desirable to have solution concentrations as large as possible above the salt crystallization line in Fig. 6(b).

The ideal COP of an absorption heat pump is equivalent to unity plus, the product of the maximum efficiency of a power producing machine operating between the generator temperature and evaporator temperature, and the maximum efficiency of a power absorbing heat pump operating between the source and sink temperatures [24] (Eq. (5)). Derivation of the ideal COP is provided in Appendix A. The real COP is expressed in terms of the useful heat output to the heat input as shown in Eq. (6). The ratio of the real COP to the ideal COP is called the efficiency factor η_{AHP} (Eq. (7)). The efficiency factor accounts for the working fluid non-ideal behaviour and inefficiencies in the system components. Temperatures in Eqs. (5)–(7) are in Kelvin (K).

$$\mathrm{COP}_{\mathrm{AHP,ideal}} = 1 + \left(1 - \frac{T_{\mathrm{COND}}}{T_{\mathrm{GEN}}}\right)\left(\frac{T_{\mathrm{EVAP}}}{T_{\mathrm{COND}} - T_{\mathrm{EVAP}}}\right) \tag{5}$$

$$\mathrm{COP}_{\mathrm{AHP,real}} = \frac{Q_{\mathrm{ABS}} + Q_{\mathrm{COND}}}{Q_{\mathrm{GEN}} + W_{\mathrm{PUMP}}} \tag{6}$$

$$\mathrm{COP}_{\mathrm{AHP,real}} = \eta_{\mathrm{AHP}} \times \mathrm{COP}_{\mathrm{AHP,ideal}} \tag{7}$$

The real COP was generated for a range of system temperatures using the thermodynamic data provided by Eisa [7]. A plot of the real COP and the ideal COP (Fig. 7(a)) shows that the efficiency factor is not constant. In order to predict the efficiency factor more accurately, it is related with the real COP in Eq. (8), also shown

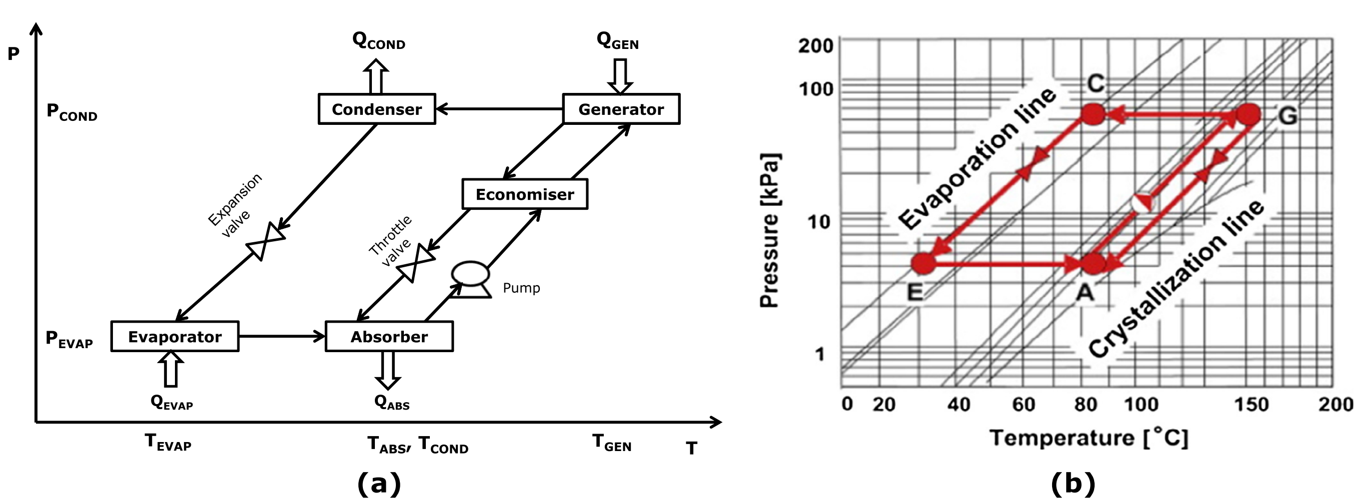

Fig. 6. (a) Absorption heat pump schematic, (b) absorption heat pump representation on refrigerant vapour pressure curve (Bakhtiari et al. [10]).

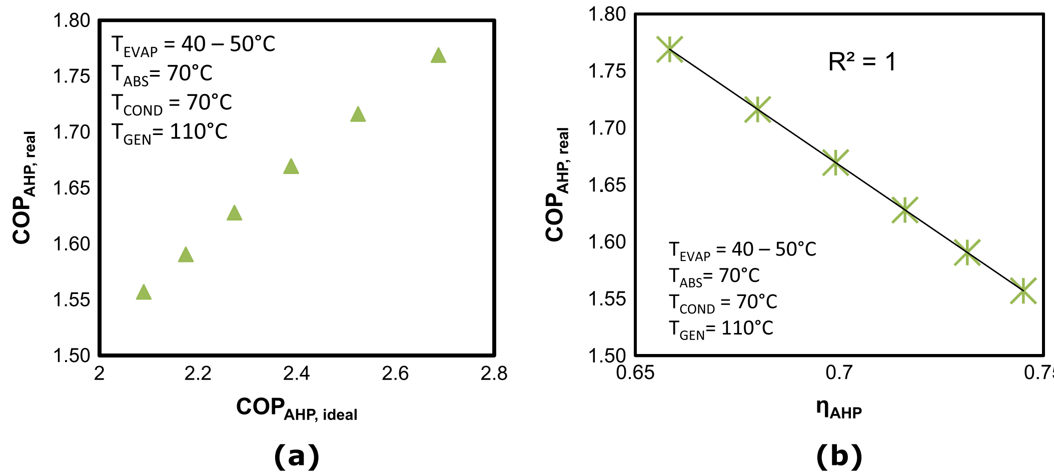

Fig. 7. (a) AHP real and ideal COP relationship, (b) linear relationship between the real COP and the efficiency factor.

Table 9
Values of *C* and *D* for a water/lithium bromide absorption heat pump.

T_{GEN} (°C)	T_{EVAP} (°C)	$T_{COND} = T_{ABS}$ (°C)	*C*	*D*
90	$20 < T_{EVAP} < 30$	50	−2.5064	3.4299
100	$20 < T_{EVAP} < 30$	50	−0.7448	2.2099
	$30 < T_{EVAP} < 40$	60	−2.9497	3.7592
110	$20 < T_{EVAP} < 30$	50	−0.5081	2.0366
	$30 < T_{EVAP} < 40$	60	−0.7478	2.2099
	$40 < T_{EVAP} < 50$	70	−2.4461	3.3795
140	$40 < T_{EVAP} < 50$	80	−1.7978	2.8816

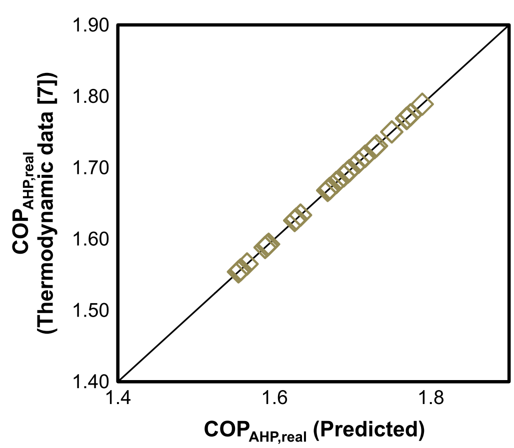

Fig. 8. Validation of absorption heat pump model.

in Fig. 7(b). The linear representation will guarantee a global optimum when embedded in complex optimisation frameworks for industrial energy systems.

$$COP_{AHP,real} = C \times (\eta_{AHP}) + D \tag{8}$$

Eqs. (7) and (8) are solved simultaneously to determine the real COP and the efficiency factor. Parameters *C* and *D* were determined from thermodynamic data provided by Eisa [7] for a range of heat source and heat sink temperatures and changing salt concentrations (Table 9). Validation of the model is shown in Fig. 8.

2.3. Absorption heat transformers (AHT)

A heat transformer consists of an evaporator, an absorber, an economiser, a generator and a condenser. The arrangement is similar to an absorption heat pump, but by contrast, the condenser and generator work at low pressure and the evaporator and absorber work at high pressure (Fig. 9(a)). Waste heat is added at a lower temperature in the generator to vaporise part of the working fluid from the weak salt solution. The vaporised working fluid is condensed, releasing heat at a reduced temperature (ambient conditions). The condenser outlet is pumped to the evaporator in the higher pressure zone. Vaporisation of the working fluid occurs in the evaporator when waste heat is added at an intermediate temperature. The vaporised working fluid then flows to the absorber, where it is absorbed in a strong salt solution from the generator, delivering heat at a high temperature. Finally, the weak absorbent solution leaving the absorber preheats the strong solution entering the absorber from the generator, prior to having its pressure reduced and returning to the generator. The AHT is shown on the thermodynamic equilibrium diagram for water/lithium bromide in Fig. 9(b). Salt concentrations are determined in a similar way with the absorption heat pump.

The ideal COP is calculated for a theoretically ideal situation where the change in entropy for the system is zero and a thermodynamically reversible process occurring in the evaporator and condenser [27]. The ideal COP is shown in Eq. (9). Derivation of the ideal COP is provided in Appendix A. The real COP is expressed in terms of the useful heat output to the heat input as shown in Eq. (10). In most cases the power input from liquid pumping is negligible [21–23,27]. An efficiency factor is introduced to represent the ratio of the real COP to the ideal COP (Eq. (11)).

$$COP_{AHT,ideal} = \left(\frac{(T_{EVAP} - T_{COND}) \times T_{ABS}}{((T_{EVAP} - T_{COND}) \times T_{GEN}) + ((T_{ABS} - T_{GEN}) \times T_{EVAP})} \right) \tag{9}$$

$$COP_{AHT,real} = \frac{Q_{ABS}}{Q_{GEN} + Q_{EVAP} + W_{PUMP}} \tag{10}$$

$$COP_{AHT,real} = \eta_{AHT} \times COP_{AHT,ideal} \tag{11}$$

Similar to the absorption heat pump, Eq. (12) is introduced. Temperatures in Eqs. (9), (11) and (12) are in Kelvin (K).

$$COP_{AHT,real} = E \times (\eta_{AHT}) + F \tag{12}$$

The working fluid non-ideal behaviour and system component inefficiencies are represented using the factor in Eqs. (11) and (12). Parameters *E* and *F* were determined from thermodynamic data provided by Eisa et al. [27] for a range of system temperatures (Table 10). Validation of the model is shown in Fig. 10.

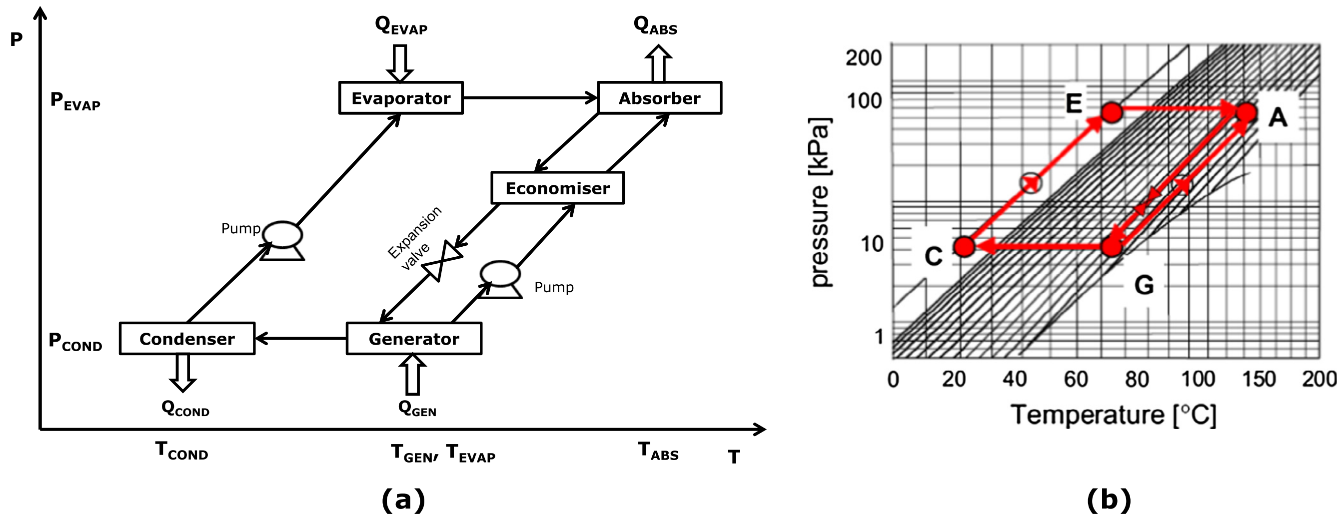

Fig. 9. (a) Absorption heat transformer schematic, (b) absorption heat transformer representation on refrigerant vapour pressure curve (Costa et al. [32]).

Table 10
Values of E and F for a lithium bromide/water absorption heat transformer for T_{COND} = 30 °C.

T_{EVAP} (°C)	T_{ABS} (°C)	T_{GEN} (°C)	E	F
40	$60 < T_{ABS} < 90$	$50 < T_{GEN} < 80$	0.6356	−0.0549
50	$70 < T_{ABS} < 100$	$50 < T_{GEN} < 80$	0.6303	−0.0461
60	$80 < T_{ABS} < 110$	$50 < T_{GEN} < 80$	0.6270	−0.0392
70	$90 < T_{ABS} < 120$	$50 < T_{GEN} < 80$	0.6190	−0.0305
80	$100 < T_{ABS} < 130$	$50 < T_{GEN} < 80$	0.5797	−0.00704
90	$120 < T_{ABS} < 140$	$60 < T_{GEN} < 80$	0.6568	−0.0407

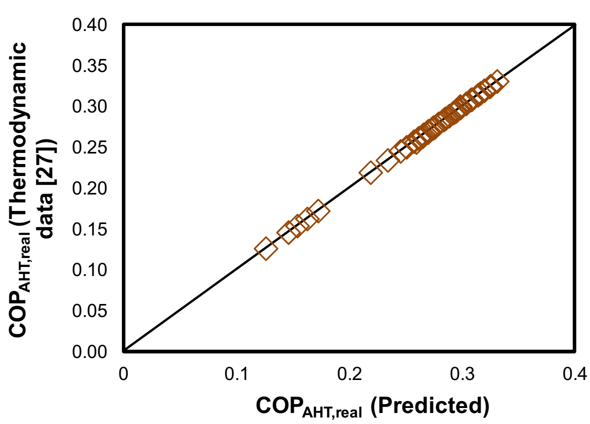

Fig. 10. Validation of absorption heat transformer model.

3. Primary fuel recovery ratio (PRR)

The coefficient of performance has been applied to evaluate and compare different heat upgrading technologies. However, applying the COP neglects the electrical power generation efficiency for a mechanical heat pump or missed opportunity for steam generation when high temperature heat separates the working fluid pair in the generator of an absorption heat pump. Therefore in this work, the primary fuel recovery ratio (PRR) is introduced for screening and comparing between technology options for low-grade heat upgrade.

Upgraded heat can reduce hot utility (for example steam) required by site processes which in turn reduces the primary fuel required in site cogeneration systems. Fig. 11 illustrates the possible interactions between technologies for low-grade heat upgrade, waste heat sources, sinks for recovered energy and interconnected systems.

Waste heat from site processes and the cogeneration system (usually rejected to cooling water and air) occurs over a wide temperature range i.e. low temperature (LT), medium temperature (MT) and high temperature (HT). Absorption heat pumps (AHP) upgrade LT and MT heat using HT heat to separate the working fluid, the quality of useful heat upgraded is between the LT (MT) and HT. There could be missed opportunities for steam generation from waste heat, especially at high temperature. In absorption heat transformers (AHT), LT heat is upgraded using MT heat to produce a higher temperature useful heat. In this case steam generation may be possible from the HT waste heat available on a site. Mechanical heat pumps (MHP) on the other hand can upgrade LT or MT heat to a higher temperature using electrical power. Generating power to drive the MHP will require additional primary energy from which waste heat is generated.

To capture these energy flows, the primary fuel recovery ratio is introduced in this work (PRR). The PRR measures the reduction in primary fuel required as a result of upgraded heat. It is defined as the savings in primary fuel per unit waste heat available. A general expression is shown in Eq. (13).

$$PRR = \frac{\Delta Q_{fuel(1)} - \Delta Q_{fuel(2)}}{Q_{WH(1)} + Q_{WH(2)}} \tag{13}$$

where $\Delta Q_{fuel(1)}$ refers to the change in primary fuel consumed in the site cogeneration system and $\Delta Q_{fuel(2)}$ is the additional primary energy required to provide power for a MHP. For the denominator terms, $Q_{WH(1)}$ refers to waste heat rejected to cooling water and air from the site processes and cogeneration system, $Q_{WH(2)}$ is the additional waste heat generated from power produced for the MHP. $Q_{WH(2)}$ depends on the power generation efficiency (η_{power}).

The change in primary fuel consumed in the site cogeneration system is determined using the cogeneration efficiency:

$$\eta_{cogen} = (Q_{steam} + W_{produced})/Q_{fuel} \tag{14}$$

This implies that additional heat upgraded has potential to reduce the primary fuel with respect to the cogeneration efficiency:

$$\Delta Q_{fuel(1)} = Q_{upgraded}/\eta_{cogen} \tag{15}$$

The change in primary fuel ($\Delta Q_{fuel(2)}$) associated with power required for a mechanical heat pump is defined by Eq. (16):

$$\Delta Q_{fuel(2)} = (Q_{upgraded})/(\eta_{power} \times COP_{MHP,real}) \tag{16}$$

The PRR is given in Eqs. (17)–(19) for a MHP, an AHP and an AHT. The real COPs are calculated from Eqs. (3), (7) and (11) respectively. The liquid pumping requirement in AHPs and AHTs are negligible. Derivations of the PRR in Eqs. (17)–(19) are provided in Appendix B.

$$PRR_{MHP} = \frac{\left[\left(\frac{Q_{EVAP}}{COP_{MHP,real}-1}\right) \times \left(\frac{COP_{MHP,real}}{\eta_{cogen}} - \frac{1}{(\eta_{power})}\right)\right]}{Q_{WH(1)} + \left[\left(\frac{Q_{EVAP}}{COP_{MHP,real}-1}\right)\left(\frac{1-\eta_{power}}{\eta_{power}}\right)\right]} \tag{17}$$

$$PRR_{AHP} = \frac{(Q_{GEN} \times COP_{AHP,real})}{\eta_{cogen} \times Q_{WH(1)}} \tag{18}$$

$$PRR_{AHT} = \frac{(Q_{EVAP} + Q_{GEN}) \times COP_{AHT,real}}{\eta_{cogen} \times Q_{WH(1)}} \tag{19}$$

Apart from being used to compare between options, the PRR can determine the best combination of heat source temperatures and duties, heat sink temperatures and duties for any heat pump application. Higher savings in hot utility and primary fuel may be obtained by applying the PRR for heat pump analysis in process sites.

4. Methodology for applying PRR for heat pump analysis in process sites

The methodology is useful for determining the best combination of heat source temperatures and heat sink temperatures for a technology and selecting between heat upgrading technologies.

The methodology begins with generating temperature–enthalpy plots for heat rejected to cooling water and air [9]. To generate the plots, data for streams on cold utility heat exchangers are extracted and the temperatures shifted by ΔT_{min} for feasible heat recovery. The enthalpy on the x-axis represents the cumulative heat transferred. To analyse the profile, temperature intervals (T_i) are introduced. These temperature intervals represent the beginning and end of a stream as illustrated in Fig. 12(a), the horizontal line in Fig. 12(b) represent the duties selected to keep hot streams hot.

Temperature–enthalpy plots for streams on hot utility similar to the site sink profile [30] are also generated. The heat sink plots are divided into temperature regions (T_r) depending on the steam distribution pressure levels (Fig. 13(a)). Within any region, the profile is subdivided into temperature intervals (T_{ri}) similar to the waste heat source profile (Fig. 12(b)). Low grade heat is upgraded to any T_{ri} below the T_r to reduce hot utility requirements, and above the T_r for possible steam generation from upgraded heat. The demand for recovered energy is between the actual duty

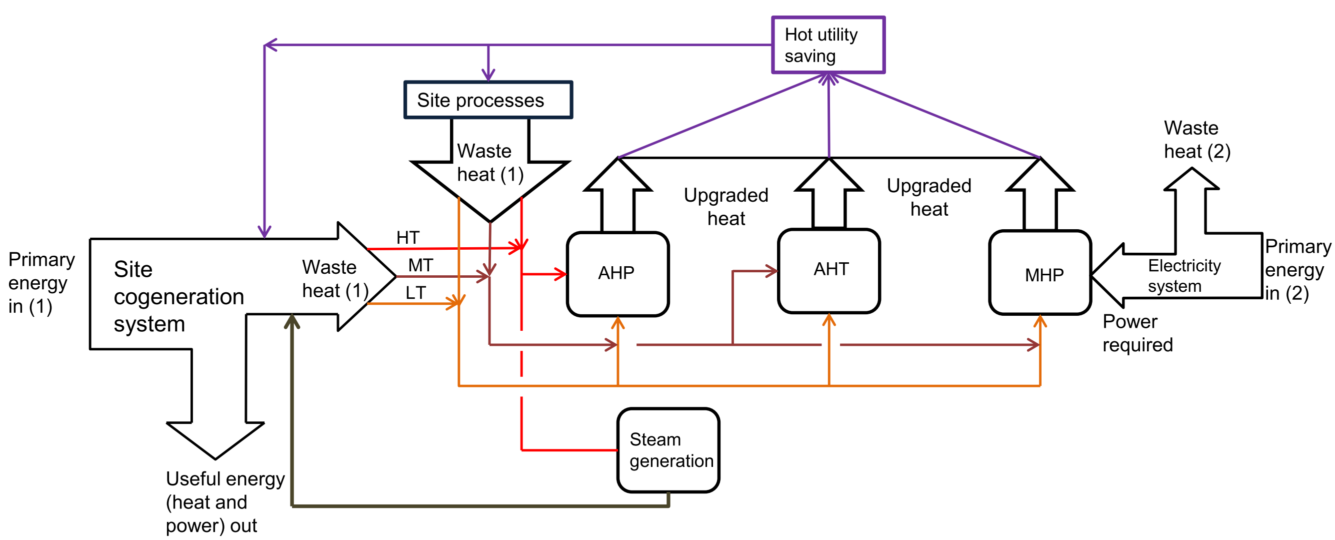

Fig. 11. Energy flows for waste heat recovery through heat upgrade.

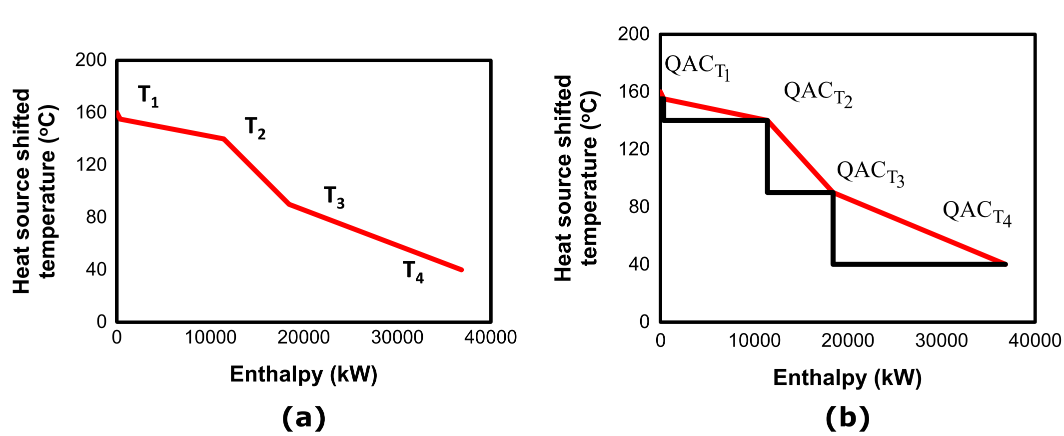

Fig. 12. (a) Example waste heat source profile, (b) profile showing temperature intervals.

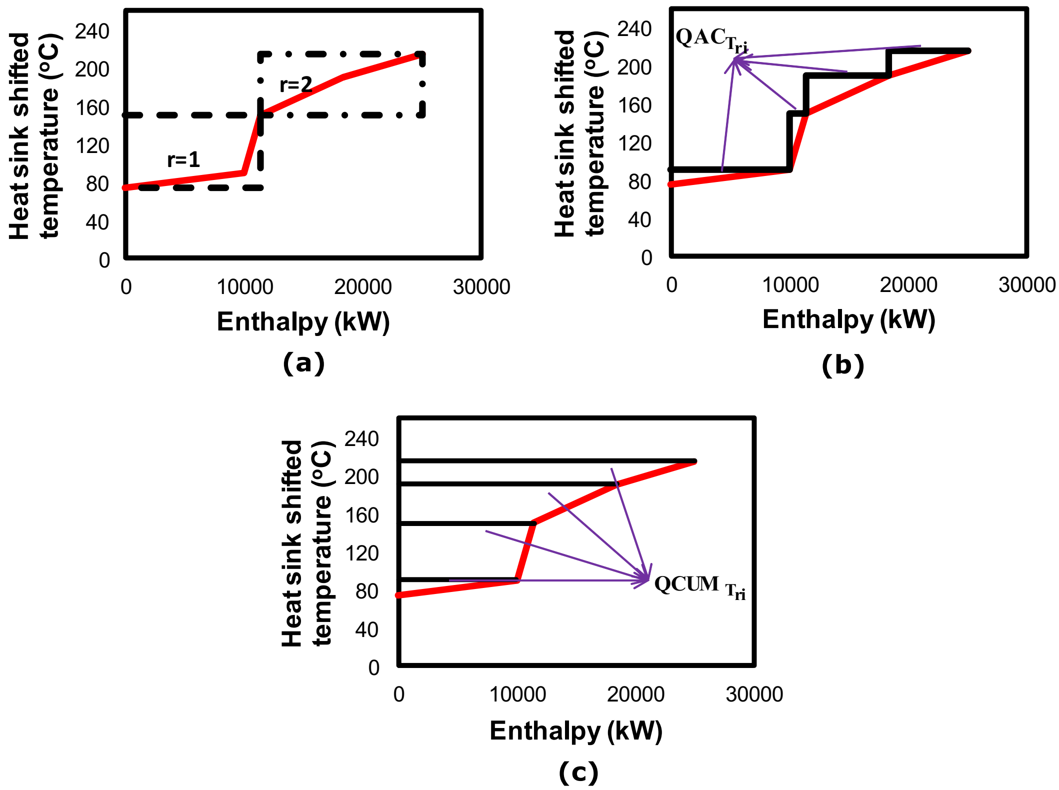

Fig. 13. Example heat sink profile (a) divided into temperature regions, T_{ri}, (b) subdivided into temperature intervals and actual duties ($QAC_{T_{ri}}$), (c) cumulative duties at the temperature intervals ($QCUM_{T_{ri}}$).

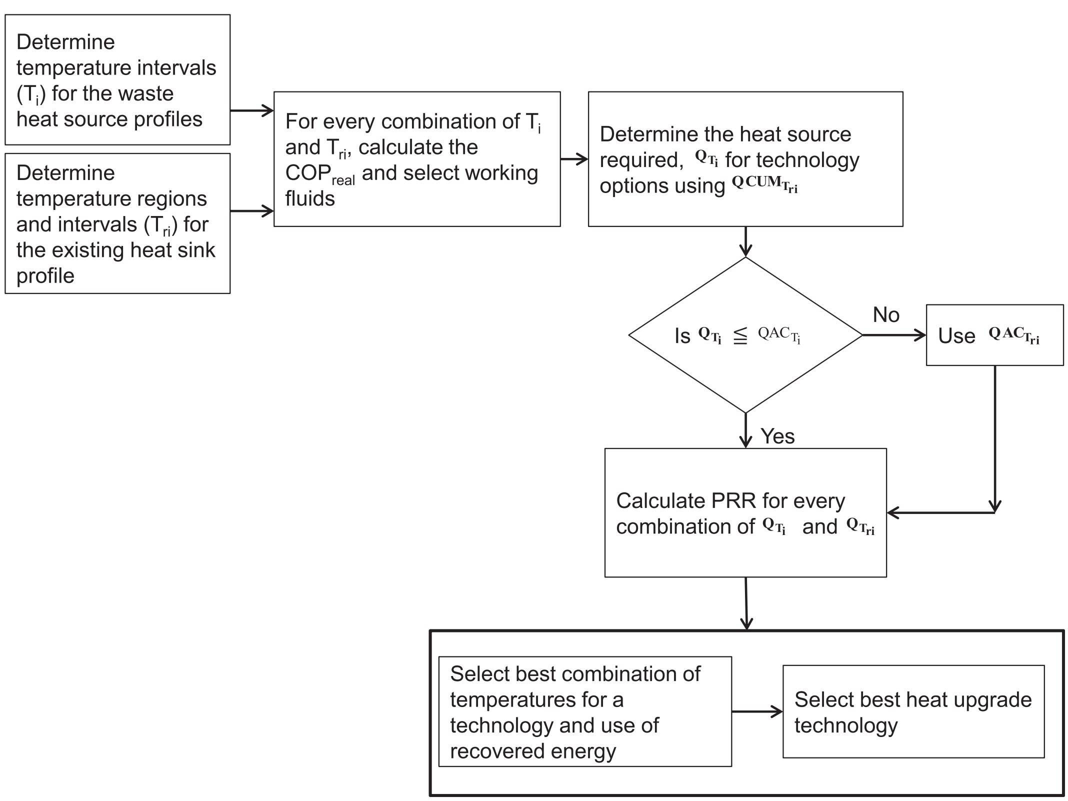

Fig. 14. Methodology flow chart for using the PRR to screen and select heat upgrade technologies and system temperatures.

QAC at T_r (T_{ri}) as shown in Fig. 13(b), and the cumulative duty, QCUM as shown in Fig. 13(c) and this depends on if there is available heat source.

The methodology is summarised in the flow chart in Fig 14.

5. Case study

The case study presented is for a medium scale petroleum refinery [31]. Stream data for heat rejected to cooling water and air from the site processes and the cogeneration system are shown in Tables 11 and 12 respectively. The heat rejected to cooling water is from the seven processing units i.e. crude/vacuum distillation unit, diesel hydrotreaters, fluidised catalytic cracking unit, kerosene hydrotreaters, platformers and visbreaker. Analysis of this refinery for power, direct heat and chilling generation from the available waste heat is done by Oluleye et al. [9].

Heat rejected to air is from the exhaust of fired heaters in some processing units (the crude distillation unit, naphtha hydrotreaters and platformer) and the coal boiler in the cogeneration system. The existing site cogeneration system (Fig. 15) comprises a coal boiler generating 66.753 kg/s of very high pressure steam, a gas turbine generating 17,500 kW electrical power with a heat recovery steam generator (HRSG) producing 31 MW of steam from the gas turbine exhaust. The system has 5 pressure levels (distribution mains) with 4 back pressure turbines, 1 extraction turbine and 4 expansion valves. In total, 76,542 kW of electrical power is generated and 52,503 kW of steam are generated from the site cogeneration system. The site cogeneration efficiency estimated using Eq. (14) is 46%.

5.1. Heat source and sink profiles

Based on the data extracted for heat rejected to cooling water in Table 11 and shifting the temperatures by an appropriate $\Delta T_{\min}$ (in this case 10 °C), the profile for heat rejected to cooling water is shown in Fig. 16(a). In order to exploit the waste heat, the profile is divided into temperature intervals (T_i) in Fig. 16(b). The temperature intervals are selected based on the target and supply temperatures of the streams; beginning from the highest target temperature ensures that high temperature heat is exploited before low temperature heat [9].

Using the same analysis for heat rejected to air in Table 12, the profile is shown in Fig. 17(a). The temperature interval is the horizontal line in Fig. 17(b). There is potential to generate 24,165 kW of LP steam (Fig. 17(c)) from the heat that was rejected to air. The available heat could also drive the separation of refrigerant/absorbent mixture in the generator of an absorption heat pump.

Sinks for the upgraded heat include the streams on hot utility. The existing heat sink profile is shown in Fig. 18(a) for all hot utility (from VHP to LP) and Fig. 18(b) for heat sinks using MP and LP steam which is considered in this work based on the feasible operating range of technologies.

The heat sink profile is divided into 2 regions representing the steam expansion levels, Fig. 18(b). It may be possible to use the heat upgraded to reduce steam demand from processes at temperatures below the steam saturation temperature as shown in Fig. 19 (a). The heat source can be upgraded to any of these temperature regions and intervals using the actual heat required in Fig. 19(a) or the cumulative heat required in Fig. 19(b).

Combinations of possible heat source and heat sink temperatures and duties from Figs. 16(b) and 19(a) and (b) are shown in Tables 13 and 14.

The objective of this case study is to determine the best combination of heat source (Q_{T_i}) and sink temperatures ($Q_{T_{ri}}$) for a technology and the best heat upgrading technology that maximises the potential to save primary fuel in the site. Water/lithium bromide is the working fluid pair for absorption systems (i.e. heat pump and heat transformer). For mechanical heat pumps, the real coefficient of performance is applied to select the working fluid (Fig. 5).

5.2. Low grade heat upgrading technology application

In this section, the COP and PRR are used to determine the best combinations of heat source and sink temperatures, and associated duties. This present work is based on the premise that taking into account interconnected systems using the PRR could yield more savings in primary fuel, compared to applying the COP for heat pump analysis in process sites. Incorporating the MHP is presented in Section 5.2.1, the AHP in Section 5.2.3 and the AHT in Section 5.2.3.

Table 11
Stream data for heat rejected to cooling water.

Stream No.	Unit	T_{SUPPLY} (°C)	T_{TARGET} (°C)	Q (kW)
Hot 1	Crude/vacuum distillation unit	116.8	31.1	5970
Hot 2		116.8	50.5	106
Hot 3		50.5	49.7	58
Hot 4		50.5	31.1	2810
Hot 5		50.5	31.1	2960
Hot 6	Diesel hydrotreaters	112.97	26	330
Hot 7		112.97	30	1240
Hot 8		112.97	34	4540
Hot 9	Fluidised catalytic cracking unit	140.9	37.51	950
Hot 10		140.9	104	220
Hot 11		104	51	810
Hot 12		140.9	104	200
Hot 13		140.9	90	1150
Hot 14		104	38	10,700
Hot 15		104	27.61	2780
Hot 16	Kerosene hydrotreaters	140.6	30	560
Hot 17		136.1	27.2	19
Hot 18		140.6	33.3	2880
Hot 19	Naphtha hydrotreaters	101.7	88.3	331
Hot 20		67.2	61.7	560
Hot 21		67.2	50	3290
Hot 22		67.2	33.9	1914
Hot 23	Platformer	67.2	36.7	1930
Hot 24		73.84	26.7	1160
Hot 25		67.2	32.2	1390
Hot 26		73.84	67.2	84.7
Hot 27		67.3	25.7	35.6
Hot 28		67.2	27.2	3020
Hot 29		67.2	32.2	330
Hot 30		43.3	26.3	81
Hot 31		73.84	65	16
Hot 32		73.84	32.2	320
Hot 33	Visbreaker	134.88	30.01	2050
Hot 34		134.88	75	1150
Hot 35	Cogeneration system	90.1	90	131,150

Table 12
Stream data for heat rejected to air.

Stream No.	Name	T_{SUPPLY} (°C)	T_{TARGET} (°C)	Q (kW)
1	Crude distillation unit fired heater exhaust	320.1	150	4440
2	Naphtha hydrotreaters fired heater exhaust	328.4	150	35
3	Platformer fired heater exhaust	320.1	150	1360
4	Coal boiler fired heater exhaust	291.3	150	18,330

5.2.1. Mechanical heat pump application

The MHP is applied to upgrade low temperature waste heat source available in this medium scale refinery (depicted in Table 13), to satisfy the heat sinks in Table 14.

The explicit thermodynamic models for the MHP developed in Eqs. (1)–(4) are applied to evaluate the real (theoretical) COP for the possible temperature combinations in Tables 13 and 14. Working fluid is selected based on Fig. 5, and parameters *A* and *B* are contained in Tables 3–8. In Fig. 20, the real COP is plotted against the heat source shifted temperature (which is the evaporator temperature for the MHP). Temperatures in the legend represent the possible heat sink temperatures from Table 14. The coefficient of performance increases as the difference between the heat sink and heat source temperature decreases.

The real (theoretical) COP is highest for a MHP upgrading heat from 92.3 °C to 95.6 °C, this occurs at the lowest temperature lift (3.3 °C). Incorporating a MHP produces 580 kW of heat at 95.6 °C to reduce the hot utility required for this site. The power required is 7.62 kW. This also implies additional 24169.1 kW of LP steam can be generated from heat that was rejected to air as shown in Fig. 17(c). However, using the COP neglects interactions with interconnected systems as shown in Fig. 11.

The Primary Fuel Recovery Ratio (PRR) developed for a MHP in Eq. (17) shows interactions with interconnected systems. Method-

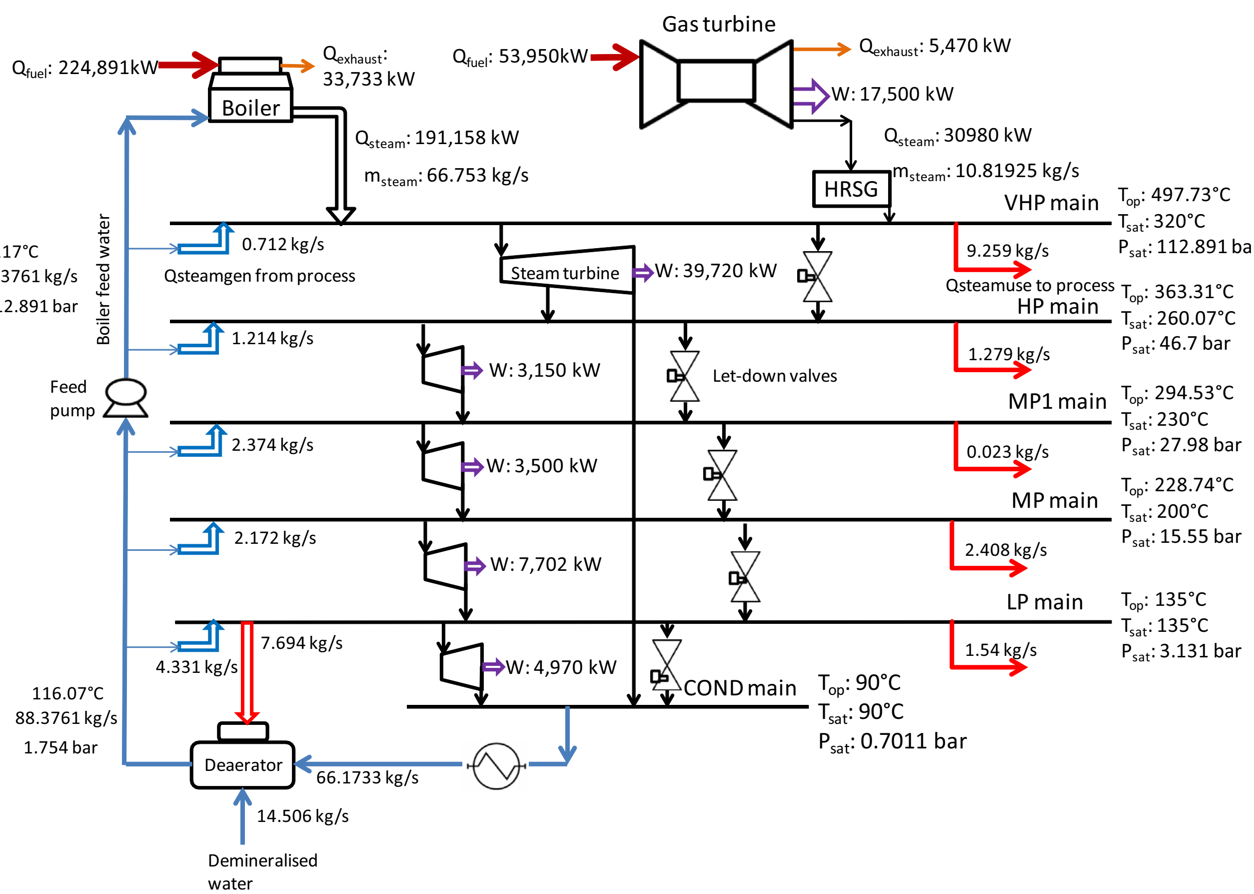

Fig. 15. Site cogeneration system configuration.

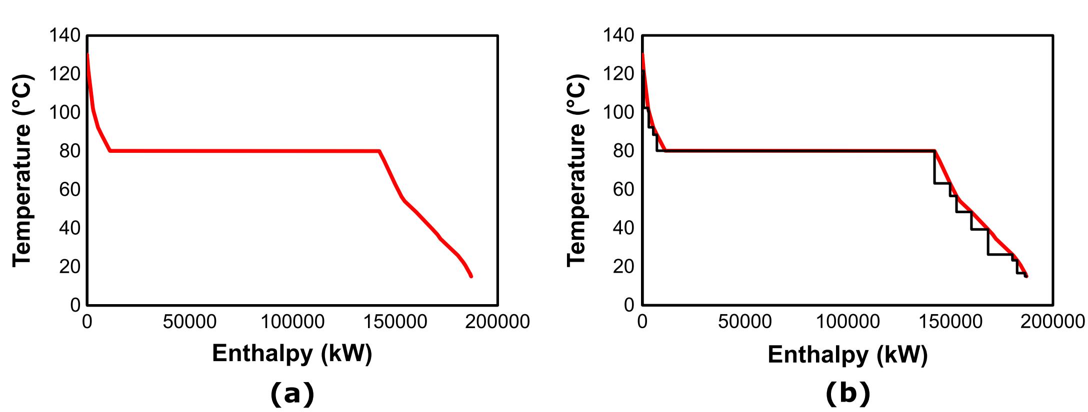

Fig. 16. (a) Profile for heat rejected to cooling water, (b) profile showing temperature intervals.

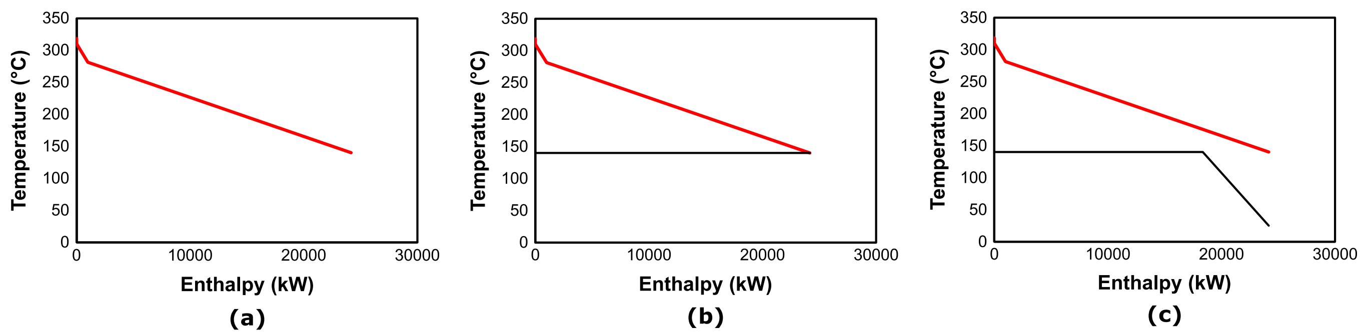

Fig. 17. (a) Profile for heat rejected to air, (b) profile showing temperature interval, (c) profile showing potential for steam generation.

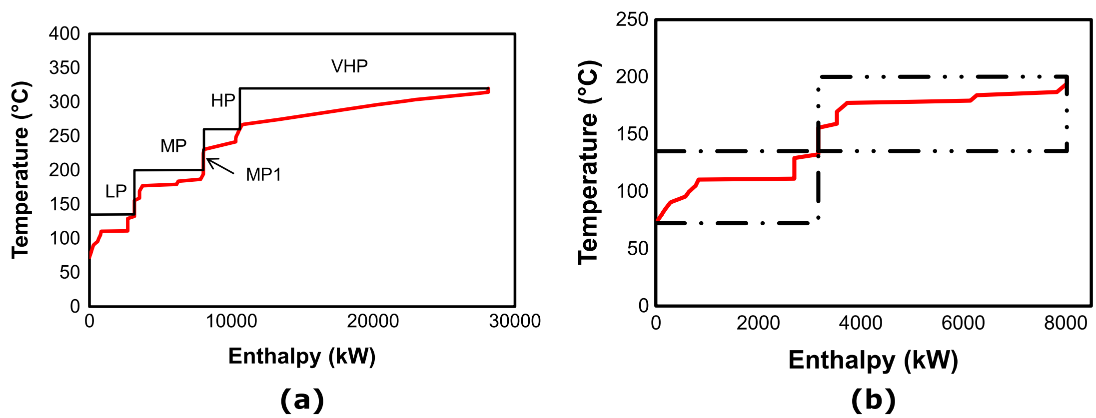

Fig. 18. (a) Site sink profile, (b) profile showing temperature regions for MP and LP steam use.

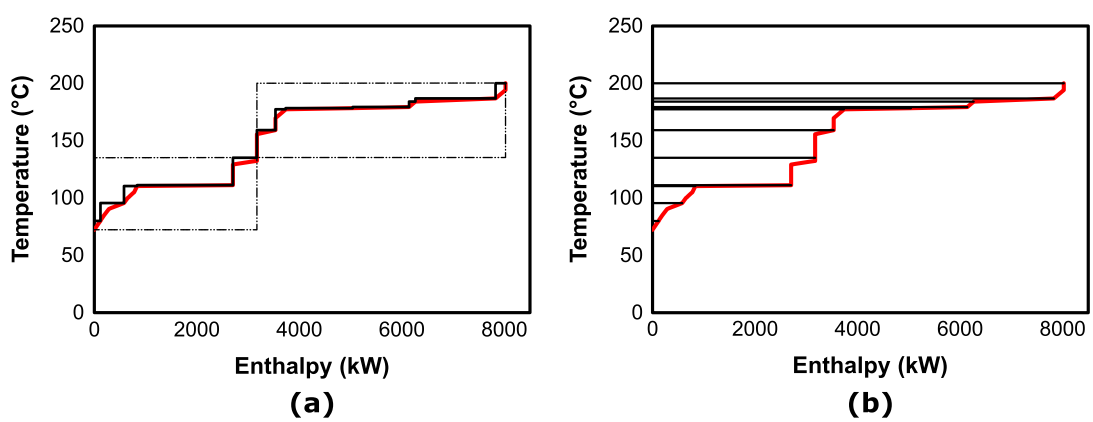

Fig. 19. Temperature regions r and interval i on the existing site sink profile for (a) actual heat required $QAC_{T_{ri}}$ (b) cumulative heat required $QCUM_{T_{ri}}$.

Table 13
Heat source profile temperature intervals and duties.

Heat source shifted temperature (°C)	QAC_{T_i} (kW)
130	0
121.58	597
102.37	2190
100.7	320
92.3	2195
88.4	1810
80.1	4050
80	131,200
63.24	7600
56.7	3090
48.4	7290
39.3	8110
26.3	11,900
23.31	2260
16.71	3860

Table 14
Heat sink profile temperature intervals and duties.

Heat sink shifted temperature (°C)	$QAC_{T_{ri}}$ (kW)	$QCUM_{T_{ri}}$ (kW)
80	120	120
95.6	460	580
110.4	260	830
111.144	1872	2706
135	466	3172
159.07	364	3540
177.2	200	3740
178.3	1308	5043
179.225	1100	6143
183.9	120	6260
200	194	8026

ology for applying the PRR was presented in Fig. 14 above. Fig. 21 shows the PRR as a function of heat source shifted temperature (equivalent to the MHP evaporator temperature). The efficiency of electrical power generation for the mechanical heat pump is assumed to be 40%. The objective is to select the combination of heat source and sink temperature to maximise primary fuel reduction.

The PRR is highest when a MHP is incorporated to upgrade heat at 102.37–111.144 °C. In this case, 2705.98 kW of hot utility is saved, 97.717 kW of electrical power is required and 24169.1 LP steam can be generated from heat rejected to air (Fig. 17(c)). An additional 2126 kW of hot utility is saved when the PRR is applied compared to the COP.

5.2.2. Absorption heat pump application

The AHP upgrades low temperature waste heat to medium temperature, using a higher temperature heat source to separate the working fluid pair in the generator. The COP is calculated using Eqs. (5), (6). Values of C and D are contained in Table 9.

Considering the possible range of water/LiBr AHP in Table 9 and the available heat source temperatures in Table 13, and heat sink temperatures in Table 14, the AHP can be incorporated to upgrade heat between 40 and 50 °C, to satisfy a hot utility at 80 °C. In this case, heat at 140 °C is required to drive the separation of the working fluid pair in the generator. The heat is available from heat rejected to air in Fig. 17(a). However, this reduces the quantity of LP steam generated from heat rejected to air.

At these operating points the COP of the AHP is 1.67 and the PRR is 0.2492 (using Eq. (18)). 120 kW of hot utility is saved and 24, 097 kW of LP steam generated from heat rejected to air. This reduces the site primary fuel by 18.8%.

5.2.3. Absorption heat transformer application

The AHT is applied to upgrade low temperature waste heat to a higher temperature using low to medium temperature heat in the

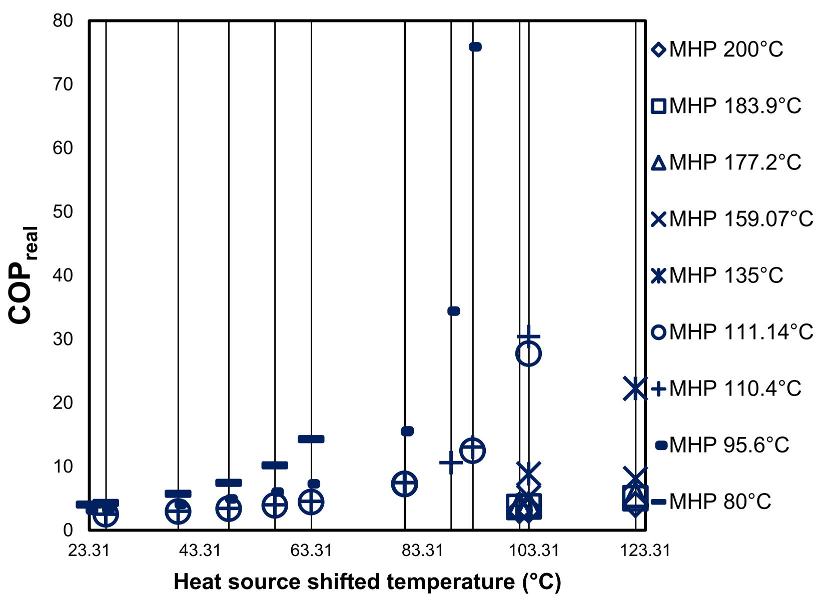

Fig. 20. Calculated real coefficient of performance for the MHP.

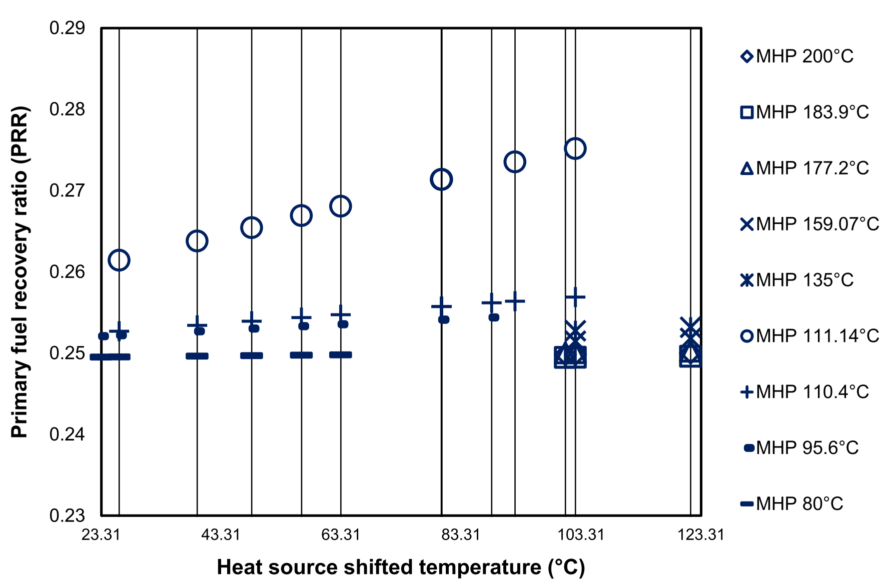

Fig. 21. Primary fuel recovery ratio for the MHP.

generator. The COP is calculated using Eqs. (9)–(12). Values of E and F are provided in Table 10.

Fig. 22 shows the real COP plotted against the heat source shifted temperature for possible temperature combinations in Tables 13 and 14. The legend in Fig. 22 shows the heat sink temperatures.

The highest COP is obtained by upgrading heat from 63.24 °C to 110.4 °C; heat at 80 °C drives the generator. 834 kW of hot utility is saved and an additional 24,169 kW of low pressure steam is generated from the heat rejected to air (Fig. 17(c)). However, the COP neglects interactions with interconnected systems. It may be possible to save more hot utility by applying the PRR for the AHT calculated using Eq. (19).

Fig. 23 shows the PRR for the AHT based on temperature combinations in Tables 13 and 14.

The PRR is highest for an AHT, when low grade heat at 63.24 °C is upgraded to the sink at 111.14 °C. The generator for the AHT is driven by heat at 80 °C. In this case, 2706 kW of hot utility is saved and an additional 24,169 kW of LP steam generated from heat that was rejected to air (Fig. 17(c)). Overall, an additional 1872 kW of hot utility is saved when a system-oriented criterion is applied to incorporate heat pumps compared to using the COP.

5.3. Case study summary

Analysis in Sections 5.2.1–5.2.3 show that using the PRR can achieve higher savings in hot utility compared to using the COP. The methodology developed can also determine the heat pump options and associated temperatures that yield the highest reduction in primary fuel.

The PRR for all heat upgrading options is shown in Fig. 24. Integrating an AHT to upgrade heat from 63.24 °C to 111.14 °C has the highest PRR. The impact on primary fuel from all three heat pumping technologies is shown in Table 15. The site cogeneration

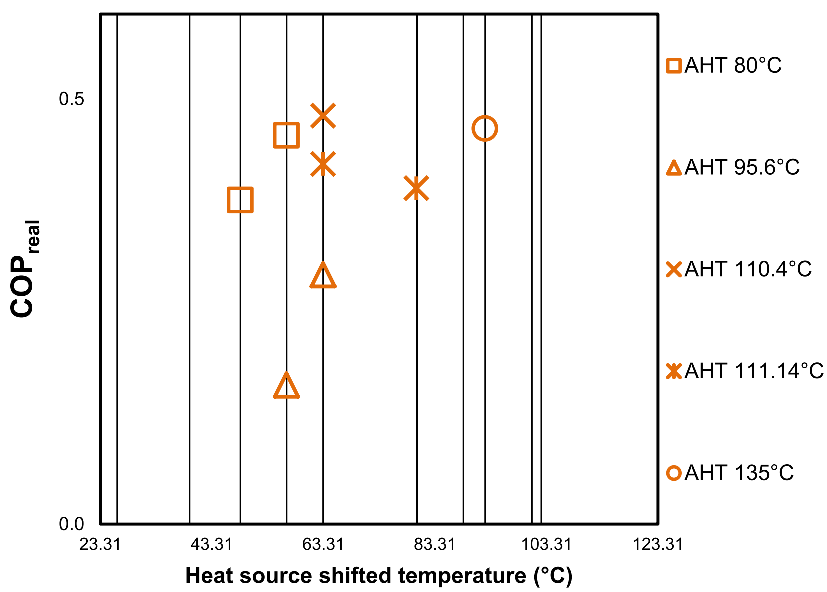

Fig. 22. Calculated real coefficient of performance for the AHT.

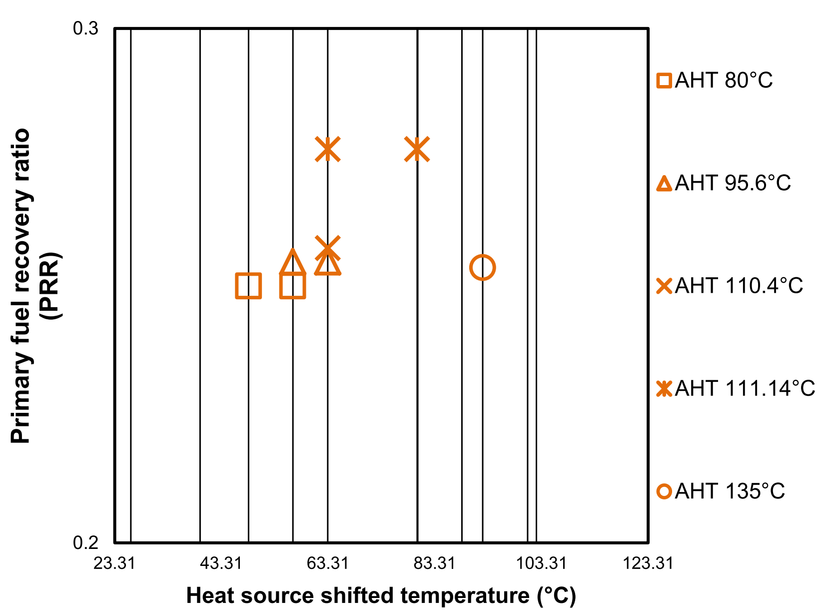

Fig. 23. Primary fuel recovery ratio for the AHT.

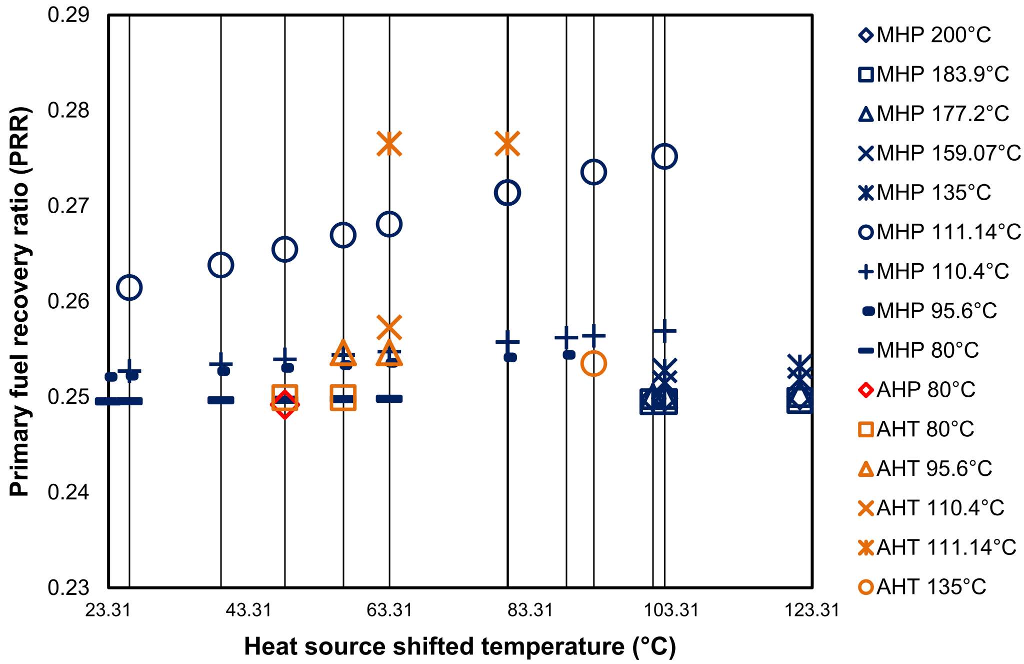

Fig. 24. Screening heat pump options using the PRR.

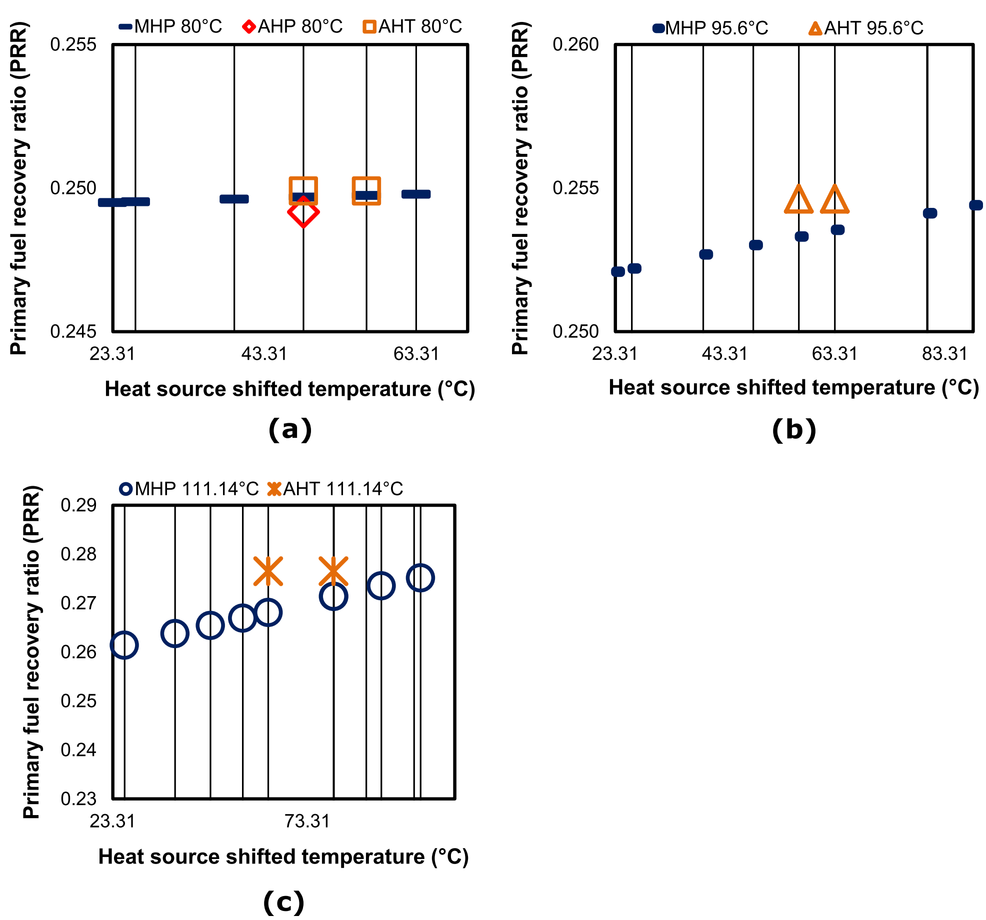

Fig. 25. Screening heat pumps options based on the same temperature lift (a) 80 °C heat sink temperature, (b) 95.6 °C heat sink temperature and (c) 111.14 °C heat sink temperature.

Table 15
Primary fuel savings from heat pumping options.

Heat pump type	Selection criterion	Hot utility saved (kW)	LP steam generated (kW)	Power required (kW)	Primary fuel saved (kW)
MHP	Highest COP	580	24,169	7.62315	53,783
	Highest PRR	2706	24,169	97.72	58,179
AHP	Highest COP	120	24,097	–	52,645
	Highest PRR	120	24,097	–	52,645
AHT	Highest COP	834	24,169	–	54,354
	Highest PRR	2706	24,169	–	58,423

efficiency is 46% and power generation efficiency for the MHP is 40%.

Additional savings in primary fuel is possible when a system-oriented criterion is used for heat pump analysis in process sites. For the MHP, an additional 8.17% reduction in primary fuel is possible when the PRR is applied compared to the COP. An additional 7.45% savings in primary fuel is achieved using the PRR compared the COP for the AHT.

A MHP is selected when the highest COP determines the heat pump option for this site. About 53,783 kW reductions in primary fuel are possible. However, an AHT is selected using the PRR, saving primary fuel by 58,423 kW. This implies additional 9.2% savings in primary fuel is possible when the PRR determines the best heat pumping scheme for this site. This implies for the whole system analysis, an AHT requires less fuel, but a MHP can achieve higher temperature lifts.

In Fig. 25 the three heat pump types are compared for the same temperature lift (i.e. difference between the heat source temperature to be upgraded and the heat sink temperature) based on the PRR. Fig. 25(a) shows the comparison for a heat sink temperature of 80 °C, 95.6 °C in Fig. 25(b) and 111.14 °C in Fig. 25(c). The heat upgraded in Fig. 25(a) is 120 kW; Fig. 25(b) is 580 kW and Fig. 25(c) 2706 kW as shown in Table 14. The PRR for mechanical heat pumps increases with a reduction in temperature lift. At low quantities of useful heat upgraded, the difference in the PRR for the technologies is negligible. However, as the quantity of useful heat upgraded increases, the influence of temperature lift on the PRR is more noticeable.

6. Conclusions and future work

Low-grade heat upgrade can indeed reduce the primary fuel requirement of process sites. The challenges associated with applying heat upgrading technologies such as mechanical heat pumps, absorption heat pumps and absorption heat transformers is in modelling of these options to analyse the diverse range of waste heat sources and sinks for upgraded heat without additional complexities, screening of technology options, selection of operating temperatures (i.e. heat source and sink) and the use to which the recovered energy is put. In this work the challenges are addressed by proposing thermodynamic models for heat upgrading technologies, a systems-oriented criterion (primary fuel recovery ratio) for screening and selecting technology options and operating conditions and a graphical based methodology for screening and integrating heat upgrading technologies in process sites. The primary fuel recovery ratio measures the primary fuel saved from low-temperature heat upgrade taking into account the available waste heat in existing sites, primary fuel required to generate power for a MHP and the associated waste heat. The primary fuel recovery ratio considers other interconnected systems. The methodology is applied to a case study of a medium scale petroleum refinery.

The absorption heat transformer has the highest potential to reduce primary fuel compared to the other thermodynamic cycles considered in the case study. The primary fuel recovery ratio is 0.277, reducing primary fuel by 21%. The advantage of using an AHT is that the power required for liquid pumping is negligible compared with mechanical heat pumping and the temperature of heat required by the generator does not compete with steam generation. However results are case specific and detailed economic analysis is required to make final decisions.

Results also show an additional 8.17% and 7.45% savings in primary fuel is possible when the PRR is applied instead of COP to select operating temperatures for the MHP and AHT respectively. Therefore, higher savings in primary fuel and hot utility is possible when a systems-oriented screening criterion is applied.

The method proposed is applicable for preliminary screening and selection of technology options. Final decisions should be made based in economics (i.e. cost and benefits), operation safety as well as physical constraints in existing process sites. Future work will consider other heat pump types such as compression/absorption heat pumps and adsorption heat pumps.

Acknowledgement

The authors acknowledge financial support granted by members of Process Integration Research Consortium (PIRC) for the development of this research.

Appendix A. Derivation of the ideal performance of AHP and AHT

The performance of absorption heat pumps are measured by the coefficient of performance:

$$\mathrm{COP}_{\mathrm{AHP,real}} = \frac{Q_{\mathrm{ABS}} + Q_{\mathrm{COND}}}{Q_{\mathrm{GEN}} + W_{\mathrm{PUMP}}} \tag{A.1}$$

For an ideal cycle, the heat pump becomes a reversible Carnot engine in which the entropy change in the evaporator and condenser are equal [24]:

$$\frac{Q_{\mathrm{EVAP}}}{T_{\mathrm{EVAP}}} = \frac{Q_{\mathrm{COND}}}{T_{\mathrm{COND}}} \tag{A.2}$$

Also for an ideal cycle, the change in entropy for the whole system is zero, thus:

$$\frac{Q_{\mathrm{EVAP}}}{T_{\mathrm{EVAP}}} + \frac{Q_{\mathrm{GEN}}}{T_{\mathrm{GEN}}} = \frac{Q_{\mathrm{ABS}}}{T_{\mathrm{ABS}}} + \frac{Q_{\mathrm{COND}}}{T_{\mathrm{COND}}} \tag{A.3}$$

Combining Eqs. (A.2) and (A.3):

$$\frac{Q_{\mathrm{GEN}}}{T_{\mathrm{GEN}}} = \frac{Q_{\mathrm{ABS}}}{T_{\mathrm{ABS}}} \tag{A.4}$$

An overall energy balance, neglecting the energy input from the liquid pumping, gives:

$$Q_{\mathrm{EVAP}} + Q_{\mathrm{GEN}} = Q_{\mathrm{ABS}} + Q_{\mathrm{COND}} \tag{A.5}$$

Combining Eqs. (A.1)–(A.5) gives:

$$\mathrm{COP}_{\mathrm{AHP,ideal}} = 1 + \left(1 - \frac{T_{\mathrm{ABS}}}{T_{\mathrm{GEN}}}\right)\left(\frac{T_{\mathrm{EVAP}}}{T_{\mathrm{COND}} - T_{\mathrm{EVAP}}}\right) \tag{A.6}$$

The performance of the absorption heat transformer is measured by the coefficient of performance:

$$COP_{AHT,real} = \frac{Q_{ABS}}{Q_{GEN} + Q_{EVAP} + W_{PUMP}} \tag{A.7}$$

Eqs. (A.2)–(A.5) also apply to the absorption heat transformer. Combining Eqs. (A.7), (A.2)–(A.5), neglecting the energy input from the liquid pump:

$$COP_{AHT,ideal} = \frac{T_{ABS}(T_{EVAP} - T_{COND})}{T_{GEN}(T_{EVAP} - T_{COND}) + T_{EVAP}(T_{ABS} - T_{GEN})} \tag{A.8}$$

Appendix B. Derivation of primary fuel recovery ratio for MHP, AHP and AHT

The primary fuel recovery ratio (PRR) is given as:

$$PRR = \frac{\Delta Q_{fuel(1)} - \Delta Q_{fuel(2)}}{Q_{WH(1)} + Q_{WH(2)}} \tag{A.9}$$

Change in primary fuel consumed in the site cogeneration system

$$\Delta Q_{fuel(1)} = Q_{upgraded}/\eta_{cogen} \tag{A.10}$$

For a mechanical heat pump,

$$Q_{upgraded} = Q_{EVAP} + W_{COMP} \tag{A.11}$$

$$COP_{MHP,real} = \frac{Q_{upgraded}}{W_{COMP}} \tag{A.12}$$

Combining Eqs. (A.11) and (A.12) gives:

$$W_{COMP} = \frac{Q_{EVAP}}{(COP_{MHP,real} - 1)} \tag{A.13}$$

The additional primary energy required to provide power for a MHP is given as:

$$\Delta Q_{fuel(2)} = \frac{W_{COMP}}{\eta_{power}} \tag{A.14}$$

Combining Eqs. (A.13) and (A.14) gives:

$$\Delta Q_{fuel(2)} = \frac{Q_{EVAP}}{\eta_{power} \times (COP_{MHP,real} - 1)} \tag{A.15}$$

The additional waste heat generated from power produced for the MHP:

$$Q_{WH(2)} = \Delta Q_{fuel(2)} - W_{COMP} \tag{A.16}$$

Combining Eqs. A.13, A.15 and A.16 gives:

$$Q_{WH(2)} = \frac{Q_{EVAP}}{(COP_{MHP,real} - 1)}\left(\frac{1 - \eta_{power}}{\eta_{power}}\right) \tag{A.17}$$

The PRR for a MHP is derived by combining Eqs. (A.9), (A.10), (A.12), (A.15) and (A.17).

$$PRR_{MHP} = \frac{\left[\left(\frac{Q_{EVAP}}{COP_{MHP,real}-1}\right) \times \left(\frac{COP_{MHP,real}}{\eta_{cogen}} - \frac{1}{(\eta_{power})}\right)\right]}{Q_{WH(1)} + \left[\left(\frac{Q_{EVAP}}{COP_{MHP,real}-1}\right)\left(\frac{1-\eta_{power}}{\eta_{power}}\right)\right]} \tag{A.18}$$

For an absorption heat pump, the COP is defined using Eq. (A.1). The liquid pumping requirement is negligible. By combining Eqs. (A.1), (A.9) and (A.10) the PRR is defined as:

$$PRR_{AHP} = \frac{(Q_{GEN} \times COP_{AHP,real})}{\eta_{cogen} \times Q_{WH(1)}} \tag{A.19}$$

For an absorption heat transformer, the COP is defined using Eq. (A.7). The liquid pumping requirement is negligible. By combining Eqs. (A.7), (A.9) and (A.10) the PRR is defined as:

$$PRR_{AHT} = \frac{(Q_{EVAP} + Q_{GEN}) \times COP_{AHT,real}}{\eta_{cogen} \times Q_{WH(1)}} \tag{A.20}$$

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Chapter 4: Comparing Technology Options for Waste Heat Utilization

The study conducted in Publications 1 and 2 show that thermodynamic cycles for waste heat recovery and heat recovery via heat exchange make waste heat utilization technically possible. In this chapter, a screening criterion and tool is developed for comparing between technology options for waste heat utilization, taking into account the heat source quality.

A comparative analysis of waste heat recovery technologies has been done based on the cycles real performance (Little and Garimella, 2011). Different first law performance definitions are used for each technology. For the organic Rankine cycle, the performance is defined as the net power output to useful heat input; which is less than 100%. The performance of absorption chillers is defined as chilling provided per unit heat input; which is less than 100%. The performance of absorption heat pumps is defined as heat upgraded in the condenser and absorber per unit heat input in the generator (greater than 100%). The performance of absorption heat transformers is defined as the useful heat upgraded in the absorber per unit heat input in the generator and evaporator (less than 100%). The performance of mechanical heat pumps is defined as the useful heat upgraded per unit power input (greater than 100%) and the performance of heat exchangers is 100% in the absence of distribution and transmission losses. Therefore, comparative analysis based on the first law performance is incoherent when multiple energy interactions occur. The energy balance provides no information on the energy degrading during a conversion process (Avanessian and Ameri, 2014).

Comparative analysis of technologies has also been done based on economics (Kwak et al., 2014). Even though an economic analysis is necessary to determine the quantity of useful energy recovered based on capital cost limitations, it does not reflect the true capabilities of the technologies. Moreover, making decisions purely on economics neglects the potential for technology improvement. The potential for technology improvement depends on the deviation of the real performance (adjusted to account for degradation of the heat sources as a result of heat transfer) from the ideal performance of technologies. Wise selection of technologies and better matching with heat source temperatures could reduce such deviations.

The deviation of the adjusted real performance from the ideal performance of technology options is defined as the exergy degradation. Using the exergy degradation as the criterion for screening is a viable and thermodynamically sound approach. The presented screening tool can provide new technological insights in waste heat utilization.

4. 1. Introduction to Publication 3

Models developed to determine the real performance in Publications 1 and 2 are extended to account for physical degradation of waste heat sources due to heat transfer.

The importance of comparing technologies and review of literature to support the literature review in Chapter 2 (section 2.3) is presented in section 1. Section 2 contains the development of the screening criterion for all technologies. Models developed for the real performance of technologies based on conservation of energy quantity in Publication 1, and Publication 2 are extended to account for irreversibilities due to finite temperature heat transfer.

A methodology for developing the screening tool is contained in section 3. The screening tool provides a visual basis to compare the technology options over a wide heat source temperature range. The objective of the comparison is to minimize the exergy degradation to improve better temperature matching with the heat sources and waste heat recovery technologies. Application of the tool to heat sources from ambient to 260°C is shown in section 4 and concluding remarks presented in section 5. Results show that the choice of technology option depends on the heat source temperature.

4. 2. Publication 3

Oluleye G., Jiang N., Smith R., Jobson M., A Novel Screening Tool for Waste Heat Utilization Technologies, Energy (under review)

A Novel Screening Tool for Waste Heat Utilization Technologies

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HIGHLIGHTS

- Analysis considers deviation from ideal thermodynamic performance of technologies
- Five thermodynamic cycles screened for waste heat utilization
- Technology choice depends on the heat source temperature
- Screening tool presented to visualise results
- Screening tool guides technology selection

Nomenclature

AbC	Absorption chiller
ABS	Absorber
AHP	Absorption heat pump
AHT	Absorption heat transformer
COMP	Compressor
COND	Condenser
COP	Coefficient of performance
DHR	Direct heat recovery
Ex_D	Exergy degradation
EVAP	Evaporator
EXP	Expander
GEN	Generator

MHP	Mechanical heat pump
ORC	Organic Rankine Cycle
Q	Quantity of heat flow (kW)
T	Temperature (°C)
T_o	Ambient temperature (°C)
VCC	Vapour compression chiller
W	Electrical power (kW)
WHS	Waste heat source

Greek letters

α	Regression coefficient for technology options
β	Regression coefficient for technology options
$\eta_{real,ORC}$	ORC real efficiency
$\eta_{ideal,ORC}$	ORC ideal efficiency
μ	efficiency factor for technology options

ABSTRACT

Recovering useful energy (in the form of heat, power and chilling) from waste heat improves the energy efficiency of process sites, ensuring lower costs and lower CO_2 emissions. Mature and commercialised technologies, such as organic Rankine cycles, absorption chillers, mechanical heat pumps, absorption heat transformers and absorption heat pumps exist to utilize the waste heat. Though these technologies can make waste heat re-use technically possible, selection of technologies taking into account different heat source temperatures, in order to utilize waste heat efficiently still needs to be addressed.

To overcome these challenges, a novel screening tool is proposed to compare between technology options taking into account the waste heat source temperature. Since multiple energy form interactions occur, the screening criterion considers the deviation of the actual performance from the ideal performance of technology options. In this case the actual (real) performance takes into account irreversibilities as a result of finite temperature heat transfer. The tool is applied to screen technologies for waste heat sources from ambient conditions to 260°C. Results show that selection of technology options depends on the heat source temperature. This analysis provides more guidance for system improvement since irreversibilities due to heat transfer are accounted for.

Keywords:
Waste heat utilization; ideal performance; real performance; thermodynamic cycles (organic rankine cycle, absorption chiller, absorption heat pump, absorption heat transformer, mechanical heat pump); comparative study.

1. Introduction

Large amounts of energy are consumed for industrial operations such as process heating and electrical power generation. However, an enormous amount of energy consumption is rejected as waste heat. For example, two-thirds of input energy for electricity generation in the USA is lost as heat during conversion processes, while 43.9% of the energy for USA consumption is converted to electricity [1]. Industrial waste heat comprises over 40% of the energy content of fuel in the UK [2]. These facts have drawn attention to waste heat utilization, along with improving equipment and system energy efficiency. Waste heat re-use is an effective way to increase energy efficiency and reduce CO_2 emissions [3].

There is a wide range of heat utilization technologies for the recovery of waste heat. Technologies considered in this work are: organic Rankine cycles (ORC) using low temperature boiling point organic fluids to produce shaft power from low to medium temperature heat sources [4], thermally driven absorption chillers (AbC) using heat to provide chilling [5], electrically driven mechanical heat pumps (MHP) for upgrading waste heat [6], thermally driven absorption heat pumps (AHP) and heat transformers (AHT) using the inverse absorption refrigeration cycle to upgrade waste heat [7], and direct heat recovery via heat exchange [8]. In addition, the available waste heat on process sites occurs over a wide range in quantity and temperature [9]. Though these waste heat recovery methods can make waste heat re-use technically possible, how to compare between options, select an option, and determine the quality (i.e. temperature of heat to use) in order to utilize waste heat efficiently on the system level still needs to be addressed.

Previous research on waste heat utilization technologies focused on working fluid screening and selection, choice of system design, and choice of operating conditions. For example Ayachi et al. [10] determined the choice of system design and working fluids for an Organic Rankine cycle through a break down thermodynamic analysis of the technology components. Also Marechal and Kalitventzeff [11] proposed the best operating conditions for an Organic Rankine cycle based on minimizing irreversibilities due to heat exchange. Impact of working fluid selection on ORC performance was studied by Long et al. [12]. Screening of working fluids and determination of the optimal expander inlet temperature, to maximize the net power output for different inlet temperature of heat sources was investigated by Wang et al. [13]. Similarly for absorption chillers, work has been done to determine the cycle component with the greatest losses [14], and also to evaluate the use of additives in water/lithium bromide absorption heat transformers [15]. However, there is very little research on screening and comparing between several thermodynamic cycles taking into account the heat source temperature. Wise selection of technology options and better matching of heat source temperature has potential to reduce irreversibilities due to finite temperature heat transfer [16].

In little and Garimella [17], thermodynamic cycles for conversion of waste heat to power, cooling and temperature upgrade were analysed and compared. The comparative assessment was based on the cycle performance based on conservation of energy quantity. Different first law efficiency definitions are used for waste heat utilization technologies. For example the performance of an organic Rankine cycle is the net power output per unit heat input, while the performance of an absorption chiller (expressed as the coefficient of performance) is the net chilling produced per unit heat input. Therefore, the analysis becomes incoherent when simultaneous energy interactions of different types such as; power, chilling, and heating occur within the same system. Furthermore, the study by Little and Garimella [17] considered only two heat source temperatures (60°C and 120°C).

A gross analysis of technology options based on the first law of thermodynamics (i.e. conservation of energy quantity) has been used to represent the non-adiabatic thermal losses [9]. However, it does not account for irreversibilities due to finite temperature heat transfer [18]. In addition, the energy balance provides no information on the energy degradation during a conversion process; neither does it quantify the usefulness of various energy streams flowing through a system [14]. There is need to adjust the real performance to account for degradation of the heat source from heat transfer.

Ajah et al. [19] compared two thermodynamic cycles for heat upgrade i.e. chemical and mechanical heat pumps. The comparison took into account the cycle's coefficient of performance (COP), economics, safety and reliability. However, the degradation of the heat sources is neglected and comparison was done for heat sources at 35 and 95°C. Kwak et al. [20] developed an optimization framework to determine the most economic options for waste heat utilization. Technologies considered include heat recovery via heat exchange, organic Rankine cycles, absorption chillers and absorption heat pumps. Even though an economic analysis can guide the determination of the quantity of heat to recover, it is not a sufficient tool for comparison since it does not reflect the true capabilities of technologies. An economic comparison between technology options such as heat recovery via heat exchange, heat pumps and absorption chillers was performed by Law et al. [21]; again making decisions based on economics neglects the potential for technology improvement. Van De Bor et al. [22] compared between mechanical heat pumps and organic rankine cycles, again only economics and the real performance is used.

A comparative analysis of technology options for waste heat utilization should account for the deviation of the actual (real performance) from the ideal thermodynamic performance. The real performance should also account for the thermal energy degraded during heat transfer. All energy conversion systems have an ideal thermodynamic performance, determined for reversible processes occurring. However, the ideal performance is not achieved due to system imperfections. Thermodynamic imperfections of systems can be explained by heat transfer irreversibilities [23]. Irreversibilities cause by heat transfer across a finite temperature difference can be minimized through better temperature matching between the heat sources and utilization technologies [16]. The objective of screening is to select technologies with minimum deviation from the ideal performance.

The aim of this paper is to develop a screening criterion and tool for comparing between technology options for waste heat utilization, taking into account different heat source temperatures. The screening criterion measure the deviation from the ideal performance of technology options i.e. the exergy degradation. Using the exergy degradation as the criterion for screening is a viable and thermodynamically sound approach. The presented screening tool can provide new technological insights in waste heat utilization.

2. Screening criterion for waste heat utilization technologies

The proposed screening criterion measures the deviation of the actual performance from the ideal performance of technology options, in this case the actual performance accounts for degradation of the heat sources as a result of heat transfer. In this section the screening criterion is developed for the five thermodynamic cycles considered and heat recovery via heat exchange.

Performance analysis of utilization technologies based on the first law (i.e. conservation of energy quantity) can serve as basis to model, and analyse technologies to consider irreversibilities due to finite temperature heat transfer [23]. Therefore, in this section models to determine the real performance of technology options based on conservation of energy quantity are extended to account for the physical degradation of the waste heat sources as a result of finite temperature heat transfer.

The ideal performance of technology options depends on assumptions about the reversible processes occurring. For example, the Carnot factor is used to represent the ideal performance of organic Rankine cycles. The deviation of the real performance (taking into account irreversibilities due to finite temperature heat transfer) from the ideal performance i.e. exergy degradation is presented for all technologies in this section. Using the exergy degradation as a screening criterion is a thermodynamically sound approach to compare technology options, since it takes into account the true capabilities of each technology. The objective is to select technologies with minimum deviation from their ideal performance.

The screening criterion for Organic Rankine cycles is presented in Section 2.1, absorption chillers in Section 2.2, absorption heat pumps in Section 2.3, absorption heat transformers in Section 2.4, mechanical heat pumps in Section 2.5 and heat recovery via heat exchange i.e. direct heat recovery in Section 2.6.

2.1 Organic Rankine cycles (ORC)

Organic Rankine cycles are a good candidate for exploitation of waste heat due to their simplicity, flexibility and relatively low driving temperature [24]. Organic Rankine cycles have simple start-up procedures, quiet operation, and good part load performance [18]. In this work, simple cycles will be considered as illustrated in Fig. 1. The energy to be exploited in the organic Rankine cycle is transferred from a heat source to vaporize the working fluid in the evaporator and vapor expansion transfers thermal energy into shaft work. Low grade thermal energy is removed from the process by condensing the working fluid to the state of saturated liquid, the working fluid is pumped and the cycle repeats.

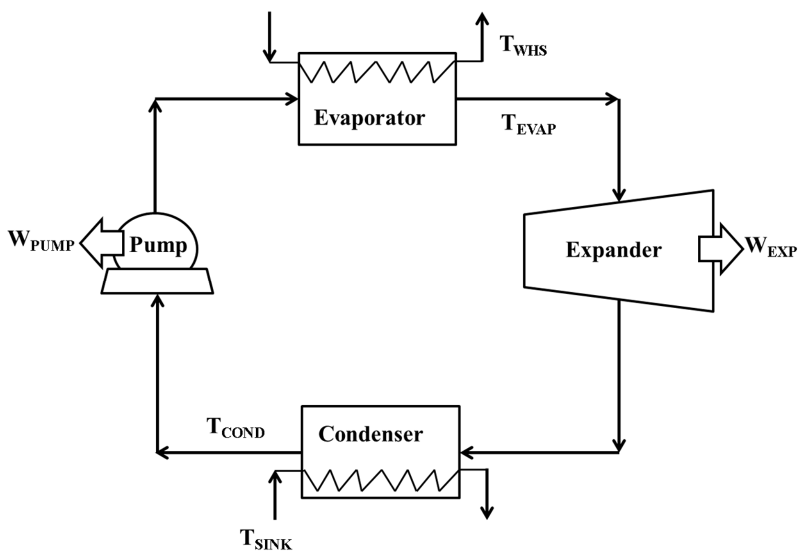

Fig. 1 Organic Rankine cycle schematic

The cycle efficiency based on the conservation of energy quantity is defined as the net power output per unit heat input (Eq. 1). This is adjusted in Eq. 2 to account for degradation of the heat sources as a result of heat transfer. In Eq. 2 exergy transfer by heat out of and into the system is taken into account. The exergy transfer by heat is used since the entropy change of a closed system during a reversible process is due to the entropy transferred across the system boundary by heat transfer. Exergy related to heat transfer is defined by the Carnot factor [25].

$$\eta_{real,ORC} = \frac{W_{EXP} - W_{PUMP}}{Q_{EVAP}} \tag{1}$$

$$\eta_{real,ORC}^{*} = \frac{W_{NET}}{Q_{EVAP} \times \left(\frac{1 - \frac{T_o}{T_{EVAP}}}{1 - \frac{T_o}{T_{WHS}}} \right)} \tag{2}$$

The ideal performance for an ORC is defined for a reversible Carnot engine in Eq. 3.

$$\eta_{ideal,\,ORC} = 1 - \frac{T_{COND}}{T_{EVAP}} \tag{3}$$

The ratio of the real performance in Eq. 1 to the ideal performance in Eq. 3 is defined as the efficiency factor [9] as shown in Eq. 4

$$\eta_{real,ORC} = \mu_{ORC} \times \eta_{ideal,ORC} \tag{4}$$

Eq. 2 can be expressed in terms of the ideal performance and efficiency factor by combining with Eqs. 1and 4:

$$\eta_{real,ORC}^{*} = \mu_{ORC} \times \eta_{ideal,ORC} \times \left(\frac{1 - \frac{T_o}{T_{EVAP}}}{1 - \frac{T_o}{T_{WHS}}} \right) \tag{5}$$

In Oluleye et al. [9], the efficiency factor was expressed as a function of the ideal efficiency as shown in Eq. 6 below.

$$\mu_{ORC} = \left(\alpha_{ORC} \times \eta_{ideal,\,ORC} \right) + \beta_{ORC} \tag{6}$$

The values of α and β were estimated based on assumptions of saturated vapour in the evaporator, saturated liquid in the condenser, negligible pressure drop in both the condenser and evaporator, and turbine and isentropic efficiency of 75% and pump isentropic efficiency of 75% [9]. The values for two working fluids (benzene and cyclopentane) are provided in Appendix A (Table A.1).

The exergy degradation is defined as the deviation of the adjusted real performance from the ideal thermodynamic performance expressed in Eq. 7.

$$Ex_{D,ORC} = \frac{\eta_{ideal,ORC} - \eta_{real,ORC}^{*}}{\eta_{ideal,ORC}} \tag{7}$$

A mathematical expression of the exergy degradation is obtained by substituting Eq. 5 into Eq. 7:

$$Ex_{D,ORC} = 1 - \left[\mu_{ORC} \times \left(\frac{1 - \frac{T_o}{T_{EVAP}}}{1 - \frac{T_o}{T_{WHS}}} \right) \right] \tag{8}$$

The screening criterion for ORC is shown in Eq. 8. This is a sound thermodynamic approach for comparing organic Rankine cycles with other utilization technologies.

2.2 Absorption chillers (AbC)

In absorption chillers, chilling is provided when a heat source stream at low temperature vaporizes the refrigerant (For example water), which is absorbed by the absorbent (For example lithium bromide), the heat given off during absorption is rejected to a sink. The weak absorbent is pumped into a generator, where waste heat separates the working fluid pair. The rich absorbent is sent back to the absorber, while the pure refrigerant is condensed, expanded in a valve and the cycle repeats. A schematic is shown in Fig. 2. The liquid pumping requirement is negligible compared to the waste heat required in the generator [5].

The use of water/ lithium bromide absorption chillers is more common than other systems since not only is the refrigerant of these systems (water) available everywhere, inexpensive and non-toxic, its latent heat of evaporation is high, which makes it possible to produce a considerable amount of cooling. In addition, since the absorbent is not evaporated there is no need for rectifiers [14].

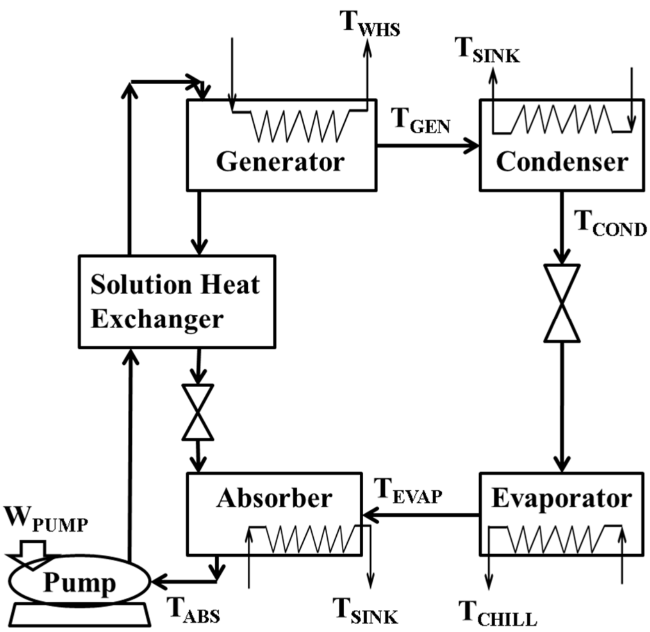

Fig. 2 Absorption chiller schematic

Based on the conservation of energy quantity, the coefficient of performance is defined as the chilling provided in the evaporator per unit waste heat input in the generator and work input in the pump (Eq. 9). The real coefficient of performance is adjusted to account for irreversibilities due to finite temperature heat transfer in the evaporator and generator in Eq. 10. In Eq. 10, the liquid pumping requirement is negligible [5] and the exergy related to heat transfer is defined by the Carnot factor [25].

$$COP_{AbC,real} = \frac{Q_{EVAP}}{Q_{GEN} + W_{PUMP}} \tag{9}$$

$$COP_{AbC,real}^{*} = \frac{Q_{EVAP} \times \left(\dfrac{1 - \dfrac{T_o}{T_{EVAP}}}{1 - \dfrac{T_o}{T_{CHILL}}} \right)}{Q_{GEN} \times \left(\dfrac{1 - \dfrac{T_o}{T_{GEN}}}{1 - \dfrac{T_o}{T_{WHS}}} \right)} \tag{10}$$

The ideal coefficient of performance can be expressed as the product of the ideal efficiency of a vapour compression heat pump operating between the evaporator and condenser temperatures, and a turbine operating between the generator and absorber temperatures [26]. Derivation of the ideal COP is presented in Appendix B.

$$COP_{AbC,ideal} = \left(1 - \frac{T_{COND}}{T_{GEN}}\right)\left(\frac{T_{EVAP}}{T_{COND} - T_{EVAP}}\right) \tag{11}$$

The ratio of the real COP in Eq. 9 to the ideal COP in Eq. 11 is the cycle efficiency factor [9]:

$$COP_{AbC,real} = \mu_{AbC} \times COP_{AbC,ideal} \tag{12}$$

In Oluleye et al. [9], a relationship between the ideal COP and the efficiency factor was developed as shown below.

$$\mu_{AbC} = \frac{\beta_{AbC}}{COP_{AbC,ideal} - \alpha_{AbC}} \tag{13}$$

Values of α and β for water/ lithium bromide absorption chiller are provided in Appendix A (Fig. A.3). The values were obtained for chilling provision between 0 to 25°C, saturation conditions and negligible pressure drop in the condenser and evaporator, and refrigerant in the condenser at 30°C [9].

The adjusted real COP in Eq. 10 can be expressed in terms of the ideal COP and efficiency factor by combining with Eqs. 9 and 12:

$$COP_{AbC,real}^{*} = \mu_{AbC} \times COP_{AbC,ideal} \times \frac{\left(\dfrac{1 - \dfrac{T_o}{T_{EVAP}}}{1 - \dfrac{T_o}{T_{CHILL}}}\right)}{\left(\dfrac{1 - \dfrac{T_o}{T_{GEN}}}{1 - \dfrac{T_o}{T_{WHS}}}\right)} \tag{14}$$

The exergy degradation for an absorption chiller is defined as the deviation of the adjusted real COP from the ideal COP, expressed as:

$$Ex_{D,AbC} = \frac{COP_{AbC,ideal} - COP_{AbC,real}^{*}}{COP_{AbC,ideal}} \tag{15}$$

By Substituting Eq. 14 into Eq. 15, a mathematical expression of the exergy degradation is shown in Eq. 16.

$$Ex_{D,AbC} = 1 - \left[\mu_{AbC} \times \frac{\left(\frac{1 - \frac{T_o}{T_{EVAP}}}{1 - \frac{T_o}{T_{CHILL}}} \right)}{\left(\frac{1 - \frac{T_o}{T_{GEN}}}{1 - \frac{T_o}{T_{WHS}}} \right)} \right] \tag{16}$$

Irreversibilities due to heat transfer are accounted for by using the exergy degradation as a screening criterion.

One of the advantages of thermally driven chilling technologies is their ability to replace vapour compression chillers. Vapour compression chillers require a large amount of high quality work to provide chilling. A combination of the absorber, desorber and solution heat exchanger replaces the compressor in a vapor compression cycle [17]. A schematic of a vapour compression chiller (VCC) is shown in Fig. 3. Integrating absorption chillers in process sites could displace the need for high quality electrical power in vapour compression chillers. Displacing high quality electrical power implies the exergy degradation accompanying VCC is saved.

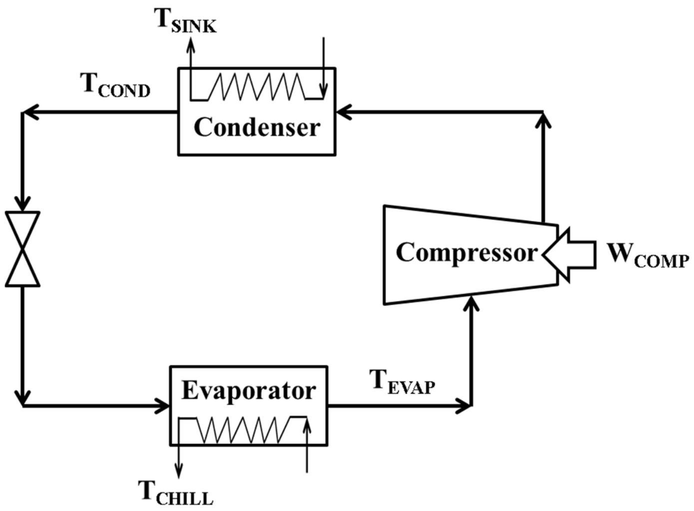

Fig. 3 Vapour compression chiller schematic

The real coefficient of performance for a vapour compression chiller, based on conservation of energy quantity is defined as the chilling provided in the evaporator per unit power input (Eq. 17). Taking into account irreversibilities due to heat transfer, the adjusted real performance is shown in Eq. 18. In Eq. 18 the exergy related to heat transfer is defined by the Carnot factor [25].

$$COP_{VCC,real} = \frac{Q_{EVAP}}{W_{COMP}} \tag{17}$$

$$COP_{VCC,real}^{*} = \frac{Q_{EVAP} \times \left(\dfrac{1-\dfrac{T_o}{T_{EVAP}}}{1-\dfrac{T_o}{T_{CHILL}}} \right)}{W_{COMP}} \tag{18}$$

The ideal coefficient of performance is that of a heat engine operating in reverse (Eq. 19). This can also be related to the real performance in Eq. 17 using an efficiency factor (as shown in Eq. 20).

$$COP_{VCC,ideal} = \frac{T_{EVAP}}{T_{COND} - T_{EVAP}} \tag{19}$$

$$COP_{VCC,real} = \mu_{VCC} \times COP_{VCC,ideal} \tag{20}$$

By combining Eqs 17 and 20, the adjusted real performance in Eq. 18 can be expressed as:

$$COP_{VCC,real}^{*} = \mu_{VCC} \times COP_{VCC,ideal} \times \left(\frac{1-\dfrac{T_o}{T_{EVAP}}}{1-\dfrac{T_o}{T_{CHILL}}} \right) \tag{21}$$

The exergy degradation for a VCC is defined as the deviation of the adjusted real COP from the ideal thermodynamic performance as expressed in Eq. 22.

$$Ex_{D,VCC} = \frac{COP_{VCC,ideal} - COP_{VCC,real}^{*}}{COP_{VCC,ideal}} \tag{22}$$

By substituting Eq. 21 into Eq. 22, the exergy degradation for a vapour compression chiller is:

$$Ex_{D,VCC} = 1 - \left[\mu_{VCC} \times \left(\frac{1-\dfrac{T_o}{T_{EVAP}}}{1-\dfrac{T_o}{T_{CHILL}}} \right) \right] \tag{23}$$

The effective exergy degradation when the chilling provided by absorption chillers replaces high quality electrical power in vapour compression chillers is expressed in Eq. 24.

$$ExD_{EFF} = ExD_{AbC} \times ExD_{VCC} \qquad (24)$$

Eq. 24 is a thermodynamically sound criterion for comparing absorption chillers with other technology options for waste heat utilization.

2.3 Absorption heat pumps (AHP)

In absorption heat pumps, low temperature heat to be upgraded vaporizes the refrigerant (water) in the evaporator. The vaporized refrigerant is absorbed, thereby giving out heat. The weak absorbent is pumped to the generator where a high temperature heat source is supplied to separate the working fluid pair. The strong absorbent flows back to the absorber, while the refrigerant is condensed, expanded and the cycle repeats. Medium temperature heat given off in the absorber and condenser is recovered. A schematic of an AHP is shown in Fig. 4. The liquid pumping requirement is negligible [27].

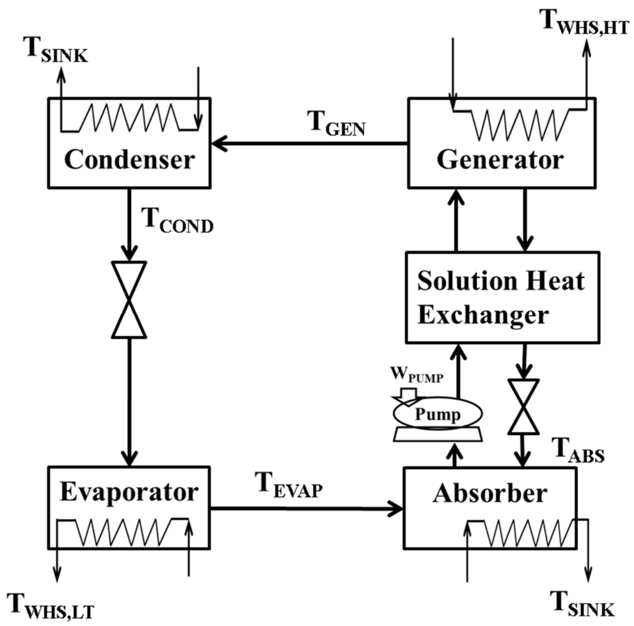

Fig. 4 Absorption heat pump schematic

The coefficient of performance (COP) based on conservation of energy quantity is defined as the sum of heat upgraded in the absorber and condenser to the sum of the heat input in the generator and liquid pumping requirement (Eq. 25). The real performance is adjusted to take into account degradation of the heat source due to heat transfer (Eq. 26). In Eq. 26 exergy related to heat transfer is defined by the Carnot factor [25].

$$COP_{AHP,real} = \frac{Q_{ABS} + Q_{COND}}{Q_{GEN} + W_{PUMP}} \quad (25)$$

$$COP_{AHP,real}^{*} = \frac{Q_{ABS} \times \left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{ABS}}} \right) + Q_{COND} \times \left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{COND}}} \right)}{Q_{GEN} \times \left(\dfrac{1 - \dfrac{T_o}{T_{GEN}}}{1 - \dfrac{T_o}{T_{WHS}}} \right)} \quad (26)$$

The ideal coefficient of performance is that of an absorption chiller plus 1 (Eq. 27). Derivation of the ideal coefficient of performance is provided in Appendix B.

$$COP_{AHP,ideal} = 1 + \left(1 - \frac{T_{COND}}{T_{GEN}} \right) \left(\frac{T_{EVAP}}{T_{COND} - T_{EVAP}} \right) \quad (27)$$

Similarly, for an absorption heat pump, the ratio of the real COP in Eq. 25 to the ideal COP is expressed as an efficiency factor in Eq. 29. The efficiency factor can also be expressed as a function of the ideal COP (Eq. 29) [33].

$$COP_{AHP,\, real} = \mu_{AHP} \times COP_{AHP,\, ideal} \quad (28)$$

$$\mu_{AHP} = \frac{\beta_{AHP}}{COP_{AHP,ideal} - \alpha_{AHP}} \quad (29)$$

Values of α and β for a steady flow system, saturated conditions in the evaporator, condenser and solutions leaving the generator and absorber, isenthalpic process in the valve, and negligible pressure losses in pipes and components are given in the Appendix (Table A.2). The real COP (Eq. 25) calculated using the expression in Eqs 28 and 29 was compared with thermodynamic data of AHP provided in Eisa et al. [27]. Validation of the model is provided in the Appendix (Figure A.5).

The adjusted real COP is Eq. 26 can be expressed as a function of the ideal COP and efficiency factor by combining Eqs. 25, 26, 27 and 28:

$$COP_{AHP,real}^{*} = \mu_{AHP} \times COP_{AHP,\,ideal} \times \frac{\left(\dfrac{1-\dfrac{T_o}{T_{SINK}}}{1-\dfrac{T_o}{T_{COND}}} \right)}{\left(\dfrac{1-\dfrac{T_o}{T_{GEN}}}{1-\dfrac{T_o}{T_{WHS}}} \right)} \tag{30}$$

Eq. 30 was simplified by assuming the temperature of heat recovered in the condenser and absorber is the same.

The exergy degradation for AHP is defined as the deviation of the adjusted real COP from the ideal COP (Eq. 31). By substituting Eq. 30 into 31, a mathematical expression for the exergy degradation is shown in Eq. 32.

$$Ex_{D,AHP} = \frac{COP_{AHP,ideal} - COP_{AHP,real}^{*}}{COP_{AHP,ideal}} \tag{31}$$

$$Ex_{D,AHP} = 1 - \left[\mu_{AHP} \times \frac{\left(\dfrac{1-\dfrac{T_o}{T_{SINK}}}{1-\dfrac{T_o}{T_{COND}}} \right)}{\left(\dfrac{1-\dfrac{T_o}{T_{GEN}}}{1-\dfrac{T_o}{T_{WHS}}} \right)} \right] \tag{32}$$

The screening criterion for AHP (i.e. the exergy degradation in Eq. 32) provides a sound thermodynamic basis to compare the AHP with other utilization technologies.

2.4 Absorption heat transformers (AHT)

Absorption heat transformers are reversed absorption heat pumps i.e. the evaporator and absorber operate at a pressure higher than the condenser and generator [28]. A heat transformer is a closed cycle system, which upgrades a fraction of the energy from an intermediate waste heat stream to a higher temperature so it may be reused [29]. A schematic is shown in Fig. 5. The arrangement is similar to absorption heat pumps, but, the condenser and generator work at low pressure and the evaporator and absorber work at high pressure.

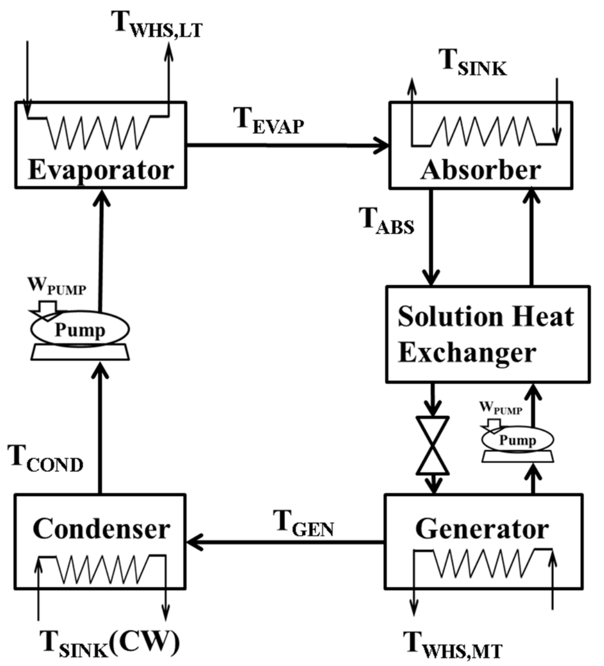

Fig. 5 Absorption heat transformer schematic

The coefficient of performance based on conservation of energy quantity is defined as the heat upgraded in the absorber divided by the sum of heat and work input into the technology (Eq. 33). This is adjusted in Eq. 34 to account for thermal degradation as a result of heat transfer. In Eq. 34, exergy related to heat transfer is defined by the Carnot factor [25]. The liquid pumping requirement is negligible [28].

$$COP_{AHT,real} = \frac{Q_{ABS}}{Q_{GEN} + Q_{EVAP} + W_{PUMP}} \qquad (33)$$

$$COP_{AHT,real}{}^{*} = \frac{Q_{ABS} \times \left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{ABS}}} \right)}{Q_{GEN} \times \left(\dfrac{1 - \dfrac{T_o}{T_{GEN}}}{1 - \dfrac{T_o}{T_{WHS}}} \right) + Q_{EVAP} \times \left(\dfrac{1 - \dfrac{T_o}{T_{EVAP}}}{1 - \dfrac{T_o}{T_{WHS}}} \right)} \qquad (34)$$

The ideal COP is for a theoretically ideal situation i.e. when a state of thermodynamic equilibrium is attained, and for thermodynamically reversible processes occurring in the evaporator and condenser [30] is shown in Eq. 35. Derivation of the ideal COP is provided in Appendix B.

$$COP_{AHT,ideal} = \left(\frac{(T_{EVAP} - T_{COND}) \times T_{ABS}}{((T_{EVAP} - T_{COND}) \times T_{GEN}) + ((T_{ABS} - T_{GEN}) \times T_{EVAP})} \right) \quad (35)$$

The ratio of the real coefficient of performance in Eq. 33 to the ideal coefficient of performance is defined as the efficiency factor as shown in Eq. 36 below (similar to that of an AHP and AbC) [33]. This can also be related to the ideal COP (Eq. 37).

$$COP_{AHT,real} = \mu_{AHT} \times COP_{AHT,ideal} \quad (36)$$

$$\mu_{AHT} = \frac{\beta_{AHT}}{COP_{AHT,ideal} - \alpha_{AHT}} \quad (37)$$

Values of α and β for a steady flow system, saturated conditions in the evaporator, condenser and solutions leaving the generator and absorber, isenthalpic process in the valve, and negligible pressure losses in pipes and components are given in the Appendix (Table A.3). The real COP (Eq. 33) calculated using the expression in Eqs 36 and 37 was compared with thermodynamic data of AHT provided in Eisa et al. [31]. Validation of the model is provided in the Appendix (Figure A.6).

By combining Eqs. 33, 34, 35 and 36 the adjusted real performance can be expressed as a function of the ideal COP and the efficiency factor (Eq. 38). To simplify Eq. 38 the evaporator and generator temperatures are assumed to be the same.

$$COP_{AHT,real}^{*} = \mu_{AHT} \times COP_{AHT,ideal} \times \frac{\left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{ABS}}} \right)}{\left(\dfrac{1 - \dfrac{T_o}{T_{EVAP}}}{1 - \dfrac{T_o}{T_{WHS}}} \right)} \quad (38)$$

The exergy degradation for an AHT is defined as the deviation of the adjusted real COP from the ideal COP (Eq. 39), also expressed mathematically in Eq. 40 by substituting Eq. 38 into Eq. 39.

$$Ex_{D,AHT} = \frac{COP_{AHT,ideal} - COP_{AHT,real}^{*}}{COP_{AHT,ideal}} \tag{39}$$

$$Ex_{D,AHT} = 1 - \left[\mu_{AHT} \times \frac{\left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{ABS}}} \right)}{\left(\dfrac{1 - \dfrac{T_o}{T_{EVAP}}}{1 - \dfrac{T_o}{T_{WHS}}} \right)} \right] \tag{40}$$

The screening criterion for an AHT is the exergy degradation in Eq. 40. This is useful for comparing AHT with also utilization technologies.

2.5 Mechanical heat pumps (MHP)

Mechanical heat pumps deliver more thermal energy than the electrical energy required to operate them. A schematic is shown in Fig. 6, low temperature waste heat vaporizes the working fluid in the evaporator, which is compressed using electrical power, and condensed, giving off heat. The working fluid is expanded in a valve and the cycle repeats. Heat given off during condensation of the working fluid is recovered at a higher temperature.

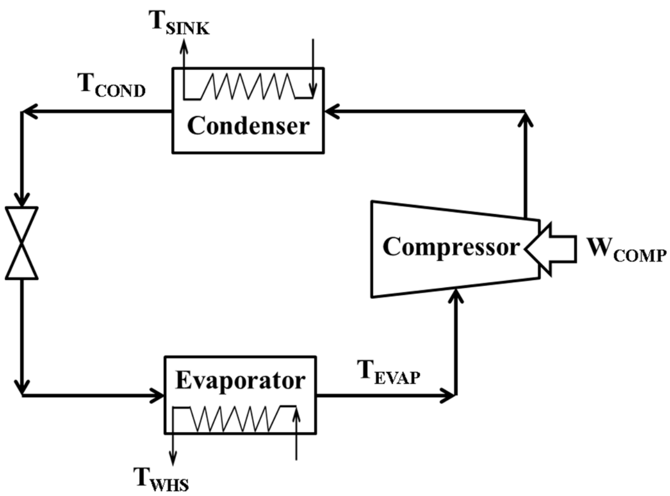

Fig. 6 Mechanical heat pump schematic

The coefficient of performance based on the conservation of energy quantity is defined as the heat upgraded in the condenser to the power input (Eq. 41), this is adjusted in Eq. 42 to account for degradation of the heat source as a result of heat transfer. In Eq. 42 exergy related to heat transfer is defined by the Carnot factor [25].

$$COP_{MHP,\ real} = \frac{Q_{COND}}{W_{COMP}} \tag{41}$$

$$COP_{MHP,real}{}^{*} = \frac{Q_{COND} \times \left(\dfrac{1 - \dfrac{T_o}{T_{SINK}}}{1 - \dfrac{T_o}{T_{COND}}} \right)}{W_{COMP}} \tag{42}$$

The ideal COP for a mechanical heat pump is 1 plus that of a vapour compression chiller as shown in Eq. 43.

$$COP_{MHP,\ ideal} = \frac{T_{COND}}{T_{COND} - T_{EVAP}} \tag{43}$$

The ratio between the real COP in Eq. 41 and the ideal COP in Eq. 43 is expressed as the efficiency factor (Eq. 44) [33]. This has also been related to the cycle temperatures as shown in Eq. 45 below [33].

$$COP_{MHP,real} = \mu_{MHP} \times COP_{MHP,ideal} \tag{44}$$

$$\mu_{MHP} = \alpha_{MHP} + \left(\beta_{MHP} \times \frac{T_{COND} - T_{EVAP}}{T_{COND}} \right) \tag{45}$$

Values of α and β for a steady flow system, saturated conditions in the evaporator, and condenser, isenthalpic process in the valve, and negligible pressure losses in pipes and components are given in the Appendix (Table A.4). The real COP (Eq. 41) calculated using the expression in Eqs 44 and 45 was compared with rigorous simulation of MHP in Aspen HYSYS [32]. Validation of the model using n-butane as working fluid is provided in the Appendix (Figure A.7).

By combining Eqs. 41, 42 and 44 the adjusted real COP can be expressed as a function of the ideal COP and the efficiency factor:

$$COP_{MHP,real}{}^{*} = \mu_{MHP} \times COP_{MHP,ideal} \times \left(\frac{1 - \frac{T_o}{T_{SINK}}}{1 - \frac{T_o}{T_{COND}}} \right) \qquad (46)$$

The exergy degradation for a MHP is defined as the deviation of the adjusted real COP from the ideal thermodynamic performance (Eq. 47). In Eq. 48, a mathematical expression for the exergy degradation is obtained by substituting Eq. 46 into Eq. 47.

$$Ex_{D,MHP} = \frac{COP_{MHP,ideal} - COP_{MHP,real}{}^{*}}{COP_{MHP,ideal}} \qquad (47)$$

$$Ex_{D,MHP} = 1 - \left[\mu_{MHP} \times \left(\frac{1 - \frac{T_o}{T_{SINK}}}{1 - \frac{T_o}{T_{COND}}} \right) \right] \qquad (48)$$

The screening criterion for MHP is the exergy degradation in Eq. 48.

2.6 Heat recovery via heat exchange

Heat recovery via heat exchange (i.e. direct heat recovery) within a process, or between processing units on process sites, or for hot water generation, or boiler feed water preheating, or steam generation is relatively inexpensive and easily implemented [31]. However, based on the conservation of energy quantity and energy quality degradation, it is necessary to compare this option with non-conventional waste heat utilization methods. Such comparison has not been done previously in the literature. Based on the conservation of energy quantity, the ratio of useful energy recovered to input heat via direct heat exchange is unity, except for transmission and distribution losses. This is not the case when degradation of energy quality is taken into account. Therefore, considering the exergy transfer by heat into and out of a heat exchanger, the exergy degradation is defined in Eq. 49. The exergy degradation expression in Eq. 49 is the screening criterion for direct heat recovery (DHR).

$$Ex_{D,DHR} = \left[1 - \left(\frac{1 - \frac{T_o}{T_{SINK}}}{1 - \frac{T_o}{T_{WHS}}} \right) \right] \qquad (49)$$

3. Screening Tool Development

The screening tool provides a visual basis to compare technology options using the screening criterion over a range of heat source temperatures. Development of the screening tool is shown in the flow chart in Fig. 7 below.

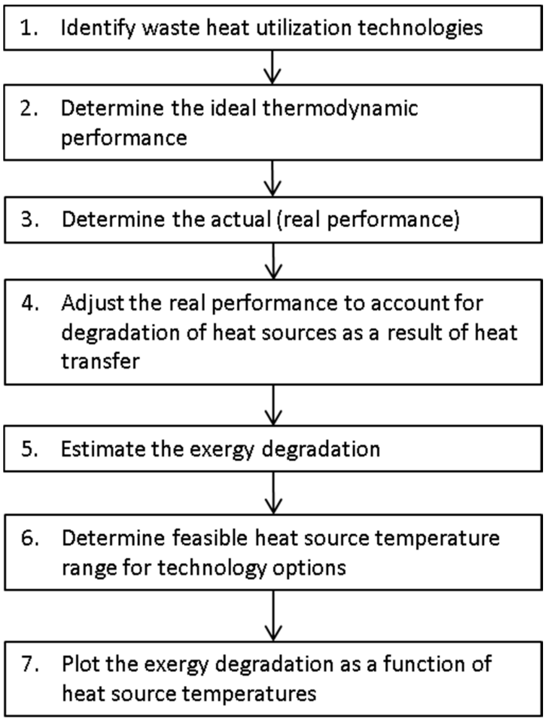

Fig. 7 Steps for screening tool development

The heat source temperature for an ORC is the temperature of the waste heat used to vaporize the working fluid. While for a mechanical heat pump, the temperature of waste heat to be upgraded is defined as the heat source temperature. For absorption systems, the heat source temperature refers to the temperature of the driving energy required in the generator to separate the working fluid pair. To provide a common basis for comparison, the same heat source temperatures are used for all technologies. For technology recovering useful heat from waste heat (either directly or via heat upgrade), the same heat sink temperature is also considered. In section 4, the screening tool is applied for a range of waste heat source temperatures and heat sink temperatures.

4. Screening tool application

Comparing between technology options is necessary to make informed design decisions by determining the most appropriate technology to utilize waste heat, taking into account waste heat source temperatures. In addition, irreversibilities cause by heat transfer across a finite temperature difference can be minimized through better temperature matching between the heat sources and utilization technologies [16]. The screening criterion for technology options is proposed in Section 2 and steps to develop the screening tool in Section 3. In this section the screening tool is applied to compare between technologies taking into account various heat source temperatures. The screening criterion for an ORC is expressed in Eq. 8, AbC in Eq. 24, AHP in Eq. 32, AHT in Eq. 40, MHP in Eq. 48 and heat recovery via heat exchange (i.e. direct heat recovery DHR) in Eq. 49.

4. 1. Waste heat sources below 100°C

The different ways to utilize waste heat below 100°C include: (1) vaporizing the working fluids in ORC to produce electrical power, (2) provide driving thermal energy to separate working fluid pair (i.e. absorbent and refrigerant) in absorption chillers and absorption heat transformers, (3) upgrading the heat to a higher temperature using mechanical heat pumps, (4) direct heat recovery via heat exchange with a heat sink (for hot water generation). For heat generation from waste heat (whether directly or via heat upgrade), different possible sink temperature considered are 40°C (denoted by (1) in the graph legend), 60°C (denoted by (2) in the graph legend), 70°C (denoted by (3) in the graph legend) and 130°C (denoted by (4) in the graph legend).

The screening tool for utilization technologies driven by heat sources below 100°C is shown in Fig. 8. It is a plot of the exergy degradation associated with the conversion processes versus the heat source temperature. The exergy degradation depends on the quality of heat source and the associated conversion technology. Operating temperatures and working fluids selected for the technology options in Fig. 8 are provided in Table 1. A minimum temperature difference of 10°C is assumed and ambient temperature of 25°C.

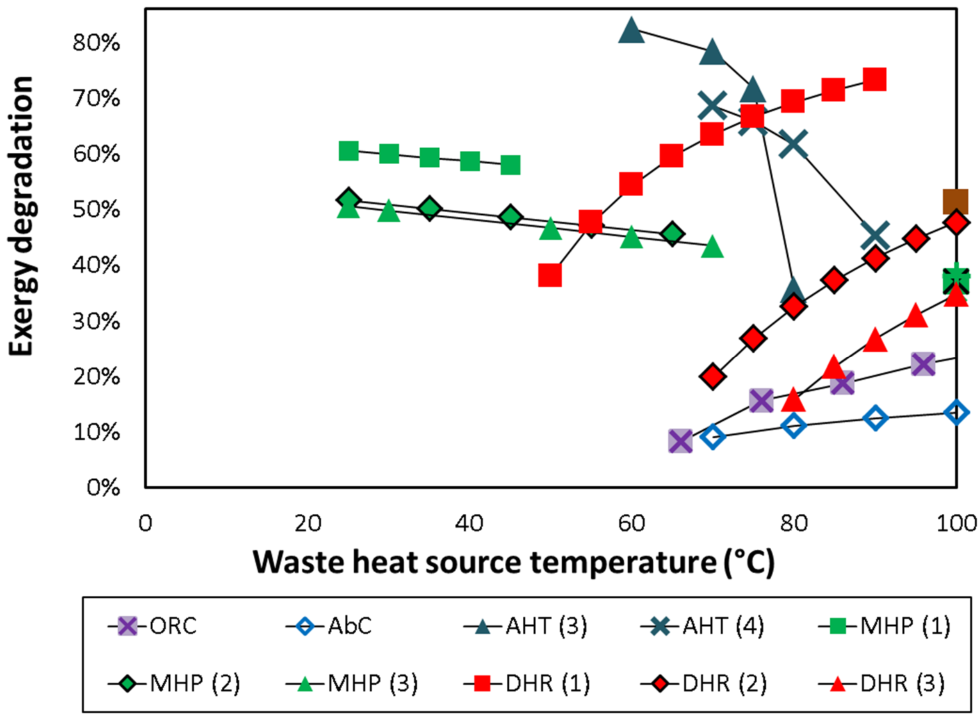

Fig. 8 Screening tool application for waste heat sources below 100°C

The objective is to minimize the exergy degradation accompanying the conversion process by appropriate matching of heat sources and technologies. For example if a heat source is available at 80°C, the technology with minimum exergy degradation is an absorption chiller (i.e. using the heat to produce chilling), followed by using the heat to generate hot water at 70°C as shown in Fig. 8.

Table 1 Operating temperatures and working fluids for utilization technologies

Technology	T_{EVAP} (°C)	T_{COND} (°C)	T_{GEN} (°C)	T_{ABS} (°C)	T_{SINK} (°C)	T_{WHS} (°C)	T_{CHILL} (°C)	Working fluid
ORC	56-90	30	-	-	-	$T_{EVAP}+\Delta T_{MIN}$	-	Cyclopentane
AbC	3	30	60-90	30	-	$T_{GEN}+\Delta T_{MIN}$	8	$H_20/LiBr$
AHT (3)	40	30	50-70	80	70	$T_{GEN}+\Delta T_{MIN}$	-	$H_20/LiBr$
AHT (4)	90	30	60-80	140	130	$T_{GEN}+\Delta T_{MIN}$	-	$H_20/LiBr$

MHP (1)	15-35	50	-	-	40	$T_{EVAP}+\Delta T_{MIN}$	-	n-butane
MHP (2)	15-55	70	-	-	60	$T_{EVAP}+\Delta T_{MIN}$	-	n-butane
MHP (3)	15-60	80	-	-	70	$T_{EVAP}+\Delta T_{MIN}$	-	n-butane
DHR (1)	-	-	-	-	40	50-90	-	-
DHR (2)	-	-	-	-	60	70-110	-	-
DHR (3)	-	-	-	-	70	80-120	-	-

The heat source temperatures in Fig. 8 can be further subdivided to taking into account the minimum exergy degradation associated with each technology option. Hierarchy of technologies based on the minimum exergy degradation for the range of heat source temperatures are shown in Table 2.

Table 2 Hierarchy of waste heat utilization technologies for heat sources below 100°C

Heat source temperature range	Technology ranking	Useful insights
< 50°C	1. Mechanical heat pumps	C1: For a MHP the exergy degradation reduces with reducing temperature lift.
50°C – 55°C	1. Heat recovery via heat exchange (for hot water generation at 40°C) 2. Mechanical heat pumps	C2: The exergy degradation for DHR reduces as the temperature difference between the waste heat source and heat sink reduces
55°C – 66°C	1. Mechanical heat pumps 2. Heat recovery via heat exchange (for hot water generation at 40°C)	C3: The ranking depends on the heat sink temperature for DHR (see C2)
66°C – 70°C	1. Organic Rankine cycle 2. Mechanical heat pumps 3. Heat recovery via heat exchange (for hot water generation at 40°C)	See C3 C4: The exergy degradation for an

	4. Absorption heat transformer	AHT reduces as the temperature difference between T_{GEN} and T_{WHS} reduces.
70°C – 80°C	1. Absorption chiller 2. Organic Rankine cycle 3. Heat recovery via heat exchange (for hot water generation at 60°C) 4. Heat recovery via heat exchange (for hot water generation at 40°C) 5. Absorption heat transformer	See C3 See C4 C5: The exergy degradation for AbC reduces as the temperature difference between T_{GEN} and T_{WHS} reduces.
80°C – 100°C	1. Absorption chiller 2. Heat recovery via heat exchange (for hot water generation at 70°C) 3. Organic Rankine cycle 4. Heat recovery via heat exchange (for hot water generation at 60°C) 5. Heat recovery via heat exchange (for hot water generation at 60°C) 6. Absorption heat transformer 7. Heat recovery via heat exchange (for hot water generation at 40°C)	See C3

4. 2. Waste heat sources between 100°C and 200°C

The different ways to utilize waste heat between 100°C and 200°C include: (1) vaporizing the working fluids in ORC to produce electrical power, (2) provide driving thermal energy to separate working fluid pair (i.e. absorbent and refrigerant) in absorption chillers and absorption heat pumps, (3) upgrading the heat to a higher temperature using mechanical heat pumps, (4) direct heat recovery via heat exchange with a heat sink. For heat generation from waste heat (whether directly or via heat upgrade), different possible sink temperatures considered are 40°C (denoted by (1) in the graph legend), 60°C (denoted by (2) in the graph legend), 70°C (denoted by (3) in the graph legend), 130°C (denoted by (4) in the graph legend) and 175°C (denoted by (5) in the graph legend).

The screening tool for utilization technologies driven by heat sources between 100°C and 200°C is shown in Fig. 9. The exergy degradation depends on the quality of heat source and the associated conversion technology. Operating temperatures and working fluids selection for the technology options in Fig. 9 are provided in Table 2. A minimum temperature difference of 10°C is assumed and ambient temperature of 25°C.

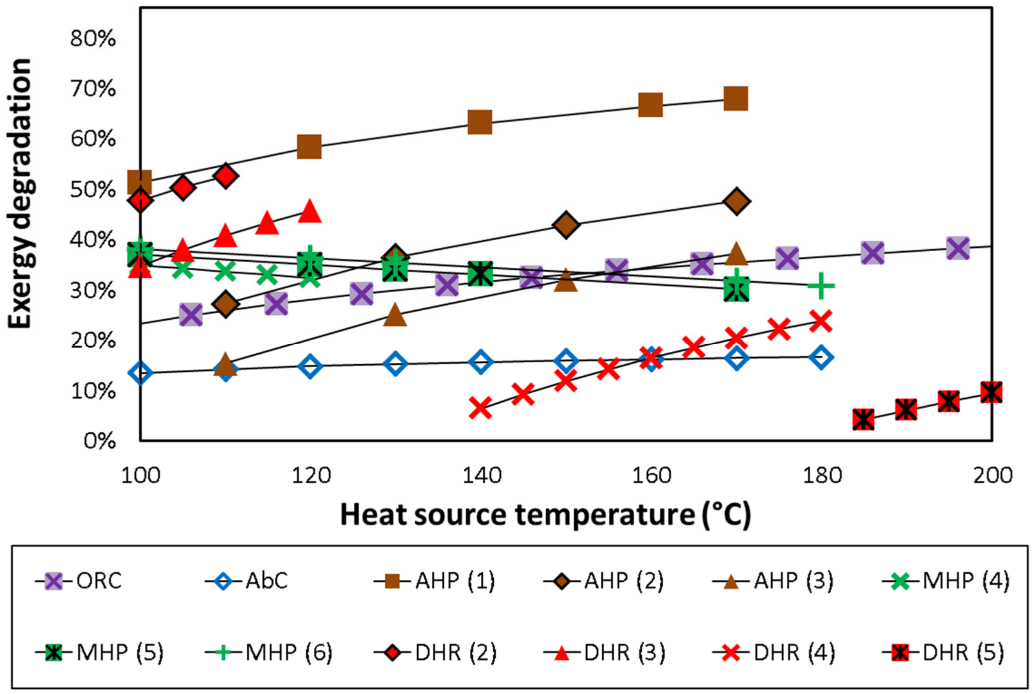

Fig. 9 Screening tool application for heat sources between 100°C and 200°C

Table 3 Operating temperatures and working fluids for utilization technologies

Technology	T_{EVAP} (°C)	T_{COND} (°C)	T_{GEN} (°C)	T_{ABS} (°C)	T_{SINK} (°C)	T_{WHS} (°C)	T_{CHILL} (°C)	Working fluid
ORC	90-190	30	-	-	-	$T_{EVAP}+\Delta T_{MIN}$	-	Benzene
AbC	3	30	90-180	30	-	$T_{GEN}+\Delta T_{MIN}$	8	$H_20/LiBr$
AHP (1)	25	50	90-160	50	40	$T_{GEN}+\Delta T_{MIN}$	-	$H_20/LiBr$
AHP (2)	35	70	100-	70	60	$T_{GEN}+\Delta T_{MIN}$	-	$H_20/LiBr$

			160					
AHP (3)	35	80	110-160	80	70	$T_{GEN}+\Delta T_{MIN}$	-	H_20/LiBr
MHP (4)	100-120	140	-	-	130	$T_{EVAP}+\Delta T_{MIN}$	-	Water
MHP (5)	100-170	185	-	-	175	$T_{EVAP}+\Delta T_{MIN}$	-	Water
MHP (6)	100-180	205	-	-	195	$T_{EVAP}+\Delta T_{MIN}$	-	Water
DHR (2)	-	-	-	-	60	100-110	-	-
DHR (3)	-	-	-	-	70	100-120	-	-
DHR (4)	-	-	-	-	130	140-180	-	-
DHR (5)	-	-	-	-	175	185-200	-	-

The heat source temperatures in Fig. 9 can be further subdivided to taking into account the minimum exergy degradation associated with each technology option. Results of the hierarchy of technologies are shown in Table 4.

Table 4 hierarchy of waste heat utilization technologies for heat sources between 100°C and 200°C

Heat source temperature range	Technology ranking	Useful Insights
100°C – 120°C	1. Absorption chiller 2. Drive an absorption heat pump (heat upgraded for use at 70°C) 3. Organic Rankine cycle 4. Drive an absorption heat pump (heat upgraded for use at 60°C) 5. Mechanical heat pumps 6. Heat recovery via heat exchange (for hot water generation at 60°C)	See C2 and C3 in Table 2 C6: The exergy degradation of AHP reduces as the temperature difference between T_{GEN} and T_{WHS} reduces. See C1 and C5 in Table 2

	7. Heat recovery via heat exchange (for hot water generation at 40°C)	
120°C – 140°C	1. Absorption chiller	See C2 and C3 in Table 2
	2. Drive an absorption heat pump (heat upgraded for use at 70°C)	
	3. Organic Rankine cycle	
	4. Mechanical heat pumps	
	5. Drive an absorption heat pump (heat upgraded for use at 60°C)	
	6. Drive an absorption heat pump (heat upgraded for use at 40°C)	
140°C – 160°C	1. Heat recovery via heat exchange (sink at 130°C)	
	2. Absorption chiller	
	3. Drive an absorption heat pump (heat upgraded for use at 70°C)	
	4. Organic Rankine cycle	
	5. Mechanical heat pumps	
	6. Drive an absorption heat pump (heat upgraded for use at 40°C)	
160°C – 180°C	1. Absorption chiller	See C2 and C3 in Table 2
	2. Heat recovery via heat exchange (sink at 130°C)	
	3. Mechanical heat pumps	
	4. Organic Rankine cycle	
180°C – 200°C	1. Heat recovery via heat exchange (sink at 175°C)	
	2. Organic Rankine cycle	

4. 3. Waste heat sources above 200°C

The different ways considered in this work to utilize waste heat above 200°C are: (1) vaporizing the working fluids in ORC to produce electrical power, and (2) direct heat recovery for steam generation). For heat generation from waste heat directly, possible sink temperatures considered are 175°C (denoted by (5) in the graph legend), 195°C (denoted by (6) in the graph legend).

The screening tool for utilization technologies driven by heat sources above 200°C is shown in Fig. 10. The exergy degradation depends on the quality of heat source and the associated conversion technology. Operating temperatures and working fluids selection for the ORC are provided in Table 5. A minimum temperature difference of 10°C is assumed and ambient temperature of 25°C. From Fig. 10 for heat sources above 200°C, direct heat recovery is ranked above ORC.

Table 5 Operating temperatures and working fluids for utilization technologies

Technology	T_{EVAP} (°C)	T_{COND} (°C)	T_{GEN} (°C)	T_{ABS} (°C)	T_{SINK} (°C)	T_{WHS} (°C)	T_{CHILL} (°C)	Working fluid
ORC	200 - 265	30	-	-	-	$T_{EVAP}+\Delta T_{MIN}$	-	Benzene
DHR (5)	-	-	-	-	175	185-200	-	-
DHR (6)	-	-	-	-	195	205-245	-	-

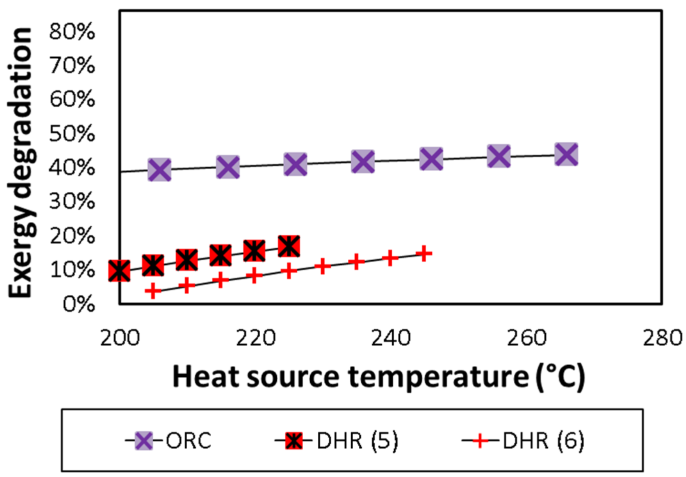

Fig. 10 Screening tool application for heat sources above 200°C

5. Concluding remarks

A novel screening tool is developed in the work to compare between technology options for waste heat utilization. The screening criterion takes into account the ideal thermodynamic performance of technologies and the actual performance (adjusted to account for irreversibilities due to finite temperature heat transfer). The screening tool visualizes the results clearly. Six technology options are screened: organic Rankine cycles, absorption chillers, absorption heat pumps, absorption heat transformers, mechanical heat pumps and heat recovery via heat exchange. The technologies are screened for varying heat sources from ambient to 260°C.

Results show that choice of technology options depend on the heat source temperature. Some general conclusions on choice of technology options are outline below:

1) Using high temperature waste heat (above 200°C) for electrical power generation via organic Rankine cycles should only be considered after direct heat recovery for medium pressure and high pressure steam generation.
2) The hierarchy of technologies such as absorption heat pumps, absorption heat transformers, mechanical heat pumps and heat recovery via heat exchange depends on the heat sink temperatures.
3) Using low temperature waste heat (below 100°C) for electrical power generation via ORC should be considered after chilling provision and hot water generation (depending on the hot water temperature).
4) The heat source quality to separate working fluids in the generator of absorption chillers, absorption heat pumps and absorption heat transformers should be separated by a minimum temperature difference from the generator temperature.
5) The heat sink for heat recovered in the condenser of mechanical heat pumps must be a minimum temperature difference colder than the condenser temperature. Where the value of the minimum temperature difference is dependent on trade-offs between capital and energy costs.

The screening tool is also useful for identifying technologies that need performance improvement. In this current work, only six technologies were screened, future work will consider other promising technologies.

Acknowledgement

The authors gratefully acknowledge: (1) the members of Process Integration Research Consortium (PIRC) for their financial support for the development of this research, and (2) the financial support provided by the European Commission 7th Framework Programme: EFENIS (296003). The second author thanks financial support from the National Natural Science Foundation of China (51206147).

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Appendix A: Values of α and β for utilization technologies and model validation for AHP, AHT and MHP

Table A.1. Selected working fluids for organic Rankine cycle application [9].

Working fluid	Chemical formula	$T_{critical}$ (°C)	$P_{critical}$ (MPa)	Boiling point (°C)	α_{ORC}	β_{ORC}	$T_{evaporator}$ (°C) range
Cyclopentane	C_5H_{10}	238.4	4.257	48.78	-0.5979	0.7622	48.78 – 238
Benzene	C_6H_6	288.9	4.894	80.10	-0.5085	0.7663	81 – 270

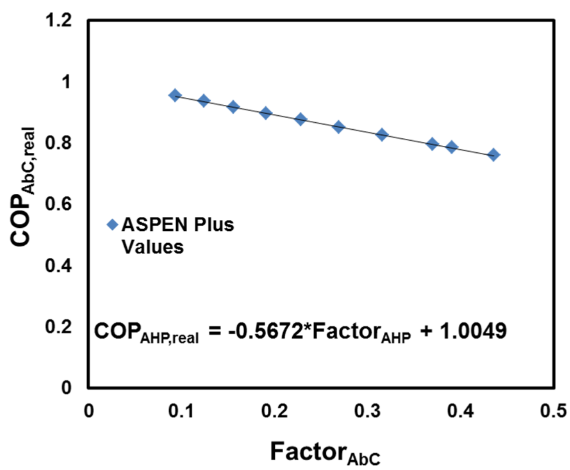

Fig. A.1 Fit for absorption chiller [9]

Table A.2 Values of regression coefficients for a water/lithium bromide absorption heat pump [33].

T_{GEN} (°C)	T_{EVAP} (°C)	T_{COND} = T_{ABS} (°C)	α_{AHP}	β_{AHP}
90	$20 < T_{EVAP} < 30$	50	–2.5064	3.4299
100	$20 < T_{EVAP} < 30$	50	–0.7448	2.2099
	$30 < T_{EVAP} < 40$	60	–2.9497	3.7592
110	$20 < T_{EVAP} < 30$	50	–0.5081	2.0366
	$30 < T_{EVAP} < 40$	60	–0.7478	2.2099
	$40 < T_{EVAP} < 50$	70	–2.4461	3.3795
140	$40 < T_{EVAP} < 50$	80	–1.7978	2.8816

Table A.3 Values of regression coefficients for a water/lithium bromide absorption heat transformer for T_{COND} = 30 °C [33].

T_{EVAP} (°C)	T_{ABS} (°C)	T_{GEN} (°C)	α_{AHT}	β_{AHT}
40	$60 < T_{ABS} < 90$	$50 < T_{GEN} < 80$	0.6356	–0.0549
50	$70 < T_{ABS} < 100$	$50 < T_{GEN} < 80$	0.6303	–0.0461
60	$80 < T_{ABS} < 110$	$50 < T_{GEN} < 80$	0.6270	–0.0392
70	$90 < T_{ABS} < 120$	$50 < T_{GEN} < 80$	0.6190	–0.0305
80	$100 < T_{ABS} < 130$	$50 < T_{GEN} < 80$	0.5797	–0.00704
90	$120 < T_{ABS} < 140$	$60 < T_{GEN} < 80$	0.6568	–0.0407

Table A.4 Values of regression coefficients for a mechanical heat pump [33].

Working Fluid	T_{cond} (°C)	T_{evap} range (°C)	α_{MHP}	β_{MHP}
n-butane	50	10 – 40	0.7319	-0.5154
	60	10 – 50	0.7259	-0.5602
	70	10 – 60	0.7181	-0.6077
	80	15 – 70	0.7081	-0.6582
	90	20 – 80	0.6952	-0.7107
	100	25 – 90	0.6781	-0.7639
	110	30 – 100	0.6551	-0.8149

	120	35 – 110	0.6217	-0.8504
	130	35 – 110	0.5586	-0.7767
Water	125	100 – 110	0.7484	-0.5518
	135	100 – 120	0.7482	-0.5363
	155	100 – 140	0.7468	-0.5014
	165	100 – 150	0.7448	-0.4729
	175	100 – 160	0.7448	-0.4746
	185	100 – 170	0.7435	-0.4639
	195	100 – 180	0.7418	-0.4547
	205	100 – 190	0.7399	-0.4474
	215	100 – 200	0.7376	-0.4410

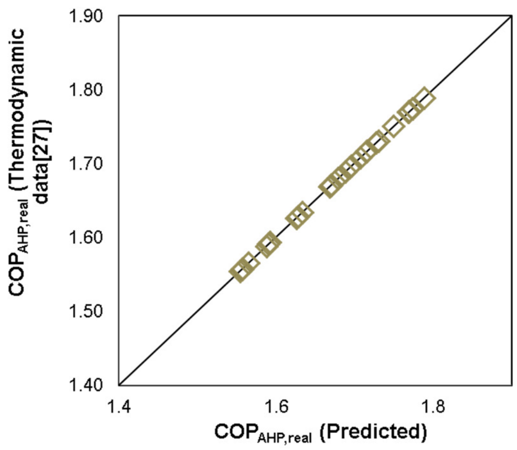

Fig. A.5 Model validation for AHP [33]

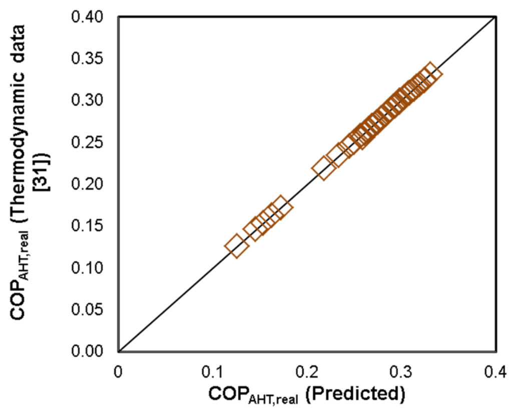

Fig. A.6 Model validation for AHT [33]

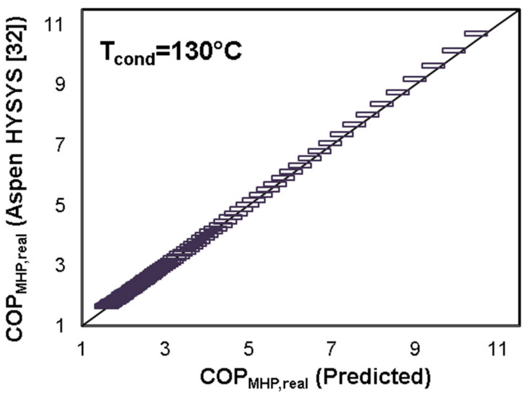

Fig. A.7 Model validation for MHP [33]

Appendix B: Derivation of ideal thermodynamic performance of AbC, AHP and AHT

The performance of the absorption chillers (AbC) is measured by the coefficient of performance:

$$COP_{AHP,real} = \frac{Q_{EVAP}}{Q_{GEN} + W_{PUMP}} \quad (A.1)$$

For an ideal cycle, the heat pump becomes a reversible Carnot engine in which the entropy change in the evaporator and condenser are equal:

$$\frac{Q_{EVAP}}{T_{EVAP}} = \frac{Q_{COND}}{T_{COND}} \quad (A.2)$$

Also for an ideal cycle, the change in entropy for the whole system is zero, thus:

$$\frac{Q_{EVAP}}{T_{EVAP}} + \frac{Q_{GEN}}{T_{GEN}} = \frac{Q_{ABS}}{T_{ABS}} + \frac{Q_{COND}}{T_{COND}} \quad (A.3)$$

Combining Equations A.2 and A.3:

$$\frac{Q_{GEN}}{T_{GEN}} = \frac{Q_{ABS}}{T_{ABS}} \quad (A.4)$$

An overall energy balance, neglecting the energy input from the liquid pumping, gives:

$$Q_{EVAP} + Q_{GEN} = Q_{ABS} + Q_{COND} \quad (A.5)$$

Combining Equations A.1 – A.5 gives:

$$COP_{AbC,ideal} = \left(1 - \frac{T_{ABS}}{T_{GEN}}\right)\left(\frac{T_{EVAP}}{T_{COND} - T_{EVAP}}\right) \quad (A.6)$$

The performance of the absorption heat pumps (AHP) is measured by the coefficient of performance:

$$COP_{AHP,real} = \frac{Q_{ABS} + Q_{COND}}{Q_{GEN} + W_{PUMP}} \quad (A.7)$$

Equations A.2 – A.5 also apply to the absorption heat pump. Combining Equations A.7, A.2 – A.5, neglecting the energy input from the liquid pump:

$$COP_{AHP,ideal} = 1 + \left(1 - \frac{T_{ABS}}{T_{GEN}}\right)\left(\frac{T_{EVAP}}{T_{COND} - T_{EVAP}}\right) \quad (A.8)$$

The performance of the absorption heat transformer is measured by the coefficient of performance:

$$COP_{AHT,real} = \frac{Q_{ABS}}{Q_{GEN} + Q_{EVAP} + W_{PUMP}} \qquad \text{(A.9)}$$

Equations A.2 – A.5 also apply to the absorption heat transformer. Combining Equations A.9, A.2 – A.5, neglecting the energy input from the liquid pump:

$$COP_{AHT,ideal} = \frac{T_{ABS}\left(T_{EVAP} - T_{COND}\right)}{T_{GEN}\left(T_{EVAP} - T_{COND}\right) + T_{EVAP}\left(T_{ABS} - T_{GEN}\right)} \qquad \text{(A.10)}$$

Chapter 5: Waste Heat Utilization Opportunities

Industrial waste heat has been defined as heat for which recovery is not viable economically (Ammar et al., 2012). The economic viability could depend on the use to which recovered energy is put i.e. waste heat utilization opportunities. Apart from economics, there could be potential to reduce CO_2 emissions by exploiting different end-uses of energy recovered from waste heat. The part of the methodological framework presented in Publications 1 – 3 enables the useful energy recovered from waste heat to be estimated, by applying the five thermodynamic cycles presented in this work. The end-use of recovered energy is addressed in this chapter.

The end-uses of recovered energy from waste heat are diverse and can occur within the boundaries of the process site (on-site) and over the fence (off-site). For example electrical power generated using organic Rankine cycles can be exported to a central grid, used to displace power imports within a site or used to displace any power produced from the site cogeneration system. Even though the same technology is applied, each of these end-uses has different financial benefits. The potential in industrial waste heat to improve economics and reduce CO_2 emissions could be dependent on the end-use of recovered energy.

In this chapter, on-site and off-site waste heat utilization opportunities are identified and ranked. The ranking criterion measure the economic potential associated with reduced CO_2 emissions resulting from waste heat recovery. Sensitivity of the hierarchy to energy prices is also studied to understand how uncertainties in energy prices affect the ranking and explore the outlook for waste heat utilization in the future. Models developed in Publication 1 and 2 are applied in this chapter. This chapter contains Publication 4.

5. 1. Introduction to Publication 4

In this paper, a hierarchy is introduced to end-uses of recovered energy from waste heat i.e. waste heat utilization opportunities. A graphical based methodology is also presented to use the hierarchy to design waste heat recovery systems. A waste heat recovery system allows for multiple end-uses of recovered energy.

Introduction to the paper and literature review to support the review in Chapter 2 (section 2.3) is provided in section 1. Both on-site and off-site waste heat utilization opportunities are identified in section 2. The ranking criterion is presented in section 3. Hierarchical ordering of utilization opportunities exploiting heat from 60°C – 260°C is presented in section 4. The hierarchy depends on the technology performance, technology capital costs, energy prices and discount rate.

In section 5, a methodology for using the hierarchy to design waste heat recovery systems is introduced and applied to a medium scale refinery case study in section 6. Conclusions are drawn in section 7.

Results show that there is potential in industrial waste heat to improve economics and reduce CO_2 emissions and this potential depends on the use to which recovered energy is put and design assumptions.

5. 2. Publication 4

Oluleye G., Jobson M., Smith R. A hierarchical approach for evaluating and selecting waste heat utilization opportunities. Energy 2015; 90: 5–23. doi: 10.1016/j.energy.2015.05.086.

Energy 90 (2015) 5–23

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

A hierarchical approach for evaluating and selecting waste heat utilization opportunities

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A R T I C L E I N F O

Article history:
Received 17 January 2015
Received in revised form
28 May 2015
Accepted 30 May 2015
Available online 26 June 2015

Keywords:
Waste heat recovery and utilization opportunities
Ranking criterion
Economic potential
Work
Chilling and heat generation
Waste heat recovery systems

A B S T R A C T

This paper presents a ranking criterion for evaluating opportunities that utilize recovered energy from the available waste heat in process sites. The ranking criterion takes into account the energy performance of waste heat recovery technologies associated with each opportunity, their potential to reduce greenhouse gas emissions (namely CO_2) and the economics (costs and benefits). Mathematical modelling of the opportunities using the ranking criterion is developed to allow for systematic evaluation of opportunities, for example within an optimization framework. A methodology using the ranking criterion to design site waste heat recovery systems is also proposed.

The methodology is applied to a case study of a petroleum refinery. Hierarchy and performance of waste heat utilization opportunities depends on the temperature of the heat available, amongst other factors. The site operating cost and CO_2 emissions reduce by 26% and 18% respectively when opportunities to use the recovered energy from waste heat within and outside the process site boundaries are explored. Sensitivity of the ranking to energy prices is studied, to explore the outlook for waste heat utilization in the future. The methodology can be applied to the process industries and other facilities producing waste heat.

1. Introduction

The process industries are responsible for 45% of global carbon dioxide emissions (the majority of which are from combustion of fuel to produce heat and electricity) [1]. Carbon dioxide emissions also account for the largest share of global greenhouse gas emissions [1]. Greenhouse gases are the major precursors of global warming, effects of global warming include: rise in sea levels, increase in global temperature, change in precipitation patterns, loss of habitat and treat to food security. There are three major ways to reduce industrial carbon dioxide emissions: (1) a shift to renewable energy, (2) carbon capture and storage, (3) improving energy efficiency. Energy efficiency has been identified as the most cost effective measure for carbon dioxide mitigation especially in the short and medium term.

As part of an energy efficiency measure, recovery of waste heat in the process industries has been identified as an effective way of improving the energy efficiency of process sites, reducing operating costs and reducing CO_2 emissions [2]. Utilization of waste heat is also described as a green, carbon neutral energy source [3]. Waste heat is defined as the residual heat after heat recovery within a process, heat recovery between several processing units on a site, and residual heat rejected to cooling water and air from a site utility system [4]. This waste heat is produced from multiple sources and occurs over a wide temperature range.

Mature and commercialised technologies exist to recover useful energy (electrical power, chilling and heating) from industrial waste heat. Examples include ORC (organic Rankine cycles) for electrical power generation, absorption chillers for chilling provision, heat exchangers and economisers. Organic Rankine cycles produces shaft work from low to medium temperature heat sources (50–220 °C [5]) using pure and mixed organic fluids [6]. The schematic of a basic cycle is shown in Fig. 1; waste heat vaporizes the working fluid in the evaporator, which expands to generate electricity. In absorption chillers, waste heat provides energy to desorb the absorption liquid in the generator which is condensed, flows through an expansion valve to the evaporator, where it is evaporated hence producing a refrigeration effect. A schematic is shown in Fig. 2. Heat exchangers (schematic shown in Fig. 3) are useful for heat transfer from a hot fluid i.e. heat source which could

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http://dx.doi.org/10.1016/j.energy.2015.05.086
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Nomenclature

Abbreviations

ACC	annualised capital cost (£/y)
AHT	after heat recovery
CEPCI	Chemical engineering plant cost index
CO_2E	site CO_2 emissions
CO_2R	CO_2 emissions reduced (kg/y)
EEx	electrical power exported (kW)
FB	financial benefits (kW)
HExN	heat exported to new buildings (kW)
HExE	heat exported to existing buildings (kW)
MC	maintenance cost (£/y)
OC	operating cost (£/y)
P	profit (£/y)
Q	quantity of energy (kW)
RC	ranking criterion
SOC	site operating costs (£/y)
T	temperature (°C)
TAC	total annualised cost (£/y)
TEC	total electricity cost (£/y)
TFC	total fuel cost (£/y)
UER	useful energy recovered (kW)
y	year

Subscripts

i	index for temperature interval
j	waste heat recovery technology
Δ	change

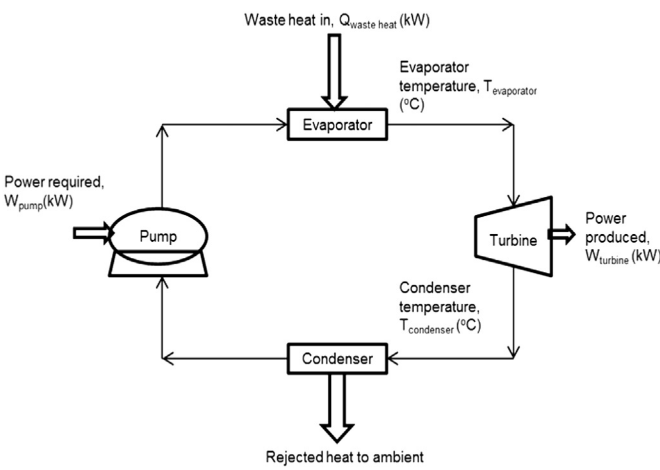

Fig. 1. Organic Rankine cycle schematic [4].

be waste heat to a cold fluid i.e. a heat sink, which could be for generating hot water. Economisers are gas–liquid tubular heat exchangers in which the hot gas (usually waste heat gas streams) flow over finned tubes containing a liquid to be heated up (for example boiler feed water) [3].

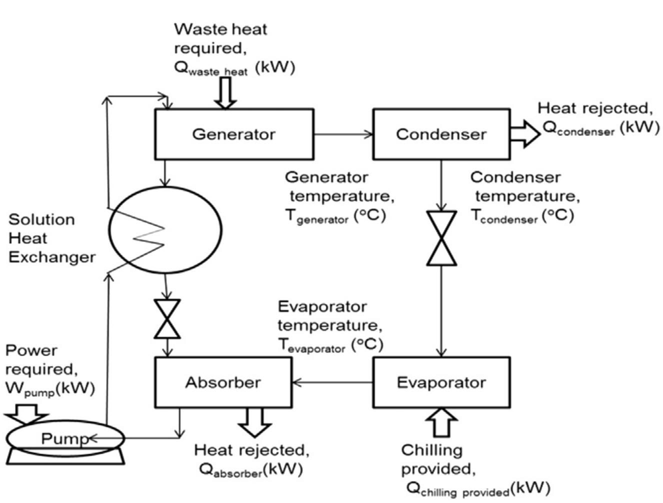

Fig. 2. Absorption chiller schematic [4].

In Hammond and Norman [8], the potential in waste heat is evaluated for the UK process industries. Technologies considered include Rankine cycles for power generation, heat exchangers for on-site waste heat recovery, mechanical heat pumps for heat upgrade, absorption chillers for chilling provision and heat transport off-site. The potential is evaluated based on primary energy saved and greenhouse gas emission saved. The economics (i.e. cost and benefits) associated with the use of recovered energy is neglected and waste heat sources are assumed to be at a single temperature. Opportunities for using waste heat in the UK food and drink industry was evaluated in Law et al. [3], the economic evaluation was limited to the cost of the technologies neglecting the value to which the recovered energy is put and the available waste heat is assumed to be at the same temperature.

For electrical power generation from industrial waste heat, Meinel et al. [9] investigated the performance and economics of an organic Rankine cycle, the economic analysis is based on total costs of operating the technology neglecting the value from using the electricity generated and the potential to reduce emissions. Song et al. [10] performed thermodynamic and economic analysis of an organic Rankine cycle for electrical power generation using five waste heat sources at different temperature levels; design was done at the same target temperature for all the heat sources. In this work, the economic criterion used is a ratio of net power output to total heat transfer area, neglecting the financial benefits associated with the use of the electricity generated and the potential to reduce CO_2 emissions. A technical, economic and market review of organic Rankine cycles was conducted in Velez et al. [11], the economic review is limited to investments in the technology also neglecting the financial benefits associated with the use of the generated electrical power, and the potential to reduce emissions.

Kapil et al. [12] considered different opportunities for using recovered energy from the available waste heat in a process site (a

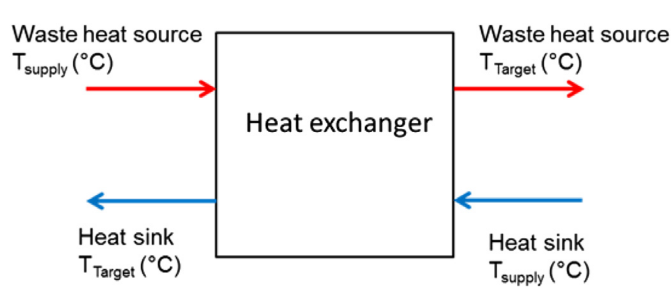

Fig. 3. Heat exchanger schematic.

petroleum refinery). Opportunities considered are boiler feed water preheating, electricity for site use and chilling for site processes. The impact on the site operating costs is used to determine the most promising opportunity. Benefits from emissions reduction and total cost, including capital, operating and maintenance costs of the heat recovery technologies are not considered, also the available waste heat sources are represented in a simplistic manner i.e. at a single temperature and from only the site processes. A similar analysis is performed for available waste heat in the UK food and drink industry [3] where saving in operating costs, and reductions in CO_2 emissions are used to evaluate opportunities to utilize waste heat. A major barrier to waste heat utilization, capital investments in technologies [2], was not considered in their work. The useful energy recovered and CO_2 emissions reduced is used in Viklund and Johansson [6] to evaluate opportunities for utilizing industrial waste heat again, the economics (costs and benefits) of waste heat recovery is neglected and the waste heat sources are assumed to be at a single temperature. Hammond and Norman [8] use only the CO_2 emissions reduction potential to evaluate waste heat utilization opportunities, also neglecting the economics (costs and benefits), again, the heat sources are represented in a rather simple manner i.e. in particular, it is assumed that all waste heat is available at one temperature. The potential in industrial waste heat to increase the energy efficiency of process sites is explored in Oluleye et al. [4]. A method is proposed to design a system taking into account the quantity of useful energy (i.e. electrical power, chilling and heat) produced; using thermodynamic models developed for organic Rankine cycles and absorption chillers. Even though the quantity and temperature of the residual waste heat, from the site processing unit and the utility system is taken into account, the use to which the recovered energy is put i.e. waste heat utilization opportunity is neglected. The use to which the recovered energy is put determines the economics of the system, and its potential to reduce CO_2 emissions.

There may be potential in industrial waste heat to increase the energy efficiency of process sites, reduce operating costs and CO_2 emissions; hence, evaluation of opportunities for waste heat utilization should take into account these issues as well as capital investment in waste heat recovery technologies.

Different opportunities have been identified to utilize the recovered energy from available waste heat in process sites [3]. Examples of such opportunities include: power for site use using an Organic Rankine cycle, boiler feed water preheating using an economiser, space heating using heat exchangers, and space cooling using absorption chillers. Even though the technologies required to implement these opportunities are mature and commercially available, with constraints on capital investment and space in existing process sites, it is important to rank these opportunities to identify the most promising technology, to support decision-making related to conserving resources and to reducing CO_2 emissions and costs.

The aim of this paper is to develop a systematic way of ranking and evaluating waste heat utilization opportunities for process sites. The ranking criterion is first introduced in Oluleye et al. [7]; however, a limited number of opportunities to use the recovered energy from waste heat were considered. Furthermore the sensitivity analysis conducted for the hierarchy introduced was limited to only changing energy prices. In this present work, the scope for utilization opportunities and sensitivity analysis is increased. In addition, a novel framework is proposed to apply the hierarchy of opportunities to select technology options and design site waste heat recovery systems.

The ranking criterion accounts for the financial benefits and capital investments in recovery technologies i.e. the economic potential. The EP (economic potential) is used to evaluate and compare design options and is suitable for use as an objective function to optimize process designs [13]. CO_2 emissions reduction potential will also be accounted for as fossil fuel combustion is responsible for over 70% of atmospheric greenhouse gas emissions [1]. The hierarchy introduced by applying the ranking criterion is applicable for screening and selecting Utilization opportunities and technology options to exploit waste heat. Evaluation of opportunities will take into account the temperatures of the heat sources from the site processes, and the site utility system. In summary, the methodology presented in this paper is focused on using the ranking criterion to identify the most promising waste heat utilization opportunity in order to support decision-making related to conserving resources and to reducing CO_2 emissions and operating costs.

2. Industrial waste heat utilization opportunities

The opportunities to utilize the recovered energy from waste heat on a site are diverse; each opportunity is associated with one or more waste heat recovery technologies. In this work, opportunities for a site are classified based on the location of the end-user (on-site or off-site e.g. for community heating and electricity to the grid). The scope of "waste heat" is defined as the residual heat after the potential for heat recovery within a process and between processing units is exhausted [4]. Therefore recovered forms of energy and utilization opportunities reflect this scope.

2.1. On-site waste heat utilization opportunities

Recovered energy can be used within the site whether directly (in form of heat) or converted to other forms of energy (electrical power and chilling). Electrical power generated from waste heat using organic Rankine cycles can reduce electricity import on-site or electricity generated from the cogeneration system; and associated financial benefits include the reduction in cost of imported electricity and fuel consumed in a cogeneration system. Environmental benefits include reduction in associated CO_2 emissions from imported electricity (using the grid emission factor) and reduction in fuel burnt to produce electricity within the site.

Site chilling demands can be supplied using waste heat to drive an absorption chiller. The chilling demand could be for a process or the inlet air to a gas turbine compressor; chilling the inlet air increases the density and mass flowrate of the air into the compressor, for a fixed volumetric flowrate thus increasing the power output [14]. When chilling provided by an absorption chiller is used in place of vapour compression systems; financial benefits results from reduction in compressor power cost, as the value of waste heat is low compared to high quality electrical power. Environmental benefits also result from saving in electricity required by the compressor. For chilling the inlet air into a gas turbine, financial benefits accrue from the power increase in the gas turbine. The electricity produced can be used to reduce electricity produced from the cogeneration system (resulting in primary energy savings). Environmental benefits are from reduction in the use of fossil fuels. Chilling provided from waste heat is applicable for space cooling thereby reducing electrical power consumption in a conventional vapour compression chiller.

Opportunities associated with using the heat directly include boiler feed water preheating (considering the boiler fuel type); resulting in a reduction in fuel consumption on-site, and space heating using hot water circulation, reducing the fuel consumption in a boiler that would otherwise be used. In summary, opportunities identified for on-site use of recovered energy considered in this work are shown in Table 1. The useful energy recovered is evaluated based on the models developed in Oluleye et al. [4] (Appendix A).

2.2. Off-site waste heat utilization opportunities

There are two forms of energy for export from a site: heat and electricity. It may be permitted for electricity produced from waste heat to be exported to the grid, thereby displacing fossil fuel consumption in power stations. Revenue can also be generated from selling electricity. Another form of energy for export is heat, even though most industrial sites are situated outside residential areas, there could still be agricultural activities and people living within 15–20 km of a process site (the distance identified as the maximum feasible distance for heat transfer [15]. Heat exported to existing buildings around the site displaces fossil fuels that would otherwise be burned to provide heating in homes, and the cost of installing and operating a boiler in new buildings around the site is off set when heat is exported. Revenue can be generated from the sale of heat to both existing and new buildings around the industrial site. The revenue generated from the sale of heat (or electricity) is determined in a way that results in a win–win situation, i.e. profit for the site and savings for off-site heat users (or the grid). In summary, opportunities for waste heat utilization off-site are shown in Table 2.

3. Ranking criterion for industrial waste heat utilization opportunities

Waste heat utilization opportunities can be ranked with respect to the useful energy recovered or the potential to reduce CO_2 emissions or the economic benefits (income less costs). Using any of these criteria alone cannot capture tradeoffs between useful energy (heat, power or cooling) produced from waste heat, emissions and economics (costs and benefits). Therefore it is important to develop a ranking criterion to capture all three. In this work, the proposed RC (ranking criterion) measures the economic potential associated with reduced CO_2 emissions resulting from waste heat recovery. The basis is emissions reduction because fossil fuel combustion is responsible for over 70% of atmospheric greenhouse gas emissions, especially CO_2 [1]. In this work, estimation of the ranking criterion depends on the location of the end-user (on or off-site).

3.1. Ranking criterion for on-site utilization opportunities

For on-site utilization opportunities, the EP (economic potential) is the difference between the annual FB (financial benefits) from operational savings associated with recovered energy and the TAC (total annualized cost) (sum of the ACC (annualized capital cost), OC (operating cost) and MC (maintenance cost)) of operating waste heat recovery technologies j required to implement the opportunity, shown as the numerator in Eq. (1). Reduced CO_2 emissions will be from savings in primary energy on-site as explained in Table 3.

Table 2
Off-site utilization opportunities.

Technology	Recovered energy	Utilization opportunity
Organic Rankine cycle	Electrical power	• Electricity export to the grid
Heat exchangers	Heat (hot water)	• Heat for new buildings • Heat for existing buildings

$$RC_{\text{on-site opportunities}}(\pounds/\text{kg}) = \frac{FB(\pounds/y) - TAC_j(\pounds/y)}{CO_2R(\text{kg}/y)} \quad (1)$$

$$TAC_j(\pounds/y) = ACC_j + OC_j + MC_j \quad (2)$$

3.2. Ranking criterion for off-site utilization opportunities

For off-site utilization opportunities, the EP is the profit (P) associated with the sale of energy (heat or power) Eq. (3).

$$RC_{\text{off-site opportunities}}(\pounds/\text{kg}) = \frac{P(\pounds/y)}{CO_2R(\text{kg}/y)} \quad (3)$$

The profits can be calculated from Eq. (4) for electricity sales, and Eqs. (5) and (6) for heat to new and existing buildings, respectively. To allow for a win–win situation, i.e. equal profit for the site and savings for off-site heat users, the constant A in Eqs. (4)–(6) is 0.5.

In Eq. (4), the site profit from electricity exported to the grid is half the difference between the cost of electricity and the total annualized cost of the organic Rankine cycle required to produce electricity from waste heat. The electricity generated from waste heat can be calculated using the model developed in Oluleye et al. [4] (shown in the Appendix). Furthermore in Eq. (5), the profit from heat exported to new heat users off-site is half the difference between the total annualized cost of installing a boiler in a new building, and the total annualized cost of heat exchangers required to generate hot water from waste heat on-site. In addition the profit from heat exported to existing building is half the difference between the operating (fuel) cost of a boiler in an existing building and the total annualized cost of heat exchangers required to generate hot water from waste heat on-site shown in Eq. (6) below.

The equation proposed in Eqs. (4)–(6) to estimate the site profit from energy (electricity or heat) exported ensures that if it is economic to export heat and power i.e. the total cost otherwise paid by the energy users off-site is greater than the total annualized cost of generating useful energy for export, then the selling price of energy (electricity or heat) will be less than what is paid by the energy users off-site making electricity or heat generated from available waste heat in a process site competitive.

Table 1
On-site utilization opportunities.

Technology	Recovered energy	Utilization opportunity
Organic Rankine cycle	Electrical power	• Electricity to reduce import on-site • Power to reduce cogeneration system fuel consumption
Absorption chiller	Chilling	• Chilling for site processes • Gas turbine compressor inlet air chilling • Space cooling
Heat exchangers	Heat (hot water)	• Space heating
Economiser	Heat	• Natural gas boiler feed water preheating • Coal boiler feed water preheating

Table 3
Financial benefits and CO_2 emissions reduction potential for on-site use of recovered energy.

Opportunity	Financial benefits	Impact on CO_2 emissions
1. Electricity for site use (reduce import and cogeneration system fuel consumption), gas turbine compressor inlet air chilling and boiler feed water preheating	Savings from reduction in site electricity imports or fuel saved from site cogeneration system	CO_2 displaced from fossil fuel combustion in the grid or directly from fuel saved in the site cogeneration system
2. Space cooling	Savings from electricity required to operate a conventional vapour compression chiller	CO_2 emissions displaced from electricity required to operate a vapour compression chiller
3. Space heating	Savings in fuel consumption from a boiler that would otherwise be used	CO_2 Emissions displaced from a boiler that would otherwise be used

$$P_{EEx}(£/y) = A.\left(TAC_{electricity}(£/y) - TAC_j(£/y)\right) \tag{4}$$

$$P_{HExN}(£/y) = A.\left(TAC_{boiler}(£/y) - TAC_j(£/y)\right) \tag{5}$$

$$P_{HExE}(£/y) = A.\left(TFC_{boiler}(£/y) - TAC_j(£/y)\right) \tag{6}$$

where TEC is the total electricity cost incurred by a domestic user, TAC_{boiler} is the total annualized cost for installing a boiler (sum of capital, fuel and maintenance cost) in a new building and TFC (total fuel cost) the total fuel cost for operating a boiler in an existing building.

The potential to reduce emissions from opportunities that involve export of heat and power is evaluated from the emissions displaced from fossil fuel combustion.

4. Hierarchical ordering of utilization opportunities

The ranking criterion developed in Sections 4.1 and 4.2 is applied to evaluate waste heat utilization opportunities, identified in Tables 1 and 2 above. This represents possible uses of recovered energy from waste heat in process sites. For this analysis, heat available over a wide range of temperatures from 60 °C–260 °C is considered.

Technology options for exploiting waste heat include Organic Rankine cycles, water/lithium bromide absorption chillers, economisers for boiler feed water preheating and shell and tube heat exchangers for hot water generation. To generate electrical power, an organic Rankine cycle using benzene and cyclopentane (below the boiling point of Benzene) as working fluids is available. Benzene and cyclopentane are selected because of their high value of thermal conductivity and latent heat of vaporization. The absorption chiller provides chilling at 8 °C and the economiser is used to preheat boiler feed water to 130 °C (maximum permissible for most boilers [18]). How water generation is at 80 °C for export to a neighbourhood 14 km away from the industrial site, and sale of electricity to the grid is permitted. Design assumptions on energy prices and emission factors are presented in Table 4 below.

Hierarchy of on-site utilization opportunities is presented in Section 4.1, off-site utilization opportunities in Section 4.2 and sensitivity analysis to the hierarchies developed performed in Section 4.3. The heat source temperature range considered in this section (60 °C–260 °C) is shifted by a minimum permissible temperature difference (−10 °C) to account for feasible heat exchange with technology options.

4.1. Hierarchy for on-site utilization opportunities

On-site utilization opportunities identified in this work are: preheating feed water into a natural gas and coal boiler, space heating, gas turbine compressor inlet air chilling, power to reduce import of electricity on-site, space cooling, chilling for site processes and electrical power generated from waste heat to reduce cogeneration system fuel consumption. The hierarchy of opportunities using Eq (1) is presented in Fig. 4 below.

Ranking of opportunities depend on the heat source temperature. There are no financial benefits when electrical power generated from waste heat off-sets power production on site from the cogeneration system. This is because the value of electricity displaced is low compared to the cost of installing an organic Rankine cycle, hence, the optimum point of most cogeneration systems is to export electrical power produced, to generate revenue for the site [25]. The economic benefit from CO_2 emissions reduced increase with temperature as seen when electrical power is produced, since the efficiency of organic Rankine cycles increase with the heat source temperature [4]. Opportunities associated with direct use of waste heat are ranked highest; the heat recovered is equal to the available waste heat (except for distribution losses). Chilling the inlet air into a gas turbine is ranked next, since for every kW of chilling provided, 2.2 kW of electricity is generated. Power to reduce import on-site is beneficial due to high savings from displacing electricity imports.

Table 4
Design assumptions on prices and emissions.

Energy prices [19]	Emission factors [19]	Investment costs	Others
Industrial electricity price: 13.4 p/kWh Industrial natural gas price: 3.2 p/kWh Industrial coal price: 1.42 p/kWh Domestic electricity price: 16.7 p/kWh Domestic natural gas price: 5.0 p/kWh	Grid emission factor: 0.485 kg/kWh Natural gas emission factor: 0.193 kg/kWh	Organic Rankine cycle: 1300 £/$kW_{electricity}$ [17] Absorption chiller: 180 £/$kW_{chilling}$ [14] Economizer: 227.5 £/m^2 [20]	Distribution network: 949 £/m [21] Discount rate: 15% Operating hours: 8600 years CEPCI 2011: 585.7 [22] CEPCI 2012: 584.6 [23] CEPCI 2013: 583.7 [24] CEPCI 2014: 586.77 [24] Retrofit factor: 3 [26] Heat transfer coefficient: 37 W/m^2K [20] Ambient temperature 25 °C

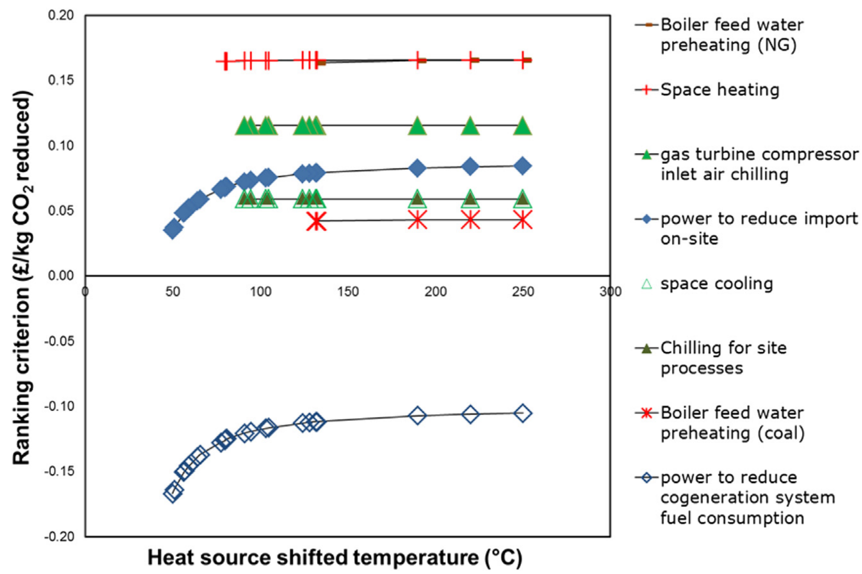

Fig. 4. Hierarchy for on-site utilization opportunities.

4.2. Hierarchy for off-site utilization opportunities

Off-site opportunities to use the recovered energy from waste heat include: hot water exported to new and existing neighbourhood, and electrical power exported to the grid. Exporting electrical power produced from waste heat could be a way to decarbonize central power stations. The hierarchy of opportunities is shown in Fig. 5.

Heat export to a new neighbourhood has a higher financial benefit from CO_2 displaced compared to an existing neighbourhood, since for a new building economical savings will be from the cost of boiler installation and maintenance compared to an existing building, where the benefits will accrue from reduction in the boiler fuel consumption.

When investment in the heating network for off-site use of recovered energy is taken into account, export of heat to both new and existing buildings become uneconomic, therefore incentives are required for this opportunity to be promising (Fig. 6).

4.3. Sensitivity analysis

Performing sensitivity analysis is necessary to understand the outlook for waste heat recovery in the future, and the impacts of uncertainties in design inputs.

The independent variables are shown in Table 5. The sensitivity involves increasing and decreasing energy prices by 20%, technology performances increase and decrease by 20%, and a high (5) and low retrofit factor (2).

4.3.1. Sensitivity of opportunities associated with electrical power generation

Sensitivity of opportunities to use electrical power within a process site and for export is shown in Fig. 7.

Reduction of electricity import on-site is the most economical way to use electricity generated from waste heat. The financial benefit from reduced CO_2 emissions when on-site import of electricity is reduced becomes negative when the retrofit factor and discount rate increases. The retrofit factor is related to how much modifications need to be made in existing process sites to fit an

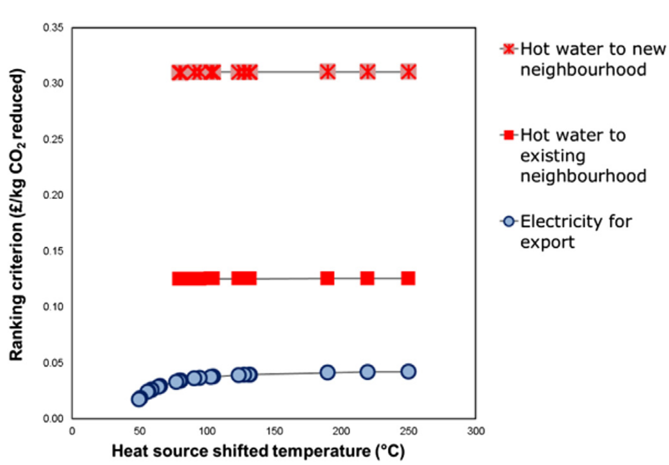

Fig. 5. Hierarchy for off-site utilization opportunities.

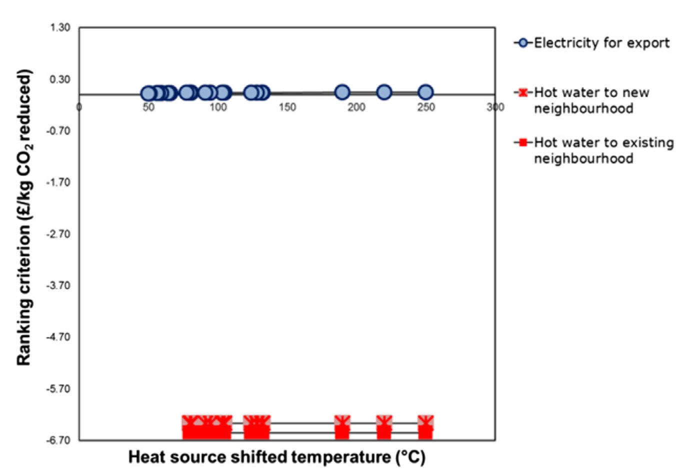

Fig. 6. Hierarchy for off-site opportunities (with investment in heating network).

Table 5
Sensitivity analysis independent variables.

1. Technology performance	2. Economic input
• Organic Rankine cycle efficiency	• Organic Rankine cycle capital cost
• Absorption chiller coefficient of performance	• Economiser capital cost
	• Absorption chiller capital cost
	• Retrofit factor
	• Industrial electricity price
	• Industrial natural gas price
	• Industrial coal price
	• Domestic natural gas price
	• Discount rate
	• Cogeneration system electricity value
	• Heating network cost over 14 km

organic Rankine cycle, while the discount rate is related to how much the investment will be paid yearly until the lifetime of the technology has elapsed. This trend is observed for other opportunities; the financial benefit from reduced CO_2 emissions associated with electrical power export becomes negative when the retrofit factor increases, and discount rate increases.

The highest financial benefit from CO_2 reduction by using electricity on-site is when the retrofit factor reduces, industrial electricity prices increases and the ORC capital cost reduces. Increasing the ORC efficiency by 20% has a negligible effect on the economics when the price of electricity does not increase. A reduction in the value of electricity imported reduces the ranking criterion compared to the base case.

There is financial loss associated with reduced CO_2 emissions when power is integrated within the cogeneration system to reduce fuel consumption; the efficiency of steam power generation from a cogeneration system is higher compared to both an ORC and the grid. Hence the value of electricity produced in a cogeneration system is low encouraging export of power, and low compared to the cost of electricity from an ORC; however, this might change if heat and power is considered. Therefore the recommended use of electrical power generated from an ORC is to reduce import of power within a process site. The temperature of the available heat should be taken into account since the ranking changes with temperature. Export of electricity to the grid is lower than reducing import on-site because the price for export is lower than import and in this case the price was determined to ensure a win–win situation between the site and the grid i.e. savings for the site and profit for the grid.

4.3.2. Sensitivity of opportunities associated with chilling provision

Hierarchy of opportunities using the chilling provided from waste heat, by an absorption chiller is shown in Fig.8. Chilling the inlet air into a gas turbine is ranked highest because for every kW of chilling provided to the inlet air, 2.2 kW of electricity is produced in the gas turbine compared to space cooling or process cooling where for every kW of chilling provided, 0.15 kW of electricity is saved. Chilling the inlet air into a gas turbine is a promising opportunity since for all sensitivities there is a positive financial benefit associated with reduced CO_2 emissions. The highest benefit is when there is an increase in the value of electricity from a cogeneration system; this could be from a decrease in the cogeneration efficiency. However, for chilling the inlet air into a gas turbine compressor, changing ambient temperature should be taken into account, since an increase in ambient temperature increases the financial benefit associated with reduced CO_2 emissions (Fig. 9) i.e. chilling the inlet air from 60 °C has a higher benefit than chilling from 25 °C.

Using the chilling provided for space cooling or process cooling has a negative RC when the retrofit factor and discount rate increases, as this makes the absorption chiller total cost more expensive compared to the value of recovered electricity. When the retrofit factor reduces and industrial electricity price increases, space cooling and process cooling become as competitive as chilling the inlet air into a gas turbine.

4.3.3. Sensitivity of opportunities associated with direct use of heat

Sensitivity analysis for opportunities associated with direct use of heat is shown in Fig. 10, the RC is positive for every case analysed. The highest financial benefit from CO_2 reduced is obtained when the price of (NG) natural gas increases for boiler feed water

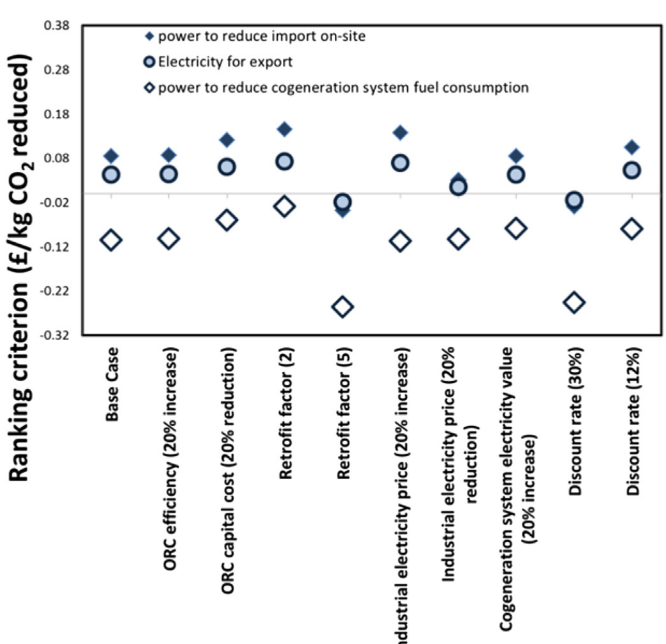

Fig. 7. Sensitivity analysis for opportunities associated with electrical power generation.

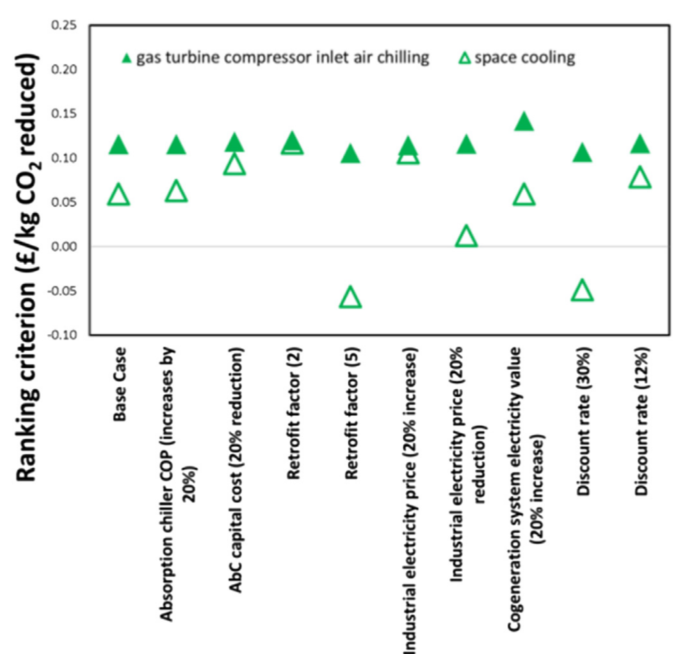

Fig. 8. Sensitivity analysis for opportunities associated with chilling provision.

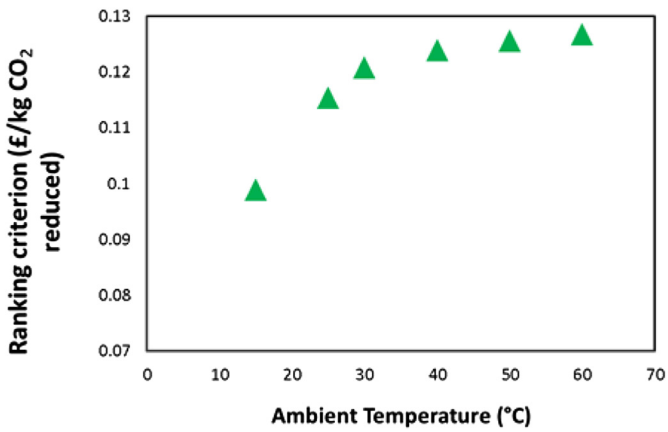

Fig. 9. Changing ambient temperature and ranking criterion for gas turbine inlet air chilling.

preheating and space heating, and when the price of coal increases for coal boiler feed water preheating. However, when the price of fuel reduces, the financial benefit from CO_2 emissions reduction reduces. Displacing natural gas results in a higher financial benefit compared to coal because the price per unit of CO_2 associated with NG is higher; therefore displacing emissions from NG gives a higher financial benefit i.e. more economic. Heat export to new buildings has a higher ranking compared to existing buildings; the benefits in new building is related to savings in installing a boiler while for an existing building the benefit is related to savings in operating a boiler.

4.3.4. Sensitivity considering both on and off-site utilisation opportunities

In this section, the hierarchy of all opportunities are considered. Key design inputs that increase the ranking of certain opportunities compared to others will be discussed. Compared to other opportunities to use recovered energy on-site:

a) Reducing the capital cost of an ORC makes it competitive with chilling the inlet air into a gas turbine compressor at temperature above 90.0 °C (Fig. 11), especially when the electrical power produced is used to reduce import of electricity within a site.
b) Reducing the retrofit factor makes space cooling and process cooling as competitive as gas turbine inlet air chilling, and electrical power generation to reduce electricity import becomes more economic than chilling provision (Fig. 12)
c) A higher electricity price increase competitiveness of ORC (Fig. 13)
d) Increasing the retrofit factor still keeps direct use of heat and gas turbine compressor inlet air chilling competitive (Fig. 14). However, space cooling, process cooling and installing an organic Rankine cycle becomes uneconomical.

Therefore for use of recovered energy on-site, the promising forms of recovered energy are chilling provision and direct heat. The promising opportunities are related to boiler feed water preheating, space heating and chilling the inlet air into a gas turbine. Using an organic Rankine cycle is only promising when the utilization opportunity is related to reducing import on-site. However, the economics depends on the cost of retrofit.

When all opportunities for using the recovered energy on-site and off-site are considered.

Heat export to new buildings has the highest RC (Fig. 15) and all opportunities associated with direct use of heat (except preheating water into a coal boiler) are ranked high compared to the others (Fig. 15). However, when investment in the heating network is considered, export of heat to both new and existing buildings become uneconomic, as was shown in Fig. 6 Even though heat export becomes uneconomics, there is still potential to reduce emissions.

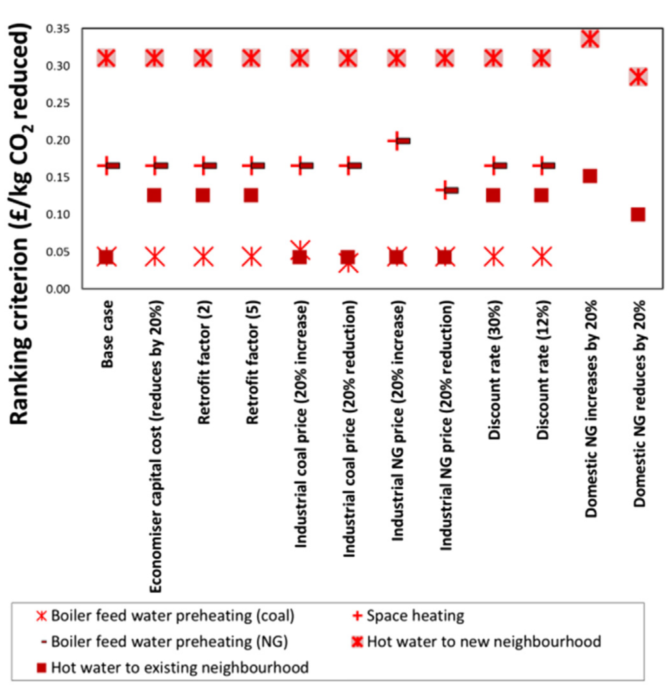

Fig. 10. Sensitivity analysis for opportunities associated with direct use of heat.

4.4. Summary for hierarchical ordering of utilization opportunities

The use to which recovered energy (whether heat, electrical power and chilling) from waste heat is put, determines the economic benefits and potential to reduce CO_2 emissions.

Heat recovery via heat exchange is still the most promising technology for waste heat recovery. However, this form of recovery becomes uneconomical when the capital cost of a heat distribution network is included especially for heat export. For opportunities such as boiler feed water preheating and space heating on-site, an increase in the equipment cost of economisers, increase in the retrofit factor, reduction in fuel prices, and increase in discount rate does not make them uneconomic.

An organic Rankine cycle is promising when equipment unit price reduces, retrofit factor reduces and industrial electricity price increases. Increasing the performance of an organic Rankine cycles alone does not improve its economic potential.

Absorption chillers are promising, because even when the equipment cost increases by 20%, retrofit factor increases to five times the equipment cost or electricity prices reduces by 20%, it is still economical to integrate them especially for chilling the inlet air into a gas turbine compressor. However, the benefits depend on ambient temperature as illustrated in Fig. 10 above.

In Section 4, the ranking criterion was used to introduce hierarchy to waste heat utilisation opportunities. The next section introduces a methodology for applying the ranking criterion to design site waste heat recovery systems.

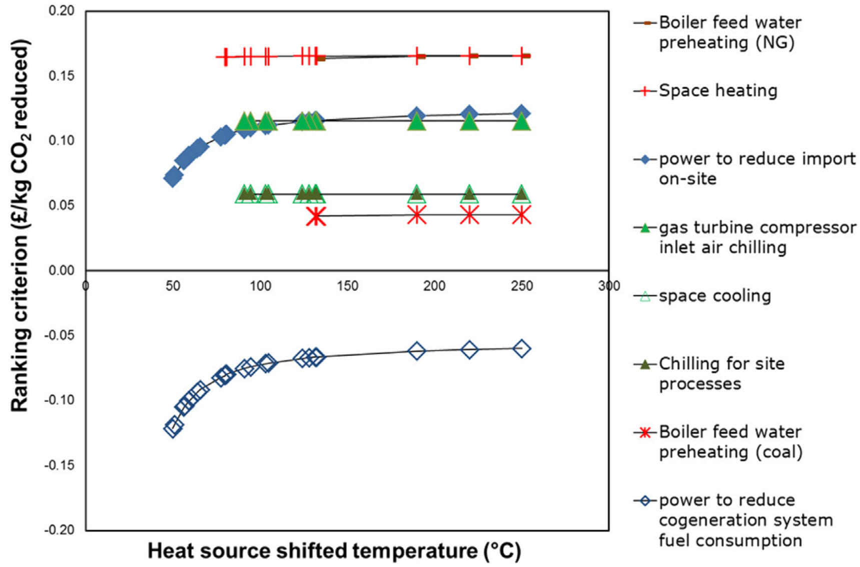

Fig. 11. Hierarchy when ORC capital cost reduces by 20%.

5. Methodology for using the ranking criterion to design site waste heat recovery systems

The ranking criterion can also determine how to combine utilization opportunities for waste heat exploitation in process sites. Combining different forms of energy has been identified as a way to maximize waste heat exploitation [4]. The method proposed in this work, takes into account the quality and quantity of heat sources from the site processes, and the site utility system. To represent the heat sources, the concept of waste heat source profiles proposed in Oluleye et al. [4] is adopted in this work. Waste heat source profiles are shifted temperature versus enthalpy plots of available waste heat in process sites. The heat source temperature are shifted by $-\Delta T_{MIN}$ for feasible heat recovery. For design purposes, the profile is divided into two; a profile for heat rejected to cooling water and heat rejected to air [4].

Temperature intervals (T_i) are introduced to analyse the profile. These intervals are kinks on the profile, the kinks represent the target temperatures of streams that make up the profile. In addition, using the kinks as temperature intervals ensures that high temperature waste heat is exploited before low temperature waste heat. The method is summarised in Fig. 16 below.

Selected utilization opportunities will be shown on the respective profiles for heat that was rejected to cooling water, and air at the final temperature intervals. Where the final temperature intervals are determined taking into account ranking of utilization opportunities, demand for recovered energy and technology size limitations. For example, industrial organic Rankine cycles are from 0.3 to 20 MW [4].

Opportunities associated with direct use of heat such as boiler feed water preheating and hot water generation are assigned against the waste heat source profile using their target

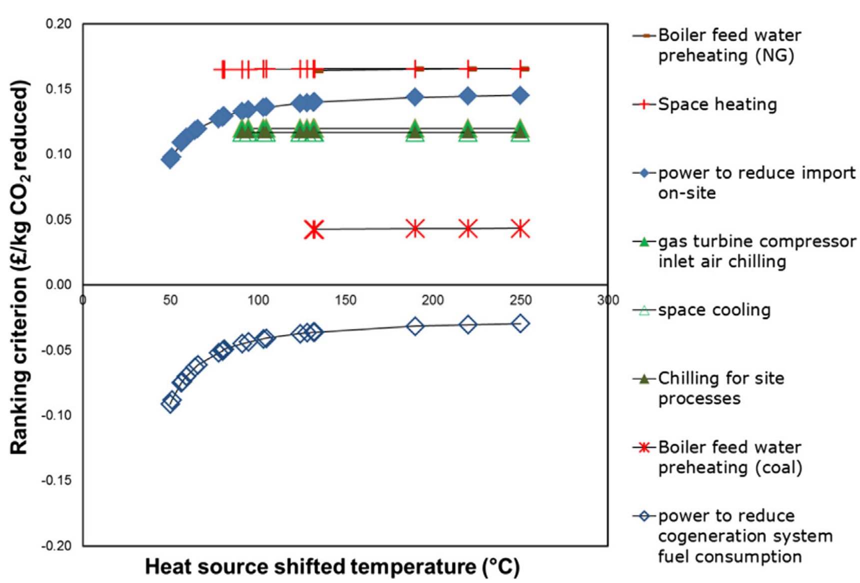

Fig. 12. Hierarchy when retrofit factor reduces by 2.

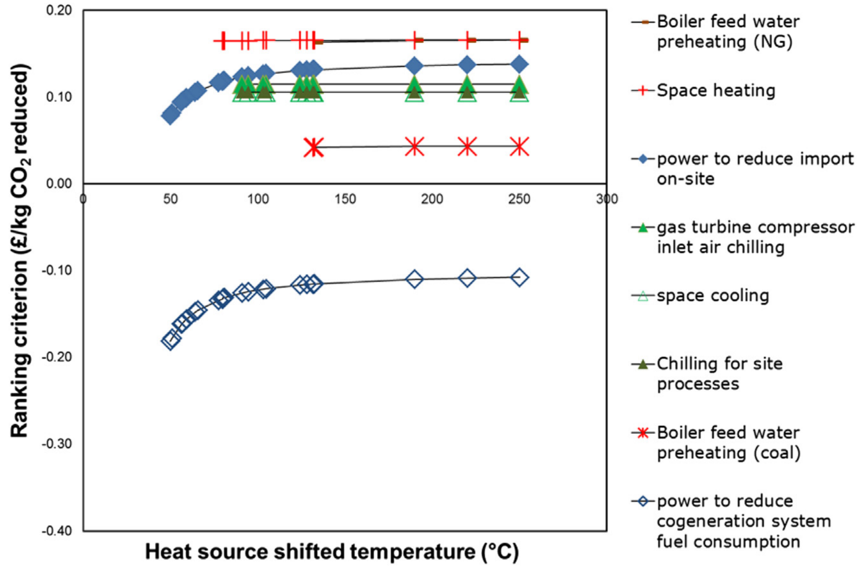

Fig. 13. Hierarchy when grid electricity price increases by 20%.

temperatures. For example if boiler feed water is preheated from ambient conditions to 130 °C using a heat source shifted temperature at 130 °C or above, the placement on the waste heat source profile will be a horizontal line at the heat source shifted temperature. Opportunities associated with chilling provision are represented using the generator temperature for absorption chillers i.e. the heat required to separate the working fluid pair. While opportunities associated with work generation are represented using the evaporator temperature of the working fluid in an Organic Rankine cycle.

The design will be evaluated based on the percentage of useful energy recovered (Eq. (7)) i.e. how much of the waste heat is recovered for use within the site and over the fence, % change in site operating cost (Eq. (8)) defined taking into account financial benefits and total cost of operating the waste heat recovery technologies and percentage change in site CO_2 emissions (Eq. (9)).

$$\mathrm{UER}(\%) = \frac{Q_{\mathrm{Recovered}}(\mathrm{kW})}{Q_{\mathrm{waste\ \ heat}}(\mathrm{kW})} \tag{7}$$

$$\Delta SOC(\%) = \frac{\mathrm{SOC}_{\mathrm{Base\ \ case}}(£/\mathrm{y}) - \mathrm{SOC}_{\mathrm{AHR}}(£/\mathrm{y})}{\mathrm{SOC}_{\mathrm{Base\ \ case}}(£/\mathrm{y})} \tag{8}$$

$$\Delta \mathrm{CO_2E}(\%) = \frac{\mathrm{CO_2E}_{\mathrm{Base\ \ case}}(\mathrm{kg/y}) - \mathrm{CO_2E}_{\mathrm{AHR}}(\mathrm{kg/y})}{\mathrm{CO_2E}_{\mathrm{Base\ \ case}}(\mathrm{kg/y})} \tag{9}$$

6. Case study

The case study presented is for a petroleum refinery with seven processing units; crude distillation unit, three hydrotreaters (for

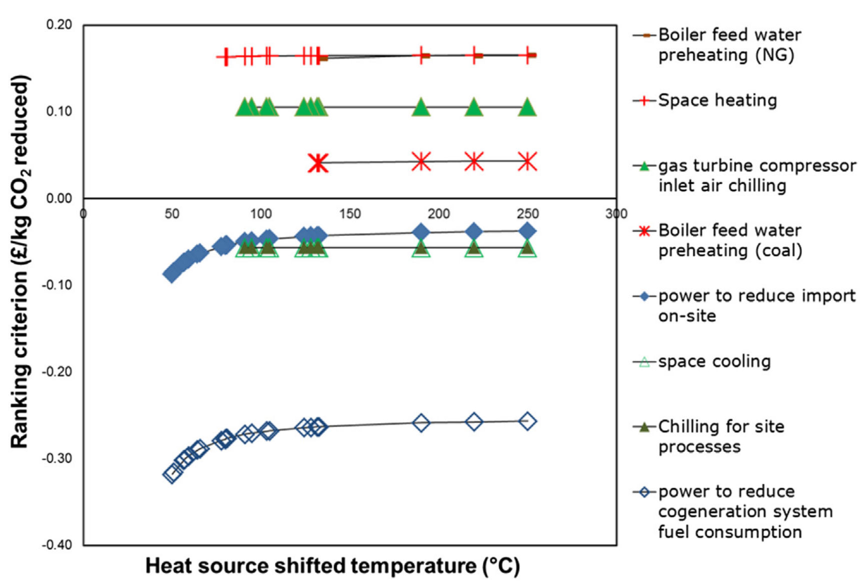

Fig. 14. Hierarchy when retrofit factor increases to 5.

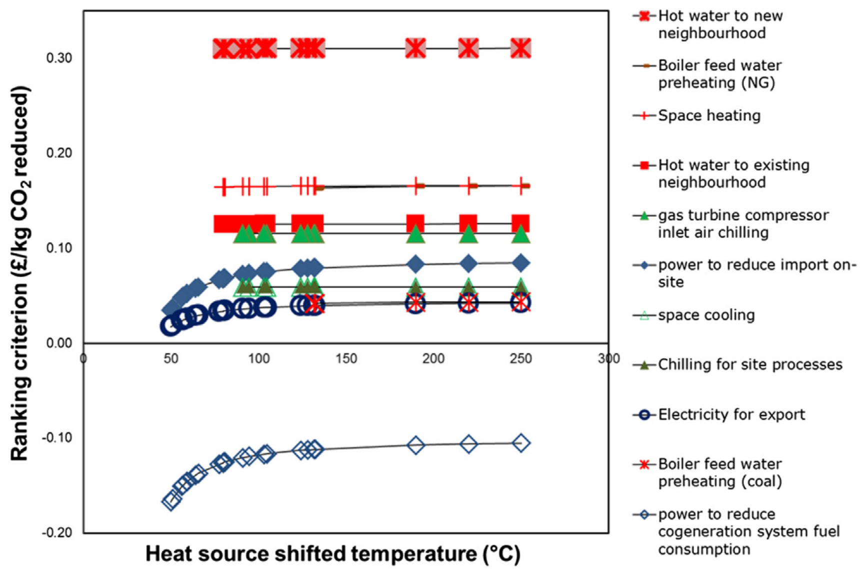

Fig. 15. Hierarchy for on-site and off-site utilization opportunities (base case).

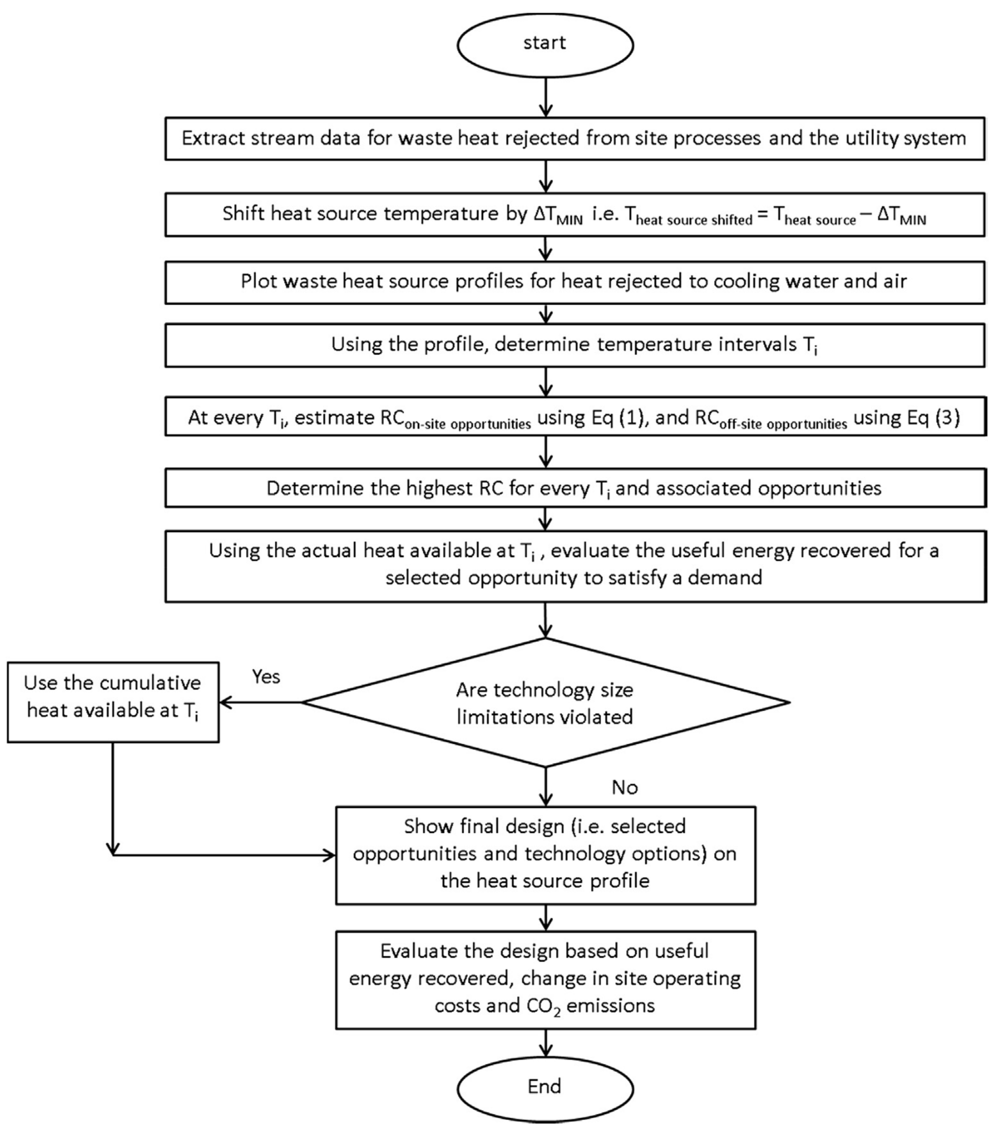

Fig. 16. Methodology for design of process sites waste heat recovery systems using the ranking criterion.

Table 6
Actual and cumulative heat at the PHRT for heat rejected to cooling water.

Shifted temperature interval T_i (°C)	Actual heat available (kW)	Cumulative heat available (kW)
250.07	1940	1940
220.00	1133	3070
190.00	1130	4210
132.50	2810	7010
131.70	39	7050
128.00	390	7440
124.08	491	7930
104.87	3260	11,190
103.20	537	11,730
94.80	2640	14,370
90.90	1850	16,220
80.80	5500	21,730
80.10	380	22,105
80.00	131,250	153,350
77.50	1240	154,590
65.74	5800	160,390
64.20	660	161,050
59.20	2330	163,380
59.10	78	163,450
56.90	1160	164,620
56.40	500	165,120

Table 7
Actual and cumulative heat at the PHRT for heat rejected to air.

Shifted temperature interval T_i (°C)	Actual heat available (kW)	Cumulative heat available (kW)
281.25	992	992
140.00	22,360	23,352

naphtha, kerosene and diesel), a vacuum distillation unit, a platformer, a visbreaker and a fluidised catalytic cracking unit [16].

Data extracted for heat rejected to cooling water and air is shown in Appendix B. the generated waste heat source profile and the existing site profiles are also shown in Appendix B. In Table 6, the temperature intervals identified as kinks on the profile for heat rejected to cooling water is presented, and Table 7 for heat rejected to air.

The refinery site currently exports electricity; has a cogeneration system consisting of a coal boiler, gas turbine and steam turbines, and a refrigeration system (vapour compression system) producing 420 kW chilling at 8 °C for the site processes. The closest off-site heat users (requiring hot water at 80 °C) are 14 km away from the site and sale of electricity to the grid is permitted. 10% distribution and transmission losses for heat export is assumed. Identified waste heat utilization opportunities for on-site and off-site use of recovered energy and actual demand for recovered energy are shown in Table 8.

The ranking criterion developed in Eqs. (1) and (3) is used to introduce hierarchy for the waste heat utilization opportunities identified for on-site and off-site opportunities in Table 8 above.

Table 8
Identified waste heat utilization opportunities and associated demand for recovered energy.

On-site utilization opportunities		Off-site utilization opportunities	
Gas turbine compressor inlet air chilling	960 $kW_{chilling}$	Electricity for export	25,000 kW (maximum)
Chilling for site processes	420 $kW_{chilling}$	Heat to existing buildings	2400 kW_{heat}
Boiler feed water preheating (Coal)			

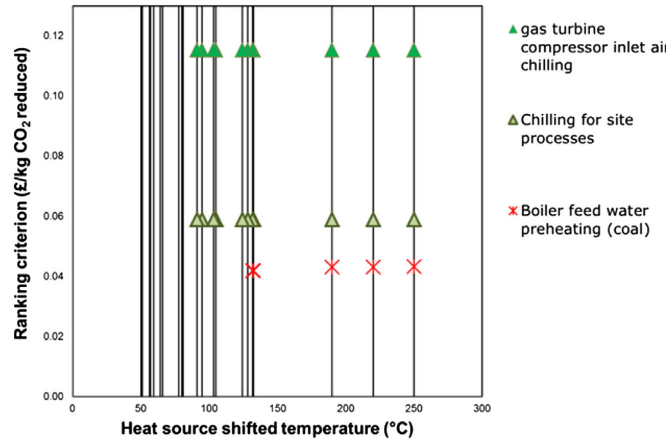

Fig. 17. Hierarchy of identified opportunities for on-site use of recovered energy.

Assumptions of UK energy prices, emissions factors and equipment capital costs are presented in Table 4. To generate electricity, an Organic Rankine cycle using benzene and cyclopentane as working fluid is available [4]; chilling using a lithium bromide/water absorption chiller, and hot water generation using a shell and tube heat exchanger. The site boiler feed water is at 116 °C (after the feed pump), it is desirable to heat it to 130 °C, and the gas turbine compressor inlet air is currently at ambient condition and is to be chilled to 8 °C. Models of technologies are shown in Appendix A. The site operating cost and CO_2 emissions before recovery are 26 million£/y and 845,208 t/y respectively. The case study will illustrate how to apply the ranking criterion to design site waste heat recovery systems.

6.1. Design for on-site use of recovered energy

Hierarchy of identified opportunities for on-site use of recovered energy is shown in Fig. 17. Vertical lines represent the temperature intervals. Based on the hierarchy chilling the inlet air into a gas turbine compressor has the highest financial benefit from reduced CO_2 emissions compared to the other opportunities; however, the amount of chilling provided is limited by the demand for recovered energy. Taking into account demand for recovered energy and technology size limitations, Figs. 18 and 19 shows placements of technologies against the profile for heat rejected to cooling water and air respectively.

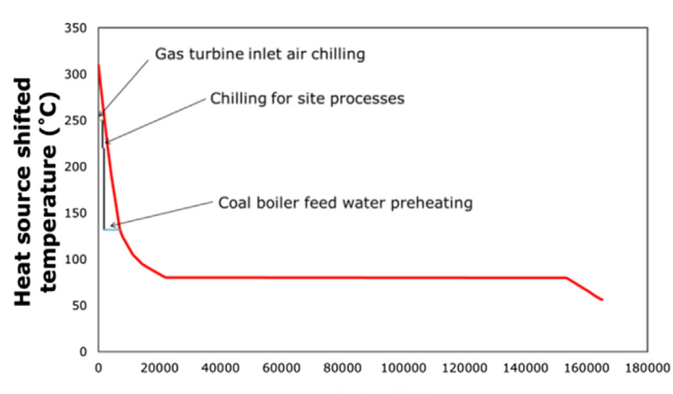

Fig. 18. Placement of technologies against the profile for heat rejected to cooling water.

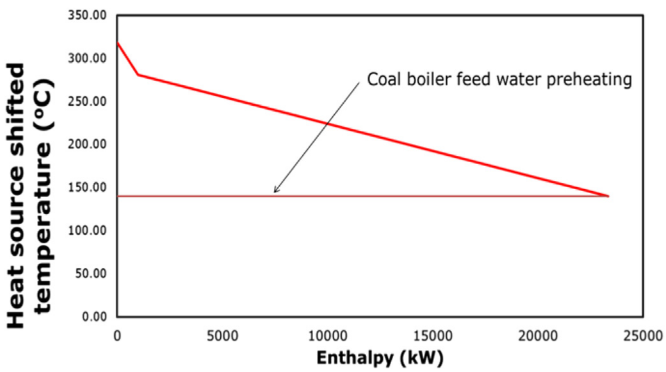

Fig. 19. Placement of technology against the profile for heat rejected to air.

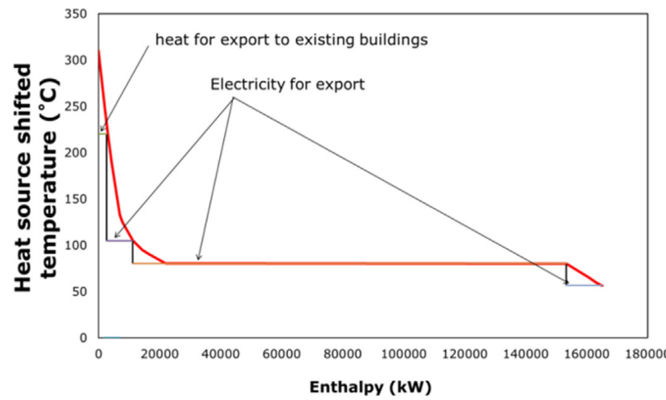

Fig. 21. Placement of off-site utilization opportunities against the profile for heat that was rejected to cooling water.

In total, 30,400 kW of useful energy was recovered (1275 kW used to drive the absorption chiller for GT (gas turbine) compressor inlet air chilling, 560 kW used to drive the absorption chiller for process chilling and 28,565 kW used for coal boiler feed water preheating). Of all the heat rejected to air and cooling water, 16% useful energy was recovered. This has potential to reduce the site operating cost by 17.8% and site CO_2 emissions by 11%.

6.2. Design for off-site use of recovered energy

Hierarchy of opportunities for off-site use of recovered energy is shown in Fig. 20 below. Based on the hierarchy, heat export to existing building should be considered before electricity export (excluding distribution costs). Placement of technologies against the profile for heat rejected to cooling water and air taking into account demand for recovered energy and technology size limitations are shown in Figs. 21 and 22 respectively.

Organic Rankine cycles are placed against the heat source profile using waste heat at 114.87 °C, 90 °C and 66.40 °C (real temperatures). A breakdown analysis of the net electrical power produced is shown in Table 9 below. Using Eq. (A.2–A.4) in Appendix A, the real efficiency (η_{Real}) i.e. net power produced per unit waste heat, is estimated from the ideal efficiency (η_{Ideal}) and a factor accounting for inefficiencies in the cycle's components, and working fluid non-ideal behaviour [4].

A total of 22,010 kW of useful energy is recovered (2650 kW heat and 19,360 kW electricity from Organic Rankine cycles) i.e. 12% useful energy recovered, this has potential to reduce site emissions by 10.3% and reduce site operating cost by 14%.

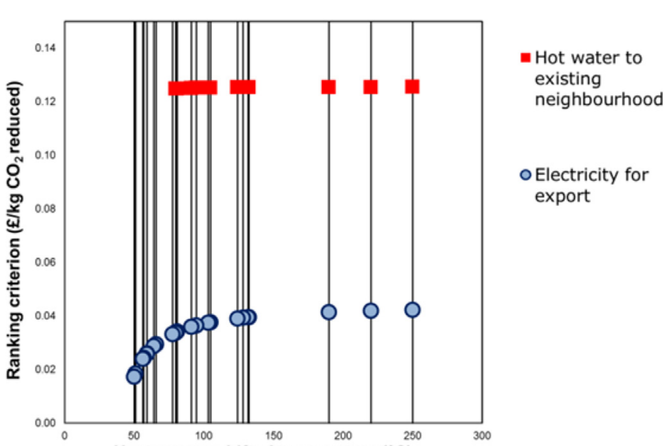

Fig. 20. Hierarchy of identified opportunities for off-site use of recovered energy.

6.3. Design for both on and off-site use of recovered energy

Hierarchy of opportunities for on and off-site use of recovered energy is shown in Fig. 23 below. Based on the hierarchy, heat export to existing buildings should be considered before electricity export (excluding distribution costs). Placement of technologies against the profile for heat rejected to cooling water and air taking into account demand for recovered energy and technology size limitations are shown in Figs. 24 and 25 respectively.

From Fig. 24, 2655 kW of available waste heat is exported, 1275.2 kW used to drive the separation of working fluids in the absorption chiller for GT compressor inlet air chilling, 560 kW for separation of working fluids in the absorption chiller for site process chilling and 2560 kW for boiler feed water preheating. The remainder heat; 4140 kW at 104.87 °C (shifted temperature), 142,160 kW at 80 °C (shifted temperature) and 11,760 kW at 56.4 °C (shifted temperature) is used to vaporize the working fluid in the evaporator of organic Rankine cycles for electrical power generation. Estimation of the net electrical power produced is shown in Table 10 below; using Eqs. (A.2–A.4) in Appendix A.

A total of 45,260 kW of useful energy is recovered (2650 kW heat, 1840 kW used to drive absorption chillers for providing chilling to the site processes and the inlet air into the gas turbine compressor, 25,910 kW for coal boiler feed water preheating and 14,860 kW electrical power using Organic Rankine cycles) i.e. 24% useful energy recovered, this has potential to reduce site emissions by 17.6% and reduce site operating cost by 26.5%.

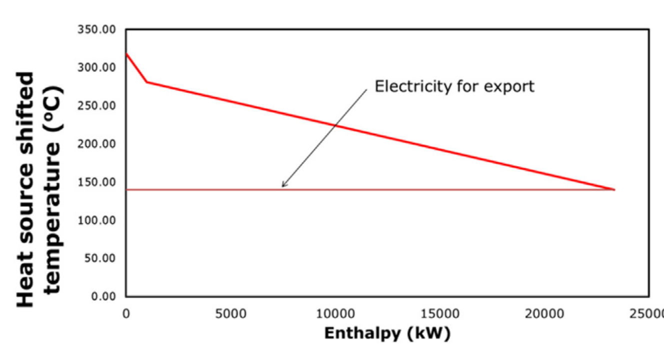

Fig. 22. Placement of off-site utilization opportunities against the profile for heat that was rejected to air.

Table 9
Net electrical power produced from available waste heat for off-site use of recovered energy.

Heat source	Opportunity	Heat available (kW)	Heat source shifted temperature (°C)	Working fluid
Heat that was rejected to cooling water	Electricity for export	8540	104.87	Benzene
		142,160	80	Cyclopentane
		11,760	56.40	Cyclopentane
Heat that was rejected to air	Electricity for export	23,350	140	Benzene

η_{Ideal} (%)	$Factor_{ORC}$ (%)	η_{Real} (%)	W_{net}^{Model} (kW)	W_{net}^{HYSYS} [27] (kW)	Error (%)
19.81	66.56	13.18	1125.54	1121.5	0.36
14.16	67.75	9.59	13,637	13,576	0.45
8.01	71.43	5.72	673.25	666.4	1.02
26.62	63.09	16.80	3922.1	3925.6	0.09

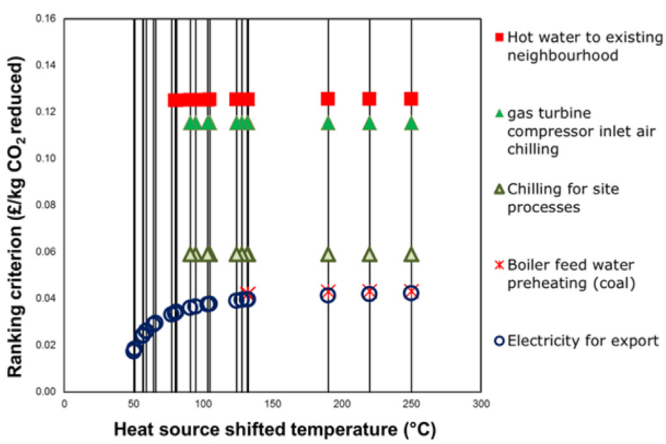

Fig. 23. Hierarchy of opportunities for both on and off-site use of recovered energy.

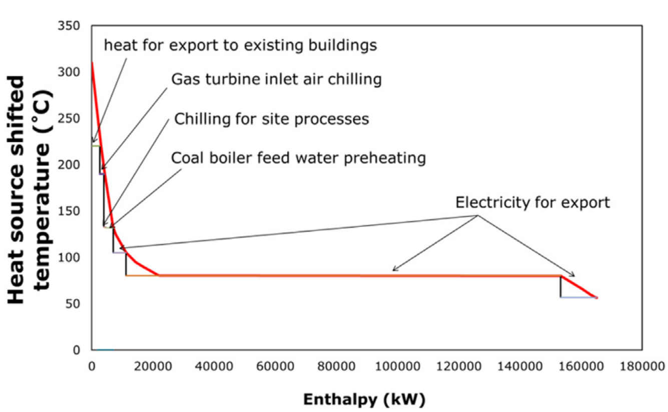

Fig. 24. Placement of opportunities against the profile for heat that was rejected to cooling water.

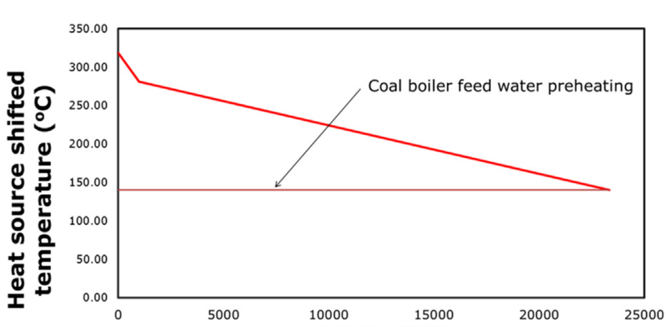

Fig. 25. Placement of opportunities against the profile for heat that was rejected to air.

6.4. Case study summary

Fig. 26 (a)–(c) shows the useful energy recovered in all cases considered above i.e. on-site use of recovered energy, off-site use of recovered energy, and on and off-site use of recovered energy. The biggest contribution to the useful energy recovered depends on the performance of technologies and demand for recovered energy.

The percentage change in useful energy recovered, site operating cost and site CO_2 emissions for all cases are shown in Fig. 27 below.

Benefits from recovered energy, reduced emissions and costs are higher when opportunities involving on and off-site use of recovered energy is considered. However, investments in heat distribution cost are not taken into account.

When investment in the heating network is taken into account, Fig. 28 shows the hierarchy of all identified opportunities. In this case, heat export to existing buildings becomes unprofitable. However, other opportunities can be harnessed such as chilling provision, boiler feed water preheating and power generation for export. Placement of technologies against the profile for this case is shown in Figs. 29 and 30 for heat rejected to cooling water and air respectively. A total of 45,260 kW of useful energy is recovered as shown in Fig. 30 (1840 kW used to drive absorption chillers for providing chilling to the site processes, and the inlet air into the gas turbine compressor; 28,560 kW for coal boiler feed water preheating and 14,860 kW electrical power using Organic Rankine cycles) i.e. 24% useful energy recovered, this has potential to reduce site emissions by 17.9% and reduce site operating cost by 25%.

Summary for both cases of on and off-site use of recovered energy with and without investment in the heating network is shown in Fig. 31 below.

Even though investing in a heating network may be uneconomic, there is still potential to reduce emissions; and numerous opportunities on and off-site also exist to use the recovered energy from waste heat.

7. Conclusions

A ranking criterion accounting for the economic value of useful energy recovered from waste heat and impact on CO_2 emissions is introduced in this work to evaluate opportunities for waste heat utilization in process sites. The RC can be used to screen and select waste heat utilization opportunities for a process site depending on the waste heat source temperature. In this work, it is applied to evaluate opportunities to reuse waste heat available in a site. In the illustration, results show that ranking of opportunities depends on the heat recovery temperature. For opportunities such as electricity generation for site use and export the value (economic and potential to reduce emissions) increases with the heat source temperature, therefore waste heat at high temperature should be

Table 10
Net electrical power produced from available waste heat for on and off-site use of recovered energy.

Heat source	Opportunity	Heat available (kW)	Heat source shifted temperature (°C)	Working fluid	η_{Ideal} (%)	$Factor_{ORC}$ (%)	η_{Real} (%)	W_{net}^{Model} (kW)	W_{net}^{HYSYS} [27] (kW)	Error (%)
Heat that was rejected to cooling water	Electricity for export	4140	104.87	Benzene	19.81	66.56	13.18	545.97	544	0.36
		142,160	80	Cyclopentane	14.16	67.75	9.59	13,637	13,576	0.45
		11,760	56.40	Cyclopentane	8.01	71.43	5.72	673.25	666.4	1.02

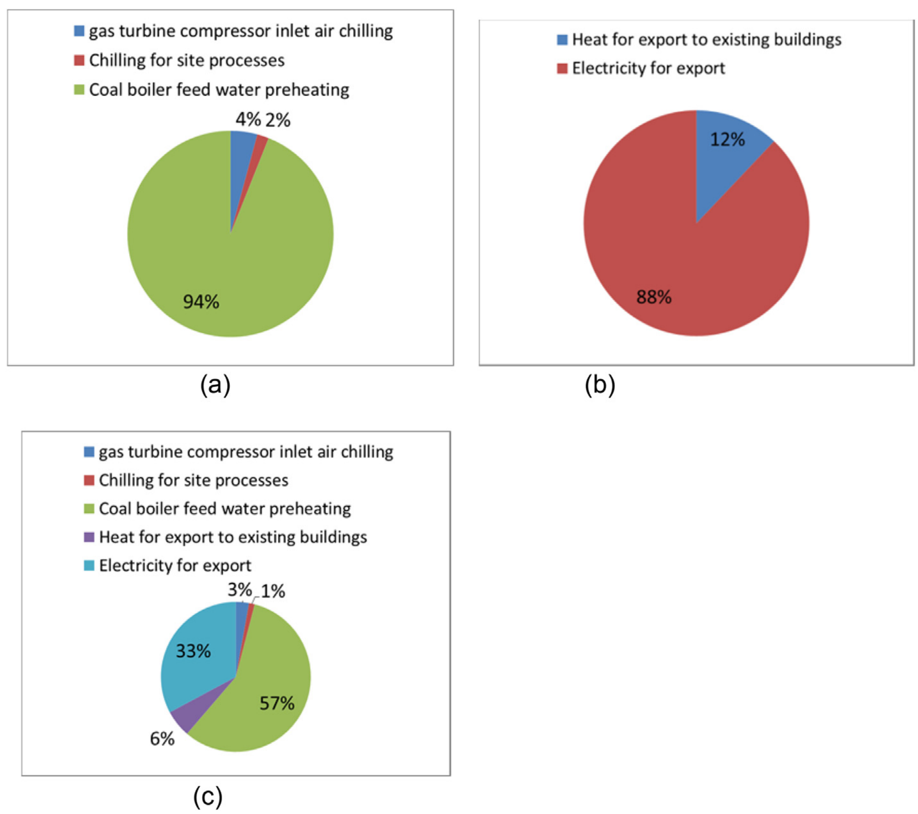

Fig. 26. Useful energy recovered in all cases (a) on-site (b) off-site (c) on and off-site.

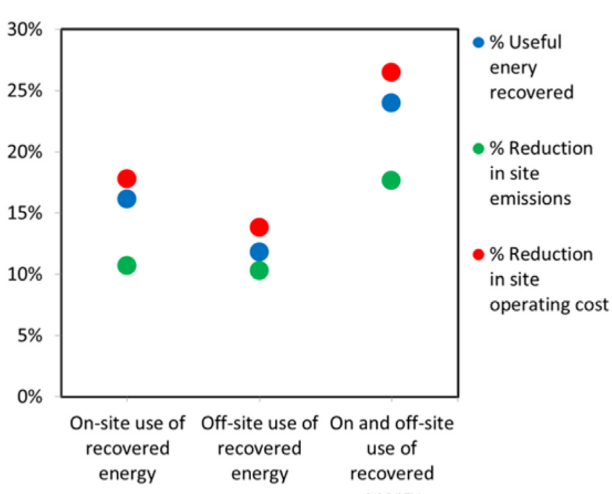

Fig. 27. Case study results summary.

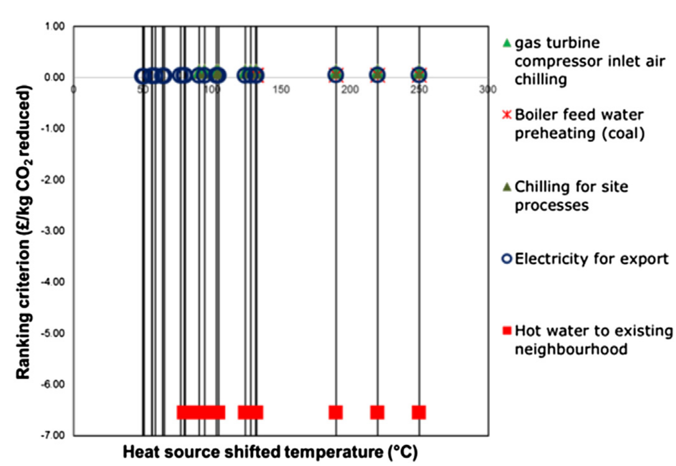

Fig. 28. Hierarchy of identified opportunities (heating network cost included).

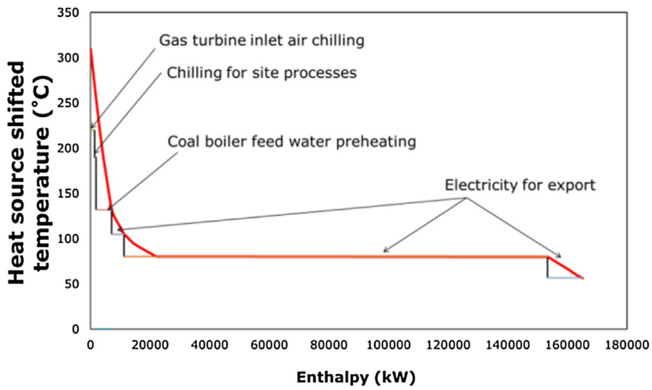

Fig. 29. Placement of opportunities against the profile for heat that was rejected to cooling water.

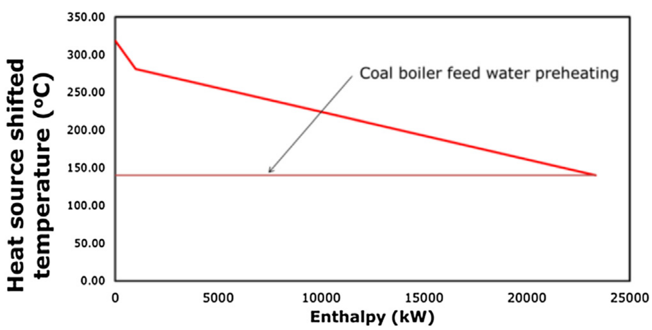

Fig. 30. Placement of opportunities against the profile for heat that was rejected to air.

exploited before low temperature waste heat, as there are more opportunities to exploit the heat and the value is higher.

A methodology was also proposed for using the Ranking criterion to design site waste heat recovery systems, taking into account the temperature of the heat sources, quantity of heat available, demand for recovered energy and technology size limitations. Results from application to a medium scale petroleum refinery show that there is potential in waste heat to increase efficiency in the use of fuel, reduce emissions and costs in process sites. The site CO_2 emissions reduce by 11%, and 16% useful energy is recovered when only economic on-site utilization opportunities are explored. For example, integrating an absorption chiller to provide chilling for site processes and the inlet air into a gas turbine, and integrating economizers for boiler feed water preheating. There is potential to reduce the site CO_2 emissions by 10.4%, from useful energy exported in form of heat to existing neighbourhoods and electrical power to the grid. Exploiting opportunities to use the energy recovered both within the process site and over the fence, results in the highest potential for CO_2 emission reduction (17.6% w.r.t the base case) and 24% useful energy was recovered. Demand for the useful energy recovered was considered in this work.

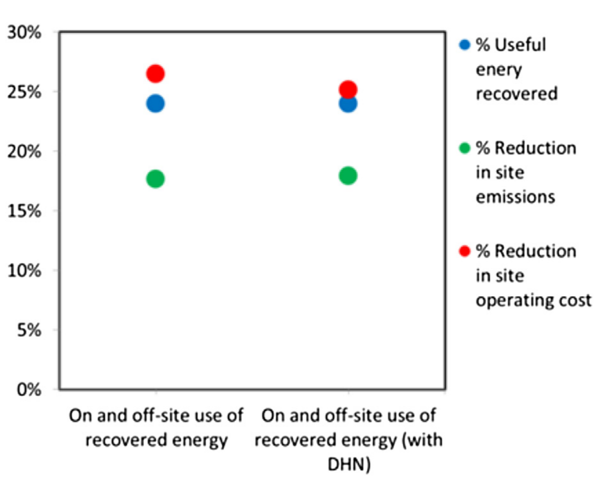

Fig. 31. Case study results summary (heating network cost included).

Sensitivity of the criterion to energy prices, technology performance and capital costs is conducted. As energy prices and technology performance increase, waste heat recovery becomes more attractive both economically and environmentally. While as the capital cost increases (especially related to the cost of installing equipment), waste heat recovery becomes less attractive economically but still has potential to reduce emissions. Therefore, in existing process sites the cost of retrofit should be taken into account.

In this work opportunities for utilization of the recovered energy from waste heat are limited to the process energy consumption; future work will include opportunities to change the process operating conditions in order to increase product yields. An optimization framework will also be developed to account for the cost of retrofitting existing process sites; to accommodate waste heat recovery technologies.

Acknowledgement

The authors gratefully acknowledge the members of Process Integration Research Consortium (PIRC) for their financial support for the development of this research.

Appendix A

Models of waste heat recovery technologies [4].

A. Organic Rankine Cycles

Efficiency (η) of an ORC is defined as the fraction of power (W) produced from heat as shown in Eq. (A.1). The ideal performance is expressed using the Carnot factor in Eq. (A.2), relating this to the real efficiency in Eq. (A.3) and a factor accounting for inefficiencies in the system components (the evaporator, turbine, condenser and pump) [4]. This factor can be correlated with the ideal efficiency for a pure working fluid Eq. (A.4). The constants α and β represent the cycle's components inefficiencies and the non-ideal behaviour of the working fluid, and are evaluated by regressing the model against rigorous simulation in HYSYS [27].

Model assumptions are outlined below;

1. Analysis for steady state conditions.
2. Negligible pressure drop in condenser and evaporator.
3. Turbine and pump adiabatic efficiency at 75%.
4. Minimum temperature difference assumed to be 10 °C.
5. Saturated vapour in evaporator.
6. Saturated liquid in condenser with a condensing temperature of 30 °C.
7. The evaporator temperature is between the boiling point and critical temperature of the working fluids.

The values of α and β depend on the working fluid as shown in Table A.1

$$\eta_{real} = \frac{W_{turbine} - W_{pump}}{Q_{waste\ \ heat}} \tag{A.1}$$

$$\eta_{ideal} = 1 - \frac{T_{condenser}}{T_{evaporator}} \tag{A.2}$$

$$\eta_{real} = Factor_{ORC} \cdot \eta_{ideal} \tag{A.3}$$

$$Factor_{ORC} = \alpha \cdot \eta_{ideal} + \beta \tag{A.4}$$

$$COP_{AbC,ideal} = \left(1 - \frac{T_{condenser}}{T_{generator}}\right)\left(\frac{T_{evaporator}}{T_{condenser} - T_{evaporator}}\right) \tag{A.5}$$

$$COP_{AbC,real} = \frac{Q_{evaporator}}{Q_{waste\ \ heat} + W_{pump}} \tag{A.6}$$

$$COP_{AbC,real} = factor_{AbC} \cdot COP_{ideal} \tag{A.7}$$

$$COP_{AbC,real} = a \cdot (factor_{AbC}) + b \tag{A.8}$$

Table A.1
Selected working fluids for organic Rankine cycle application.

Working fluid	Chemical formula	$T_{critical}$ (°C)	$P_{critical}$ (MPa)	Boiling point (°C)	α	β	$T_{evaporator}$ (°C) range
Cyclopentane	C_5H_{10}	238.4	4.257	48.78	−0.5979	0.7622	48.78–238
Benzene	C_6H_6	288.9	4.894	80.10	−0.5085	0.7663	81–270

B. Absorption chillers

The ideal COP (coefficient of performance) is the product of the ideal efficiency of a turbine operating between the generator and absorber temperatures and a vapour compression heat pump operating between the sink (evaporator) and source (condensing) temperatures [4] as shown in Eq. (A.5).

The actual COP is the fraction of the energy input converted to chilling Eq. (A.6), expressed in terms of the ideal COP and a factor that accounts for inefficiencies in the system components and working fluid non-ideal behaviour in Eq. (A.7). To determine the factor and the real COP, Eqs. (A.7) and (A.8) can be solved simultaneously, where the parameters in Eq. (A.8) are determined from rigorous simulation or manufacturer data. In this work the parameters were determined from rigorous simulation of an absorption chiller in ASPEN PLUS [28].

The calculations were performed based on the following assumptions:

1. The refrigerant in the condenser is saturated liquid at 30 °C.
2. At the evaporator outlet, the refrigerant is a saturated vapour.
3. Pressure drops in pipes and other components are negligible.
4. All components are externally adiabatic.

The generator temperature is determined from the system saturation pressure set to prevent the working fluid from crystallizing [4]. Values of a and b for lithium bromide absorption chillers are −0.5672 and 1.0049 respectively for producing chilling between 0 and 25 °C driven by 89.9 °C waste heat and rejecting heat at 30 °C in the condenser.

Appendix B

Case study data.

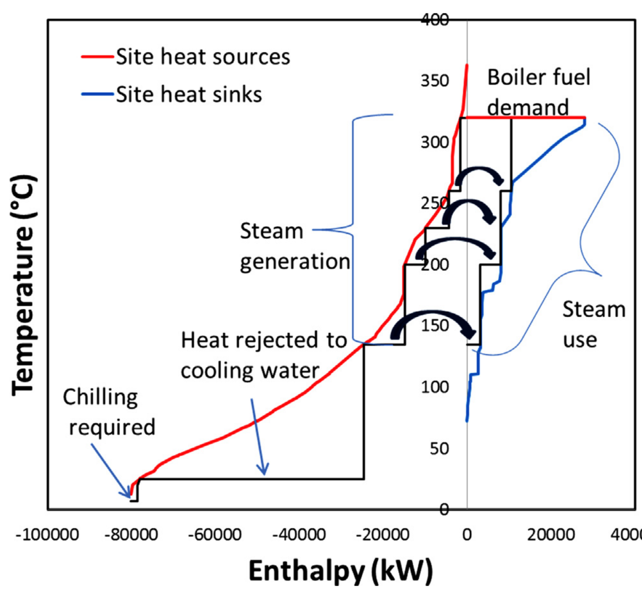

Fig. B.1Refinery total site profile [4].

Table B.1
Data extracted for heat rejected to cooling water [4].

Stream	Unit	Name	T_{supply} (°C)	T_{target} (°C)	Enthalpy (kW)
1	Crude/vacuum distillation unit	CDUVDU 9	116.8	31.1	5970
2		CDUVDU 5	116.8	50.5	106
3	Diesel hydrotreaters	DHT 3	112.97	26	333
4		DHT 2	112.97	30	1235
5		DHT 1	112.97	34	4540
6	Fluidised catalytic cracking unit	FCCU 3	140.9	37.51	950
7		FCCU 10	140.9	104	220

(*continued on next page*)

Table B.1 (*continued*)

Stream	Unit	Name	T_{supply} (°C)	T_{target} (°C)	Enthalpy (kW)
8		FCCU 10.1	104	51	810
9		FCCU 8	140.9	104	200
10		FCCU 1	140.9	90	1150
11		FCCU 9	104	38	10,700
12		FCCU 4	104	27.61	2783
13	Kerosene hydrotreaters	KHT 2	140.6	30	560
14		KHT 3	136.1	27.2	19.4
15		KHT 4	140.6	33.3	2880
16	Naphtha hydrotreaters	NHT 4	101.7	88.3	331
17		NHT 3	67.2	61.7	560
18		NHT 2	67.2	50	3290
19		NHT 1	67.2	33.9	1914
20	Platformer	PLAT 4	67.2	36.7	1930
21		PLAT 5	73.84	26.7	1160
22		PLAT 7	67.2	32.2	1390
23		PLAT 7.1	73.84	67.2	84.7
24		PLAT 8	67.3	25.7	35.6
25		PLAT 9	67.2	27.2	3020
26		PLAT 10	67.2	32.2	330
27		PLAT 11	43.3	26.3	81.1
28		PLAT 12	73.84	65	16
29		PLAT 13	73.84	32.2	320
30	Visbreaker	VBU 1	134.88	30.01	2050
31		VBU 2	134.88	75	1150
32	Utility system	VHP COND	320	76.32	7900
33		HP COND	260.07	76.32	970
34		MP1 COND	230	76.32	8
35		MP COND	200	76.32	1370
36		COND	90.1	90	131,150

Table B.2
Data extracted for heat rejected to air [4].

Stream	Name	T_{supply} (°C)	T_{target} (°C)	Enthalpy (kW)
1	Crude distillation unit fired heat exhaust	320.1	150	4440
2	Naphtha hydrotreaters fired heat exhaust	328.4	150	35
3	Platformer fired heat exhaust	320.1	150	1360
4	Coal boiler fired heat exhaust	291.3	150	18,330

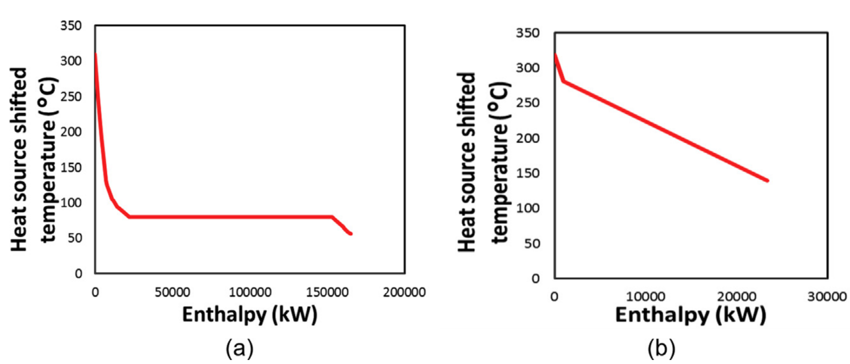

Fig. B.2. (a) Profile for heat rejected to cooling water and (b) profile for heat rejected to air [4].

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Chapter 6: Design of Waste Heat Utilization Systems

A waste heat utilization system comprises one or more technologies exploiting waste heat in process sites, to satisfy one or more end-uses of recovered energy within the site and over the fence. Additional savings in primary fuel, reductions in CO_2 emissions and costs could be obtained when waste heat recovery concepts are combined. Allowing for concepts to be combined implies a technology is selected when it is most efficient (depending on the heat source temperature) and most economic (depending on the end-use of recovered energy).

Previous researchers focus on integrating a single technology to utilize all the available waste heat from the processing unit (Bakhtiari et al., 2010; Donnellan et al., 2014; Chen et al., 2014) and from the site utility system (Popli et al., 2013; Zhang et al., 2015). However, a single technology may not be the best option to exploit all the available waste heat.

In the energy intensive process industries like refineries and chemical industries, the quantity of waste heat may be large and temperature over a wide range; therefore, there is a need to develop a generic design framework that systematically allows for selection of one or more technology options, waste heat sources and end-uses of recovered energy.

Publication 1 shows that a higher increase in efficiency (related to improving availability of energy) is possible through integrating more than one technology. The hierarchy of waste heat utilization opportunities (i.e. end-uses of recovered energy) presented in Publication 4 shows how the end-use of recovered energy determines the economics (i.e. costs and benefits) and potential to reduce CO_2 emissions. Also, the analysis in Publication 4 shows that additional savings in costs and reduction in CO_2 emissions are possible when multiple end-uses of recovered energy are explored.

Models of technology options that are easily embeddable in design frameworks for energy systems are provided in Publications 1 and 2. A comparison of the five thermodynamic cycles and heat recovery via heat exchange is provided in Publication 3; the results show that the heat source temperature should be taken into account. The analysis in Publication 3 also establishes the allowable temperature difference between the heat sources and technology operating temperatures.

In Publication 2, a systems-oriented criterion (primary fuel recovery ratio) is developed to determine the working temperatures for heat upgrading technologies and screen heat upgrading technologies. The primary fuel recovery ratio takes into consideration interconnected systems. Results show that higher savings in primary fuel is possible using a systems-oriented criterion compared to the coefficient of performance.

Heat recovery between several processing units on a site is possible through the site utility system. Steam may be generated from processing units and fed into the site utility system; heat is supplied to processing units by the site utility system or fired heaters in the processing units, especially for high temperature hot utility requirement. Power may also be produced from cogeneration systems or imported from the grid; in the case of heat only utility systems. Therefore, design of waste heat utilization systems should consider interactions with the site utility system. Such as exploiting waste heat produced from the site utility system; and end-uses of recovered energy within the site utility system. Some of the end-uses of recovered energy within the site utility system are: gas turbine compressor inlet air chilling, boiler feed water preheating, steam generation into the site utility system, hot utility savings and power generation. Simultaneous optimization with the site utility systems explores and accurately predicts the benefits of the end-uses listed above. Simultaneous optimization with the site utility system also provides a degree of freedom to reduce the quantity of waste heat produced since the flows of fuel steam and power are allowed to change.

A holistic design approach for waste heat utilization systems considering interactions with the site utility system could yield additional savings in costs, reductions in CO_2 emissions and increase in efficiency. Previous studies on process integration of waste heat recovery technologies neglect interactions with the site utility system.

Graphical techniques for integrating waste heat recovery in process sites were developed in Publications 1, 2 and 4. Even though these techniques were applied to show the benefits from combining technologies, interactions with the site utility system are neglected. The solution provided from applying the graphical techniques gives a designer multiple choices to evaluate with regards to practical considerations. However, their results are sub-optimal.

In this chapter optimization techniques are applied to design site waste heat utilization systems. The chapter contains Publication 5, 6 and 7. A Mixed Integer Linear Programming (MILP) model is developed to allow for simultaneous optimization of structural and operational variables. Structural variables are introduced for selection of end-uses of recovered energy and associated technologies. Operational variables are introduced to determine what quantity of useful energy to recover and change the current operating condition of the site utility system.

A spreadsheet modelling environment is used in this work to implement the model due to ease of replicability (i.e. allows provision of the application in a form that is best suited to the user) and ease of automation.

Enumerative algorithms like the branch-and-bound algorithm (Land and Doig, 1960) exist to solve deterministic MILP problems. The branch-and-bound algorithm in Lindo's systems What's Best! is adopted in this work.. The MILP problem is solved in two stages; first, What's Best! solves a continuous approximation of the problem to give a theoretical limit on the objective function, secondly the branch-and-bound algorithm is used to enumerate all possible integer solutions to find the optimal integer solution. What's Best license can be included as an add-in in Microsoft Excel

6. 1. Introduction to Publication 5

A multi-period MILP model is developed in this paper to design waste heat recovery systems. Technologies considered include organic Rankine cycles, absorption chillers and heat exchangers. End-uses of recovered energy within the process site and over the fence (for heat and power export) are considered. A multi-period adaptation shows the variability of hot water demand for export and the electrical power tariff. The methodology is applied to a medium scale refinery case study. Results show that there is potential to reduce CO_2 emissions and costs when a site is pinched (i.e. reached its maximum limit for heat recovery via heat exchange). A higher reduction is possible when technologies are combined. Results also show the economic potential of the ORC depends on the electricity tariff amongst other factors.

6. 2. Publication 5

Oluleye G., Jobson M., Smith R. Optimization-based Design of Waste Heat Recovery Systems, conference proceeding for the 28th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, 2015 (lecture number 50219).

Optimisation-based Design of Site Waste Heat Recovery Systems

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Abstract:

Waste heat recovery has received interest in recent years due to increasing energy prices, rising CO_2 emissions, and decreasing availability of fossil fuels. Technologies exist to recover useful energy from the available waste heat in process sites. Examples include absorption chillers for chilling provision, and Organic Rankine cycles for power generation.
Opportunities also exist to utilise the recovered energy from waste heat; these are classified based on the end users, namely on-site and off-site users. For example, if the recovered heat provides chilling, utilisation opportunities include: space cooling, chilling for site processes, and chilling the air before it is compressed in a gas turbine, to increase power throughput.
Together, the recovered forms of energy and utilisation opportunities form waste heat recovery systems. A key challenge is deciding how best to design the system taking into account: (1) waste heat available on sites; (2) temperatures of waste heat sources; (3) demand for recovered energy; (4) capital cost of heat recovery technologies; (5) financial benefits associated with utilisation opportunities; (6) the impact on CO_2 emissions and; (7) the variability of utilisation opportunities through the year. The methodology developed in this work to design site waste heat recovery systems takes all of the above into account. The design is formulated as a multi-period mixed integer linear programming problem, where the objective is to maximise the economic potential i.e. the difference between the financial benefits associated with utilisation opportunities and total cost of recovery technologies.
The methodology is applied to the case study of a medium-scale petroleum refinery, where 22% useful energy is recovered from waste heat, reducing the site CO_2 emissions by 15.6%. The methodology is effective for identifying the best combinations of heat source temperatures and duties as well as the best set of technologies to utilise energy recovered from waste heat.

Keywords:

Mixed integer linear programming, Multi-period optimisation, Waste heat recovery, Waste heat recovery technologies, Waste heat utilisation opportunities.

1. Introduction

The industrial sector is responsible for over 35% of world energy consumption [1], generating at least 30% of global greenhouse gases in the form of carbon dioxide (CO_2) released from combustion of fossil fuels. In spite of this, a considerable amount of heat is wasted in the process industries. In the United States, heat wasted below 200°C is 20 – 50% of the energy content of fuel [2]. Also, in the UK, heat wasted below 250°C is about 40% of the energy content of fuel [3]. The majority of the heat wasted is from petrochemicals production sites and refineries [3].

Waste heat utilisation is a measure to increase efficiency in the use of fuel; increasing energy efficiency is also a low-cost method of reducing carbon emissions [4]. Waste heat recovery and reuse can simultaneously reduce energy costs and CO_2 emissions [5] since additional fuel is not required and no additional emissions are emitted [6].

There are diverse sources of waste heat in process sites, including those from the site processes and from the site cogeneration system designed to satisfy demand for power to drive process units, and to provide steam at different pressure levels. Conventional sinks for waste heat include cooling towers and stacks for disposal of flue gases. Waste heat recovery has the potential to reduce investments in cooling towers and stacks for disposal of flue gases.

Waste heat from the site processes is defined for when the site has reached its limit for heat recovery [7]i.e. when heat recovery within a process and between processes are maximized based on pinch analysis [8,9]. For process sites, direct heat exchange between processes or within processes is relatively cheap and easy to implement [10]. However, if maximum heat recovery within a process or between processes cannot be achieved due to technical limitations, the residual heat can be regarded as waste heat. For a cogeneration system, heat that is rejected to air or to cooling water is classified as waste heat. The waste heat from the site processes and the cogeneration system occurs over a wide temperature range [7].

Mature technologies exist to recover useful energy from waste heat. For example, absorption chillers provide chilling, Organic Rankine cycles generate power, and economisers exchange heat directly and generate hot water. Absorption chillers are thermally activated chilling technologies that use waste heat to fulfill a chilling demand, organic Rankine cycles produce power from low to medium temperature heat sources using low boiling point organic fluids. Economisers are shell and tube gas-liquid or liquid-liquid heat exchangers for hot water generation.

Opportunities also exist within a process site and 'over the fence' (off-site) to use the energy (power, heat or chilling) recovered from waste heat. For example, if power is generated using an organic Rankine cycle, the electricity generated can reduce site electricity import, be exported to the grid or be used to reduce power generated from the site cogeneration system [15].

To evaluate the potential in industrial waste heat, Hammond and Norman [11] examined technologies such as absorption chillers, organic Rankine cycles and heat exchangers for heat recovery on-site for the UK process industry. The technologies were analysed in a single and combined mode. It was shown that combination of technologies, i.e. allowing the use of more than one technology for heat recovery, could decrease CO_2 emissions more than the single technologies could. A more detailed analysis is required at a site level to consider the temperature of the heat sources, opportunities for using the recovered energy and the economics (i.e. costs and benefits) associated with combining technologies.

At site level, Kapil et al. [12] examined absorption chillers, organic Rankine cycles and economisers for boiler feed water preheating; the analysis considered only heat sources from site processes, and assumed all the heat sources to be at the same temperature. Furthermore, combining technologies and utilisation opportunities are not explored. Oluleye et al. [7] combined technologies at a site level using heat sources at various temperatures from the site processes, and the site cogeneration system; the recovery of useful energy is highest when different forms of energy are recovered. However, in this work decisions-making criterion consider only efficiency, neglecting the economics associated with the design. Kwak et al. [6] compared the potential energy savings and cost associated with implementing these technologies for heat available at fixed and varying temperatures. Only the heat source from the site processes are considered, and the aim was to compare options, rather than to combine them to determine which technologies to use for given heat source temperatures and quantities. Liew et al. [18] presented a framework for total sites, to determine cost-effective retrofit options. The potential to exploit the residual low quality heat after individual process integration, total site integration, or residual heat from the site cogeneration system is not explored. The utilization of this excess heat is considered in Hackl and Harvey [19], where a holistic approach is presented to identify opportunities for increased energy efficiency in industrial clusters. Even though the temperature range of the waste heat sources was considered, only excess heat from the clusters processing units were considered. Furthermore, the possibility of recovering and combining diverse forms of energy and utilisation opportunities, depending on the quality of the heat is not considered. Installation of absorption chillers can reduce/ eliminate the need for conventional refrigeration systems thereby saving shaft power demand.

Waste heat recovery technologies and utilisation opportunities can be integrated to exploit waste heat, the combining of technologies is analogous to that in existing site cogeneration systems. In combining technologies, a multi-criteria decision making process may be involved; hence, optimisation tools are required due to the large number of decisions and degrees of freedom relating to choice of technologies and utilisation opportunities, as well as trade-offs [13]. Optimisation strategies have proven useful for the synthesis and design of combined cooling , heating and power systems [13], and for synthesis and design of utility systems providing fixed demands of power and steam at various pressure levels [14]. Becker and Maréchal [20] applied a mixed integer linear optimisation framework to identify options for optimal energy conversion and heat recovery in industrial process sites. The framework calculates both the flow rates of the cogeneration system and heat transfer units to minimise operating costs. However, exploitation of the residual heat from the cogeneration system (such as exhaust of combustion equipments and heat of condensation) is not considered. To account for changing inputs and energy prices, a multi-period MILP framework is applied in Becker and Maréchal [21]. This formulation targets integration of energy conversion systems like heat pumps and storage tanks to maximise heat recovery, again, residual heat available in the site cogeneration system designed to satisfy energy demands of site processing units is not considered. Furthermore, the potential to combine technology options for waste heat recovery, depending on the temperature of the available heat is not explored. In the multi-period optimisation framework adapted by Marechal and Kalitventzeff [22], models for targeting optimal operational strategy of cogeneration systems are included. However the scope for waste heat recovery is limited to the site processing unit, neglecting residual heat from cogeneration systems. A system consisting of diverse recovered forms of energy and utilisation opportunities (i.e. the use to which the recovered energy is put), can be designed to exploit the excess heat from site processing units and the cogeneration system. Design of this system has not been explored in the open literature.

This present work therefore applies modelling and optimisation for the synthesis, and design of site waste heat recovery systems. A mixed integer linear programming (MILP) formulation is proposed as it allows simultaneous structural and parameter optimisation in process synthesis. To account for variable operating conditions, demands and energy prices, a multi-period approach is applied to design the system. The model takes into account: (1) amount of waste heat available from the site and temperatures of the waste heat sources; (2) demand for recovered energy in various forms; (3) capital cost of technologies, financial benefits associated with utilisation opportunities and their potential to reduce emission; (4) variation in utilisation opportunities and energy prices throughout the year. The first step in formulating the problem is to define a general configuration or superstructure that embeds all the design alternatives considered, and from which the optimal solution will be selected. The superstructure is commonly derived by making use of thermodynamic considerations and engineering judgement [14]. The second step involves reducing the superstructure in order to select the design to satisfy an objective function. The optimisation is done for an existing process site. In this work, the organic Rankine cycle for electrical power generation from waste heat is run on dry fluids. Since the condition of the fluid after expansion is dry, mechanical damage from turbine blades wearing will not occur. In addition, highest efficiency values are obtained from dry high boiling substances [23]. Detailed analysis for ORC working fluid selection is beyond the scope of this study.

2. Waste heat sources

The sources of waste heat from site processes, and the site cogeneration system are typically diverse. The energy profile for a single process, showing streams requiring heat (heat sinks, represented by the cold composite curve) and heat sources (represented by the hot composite curve)

[8] is shown in Fig. 1. The overlapping region represents the heat recovery target within a process, while the cooling requirement, as depicted in Fig. 1, represents the potential for waste heat recovery. Total site profiles [9], is used to combine different processes to provide an overall picture of the steam demand and steam generation on a site. The total site profile is plotted by taking the residual heat sinks and sources from different processes (after heat recovery within a process). The total site profiles are used to set targets for heat recovery and utility for a new process and for an existing process; the potential for direct heat recovery between the process heat sources and heat sinks may be exploited. The heat rejected to cooling water using the total site profiles determines the potential for heat recovery. Some of the heat rejected to cooling water in the composite curve in Fig. 1 and the total site profile in Fig. 2 can be recovered. How much of the heat is recoverable depends on the operating conditions of recovery technologies, the physical limitations of a site, characteristics of the waste heat sources and the demand for recovered energy [7].

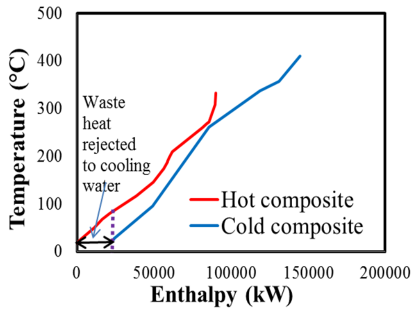


Fig. 1. Composite curves.

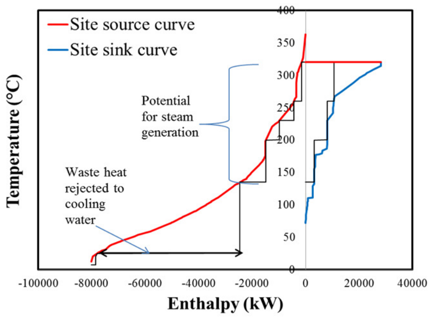


Fig. 2. Total site profiles.

Waste heat from a site cogeneration system is from the exhaust of fired heaters providing high temperature heating to the site processes, exhaust of boilers and gas turbines, condensate returned from the process, condensate from the condensing main and vented steam. Fig. 3 represents a site cogeneration system showing some sources of waste heat.

The available waste heat on a site occurs over a range of temperatures. In Oluleye et al. [7], the concept of energy profiles was extended to generate temperature–enthalpy plots for heat rejected to air and cooling water that represent available waste heat in terms of quantity and quality. However, in this present work, an assumption is made that heat sources can be collected for system design. Therefore, for feasible heat recovery, the heat source temperature is shifted by ΔT_{min} to an intermediate fluid and another ΔT_{min} for the heat recovery technologies. For analysis of the profile, the kinks were used as preliminary heat recovery temperatures (PHRT) i.e. T_j, ensuring that waste heat at high temperature is exploited before lower temperature waste heat. Depending on the number of kinks and taking into account the quantity of available heat, the heat sources can be combined at different PHRT's to determine the final heat recovery temperature (i.e. the final temperatures at which useful energy i.e. heat, chilling or power is recovered.

As an illustration, a heat source profile with four kinks (i.e. 4 PHRT) is shown in Fig. 4(a). Technologies may be assigned against this profile using the four PHRT and associated duties (Fig. 4 (b)), or using three PHRT and associated duties (Fig. 4 (c)), or two PHRT and associated duties in (Fig. 4(d)) or the heat can be collected at the lowest temperature level using all the heat available in Fig. 4 (e).

The design problem therefore requires multiple options such as in Figs 4 (a-e) to be evaluated, where several technologies could be used to recover the waste heat at each heat recovery temperature. This work proposes an optimisation framework to identify the best combination of heat source temperatures and duties as well as the best set of technologies and opportunities to utilise energy recovered from waste heat. A multi-period approach is used to account for changing energy prices and variations in demand for recovered energy.

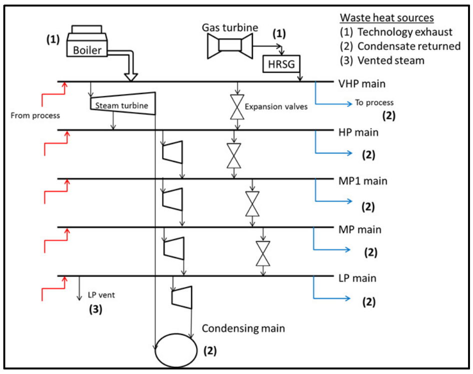


Fig. 3. Site cogeneration system.

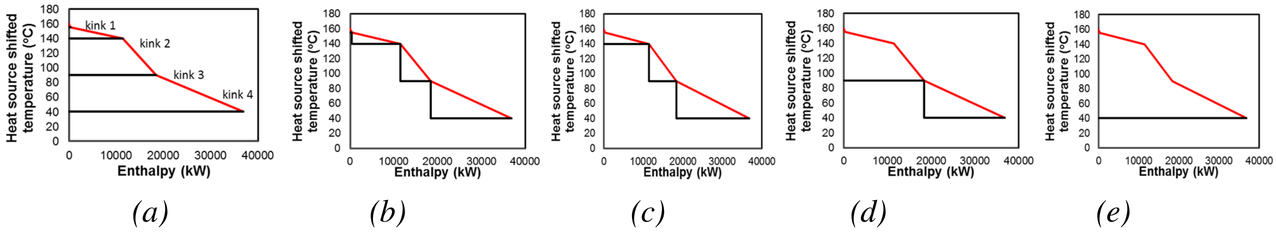


Fig. 4. Different ways for combining the heat source temperature and duties.

3. Modelling framework

The modelling framework is formulated to assess options that exploit recoverable waste heat in process sites, taking into account the temperatures and duties of the heat sources and assuming they can be collected using an intermediate working fluid (for example water). The framework involves the creation of a superstructure consisting of various combinations of waste heat sources and utilisation opportunities to use recovered energy within the process site and over the fence, as shown in Fig. 5.

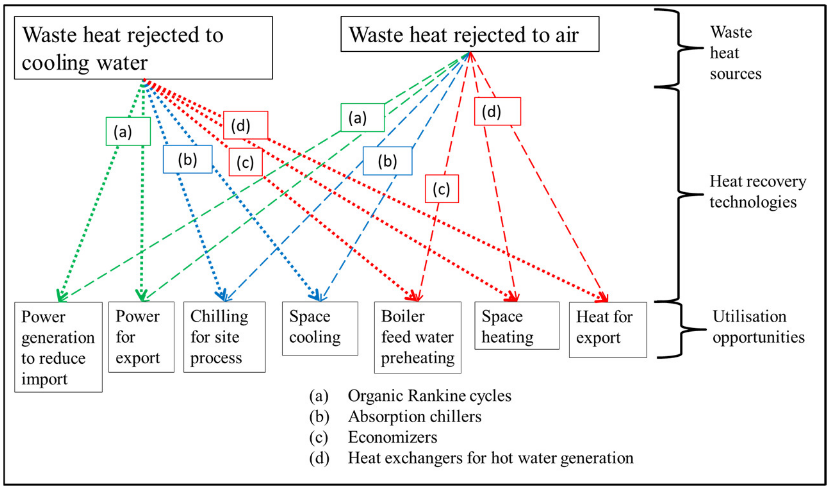


Fig. 5. Superstructure for waste heat recovery system design.

The framework comprises: (1) a scalar quantitative measure of performance i.e. the objective function, (2) decision variables (degrees of freedom) consisting of operational (continuous) and structural (binary) variables and (3) a predictive model describing the behaviour of the system i.e. inequality constraints, equations and performance models for technologies relating the energy inputs and energy outputs. Further information on the performance models for technologies is presented by Oluleye et al [7]. By using suitable linear relationships to represent costs, energy conversion, etc., and integer variables to represent discrete choice, a mixed-integer linear model is created.

The objective is to maximise the economic potential i.e. the difference between the financial benefits (FB) and total costs associated with the design. The total cost is the sum of the capital costs (CC), operating costs (OC) and maintenance costs (MC) of the heat recovery technologies:

$$\text{Maximize}: \sum_{i=1}\sum_{j=1}\left\{\left[\left[\frac{\sum_{t=1}\left(FB_{i,k,T_j,t} * h_t * day_t\right)}{h_{year}}\right] - \left(CC_{i,k,T_j} + OC_{i,k,T_j} + MC_{i,k,T_j}\right)\right]\right\}, \forall k \qquad (1)$$

Where i represents the utilisation opportunities i.e. on-site and off-site users of energy recovered from waste heat, j, the 'kinks' on the heat source profiles i.e. PHRT, k represents heat rejected to cooling water and air, and t, time scenarios defined to represent variations in demand, energy price etc. of a typical weekday (WD), weekend day (WE), time of day, season; winter (W), transition (T) and summer (S), h_t represents number of hours in a particular time scenario, day_t, number of days in a time scenario and h_{year}, number of hours in a year. An explanation for estimating the financial benefits (FB) is shown in Table 1.

Decision variables include continuous and binary variables:

- Continuous variables $P_{i,k,T_j,t}, C_{i,k,T_j,t}, H_{i,k,T_j,t}$; representing energy flows for opportunities utilizing power (P), chilling (C) and heat (H) from waste heat rejected to cooling water (cw) and air (a), at the PHRT (T_j) in a particular time scenario (t). Where k ϵ [cw, a], i ϵ I, j ϵ J, t ϵ T.
- Binary variables for existence of technologies associated with opportunities utilizing power, chilling and heat generated from waste heat.

$$Y_{P_{i,k,T_j,t}}, Y_{C_{i,k,T_j,t}}, Y_{H_{i,k,T_j,t}} \in 0,\ 1$$

The system is subject to the following constraints:

1. Energy balance for the waste heat required to operate technologies, and the available waste heat;

$$\sum_{i=1}\sum_{j=1}\left[\frac{\sum_{t=1}\left(Q_{P_i,k,T_j,t} * h_t * day_t\right)}{h_{year}}\right] + \left[\frac{\sum_{t=1}\left(Q_{C_i,k,T_j,t} * h_t * day_t\right)}{h_{year}}\right] + \left[\frac{\sum_{t=1}\left(Q_{H_i,k,T_j,t} * h_t * day_t\right)}{h_{year}}\right] \le Q_{available_k}, \forall k \qquad (2)$$

Where Q represents the heat flow (kW).

2. Feasible combinations of heat recovery temperatures and heat duties.

$$0 \le Q_{k,T_j,t} \le \left(Q^*_{CU_j} + Q_{CU_{j-1},t} + Q_{CU_{j-2},t} + Q_{CU_{j-3},t} + Q_{CU_{j-(j-1)},t}\right), \quad \forall k, t, j \qquad (3)$$

The heat consumed by all opportunities at a particular temperature level T_j, and time scenario t, is given by:

$$Q_{k,T_j,t} = \sum_{i=1}\left(Q_{P_i,k,T_j,t} + Q_{C_i,k,T_j,t} + Q_{H_i,k,T_j,t}\right), \quad \forall k \qquad (4)$$

3. Implicit constraint for technology sizes: technologies associated with power generation in (6-7), chilling provision in (7-8), and heat provision in (9-10):

$$P_{i,k,T_j,t} - U * Y_{P_{i,k,T_j,t}} \le 0, \forall k, t, i, j \qquad (5)$$

$$P_{i,k,T_j,t} - L * Y_{P_{i,k,T_j,t}} \ge 0, \forall k, t, i, j \qquad (6)$$

$$C_{i,k,T_j,t} - U * Y_{C_{i,k,T_j,t}} \le 0, \forall k, t, i, j \qquad (7)$$

$$C_{i,k,T_j,t} - L * Y_{C_{i,k,T_j,t}} \ge 0, \forall k, t, i, j \qquad (8)$$

$$H_{i,k,T_j,t} - U * Y_{H_{i,k,T_j,t}} \leq 0, \forall\, k, t, i, j \tag{9}$$

$$H_{i,k,T_j,t} - L * Y_{H_{i,k,T_j,t}} \geq 0, \forall\, k, t, i, j \tag{10}$$

Where U is a large number and L is the minimum size of a technology for industrial application. If an opportunity is selected, Y=1; implying the technology exists in the superstructure.

4. Finite demand (D) for recovered energy:
   - Demand for recovered heat

$$\sum_{j=1}\left(H_{i,k,T_j,t}\right) \leq Q_{DH_{i,t}}, \forall\, k, i, t \tag{11}$$

   - Demand for chilling

$$\sum_{j=1}\left(C_{i,k,T_j,t}\right) \leq Q_{DC_{i,t}}, \forall\, k, i, t \tag{12}$$

   - Electricity demand

$$\sum_{j=1}\left(P_{i,k,T_j,t}\right) \leq Q_{DP_{i,t}}, \forall\, k, i, t \tag{13}$$

Performance correlations for waste heat recovery technologies developed in Oluleye et al. [7] are used to determine the useful energy (power, chilling and heat) recovered. An organic Rankine cycle and an absorption chiller are illustrated in Figs 6 and 7, respectively.

1. Power produced using an organic Rankine cycle:

$$P_{i,k,T_j,t} = Q_{P_i,k,T_j,t} * \left[\alpha * \left(1 - \frac{T_{condenser}}{T_j}\right)^2 + \beta * \left(1 - \frac{T_{condenser}}{T_j}\right)\right], \forall\, k, i, j, t \tag{14}$$

2. Chilling produced from an absorption chiller:

$$C_{i,k,T_j,t} = Q_{C_i,k,T_j,t} * \left\{ \frac{\lambda * \left[\left(1 - \frac{T_{condenser}}{T_j}\right)\left(\frac{T_{evaporator}}{T_{condenser} - T_{evaporator}}\right)\right]}{\left[\left(1 - \frac{T_{condenser}}{T_j}\right)\left(\frac{T_{evaporator}}{T_{condenser} - T_{evaporator}}\right)\right] - \gamma} \right\}, \forall\, k, i, j, t \tag{15}$$

   Values of α, β, γ, and λ depend on the working fluid selected for the technologies and are shown in Table A.2 (Appendix A). Non-linearity's in (14 – 15) were handled with the introduction of discrete and semi-continuous variables.

3. Recovered Heat

$$Q_{H_i,k,T_j,t} = H_{i,k,T_j,t} * (1 + DL), \forall\, k, i, j, t \tag{16}$$

   Where DL is the distribution loss associated with heat export

The calculations are carried out using What's Best! (a Lindo systems modelling environment) [17].

CO_2 emissions associated with the design are also evaluated as shown in Table 1 below:

Table 1. Financial benefits and CO_2 emissions reduced from use of recovered energy [15]

Opportunity	Financial Benefits (£/y)	Potential to reduce emissions (t/h)
Power for site use and export	Value of fuel saved from site cogeneration system and the grid when energy is exported	CO_2 displaced directly from fuel not consumed in the site cogeneration system and from fossil fuel combustion in the grid
Space cooling/	Savings from electricity costs	CO_2 emissions displaced from

process chilling	required to operate a conventional vapour compression chiller	electricity required to operate a vapour compression chiller
Space heating/ boiler feed water preheating	Value of fuel not consumed in a boiler that would otherwise be used	CO_2 emissions displaced from a boiler that would otherwise be used

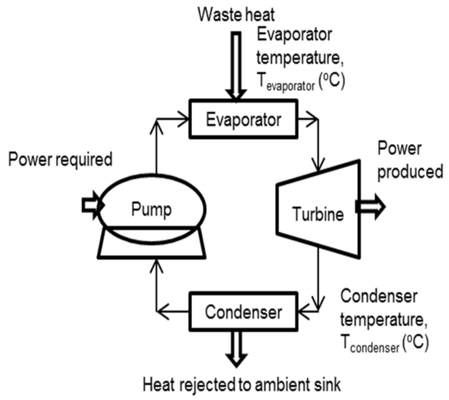


Fig. 6. Organic Rankine cycle [7].

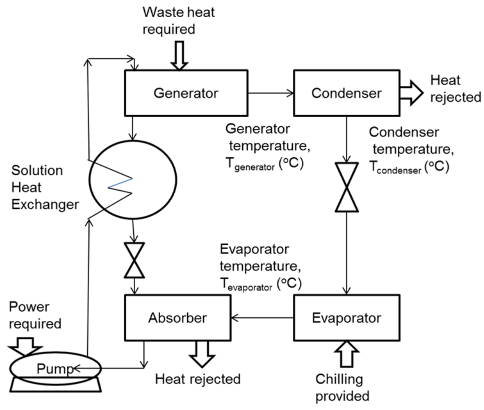


Fig. 7. Absorption chiller [7].

4. Design methodology

The design methodology presented in this paper selects the form of energy recovered, the temperatures at which heat is recovered and utilisation opportunities to maximise the economic potential and satisfy imposed constraints. This involves five stages: (i) data extraction stage; (ii) identification stage; (iii) Modelling stage; (iv) optimisation stage and (v) design evaluation stage. The design is evaluated in terms of the economic potential using (2) and the potential to reduce CO_2 emissions (kg/s) (Table 1).

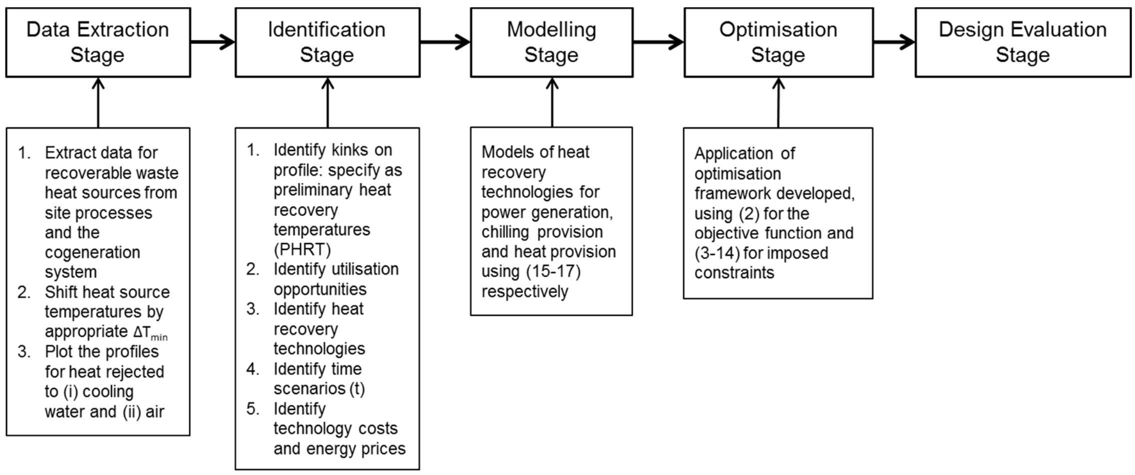
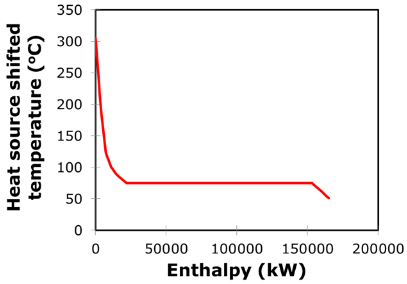


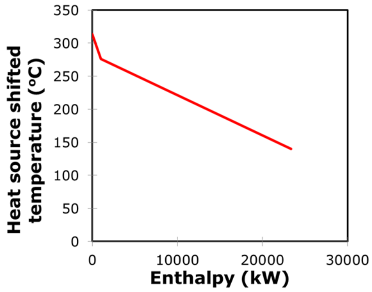
Fig. 8. Design methodology flow chart.

5. Case study

The case study pertains to a medium scale petroleum refinery. Data extracted for the recoverable waste heat are given in Fig. 9(a) for heat rejected to cooling water, and Fig. 9(b) for heat rejected to air [7]. The site is permitted to export electricity, and 420 kW chilling at 8°C is required by the site processes (currently satisfied by a vapour compression chiller). A coal boiler also exists on site the temperature of boiler feed water after the feed pump is 116 °C, it is desirable to heat it to 130 °C (maximum permissible for some boilers [16]). The closest off-site heat users (requiring 2,400 kW of hot water at 80°C) are 14 km away from the site. 10% distribution and transmissions losses are assumed for heat export. The minimum permissible temperature difference for collecting the heat sources using an intermediate fluid is 5°C, while that for the heat recovery technology is 10°C. Note that heat source temperatures in Figs 9(a) and (b) have been shifted by 15°C. Identified utilisation opportunities relevant to this case include: (1) power for export, (2) chilling for site processes, (3) boiler feed water preheating, (4) heat for export. Assumptions on technology capital cost, energy prices and emission factors are presented in Table A.1 (Appendix A).



(a)



(b)

Fig. 9. Heat source profile for: (a) heat rejected to cooling water and (b) heat rejected to air.

The objective is to design a site waste heat recovery system taking into account the temperature and duty of the heat sources, demand for recovered energy and the size limitations of the various technologies. There are 256 possible combinations of heat source temperature and duties (see (1)). The best quality of heat to use and quantity of heat to recover power, chilling and heat is determined when the objective function is maximised. The model involves the use of 8786 continuous variables and 7839 binary variables; solved in less than one second.

The economic potential is plotted against the potential to reduce CO_2 emissions in Fig. 10 for designs done for a single utilisation opportunity and multiple opportunities. Chilling provision has the lowest economic potential and potential to reduce CO_2 emissions, since the demand for chilling is low (420 kW); making it less economic to provide chilling using an absorption chiller compared to a conventional vapour compression system, due to the small amount of electricity (62 kW) displaced. Hence in the combined system (Fig. 11), chilling provision is not selected.

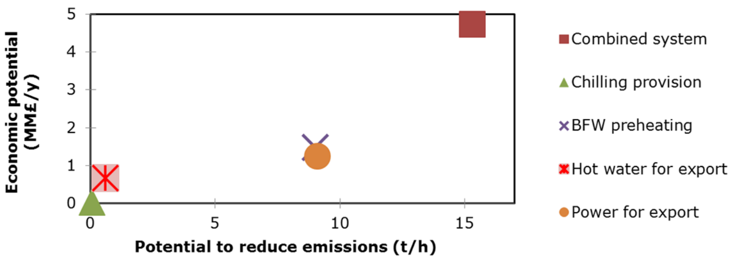


Fig.10. Optimisation results for a single user and multiple users of recovered energy

Combining different waste heat utilisation opportunities results in a higher economic and CO_2 emissions reduction potential. However, a more detailed analysis is required to account for practical issues, such as availability of space to install equipment in process sites.

For the combined system, 22% useful energy is recovered from waste heat and this has the potential to reduce site emissions by 15.6%, and site operating costs by 21.5% (excluding complexity in collecting heat sources and distribution costs for heat export). The grid representation in Fig. 11 shows the best combination of technologies selected for all temperatures at which waste heat is recovered in the combined system.

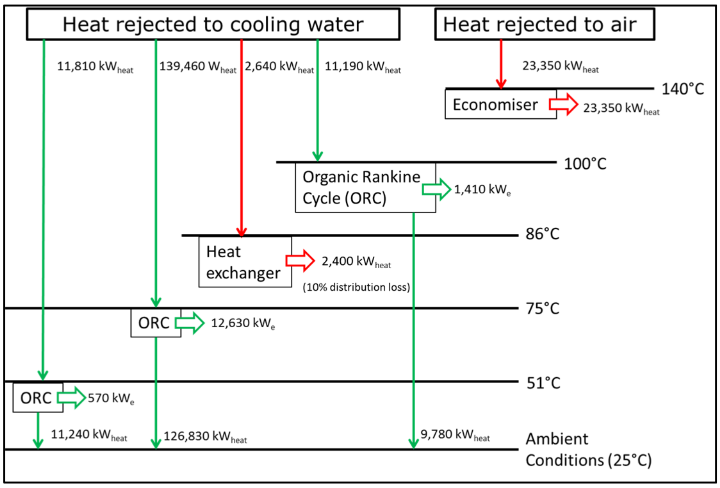
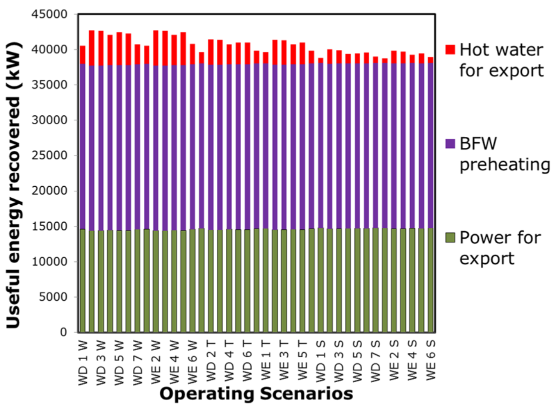


Fig.11. Grid diagram for waste heat recovery system (combined system).

A considerable amount of heat is still rejected at ambient conditions due to low electricity conversion efficiencies in the ORC. Therefore, future work will consider technologies to upgrade low temperature waste heat, for example mechanical heat pumps and absorption heat pumps. The operation of the system by time scenarios is shown in Fig. 12(a) for a base case scenario (i.e. for the combined system in Fig. 11). When the off-peak electricity price reduces to 4.55 p/kWh, the operation of the system is shown in (Fig. 12(b)). It is found that using the organic Rankine cycle during off-peak times (00.00-07.00am) is uneconomic. In this case, 19% useful energy is recovered reducing the site emissions by 13.48%.



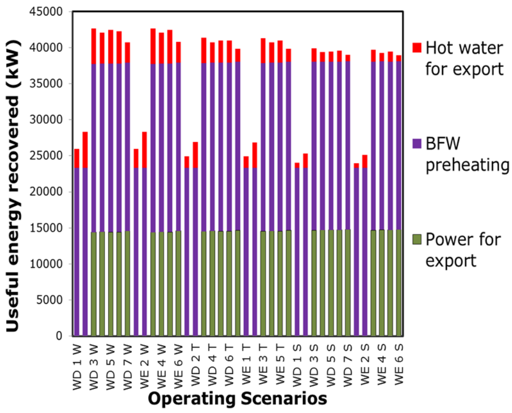


Fig. 12. Operation of heat recovery system in each time scenario: (a) base case electricity tariff (b) lower off-peak electricity tariff.

6. Conclusions

A generic methodology for design of waste heat recovery systems is proposed to utilise waste heat available from site processes and the site cogeneration system. The design methodology takes into account the temperature and duties of the heat sources, various opportunities to use recovered energy from waste heat, varying energy prices and useful energy demand. The problem is formulated as a multi-period mixed integer linear program and solved using What's Best! [17]. A case study is presented to illustrate the application of the methodology, results show that combining heat recovery technologies and opportunities to exploit the energy recovered from waste heat results in the highest financial and environmental benefits compared to designs that convert waste heat into only single forms of recovered energy. Results also show that the economic potential of organic Rankine cycles depend on the electricity tariff amongst other factors.

Future research will consider practical aspects of installing waste heat recovery technologies especially relating to space constraints on existing sites. Models of waste heat recovery technologies will be further developed to reflect part load performance. Including heat upgrade technologies in the optimisation framework, existing cooling water systems and the existing cogeneration system will also be considered.

Appendix A

Table A.1. Design assumptions on prices and emissions [15]

Energy Prices	**Emission factors**	**Investment costs**	**Others**
Industrial coal price: 1.42 p/kWh Domestic natural gas price: 5.0 p/kWh Industrial electricity price: Off peak (00.00-7.00am: 9.11 p/kWh) Peak (7.00-23.59pm: 13.4 p/kWh)	Natural gas emission factor: 0.193 kg/kWh Grid emission factor: 0.485 kg/kWh	Absorption chiller: 180 £/$kW_{chilling}$ Organic Rankine cycle: 1300 £/$kW_{electricity}$ Economizer: 227.5 £/m^2	Discount rate: 15% Operating hours: 8,600 Retrofit factor: 3 Heat transfer coefficient for economiser: 37 W/m^2K Ambient temperature 25°C CEPCI 2011: 585.7 CEPCI 2012: 584.6 CEPCI 2013: 583.7 CEPCI 2014: 586.77

Table A.2. Model parameters for organic Rankine cycle and absorption chillers [7]

Technology	**Working fluid**	**α**	**β**	**γ**	**λ**
Organic Rankine cycle	Benzene	-0.5085	0.7663		
	Cyclopentane	-0.5979	0.7622		
Absorption chiller				0.5672	1.0079

Nomenclature

CU cumulative heat, kW

Q heat, kW

T temperature, °C

Greek symbols

α correlation for Organic Rankine cycle

β correlation for Organic Rankine cycle

γ correlation for absorption chiller

λ correlation for absorption chiller

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6. 3. Introduction to Publication 6

A considerable amount of low temperature waste heat is produced in process sites. Technologies such as mechanical heat pumps, absorption heat pumps and absorption heat transformers can upgrade the heat to a higher temperature. The high temperature heat can be used to reduce hot utility required by the site processing units at various temperature levels, generate steam into the site cogeneration system at various temperature levels and preheat boiler feed water.

Previous researches on heat upgrading assume the price of hot utility saved at different pressure levels is the same or predict the price irrespective of the existing utility system (Costa et al., 2009; Donnellan et al., 2014; Miah et al., 2015). The best way to accurately predict hot utility savings is to optimize the site utility system simultaneously with the heat upgrading technologies. A simultaneous optimization also takes into account the configuration of the existing system to predict the maximum amount of steam generated depending on the temperature levels.

A MILP model is developed in this paper for integration of heat upgrading technologies in existing process sites. The site utility system is simultaneously optimized. The methodology is applied to a medium scale refinery case study. Results show that savings in fuel and reductions in CO_2 emissions is possible through low temperature heat upgraded. However, the economics depends on the difference between the electrical power price and fuel price. Upgrading heat to reduce primary fuel competes with generating additional electrical power (from the fuel saved) for export. When the price of fuel is expensive relative to power, waste heat upgrade is viable economically and when the price of fuel is cheap relative to power waste heat upgrade in not viable economically.

6. 4. Publication 6

Oluleye G., Jobson M., Smith R., Process integration of waste heat upgrading technologies, Process Safety and Environmental Protection (2016), http:/dx.doi.org/10.1016/j.psep.2016.02.003.

Process Safety and Environmental Protection xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Process Safety and Environmental Protection

journal homepage: www.elsevier.com/locate/psep

Process integration of waste heat upgrading technologies

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ARTICLE INFO

Article history:
Received 31 August 2015
Received in revised form 2 February 2016
Accepted 7 February 2016
Available online xxx

Keywords:
Industrial waste heat
Mechanical heat pump
Absorption heat pump
Absorption heat transformer
Site cogeneration system
Mixed integer linear programming

ABSTRACT

Technologies such as mechanical heat pumps, absorption heat pumps and absorption heat transformers allow low-temperature waste heat to be upgraded to higher temperatures. This work develops a comprehensive Mixed Integer Linear Program (MILP) to integrate such technologies into existing process sites. The framework considers interactions with the associated cogeneration system (in order to exploit end-uses of upgraded heat within the system and determine their true value), temperature and quantity of waste heat sources and of sinks for the heat upgraded as well as process economics and the potential to reduce carbon dioxide (CO_2) emissions. The methodology is applied to an industrially relevant case study. Integration of heat upgrading technologies has potential to reduce total costs by 23%. Sensitivity analysis is also performed to illustrate the effect of changing capital costs and energy prices on the results, and demonstrate the model functionality.

1. Introduction and previous works

Adoption of technologies to upgrade low temperature waste heat to higher temperatures are becoming more relevant due to limitations on CO_2 emissions and depleting reserves of fossil fuels (Van de Bor and Ferreira, 2013). Examples of such technologies include mechanical heat pumps, absorption heat pumps and absorption heat transformers.

In mechanical heat pumps (MHP), waste heat vaporizes the working fluid in the evaporator, which is compressed to a higher temperature by electrical power. The working fluid is condensed and expanded in a valve, and then the cycle repeats. Different refrigerants such as ammonia and n-butane are suitable working fluids for the mechanical heat pump (Smith, 2005). A schematic is shown in Fig. 1. Absorption heat pumps (AHP) and heat transformers (AHT) are thermally activated heat upgrading technologies i.e. compression of the working fluid is achieved in a solution circuit consisting of a generator, an expansion valve, a solution pump and an absorber (Figs. 2 and 3) (Oluleye et al., 2016). The difference between AHP and AHT is that in an AHT, thermal energy required to vaporize the working fluid in the evaporator is supplied at a higher temperature than that of the waste heat required for separating the working fluid pair in the generator (Lazzarin, 1994). The most common working fluid pair for both technologies in industrial applications is water/lithium bromide (Donnellan et al., 2015). MHP, AHP and AHT could provide considerable reductions in CO_2 emissions and possible energy savings in the process industry (USDOE, 2003).

Previous research in this area focused on making heat pump systems more energy efficient (Grossman and Perez-Blanco, 1982; Romero et al., 2011), developing performance models for these technology options (Oluleye et al., 2016), and selection of working fluids (Oluleye et al., 2016; Angelino and Invernizzi, 1988). Optimal integration in existing process sites remains a challenging task (Chua et al., 2010).

In earlier work in this area, Wallin and Berntsson (1994) proposed using the grand composite curve (GCC) to guide

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http://dx.doi.org/10.1016/j.psep.2016.02.003
0957-5820/

Nomenclature

Sets

$i \in I$	Heat source streams
$j \in J$	Temperature intervals on heat source streams
$k \in K$	Sinks for upgraded heat
$pl \in PL$	Pressure distribution levels in the site cogeneration system
$t \in TT$	Technologies burning fuel to generate steam in the site cogeneration system

Independent variables

$mfuel_t$	Mass flow of fuel consumed by technologies in the site cogeneration system, kg/s
$mturbine_{pl}$	Mass flow of steam into a stream turbine at different pressure levels in the site cogeneration system, kg/s
$Qout^{MHP}_{i,j,k}$	Flow of heat upgraded to heat sink k, from a MHP using heat source stream i, in temperature interval j, kW
$Qout^{AHP}_{i,j,k}$	Flow of heat upgraded to heat sink k, from an AHP using heat source stream i, in temperature interval j, kW
$Qout^{AHT}_{i,j,k}$	Flow of heat upgraded to heat sink k, from an AHT using heat source stream i, in temperature interval j, kW
W_{Import}	Total electrical power imported from the grid for site use, kW
W_{Export}	Total electrical power exported to the grid, kW
$Y^{MHP}_{i,j,k}$	Binary variable for existence of a MHP to upgrade heat from stream i in temperature interval j to satisfy heat sink k.
$Y^{AHP}_{i,j,k}$	Binary variable for existence of an AHP to upgrade heat from stream i in temperature interval j to satisfy heat sink k.
$Y^{AHT}_{i,j,k}$	Binary variable for existence of an AHT to upgrade heat from stream i in temperature interval j to satisfy heat sink k.

Dependent variables

ACC	Annualized capital cost, £/y
FC	Overall site fuel cost, £/y
MC	Maintenance cost, £/y
mQ^{STG}	Mass flow of steam generated from heat recovered, kg/s
OC	Operating costs, £/y
PER	Overall revenue from electrical power export, £/y
PIC	Overall cost of electrical power import, £/y
Qin	Heat input into technology options from waste heat source streams, kW
Qout	Useful heat upgraded, kW
Qsteam	Heat flow of steam generated by burning fuel, kW
Q_{COND}	Heat loss from steam condensation, kW
T_{EVAP}	Evaporator temperature of heat upgrading technology, °C
T_{COND}	Condensing temperature of heat upgrading technology, °C
T_{ABS}	Absorber temperature of heat upgrading technology, °C
T_{GEN}	Generator temperature of heat upgrading technology, °C
TAC	Total annualized costs, £/y
TCO_2E	Total CO_2 emissions, t/y
WaterC	Overall cost of water, £/y
W_{MHP}	Electrical power required by the mechanical heat pump, kW
W_{Demand}	Site electrical power demand, kW
$W_{turbine}$	Total power produced from the steam turbines in the cogeneration system

Parameters

AF	Annualization factor
CP	Heat capacity flow rate, kW/°C
CW_{price}	Specific cost of cooling water, £/kWh
DW_{price}	Specific cost of demineralized water, £/kg
EC	Specific equipment cost, £/kW
FEF	CO_2 produced per kW of fuel consumed, kg/kWh
FP	Specific price of fuel consumed, £/kWh
GEF	CO_2 produced per kWh of electrical power distributed in the grid, kg/kWh
IR	Interest rate
L	Lower limit for technology size (basis is the useful heat upgraded), kW
LHVfuel	Lower heating value of fuel consumed, kJ/kg
msteamgen	Mass flow of steam generated from the site processes into the cogeneration system, kg/s
msteamuse	Mass flow of steam consumed by the site processes, kg/s
n	Technology life time (y)
PImp	Electrical power import tariff, £/kWh
PExp	Electrical power export tariff, £/kWh
Qac	Actual heat available, kW
Qcum	Cumulative heat available, kW
Qsteamgen	Heat flow of steam generated from site processes, kW
Qsteamuse	Heat flow of steam consumed by site processes, kW
RF	Retrofit factor to account for installation of equipment
T_{Supply}	Stream supply temperature, °C
T_{Target}	Stream target temperature, °C
$T_{i,j}$	Shifted temperature in interval j on heat source stream i, °C
T_{BFW}	Boiler feed water preheat temperature, °C
U	Upper limit for heat upgraded, kW

Greek letters

α	Regression parameter for heat upgrade technologies
β	Regression parameter for heat upgrade technologies
ΔT_{MIN}	Minimum permissible temperature difference, °C
η_t	Energy conversion efficiency of technology t, %

Abbreviations

ABS	Absorber
AHP	Absorption heat pump
AHT	Absorption heat transformer
BFW	Boiler feed water
COND	Condenser
COMP	Compressor

COP	Coefficient of performance
EVAP	Evaporator
GCC	Grand composite curve
GEN	Generator
HP	High pressure
HT	High temperature
HUR	Hot utility reduced
LP	Low pressure
LT	Low temperature
MHP	Mechanical heat pump
MP	Medium pressure
MT	Medium temperature
STG	Steam generation
VHP	Very high pressure

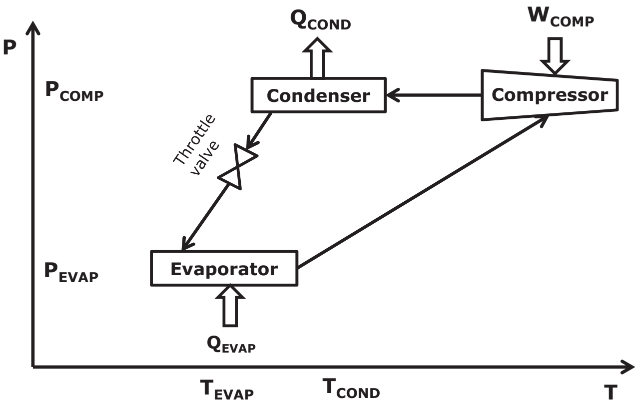


Fig. 1 – Mechanical heat pump schematic (Oluleye et al., 2016).

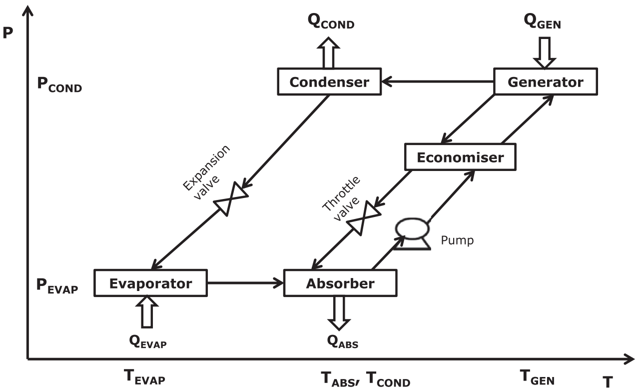


Fig. 2 – Absorption heat pump schematic (Oluleye et al., 2016).

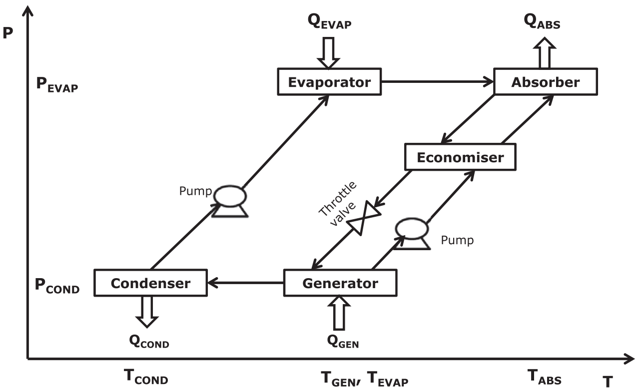


Fig. 3 – Absorption heat transformer schematic (Oluleye et al., 2016).

the integration of heat pumps in industrial processes. The GCC is a graphical representation of the net heat flow against shifted temperatures (using a minimum approach temperature for feasible heat recovery). This divides the process into two regions relative to the pinch i.e. where the design is most constrained. Below the pinch is the heat source region (representing streams that require cold utility), and above the pinch is the heat sink region (i.e. streams requiring hot utility). In integrating heat pumps, the heat below the pinch was upgraded and used to satisfy the energy demand above the pinch. The idea is to reduce the temperature lift associated with technologies. However, the thermodynamic temperature lift may not be the economic temperature lift, since the value of hot utility above the pinch depends on the pressure levels of hot utility required (Varbanov et al., 2004a). Therefore, the most efficient design depends on the economics of the system, which depends on the value of the heat sink as well as the quantity of the heat sinks and sources (Modla and Lang, 2013). Later work confirmed that the smallest temperature lift may not be the most economic (Matsuda et al., 2012).

The goal in integration is to design a system in which the costs associated with operating the heat pump are less than the benefits of using the upgraded waste heat (USDOE, 2003). In order to assess properly the cost and benefits of applying heat pumps for waste heat recovery, Ranade (1988) presented a general equation for the maximum economic lift (i.e. feasible temperature range within which the optimum lift must lie). Computation of the maximum economic lift requires assessment of the marginal costs of site utility levels i.e. the total cost avoided when reducing by one unit the amount of that level of thermal energy being provided under the current operating conditions (Ranade, 1988). However, as utility is reduced, the operating conditions and the marginal cost changes, and several iterations are required to properly evaluate the maximum economic lift. In addition, the marginal cost of hot utility reduced may be different from the marginal cost of steam generated into the existing site utility system. Hot utility reduction is limited by the process demand for hot utility, the limits for steam generation from upgraded heat into the existing cogeneration system depends on the system configuration. Therefore this method (Ranade, 1988) is useful for preliminary screening but not robust enough to make a final design decision. A robust design approach will involve optimizing the cogeneration system simultaneously to determine the true value of hot utility saved or steam generated. Furthermore, selection of heat sources (from both the processing units and the cogeneration system), sinks for recovered heat and technology options was not addressed.

Wallin et al. (1990) developed an optimization methodology for the integration of mechanical heat pumps in process sites. In this method, composite curves serve as a guide to determine the correct placement of heat pump types. Composite curves are formed by combining the temperatures and enthalpies of streams requiring hot utility (cold composite curves) and streams requiring cold utility (hot composite curves) (Smith, 2005). The method involves matching the shape of the composite curves against the specific characteristics of certain heat pump sizes. The optimization objective was to minimize annualized costs by selecting temperature levels for the heat source and heat sink. However, the model of the mechanical heat pump neglects the effect of changing working fluids, and changing system temperatures. Furthermore, a constant value was associated with the use of recovered heat at different steam pressure levels and interactions with the site cogeneration system were neglected.

Most research on heat pump integration focuses on using the composite curves (Wallin et al., 1990), and the grand composite curve (Wallin and Berntsson, 1994; Becker et al., 2011) neglecting the context of total sites. Kapil et al. (2011) screened and compared different technology options for waste heat recovery, including mechanical heat pumps in the context of total sites. The advantage of this approach is that existing heat recovery between processes is taken into account by using the total site profiles. However, in their work the waste heat available was assumed to be at a single temperature, treated as a single source stream and only MHP was considered for upgrading heat. Furthermore the heat available from the site cogeneration system was omitted and only one heat sink (related to low pressure steam reduction) was considered.

Still applying a total site perspective, Kwak et al. (2014) performed techno-economic analysis for the integration of waste heat recovery technologies into a site. In this work, a mechanical heat pump is applied to upgrade waste heat to provide the lowest level of steam use, neglecting other sinks for recovered heat. The design approach assumes a single temperature heat source, neglects heat sources from the site cogeneration system and fired heaters, and the possibility of using electrical power from the cogeneration system for the MHP. Appropriate integration of heat pumps requires the identification of the best heat upgrade technology and its operating conditions (Becker et al., 2011); in Kapil et al. (2011) and Kwak et al. (2014) the conditions were fixed.

In this present work, heat pump integration is addressed in the context of existing total sites, so as to recognize the potential for direct heat recovery within a process and between processes. This form of recovery is relatively inexpensive and easy to implement (Viklund and Johansson, 2014). 'Waste heat' is defined as the residual heat rejected to cooling water or air after maximizing heat recovery within a process and between processes on a site. Design will be done on a stream level (i.e. using the residual heat source streams rejected to cooling water and air after direct heat recovery). In addition, the methodology developed in this work explores interactions with the site cogeneration system as a clear understanding of utility system–process interactions are important for heat pump integration (Ranade, 1988). Waste heat sources from the cogeneration system include heat loss during steam condensation, exhaust of combustion technologies and vented steam.

Many researchers have carried out optimization of existing site cogeneration systems for fuel and cost savings, but few have considered integrating heat upgrade technologies into existing process sites by exploring interactions between the technologies, the site cogeneration system and the site processes. Varbanov et al. (2004b) developed a successive mixed integer linear programming procedure for operational optimization of existing site cogeneration systems. A linear optimization model was obtained by fixing the values of some system properties followed by rigorous simulations until the fixed values converge. Mixed integer linear programming (MILP) representation for site cogeneration systems is sufficiently accurate especially when the pressure and temperature at each of the steam mains is considered constant (Micheletto et al., 2008). The framework exploited various degrees of freedom relating to changes in fuel flows and fuel type in firing machines (Varbanov et al., 2004b). However, degrees of freedom relating to exploiting the waste heat available was not explored. Taking into account low-temperature heat recovery, Zhang et al. (2012) developed an optimization procedure for industrial refinery complexes based on insights of process production and energy utilization. The low temperature heat recovery and utilization options were limited to sources from the site processes neglecting residual heat from the cogeneration system. Furthermore, only a single sink for use of recovered heat was considered.

This work proposes a novel generic mixed integer linear modeling and optimization framework for integration of heat pump options (mechanical heat pumps, absorption heat pumps and absorption heat transformers) in existing process sites. The proposed method takes into account: (1) low-grade heat available from the site processing units, cogeneration system and any fired heaters, (2) selection of heat source streams and technology options, and (3) multiple sink types for recovered heat relating to process hot utility savings, steam generation (into the site cogeneration system), and boiler feed water preheating. To estimate the correct value of hot utility saved, steam generated and boiler feed water preheated, the cogeneration system is optimized simultaneously. The framework involves the creation of a superstructure of all possible combinations of heat sources, sinks for recovered heat and technology options. The superstructure is reduced to an optimal design subject to an objective function and sets of constraints. The model is solved using the branch and bound algorithm in Lindo's systems what's Best! (What's Best, 2013). Thermodynamic models of mechanical heat pumps, absorption heat pumps and heat transformers developed and validated by Oluleye et al. (2016) are applied. For the cogeneration system, generic linear models for energy equipment such as boilers, steam turbines and gas turbines developed and validated by Aguilar et al. (2007) are also applied in this work.

2. Problem statement

A framework for integrating heat upgrading technologies in existing process sites that can identify the most suitable technology, by optimizing its economic and thermodynamic performance for different heat sources, and sink temperatures (and associated duties) is an essential tool in assessing the potential for heat pumps in process sites. A more specific definition of the problem is:

- Given:
  - A set of streams rejecting heat to cooling water and air from the site processing units and the cogeneration system. The stream data includes supply (inlet) temperatures, target (outlet) temperatures and the thermal energy content.
  - A set of heat upgrading technologies (MHP, AHP and AHT) capable of upgrading the heat sources to higher temperatures. Properties provided for the heat upgrading technologies are the equipment costs and economic lifetime.
  - The existing site utility consumption. This includes:
    - Existing process steam requirements in quantity and temperature.
    - Existing quantities and temperatures of steam generated from the site processing units.
    - Technologies for combustion of fuel in the site cogeneration system.
    - Site cogeneration system components.

- Site electrical power demand.
- Fuel prices, electrical power tariffs, CO_2 emission factors.

- Determine:
  - Temperature and associated duty of heat source stream to upgrade.
  - Suitable sink to dump the upgraded heat.
  - Selection and operation of heat upgrading technologies.
  - Impact on the existing site cogeneration system.
  - How changes in fuel price, power tariff and capital cost affects the integration scheme.
- Subject to:
  - Overall energy balances for the site cogeneration system and heat upgrading technologies.
  - Determining the operation of heat upgrading technologies only when they are selected.
  - Steam flow mass balance per pressure distribution level in the site cogeneration system.
- In order to:
  - Minimize an objective function.

3. Methodology

This paper focuses on the development of a Mixed Integer Linear Program for integrating heat upgrading technologies in process sites. Applying optimization techniques allows multiple degrees of freedom to be exploited to reduce capital and operating costs whilst exploring interactions with the existing site cogeneration system. Good solutions can be guaranteed since all aspects of the design (both operational and structural) are considered simultaneously (Smith, 2005). The methodology involves the below steps (each step is described in detail in Sections 3.1–3.7):

Step 1: This involves representing the heat source streams to account for the temperature and thermal energy content.
Step 2: Thermodynamic modeling of heat upgrading technologies and the site cogeneration system.
Step 3: Create an irreducible superstructure involving all technology options, heat sources and sinks for upgraded heat.
Step 4: Define the system variables i.e. degrees of freedom.
Step 5: Define the objective function. The superstructure created in Step 3 is reduced subject to the objective function and set of constraints.
Step 6: Define the system constraints.
Step 7: Evaluate the results generated.

3.1. *Representing waste heat source streams and sinks for upgraded heat*

Heat sources for upgrading technologies include heat rejected to cooling water and air by the site processes, and the site cogeneration system (Oluleye et al., 2014). The analysis of heat sources begins with extracting the supply temperature, target temperature and heat contained in the heat source streams. The temperature of the heat sources is shifted by $-\Delta T_{MIN}$ to allow for feasible heat exchange. The extracted streams data are plotted on a grid diagram in order to identify suitable temperature intervals to represent them. The temperature intervals j can be created from a combination of supply and target temperatures as illustrated in Fig. 4. This ensures that heat is extracted from a stream i above the target temperature but below the supply temperature (Eq. (1)). In this case, exploitation of high quality heat (relative to the target temperature) is encouraged in every stream.

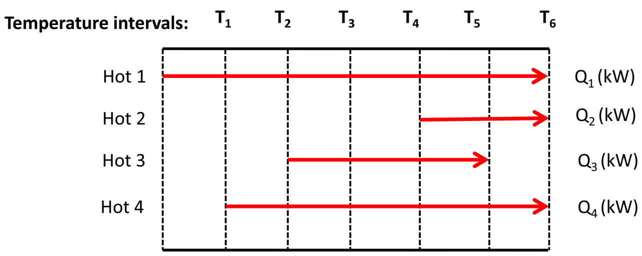


Fig. 4 – Grid diagram for heat source streams (Illustration).

$$T_{\mathrm{Target},i} \le T_{i,j} \le T_{\mathrm{Supply},i} \tag{1}$$

The modeling framework is written to select a stream for a heat upgrade technology option using the actual heat available (Qac) in any $T_{i,j}$ or the cumulative heat available (Qcum) from $T_{i,j-1}$ to $T_{i,j}$.

Sinks for upgraded heat considered in the work are: (1) reducing process demand for hot utility at different pressure levels *pl*, (2) steam generated into the cogeneration system at different pressure levels *pl*, and (3) boiler feed water preheating. Reducing process demand for hot utility is limited by the quantity of hot utility required by the chemical processes, while steam generation into the cogeneration system is limited by the capacity of the cogeneration system. The modeling framework is formulated to select sinks k for upgraded heat, where:

$$Q^{\mathrm{HUR}}_{k(pl)}, Q^{\mathrm{STG}}_{k(pl)}, Q^{\mathrm{BFW}} \in \mathrm{Qout}_k \tag{2}$$

3.2. *Modeling technology options*

In order to assess alternatives for waste heat upgrade, models are needed to predict the performance of the technology options. Oluleye et al. (2016) developed thermodynamic models for mechanical heat pumps, absorption heat pumps and absorption heat transformers. In their work, the real (actual) coefficient of performance is correlated with an ideal reference case. The models are adopted in this work to determine the useful heat upgraded (Qout).

For a mechanical heat pump (Fig. 1), the heat upgraded is a function of the flow of low temperature waste heat in the evaporator and the technology ideal performance ($COP_{MHP,ideal}$) as shown in Eqs. (3) and (4) (Oluleye et al., 2016).

$$\mathrm{Qout}^{\mathrm{MHP}} = \mathrm{Qin}^{\mathrm{MHP,EVAP}} \times \left(\frac{(\alpha_{\mathrm{MHP}} \times \mathrm{COP}_{\mathrm{MHP,ideal}}) + \beta_{\mathrm{MHP}}}{(\alpha_{\mathrm{MHP}} \times \mathrm{COP}_{\mathrm{MHP,ideal}}) + \beta_{\mathrm{MHP}} - 1} \right) \tag{3}$$

$$\mathrm{COP}_{\mathrm{MHP,ideal}} = \left(\frac{T^{\mathrm{MHP}}_{\mathrm{COND}}}{T^{\mathrm{MHP}}_{\mathrm{COND}} - T^{\mathrm{MHP}}_{\mathrm{EVAP}}} \right) \tag{4}$$

where $\mathrm{Qout}^{\mathrm{MHP}}$ is the flow of high temperature heat released during condensation of working fluid in the MHP; $\mathrm{Qin}^{\mathrm{MHP,EVAP}}$ denotes low temperature heat required to vaporize working fluids; α and β are regression parameters for the mechanical heat pump; $T^{\mathrm{MHP}}_{\mathrm{COND}}$ is the temperature of heat upgraded; $T^{\mathrm{MHP}}_{\mathrm{EVAP}}$ is the temperature of heat required to vaporize the working fluid in the evaporator. The selection of working fluids for the mechanical heat pump was addressed by Oluleye et al. (2016) and Fig. A4 in Appendix provides a summary. The temperatures in Eq. (4) are in Kelvin.

For an absorption heat pump (Fig. 2), the heat upgraded in the condenser and absorber is a function of the flow of medium to high temperature waste heat supplied to the generator:

$$\mathrm{Qout}^{\mathrm{AHP}} = \mathrm{Qin}^{\mathrm{AHP,GEN}} \times \left(\frac{\beta_{\mathrm{AHP}} \times \mathrm{COP}_{\mathrm{AHP,ideal}}}{\mathrm{COP}_{\mathrm{AHP,ideal}} - \alpha_{\mathrm{AHP}}}\right) \tag{5}$$

$$\mathrm{COP}_{\mathrm{AHP,ideal}} = 1 + \left(1 - \frac{T^{\mathrm{AHP}}_{\mathrm{COND}}}{T^{\mathrm{AHP}}_{\mathrm{GEN}}}\right)\left(\frac{T^{\mathrm{AHP}}_{\mathrm{EVAP}}}{T^{\mathrm{AHP}}_{\mathrm{COND}} - T^{\mathrm{AHP}}_{\mathrm{EVAP}}}\right) \tag{6}$$

where $\mathrm{Qout}^{\mathrm{AHP}}$ is the medium temperature heat released; $\mathrm{Qin}^{\mathrm{AHP,GEN}}$ denotes the high temperature heat required to separate the working fluid pair in the generator; α and β are regression parameters for the absorption heat pump; $T^{\mathrm{AHP}}_{\mathrm{COND}}$ is the temperature of heat upgraded; $T^{\mathrm{AHP}}_{\mathrm{GEN}}$ is the temperature of heat required to separate the absorbent (lithium bromide) and refrigerant (water) in the generator; $T^{\mathrm{AHP}}_{\mathrm{EVAP}}$ is the temperature of heat required to vaporize the refrigerant in the evaporator. Possible combinations of systems temperatures for the AHP are presented in Appendix. The temperatures in Eq. (6) are in Kelvin.

For an absorption heat transformer (Fig. 3), the heat upgraded in the absorber is a function of the flow of low and medium temperature heat in the evaporator, the generator and the cycle ideal performance ($\mathrm{COP}_{\mathrm{AHT,ideal}}$):

$$\mathrm{Qout}^{\mathrm{AHT}} = (\mathrm{Qin}^{\mathrm{AHT,EVAP}} + \mathrm{Qin}^{\mathrm{AHT,GEN}}) \times \left(\frac{\beta_{\mathrm{AHT}} \times \mathrm{COP}_{\mathrm{AHT,ideal}}}{\mathrm{COP}_{\mathrm{AHT,ideal}} - \alpha_{\mathrm{AHT}}}\right) \tag{7}$$

$$\mathrm{COP}_{\mathrm{AHT,ideal}} = \left(\frac{(T^{\mathrm{AHT}}_{\mathrm{EVAP}} - T^{\mathrm{AHT}}_{\mathrm{COND}}) \times T^{\mathrm{AHT}}_{\mathrm{ABS}}}{((T^{\mathrm{AHT}}_{\mathrm{EVAP}} - T^{\mathrm{AHT}}_{\mathrm{COND}}) \times T^{\mathrm{AHT}}_{\mathrm{GEN}}) + ((T^{\mathrm{AHT}}_{\mathrm{ABS}} - T^{\mathrm{AHT}}_{\mathrm{GEN}}) \times T^{\mathrm{AHT}}_{\mathrm{EVAP}})}\right) \tag{8}$$

where $\mathrm{Qout}^{\mathrm{AHT}}$ is the high temperature heat released; $\mathrm{Qin}^{\mathrm{AHT,EVAP}}$, $\mathrm{Qin}^{\mathrm{AHT,GEN}}$ are the medium to low temperature heat required to vaporize the working fluid and separate the working fluid pair in the generator respectively; α and β are regression parameters for the absorption heat transformer; $T^{\mathrm{AHT}}_{\mathrm{ABS}}$ is the temperature of heat upgraded; $T^{\mathrm{AHT}}_{\mathrm{GEN}}$ is the temperature of heat required to separate the absorbent (lithium bromide) and refrigerant (water) in the generator; $T^{\mathrm{AHT}}_{\mathrm{EVAP}}$ is the temperature of heat required to vaporize the refrigerant in the evaporator. Possible combinations of system temperatures for the AHT are presented in Appendix. The temperatures in Eq. (8) are in Kelvin.

For estimation of the ideal coefficient of performance in Eqs. (4), (6) and (8):

$$T^{\mathrm{MHP}}_{\mathrm{EVAP}}, T^{\mathrm{AHP}}_{\mathrm{EVAP}}, T^{\mathrm{AHP}}_{\mathrm{GEN}}, T^{\mathrm{AHT}}_{\mathrm{EVAP}}, T^{\mathrm{AHT}}_{\mathrm{GEN}} \in T_{i,j} \tag{9}$$

$$T^{\mathrm{MHP}}_{\mathrm{COND}}, T^{\mathrm{AHP}}_{\mathrm{COND}}, T^{\mathrm{AHT}}_{\mathrm{ABS}} \in T_{k(\mathrm{pl})} \tag{10}$$

$T^{\mathrm{AHT}}_{\mathrm{COND}}$ is dependent on ambient conditions. Values of α and β in Eqs. (3), (5) and (7) are provided in Appendix (Tables A1–A3).

Models of the cogeneration system components such as steam turbines, gas turbines and boilers proposed by Aguilar et al. (2007) are provided in Appendix. To represent the cogeneration system in a linear way, the saturation temperature and pressure of the steam distribution mains are fixed (Micheletto et al., 2008). In addition, introducing binary variables to represent existence of technology options exploiting waste heat from stream i at temperature interval j to satisfy heat sink k, means that the models for heat upgrading technologies in Eqs. (3), (5) and (7) are discretized. This implies that once a technology is selected; the operating temperatures and the flow of heat will also be determined.

3.3. *Superstructure creation*

The next step is to create a superstructure representing possible connections between the heat pump technologies, the site processes and the site cogeneration system (Fig. 5) by careful description of the variables (Section 3.4).

Waste heat vaporizes the working fluid in heat upgrade technology options, and separates the working fluid pair in the generators of absorption heat pumps and absorption heat transformers. Sinks for upgraded heat are for boiler feed water preheating, steam generation, and hot utility savings.

The main design and operational issues to address are:

1. Selection of heat source streams from both the site processes and the site cogeneration system.
2. Selection of technology options: mechanical heat pumps, absorption heat pumps and absorption heat transformers.
3. Selection of sinks for upgraded heat: boiler feed water preheating, hot utility savings and steam generation at different pressure levels.
4. Power required for the mechanical heat pump: imported from a central grid or produced from the site cogeneration system.

3.4. *System variables*

Binary (structural) and continuous (operational) variables are introduced to represent degrees of freedom.

- Binary variables are introduced for existence of technology options upgrading heat from heat source stream i in temperature interval j to satisfy heat sink k. The total number of binary variables is the product of i, j, k and the number of technology options.

$$Y^{\mathrm{MHP}}_{i,j,k}, Y^{\mathrm{AHP}}_{i,j,k}, Y^{\mathrm{AHT}}_{i,j,k} = \{0, 1\} \tag{11}$$

- Continuous variables are described below:
  $\mathrm{Qout}^{\mathrm{MHP}}_{i,j,k}$: Heat upgraded to heat sink k, from a MHP using heat source stream i, in temperature interval j.
  $\mathrm{Qout}^{\mathrm{AHP}}_{i,j,k}$: Heat upgraded to heat sink k, from an AHP using heat source stream i, in temperature interval j.
  $\mathrm{Qout}^{\mathrm{AHT}}_{i,j,k}$: Heat upgraded to heat sink k, from an AHT using heat source stream i, in temperature interval j.
  $mfuel_t$: Fuel consumed by technologies in the site cogeneration system.
  $mturbine_{pl}$: Mass flow of steam into steam turbines at pressure level pl in the site cogeneration system.
  W_{Import}: Electrical power imported from the grid to satisfy site demand.
  W_{Export}: Electrical power exported to the grid.

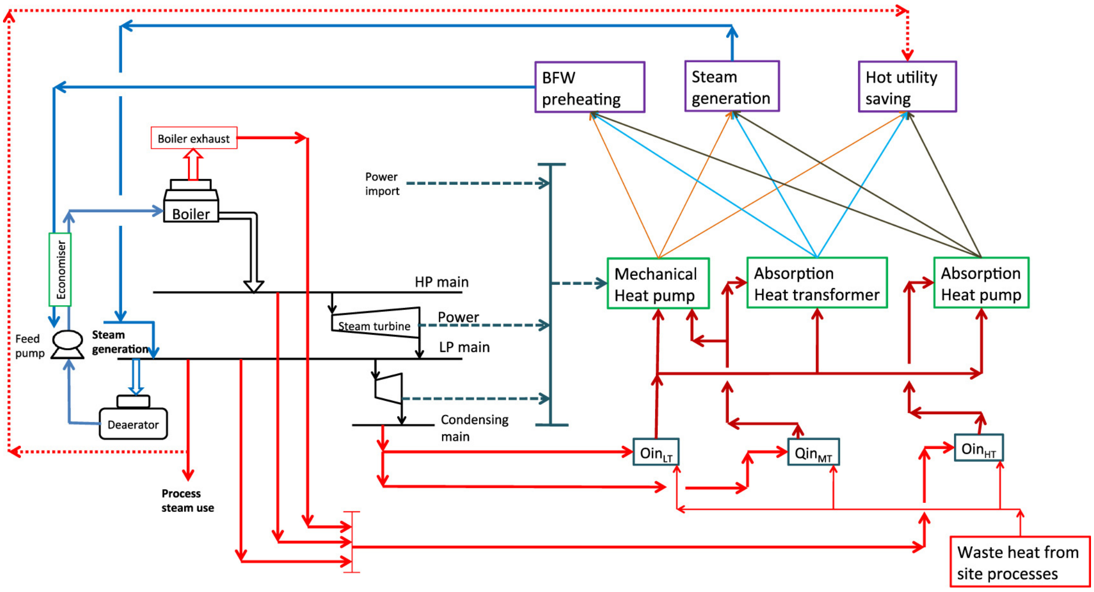


Fig. 5 – Superstructure showing the cogeneration system, steam distribution levels, waste heat sources and heat upgrade technologies.

3.5. *Objective function*

The objective function is to minimize the total annualized costs (TAC) defined as the sum of the annualized capital costs (ACC), maintenance cost (MC) and operating costs (OC):

$$\textit{Minimize}: (\mathrm{ACC} + \mathrm{MC} + \mathrm{OC}) \tag{12}$$

The capital cost (Eq. (13)) is calculated taking into account the equipment cost (EC) for new technology installations, the retrofit factor (RF) to account for costs of installing new equipment and retrofitting existing facilities and the annualization factor (AF) to spread the cost over the lifetime of a technology. Simple economic models in published works can be used to represent the equipment cost.

$$\mathrm{ACC} = \mathrm{AF} \times \mathrm{RF} \times \left\{ \left[\left(\left(\sum_i \sum_j \sum_k \mathrm{Qout}^{\mathrm{MHP}}_{i,j,k} \right) \times \mathrm{EC_{MHP}} \right) \right] + \left[\left(\left(\sum_i \sum_j \sum_k \mathrm{Qout}^{\mathrm{AHP}}_{i,j,k} \right) \times \mathrm{EC_{AHP}} \right) \right] + \left[\left(\left(\sum_i \sum_j \sum_k \mathrm{Qout}^{\mathrm{AHT}}_{i,j,k} \right) \times \mathrm{EC_{AHT}} \right) \right] \right\} \tag{13}$$

The annualization factor is calculated as shown below (Smith, 2005):

$$\mathrm{AF} = \frac{\mathrm{IR} \times (1 + \mathrm{IR})^n}{(1 + \mathrm{IR})^{n-1}} \tag{14}$$

The maintenance cost of the technologies is assumed to be 2% of the equipment capital cost (Aguilar et al., 2007). The operating cost is defined as the sum of the fuel costs (FC), water costs (WaterC), power imports costs (PIC) minus revenue from power export (PER) Eq. (15). The fuel cost is associated with fuel consumed in the site cogeneration system and other auxiliary equipment including fuel consumed by fired heaters for high temperature process heating (Eq. (16)).

$$\mathrm{OC} = \mathrm{FC} + \mathrm{WaterC} + \mathrm{PIC} - \mathrm{PER} \tag{15}$$

$$\mathrm{FC} = \sum_t (\textit{mfuel}_t \times \mathrm{FP}_t) \tag{16}$$

where FP_t denotes the unit price of fuel consumed by a technology in the site cogeneration system. Water costs include costs for cooling water (for the site processes and the site cogeneration system) and demineralized water (DW) consumed in the site cogeneration system:

$$\mathrm{WaterC} = \left[\left(\sum_i \sum_j \mathrm{Qin}_{i,j} \right) \times \mathrm{CW_{price}} \right] + [m_{\mathrm{DW}} \times \mathrm{DW_{price}}] \tag{17}$$

Overall electrical power import cost and revenue from export are calculated as shown below:

$$\mathrm{PIC} = \mathrm{W_{Import}} \times \mathrm{PImp} \tag{18}$$

$$\mathrm{PER} = \mathrm{W_{Export}} \times \mathrm{PExp} \tag{19}$$

where PImp is the electrical power import tariff, PExp is the electrical power export tariff.

3.6. *System constraints*

Sets of equality and inequality equations defining various limits of the developed modeling framework are presented below.

1. Constraint to ensure that the heat consumed by technologies (Qin) is available from the waste heat source streams:

$$\sum_k (Qin^{MHP,EVAP}_{i,j,k} + Qin^{AHP,GEN}_{i,j,k} + Qin^{AHP,EVAP}_{i,j,k} + Qin^{AHT,EVAP}_{i,j,k} + Qin^{AHT,GEN}_{i,j,k}) = Qin_{i,j}, \quad \forall i \in I, \quad j \in J \tag{20}$$

$$0 \le Qin_{i,j} \le (Qcum_{i,j} - Qac_{i,j-1} - Qac_{i,j-2} - Qac_{i,j-3} - Qac_{i,j-(j-1)}), \quad \forall i \in I, \quad j \in J \tag{21}$$

The terms in Eqs. (20) and (21) are summarized below:

- $Qin^{MHP,EVAP}_{i,j,k}$, $Qin^{AHP,EVAP}_{i,j,k}$ and $Qin^{AHT,EVAP}_{i,j,k}$ are the quantities of heat required to vaporize the working fluid in the evaporators of mechanical heat pumps, absorption heat pumps and absorption heat transformers respectively, to satisfy sink k. The heat is provided from heat source stream i in temperature interval j.
- $Qin^{AHP,GEN}_{i,j,k}$ and $Qin^{AHT,GEN}_{i,j,k}$ are the quantities of heat required to separate the absorbent and refrigerant in the generators of absorption heat pumps and absorption heat transformers respectively, to satisfy sink k. The heat is provided from heat source stream i in temperature interval j.
- $Qcum_{i,j}$ is the cumulative heat available at temperature interval j from heat source stream i.
- $Qac_{i,j}$ is the actual heat available at temperature interval j from heat source stream i.

2. Sinks for upgraded heat
Sinks k for upgraded heat considered are: hot utility reduction (i.e. heat upgraded reduces process requirement for hot utility), steam generation into the site cogeneration system and boiler feed water preheating.
When k is related to reducing the hot utility required by the site processing units:

$$\sum_i \sum_j (Qout^{MHP}_{i,j,k} + Qout^{AHP}_{i,j,k} + Qout^{AHT}_{i,j,k}) = Q^{HUR}_{k(pl)} \quad \forall k \in K, \quad pl \in PL \tag{22}$$

$$0 \le Q^{HUR}_{k(pl)} \le Qsteamuse_{pl} \quad \forall k \in K, \quad pl \in PL \tag{23}$$

When k is related to steam generation into the site cogeneration system at different pressure levels pl:

$$\sum_i \sum_j (Qout^{MHP}_{i,j,k} + Qout^{AHP}_{i,j,k} + Qout^{AHT}_{i,j,k}) = Q^{STG}_{k(pl)} \quad \forall k \in K, \quad pl \in PL \tag{24}$$

$$0 \le Q^{STG}_{k(pl)} \quad \forall k \in K, \quad pl \in PL \tag{25}$$

The upper limit for steam generation depends on the configuration of the site cogeneration system. Since both systems are optimized simultaneously, this limit is taken into account.

When k is related to boiler feed water preheating:

$$\sum_i \sum_j \sum_k (Qout^{MHP}_{i,j,k} + Qout^{AHP}_{i,j,k} + Qout^{AHT}_{i,j,k}) = Q^{BFW} \tag{26}$$

$$0 \le Q^{BFW} \le Q^{BFW}_{Demand} \tag{27}$$

The terms in Eqs. (22)–(27) are described below:

- $Qout^{MHP}_{i,j,k}$, $Qout^{AHP}_{i,j,k}$ and $Qout^{AHT}_{i,j,k}$ are the quantities of heat released from the condensers of MHP, absorbers and condensers of AHP and absorbers of AHT respectively, to satisfy heat sink k, using heat source stream i in temperature interval j. The temperature of the heat sink depends on the steam distribution pressure levels pl in the site cogeneration system.
- $Q^{HUR}_{k(pl)}$ is the flow of heat associated with reducing the process demand for hot utility at pressure level pl.
- $Qsteamuse_{pl}$ is the heat flow of existing steam consumed by the site processes at different pressure levels.
- $Q^{STG}_{k(pl)}$ is the flow of heat associated with generating steam into the site cogeneration system at different pressure levels.
- Q^{BFW} is the flow of heat associated with preheating boiler feed water.

3. The heat source streams are already shifted by ΔT_{MIN} to account for feasible heat recovery (Section 3.1 above). For sinks of upgraded heat:

$$T^{MHP}_{COND} \ge T_{k(pl)} + \Delta T_{MIN} \quad \forall k \in K, \quad pl \in PL \tag{28}$$

$$T^{AHP}_{COND} \ge T_{k(pl)} + \Delta T_{MIN}, \quad \forall k \in K, \quad pl \in PL \tag{29}$$

$$T^{AHT}_{ABS} \ge T_{k(pl)} + \Delta T_{MIN} \quad \forall k \in K, \quad pl \in PL \tag{30}$$

where $T_{k(pl)}$ is the temperature associated with steam distribution pressure levels pl in the site cogeneration system.

4. Implicit constraints for existence of technologies within specified size limits. L represents the lower bound for technology sizes and U represents an upper bound. Note that ‘size’ is expressed in terms of heat flow in this work. Implicit constraints also show the relationship between the binary and operational variables.

$$Qout^{MHP}_{i,j,k} - (U_{MHP} \times Y^{MHP}_{i,j,k}) \le 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{31}$$

$$Qout^{MHP}_{i,j,k} - (L_{MHP} \times Y^{MHP}_{i,j,k}) \ge 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{32}$$

$$Qout^{AHP}_{i,j,k} - (U_{AHP} \times Y^{AHP}_{i,j,k}) \le 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{33}$$

$$Qout^{AHP}_{i,j,k} - (L_{AHP} \times Y^{AHP}_{i,j,k}) \ge 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{34}$$

$$Qout^{AHT}_{i,j,k} - (U_{AHT} \times Y^{AHT}_{i,j,k}) \le 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{35}$$

$$Qout^{AHT}_{i,j,k} - (L_{AHT} \times Y^{AHT}_{i,j,k}) \ge 0 \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{36}$$

Constraint to ensure that a heat source stream is not used twice:

$$\sum_i \sum_j (Y^{MHP}_{i,j,k} + Y^{AHP}_{i,j,k} + Y^{AHT}_{i,j,k}) = 1 \forall k \in K \tag{37}$$

Constraint to allow for more than one technology in the system using unique heat source streams:

$$\sum_{i}\sum_{j}\sum_{k}(Y^{MHP}_{i,j,k} + Y^{AHP}_{i,j,k} + Y^{AHT}_{i,j,k}) \geq 0 \tag{38}$$

5. Overall energy balance for the site cogeneration system:

$$\left\{\left[\sum_{t}((mfuel_t \times LHVfuel_t) - Q^{BFW}) \times \eta_t\right] + \sum_{pl}(Qsteamgen_{pl} + Q^{STG}_{k(pl)}) - \sum_{pl}(Qsteamuse_{pl} + Q^{HUR}_{k(pl)}) - \sum_{pl}W_{turbine_{pl}} - \sum_{pl}Q_{cond_{pl}}\right\} = 0 \tag{39}$$

The terms in Eq. (39) are summarized below:

- $mfuel_t$ is the mass flow of fuel consumed by technology t in the site cogeneration system.
- $LHVfuel_t$ is the lower heating value of fuel consumed by a technology in the site cogeneration system.
- η_t is the energy conversion efficiency of technology t in the site cogeneration system.
- $Qsteamgen_{pl}$ is the heat flow of existing steam generation from the site processes into the cogeneration system at different pressure levels.
- $W_{turbine}$ is the total power produced from steam turbines in the site cogeneration system.
- Q_{cond} is the heat loss from steam condensation in the site cogeneration system.

6. Energy balances for each heat upgrade technology: MHP is given in Eq. (40), AHP in Eq. (41) and AHT in Eq. (42).

$$Qout^{MHP}_{i,j,k} = Qin^{MHP,EVAP}_{i,j,k} + W^{MHP,COMP}_{i,j,k} \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{40}$$

$$Qout^{AHP}_{i,j,k} = Qin^{AHP,GEN}_{i,j,k} + Qin^{AHP,EVAP}_{i,j,k} + W^{AHP,PUMP}_{i,j,k} \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{41}$$

$$Qout^{AHT}_{i,j,k} = Qin^{AHT,GEN}_{i,j,k} + Qin^{AHT,EVAP}_{i,j,k} + Qin^{AHT,COND}_{i,j,k} + W^{AHT,PUMP}_{i,j,k} \quad \forall i \in I, \quad j \in J, \quad k \in K \tag{42}$$

where $W^{MHP,COMP}$ represents the compression power requirements of the MHP, $W^{AHP,PUMP}$ and $W^{AHT,PUMP}$ represents the liquid pumping requirements of AHPs and AHTs respectively. The liquid pumping requirements of AHPs and AHTs can be assumed to be negligible (Donnellan et al., 2015; Grossman and Perez-Blanco, 1982).

7. Mass balance per pressure level *pl* in the site cogeneration system:

$$m_{in,pl} = m_{out,pl} \quad \forall pl \in PL \tag{43}$$

8. Technology flow boundaries (on a mass basis) in the cogeneration system:

$$m_{L,t} \leq m_t \leq m_{U,t} \quad \forall t \in TT \tag{44}$$

Where *L* and *U* represents the lower and upper limit of steam flow (on a mass basis) into technologies in the site cogeneration system.

9. Electrical power import and export: Eq. (45) is formulated to allow for generation of additional power from the cogeneration system to drive the mechanical heat pump; when this is done the net power exported is reduced.

$$\sum_{pl}W_{turbine_{pl}} - W_{Demand} + W_{Import} - W_{Export} + W^{MHP,COMP} = 0 \tag{45}$$

$$W^{MHP,COMP} = \sum_{i}\sum_{j}\sum_{k}(Qout^{MHP}_{i,j,k} - Qin^{MHP}_{i,j,k}) \tag{46}$$

where W_{Demand} is the site electrical power demand.

3.7. *Evaluating the design*

The design is formulated to minimize total costs i.e. sum of annualized capital costs, operating costs and maintenance costs, subject to constraints. Results generated by applying the modeling and optimization framework will be evaluated based on the difference between the total cost of the base case (without heat recovery) and the optimized case. The total cost is formulated as the objective function in Eq. (12). A positive difference indicates a gain and a negative difference indicates that upgrading waste heat is uneconomic. In addition to the costs, the total CO_2 emissions will also be determined. To account for the potential to reduce CO_2 emissions, the difference between the CO_2 emissions of the base case and the optimum design will also be estimated to evaluate the design. The total CO_2 emissions (TCO_2E) is estimated considering: (1) CO_2 emissions from fuel combustion in the site cogeneration system, (2) emissions associated with electrical power imported (as fuel is combusted in a central grid to provide the electricity), and (3) CO_2 offset when electricity is exported (since fossil fuel is displaced in a central grid when electricity is exported). The mathematical expression for the overall CO_2 emitted is:

$$TCO_2E = (mfuel_t \times LHVfuel_t \times FEF_t) + ((W_{Import} - W_{Export}) \times GEF) \tag{47}$$

The optimization framework is solved using Lindo's system What's Best! software (What's Best, 2013). The problem is solved in two stages: (1) a continuous approximation of the model is solved to give a theoretical limit on the objective and (2) branch and bound algorithm is applied to find an optimal integer solution. The branch and bound algorithm implicitly identifies all possible integer solutions in a robust way (What's Best, 2013).

4. Case study

The case study presented is for a medium scale petroleum refinery (Fraser and Gillespie, 1992). The refinery has seven processing units: crude/vacuum distillation unit, diesel hydrotreaters, fluidised catalytic cracking unit, platformer, kerosene hydrotreaters, Naphtha hydrotreaters and visbreaker unit. The grid diagrams for heat source streams rejecting heat to cooling water and to air from each of

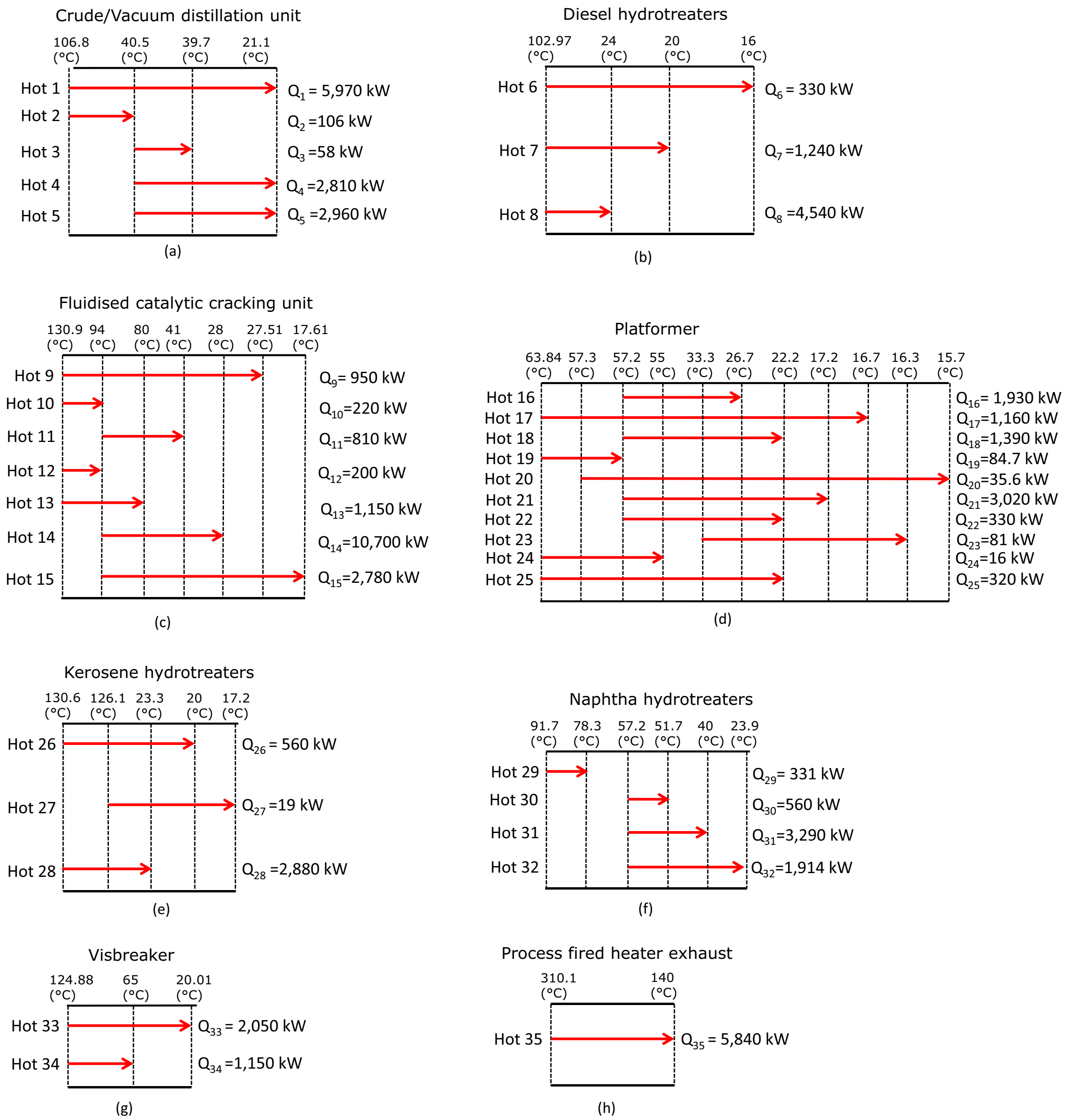


Fig. 6 – Heat source streams grid diagrams for the processing units considered in the medium scale petroleum refinery: (a) crude/vacuum distillation unit, (b) diesel hydrotreaters, (c) fluidised catalytic cracking unit, (d) platformer, (e) kerosene hydrotreaters, (f) Naphtha hydrotreaters, (g) Visbreaker, and (h) process fired heater exhaust.

the seven processing units are shown in Fig. 6(a–g). Heat rejected by the fired heater providing high temperature heat to the crude oil distillation unit, Naphtha hydrotreaters and the platformer is shown in Fig. 6(h). Temperature intervals ($T_{i,j}$) for the source streams are also indicated in Fig. 6(a–h). The data in Fig. 6(a–h) can be obtained by extracting the beginning (supply) temperature and end (target) temperature for all heat exchangers rejecting heat to cooling water and air.

In total 61,785 kW of heat is rejected to cooling water and air from the site processing units. The existing cogeneration system consists of a coal boiler, a gas turbine (GT) with a heat recovery steam generator (HRSG) for steam generation from the GT exhaust, four back pressure turbines, one extraction turbine, four expansion valves, and a deaerator as shown in Fig. 7. The site power demand is 50,000 kW. The demand for hot utility (steam) at different pressure levels and the steam generated from the site processing unit at the existing operating conditions are also shown in Fig. 7.

Based on the saturation temperatures of steam distribution mains in Fig. 7, there is no potential for direct steam generation (into the cogeneration system) from process heat rejected to cooling water. Sources of waste heat from the cogeneration system include exhaust of technologies such as GT and boilers, and latent heat loss from steam condensation. Waste heat available in equipment exhaust is extracted above the acid dew point to prevent condensation of the gases (Smith, 2005). 150 °C (shifted to 140 °C) is assumed as the stack temperature (Oluleye et al., 2014). In total 104,136 kW of waste heat is rejected from the site utility system to cooling water and air, based on the assumed stack temperature only 88% is recoverable.

Taking into account the operating temperature range of technologies for heat upgraded (as seen in Tables A1–A3 in Appendix), the maximum heat upgrade temperature is 215 °C. This temperature is within the saturation temperature of the medium pressure main (200 °C). Therefore, using the upgraded heat to reduce hot utility (i.e. steam required by the site

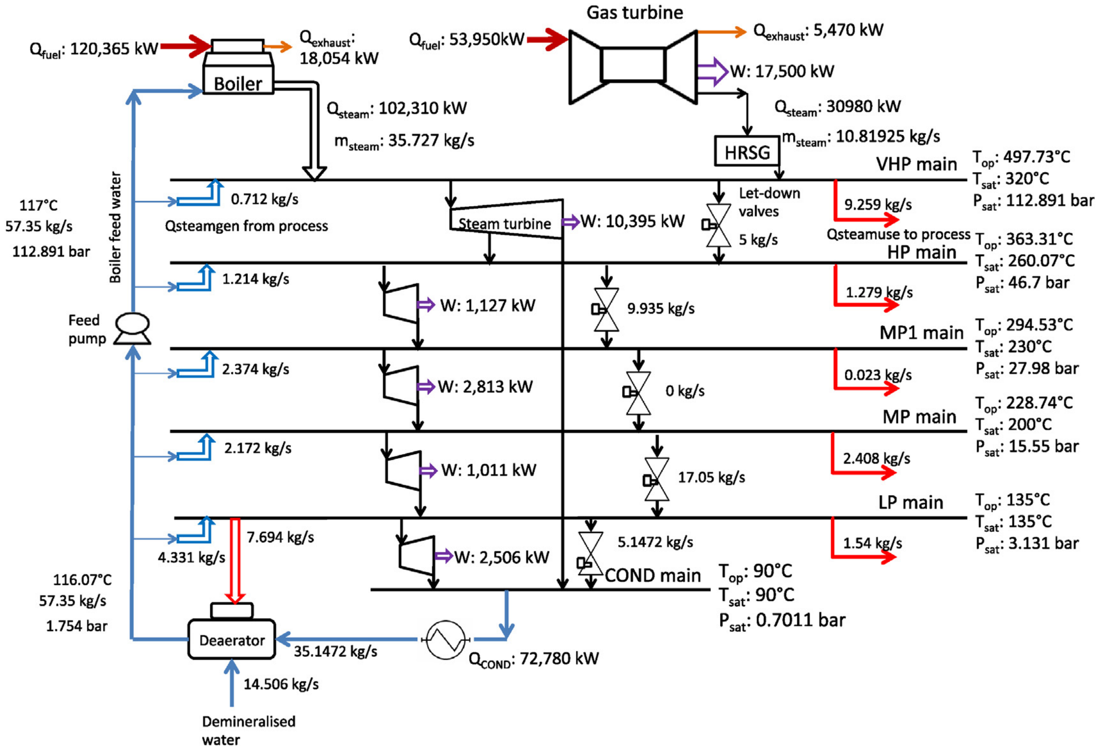


Fig. 7 – Site cogeneration system (base case).

Table 1 – Design assumptions on prices and emissions.

Energy Prices (DECC, 2012)	Emission factors (DECC, 2012)	Equipment costs	Others
Electrical power tariff: 13.4 p/kWh Industrial coal price: 1.42 p/kWh	Grid emission factor: 0.485 kg/kWh Coal emission factor: 0.327 kg/kWh	Mechanical heat pump: 333 £/kW (Macro DE Project, 2012) Absorption heat pump: 265 £/kW (Keil et al., 2008) Absorption heat transformer: 359 £/kW (Aly et al., 2007)	Interest rate (IR): 15% Operating hours: 8600 hours Assumed retrofit factor: 3 (Aguilar et al., 2007) Ambient temperature 25 °C Technology life time (n): 10 yrs

processing units) and steam generation into the site cogeneration system is feasible at the low pressure (LP) and medium pressure (MP) levels.

The case study aims to apply the developed methodology to integrate heat upgrade technologies into this refinery site in order to exploit the waste heat rejected by the site processes and the site cogeneration system. The heat upgraded can reduce hot utility requirement, generate steam into the site cogeneration system, and preheat BFW after the feed pump. Assumptions about energy prices, emission factors and equipment cost are presented in Table 1. The cogeneration system performance before heat recovery is presented in Table 2.

The total fuel cost consists of fuel consumed in the site cogeneration system and fuel consumed by fired heaters for high temperature process heating. Fuel consumed by the site cogeneration system is 76% of the total fuel cost. The site cogeneration system produces the heat required to satisfy the existing demand for hot utility. 35,355 kW of power is produced from the same fuel source, and in order to satisfy the total power demand for the site (50,000 kW); 14,646 kW of power is imported. Results of applying the developed methodology are presented in Section 4.1 and sensitivity analysis performed in Section 4.2 to explore how changes in capital cost, fuel price and electrical power tariff can influence the choice of technology and the quantity of heat upgraded.

4.1. *Case study results and discussion*

4.1.1. *Base case optimized with heat pump integration*

The optimization framework proposed in Section 3 above was applied to integrate heat upgrading technologies into this refinery site, taking into account interactions with the site

Table 2 – Cogeneration system performance before heat recovery.

		Base case
Economics	Total fuel cost (£/y)	38,765,733
	Total cooling water cost (£/y)	2,460,603
	Power export value (£/y)	0
	Power import cost (£/y)	17,199,855
	Total cost (£/y)	58,426,191
Emissions	Cogeneration system fuel CO_2 emissions (t/y)	427,810
	CO_2 emissions offset from power export (t/y)	0
	CO_2 associated with power import (t/y)	61,083
	Process fired heater CO_2 emissions (t/y)	212,170
	Total CO_2 emissions (t/y)	701,063

Please cite this article in press as: Oluleye, G., et al., Process integration of waste heat upgrading technologies. Process Safety and Environmental Protection (2016), http://dx.doi.org/10.1016/j.psep.2016.02.003

Table 3 – Results for optimized design after heat recovery.

		Base case	Optimized with heat pump integration
Economics	Total fuel cost (£/y)	38,765,733	41,424,064
	Total cooling water cost (£/y)	2,460,603	2,597,782
	Power export value (£/y)	0	0
	Power import cost (£/y)	17,199,855	0
	Total cost (£/y)	58,426,191	44,930,932
Emissions	Cogeneration system fuel CO_2 emissions (t/y)	427,810	488,985
	CO_2 emissions offset from power export (t/y)	0	0
	CO_2 associated with power import (t/y)	61,083	0
	Process fired heater CO_2 emissions (t/y)	212,170	212,170
	Total CO2 emissions (t/y)	701,063	701,155

cogeneration system. The site cogeneration system was optimized simultaneously in order to properly assess the value of hot utility (i.e. steam) saved, steam generated and boiler feed water preheated. The model involves the use of 544 continuous variables and 500 binary variables; solved in 18 s. In total, there are 34 heat source streams from the site processing units, 3 heat source streams from the site cogeneration system and 5 sinks for upgraded heat. The heat sinks are: (1) boiler feed water preheating (BFW), (2) LP steam savings denoted as HUR (LP), (3) MP steam savings denoted as HUR (MP), (4) LP steam generation denoted as STG (LP), and (5) MP steam generation denoted as STG (MP).

Results obtained after heat recovery are provided in Table 3. A mechanical heat pump was selected to upgrade waste heat. About 4349 kW of MP steam is generated from heat released during condensation of the working fluid. Power required to operate the MHP is produced from the site cogeneration system. This has potential to reduce the total cost by £13,495,260/y. The total capital cost and maintenance cost of the MHP is £909,086/y. The total cost in Table 3 for the optimized design with heat pump integration includes investments in the heat upgrading technology.

Fig. 8 shows the configuration of the site cogeneration system after heat recovery. The site cogeneration system produces all the power required by the site and the MHP (50,806 kW), thereby saving £17,199,855/y associated with power imports in the base case. Even though the cogeneration system fuel cost and cooling water cost increases by £2,795,510/y, the savings from power import is enough to

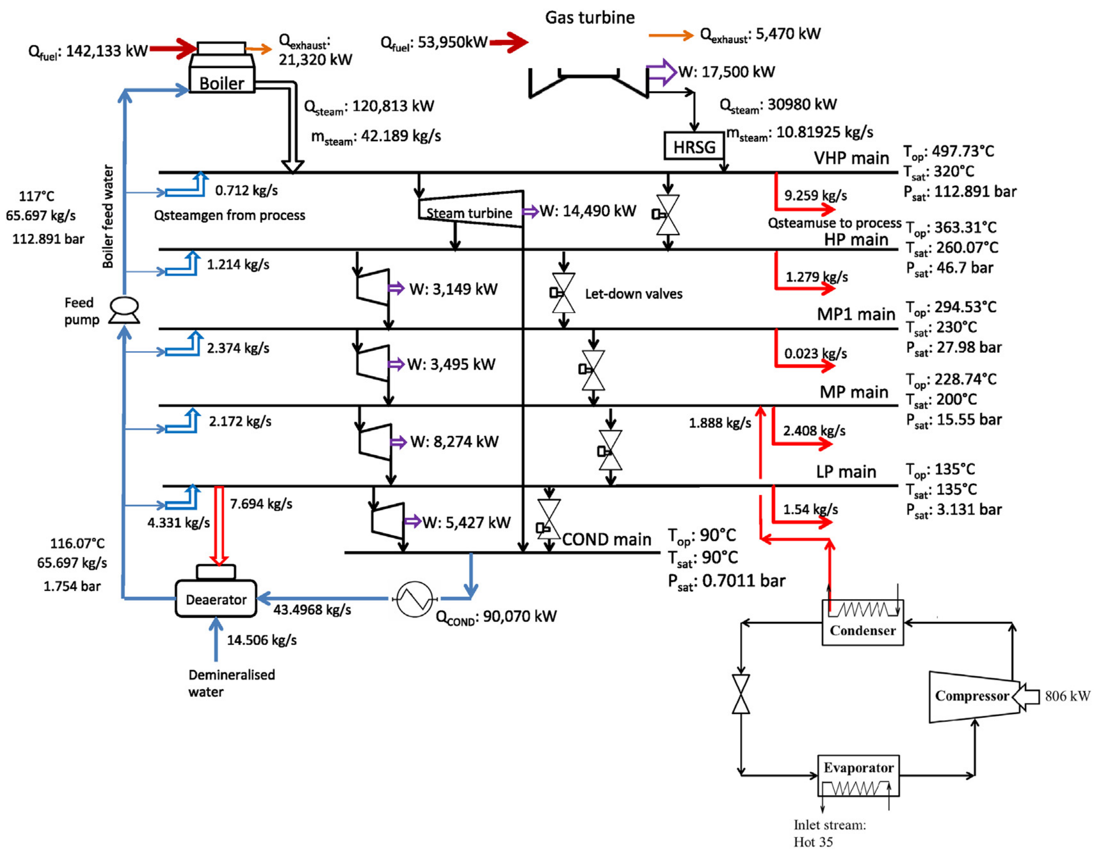


Fig. 8 – Optimized site cogeneration system with heat pump integration.

Table 4 – Results obtained from operational optimization of the site cogeneration system.

		Base case	Optimized without integrating heat pump
Economics	Total fuel cost (£/y)	38,765,733	51,530,490
	Total cooling water cost (£/y)	2,460,603	3,201,400
	Power export value (£/y)	0	28,825,450
	Power import cost (£/y)	17,199,855	0
	Total cost (£/y)	58,426,191	25,906,440
Emissions	Cogeneration system fuel CO_2 emissions (t/y)	427,810	721,560
	CO_2 emissions offset from power export (t/y)	0	104,270
	CO_2 associated with power import (t/y)	61,083	0
	Process fired heater CO_2 emissions (t/y)	212,170	212,170
	Total CO_2 emissions (t/y)	701,063	829,450

offset this increase in costs, making the design economically attractive.

4.1.2. *Based case optimized without heat pump integration*

The optimization framework proposed in this work can also be applied to improve the existing operation of the cogeneration system without need for capital investment. In this case, the objective function is the minimization of the cogeneration system operating cost in Eq. (15), subject to constraints in Eqs. (39) and (43)–(45). The continuous variables are: the fuel consumed by technologies in the site cogeneration system, mass flow of steam into steam turbines at different pressure levels, electrical power imported from the grid to satisfy site demand and electrical power exported to the grid. All binary variables and continuous variables associated with the heat pumps are set to zero. Table 4 shows the results obtained from changing the current operating conditions of the system without integrating heat pumps.

The operational improvements made to the site cogeneration system are summarized below:

- Increase in power produced from cogeneration. The total power produced is enough to eliminate the need for power import and the system exports 25,000 kW of power to the grid. Revenue generated from power export offsets the total operating costs by 53% (Table 4).
- Increase in fuel consumed and cooling water required as a result of the additional power produced for export. Since more fuel is consumed, the heat given off from steam condensation increases as shown in Fig. 9, thereby increasing the cooling water cost (Table 4). Even though the total cost

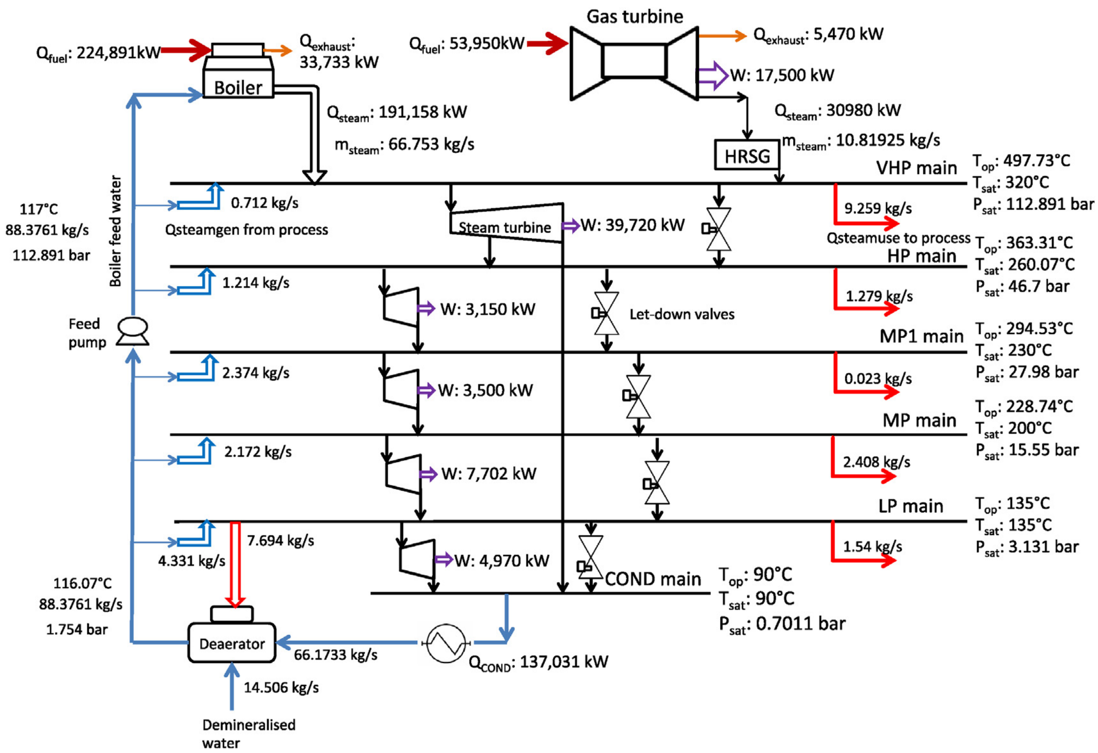


Fig. 9 – Optimized site cogeneration system without heat pump integration.

for fuel and cooling water increases by £13,505,554/y, the revenue from power export is high enough to offset the increased cost.

- A menace of increased fuel consumption is the increase in CO_2 emissions from fuel combustion (Table 4). CO_2 emissions offset from power export are not enough to make this improvement environmentally attractive.

Fig. 9 shows the configuration of the site cogeneration system after optimization.

Operational improvements to the existing system increase the CO_2 emissions by 18.3% and reduce costs by 55%. Since the heat requirements for the processing units are already satisfied, benefits were gained from exporting power. On the other hand, integrating heat pumps (Section 4.1.1) can achieve a 23.1% reduction in costs with negligible increase in the total CO_2 emissions as shown in Fig. 10.

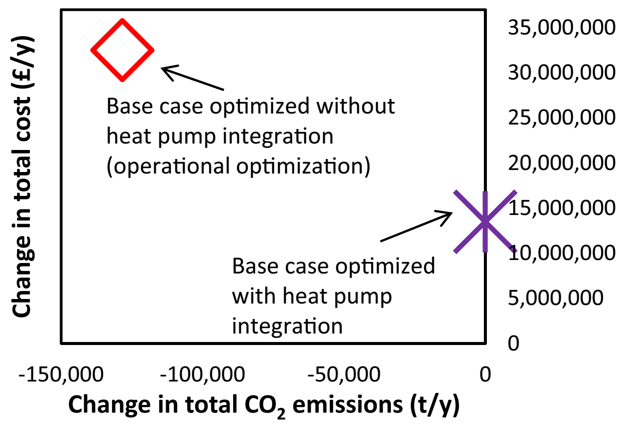


Fig. 10 – Comparison between the optimized designs.

4.2. *Sensitivity analysis*

Sensitivity analysis is performed to explore the impact of changes in capital cost assumptions, fuel price and electrical power tariff on the choice of heat upgrading technologies and sinks for upgraded heat. Varying the retrofit factor (RF) in Eq. (13) takes into account changes in total capital costs. Two major inputs affecting the economics of site cogeneration systems are the value of electrical power and the fuel prices (Smith, 2005). The difference between them is called the spark gap. Due to the long lifetimes of cogeneration systems, trends in the spark gap could influence the uptake of heat pumps and the economic viability of only operational optimization (Section 4.1.2). Data for the sensitivity analysis

Table 5 – Data for sensitivity analysis.

	Independent variables	Value	Spark gap (p/kWh)
Case 1	Retrofit factor	1.5	11.98
Case 2	Retrofit factor	3	11.98
Case 3	Retrofit factor	5	11.98
Case 4	Coal price Electrical power price	0.71 p/kWh 9.3 p/kWh	8.59
Case 5	Coal price Electrical power price	2.84 p/kWh 9.30 p/kWh	6.46
Case 6	Coal price Electrical power price	5.68 p/kWh 7.00 p/kWh	1.32

Table 6 – Results of re-simulated base case.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
Total fuel cost (£/y)	38,765,733	38,765,733	38,765,733	26,806,360	62,684,485	110,521,985
Total cooling water cost (£/y)	2,460,603	2,460,603	2,460,603	2,203,523	2,203,523	2,059,559
Power export value (£/y)	0	0	0	0	0	0
Power import cost (£/y)	17,199,855	17,199,855	17,199,855	17,199,855	11,712,902	8,816,163
Total cost (£/y)	58,426,191	58,426,191	58,426,191	46,209,738	76,600,910	121,397,707

Table 7 – Optimized results of base case with heat pump integration.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
Total fuel cost (£/y)	40,487,349	41,424,064	41,424,066	28,135,526	66,611,225	81,975,005
Total cooling water cost (£/y)	2,570,570	2,597,782	2,659,964	2,060,344	2,009,685	1,464,956
Power export value (£/y)	0	0	0	0	0	0
Power import cost (£/y)	0	0	0	0	0	14,206,775
Total capital (£/y)	1,344,755	890,904	1,409,960	842,227	2,219,016	3,049,548
Maintenance cost (£/y)	27,444	18,182	28,775	17,188	45,286	62,236
Total cost (£/y)	44,430,118	44,930,932	45,522,765	31,055,285	70,885,212	100,758,520
Cogeneration system fuel CO_2 emissions (t/y)	467,428	488,985	488,985	488,985	472,992	263,576
CO_2 emissions offset from power export (t/y)	0	0	0	0	0	0
CO_2 associated with power import (t/y)	0	0	0	0	0	98,433
Process fired heater CO_2 emissions (t/y)	212,170	212,170	212,170	212,170	212,170	212,170
Total CO_2 emissions (t/y)	679,598	701,155	701,155	701,155	685,162	574,178

Table 8 – Optimized results of base case without heat pump integration.

	Case 4	Case 5	Case 6
Total fuel cost (£/y)	33,188,740	86,881,619	158,916,253
Total cooling water cost (£/y)	3,139,217	2,392,780	1,974,781
Power export value (£/y)	28,825,450	19,994,956	15,049,967
Power import cost (£/y)	0	0	0
Total cost (£/yr)	7,502,510	69,279,443	145,841,067
Cogeneration system fuel CO_2 emissions (t/y)	721,560	706,228	706,228
CO_2 emissions offset from power export (t/y)	104,270	104,275	104,275
CO_2 associated with power import (t/y)	0	0	0
Process fired heater CO_2 emissions (t/y)	212,170	212,170	212,170
Total CO_2 emissions (t/y)	829,450	814,123	814,123

and cases developed to reflect changes in the spark gap are provided in Table 5.

The price of fuel (coal) and electrical power price for Cases 1–3, and the retrofit factors in Cases 4–6 are the same as the base case presented in Table 1. The re-simulated base case of the cogeneration system using the fuel prices and power tariffs in Table 5 for Cases 1–6 is presented in Table 6.

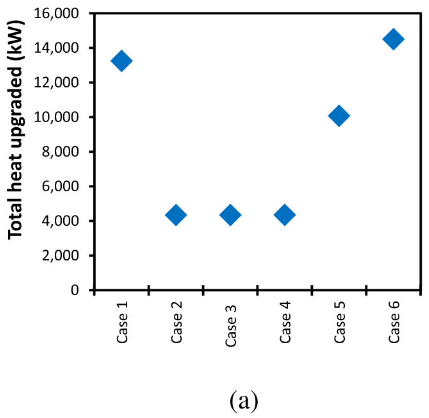
The total operating costs (calculated using Eq. (15)) increases as the difference between the electrical power price and fuel price reduces (Table 6). Therefore, a large spark gap improves the economic viability of cogeneration schemes. Integrating heat upgrading technologies could improve the economic viability when the spark gap is low.

The optimization framework developed in Section 3 was applied to the re-simulated cases in Table 6. Optimized results are presented in Table 7. There is potential to reduce the total costs and CO_2 emissions when heat pumps are integrated. Integrating heat pumps provides both structural and operational degrees of freedom to reduce the total operating costs when the spark gap reduces. In cases 1, 5 and 6; AHTs were selected for boiler feed water preheating, and MHPs selected to reduce hot utility required at the MP steam level and generate MP steam into the site cogeneration system. In cases 2–4, MHPs were selected to generate MP steam into the site cogeneration system. The quantity of heat upgraded for all cases is presented in Fig. 11(a) and contribution of technologies to the total heat upgraded presented in Fig. 11(b).

A breakdown of the heat upgraded for all sinks is shown for case 1 in Fig. 12(a); cases 2–4 in Fig. 12(b); case 5 in Fig. 12(c); case 6 in Fig. 12(d). The x-axis labels represent the sinks for upgraded heat. BFW means boiler feed water preheating, HUR (LP) and HUR (MP) represents hot utility savings at the low pressure steam level and medium pressure steam level respectively, STG (LP) and STG (MP) denotes steam generation into the cogeneration system at the low pressure steam level and medium pressure level respectively. In most cases presented in Fig. 12, the sinks with the most value i.e. higher temperature sinks were selected.

The difference between the total cost and CO_2 emissions of the re-simulated base cases in Table 6 and optimized design with heat pump integration in Table 7 are presented in Fig. 13. Reducing the capital cost of heat pumps, increasing fuel price and reducing the value of power export increases the economic viability of heat upgrade schemes. Furthermore, increased uptake of heat pumps reduces CO_2 emissions produced since less fuel is required due to the useful heat upgraded from waste heat.

In Section 4.1.2, the methodological framework was applied to improve the current operating conditions of the cogeneration system without integrating heat pumps. This has potential to reduce the total costs by 55%. However, the CO_2 emissions produced was 18.3% higher than the base case (Table 2). Even though the economic benefits seem attractive at the current conditions, it is necessary to investigate how the benefits change over time. For this sensitivity analysis, operational optimization of the utility system was performed using the assumptions of fuel price and power price in Table 5 for cases 4–6. Results are presented in Table 8. Revenue generated from power export reduces due to a decrease in the price of



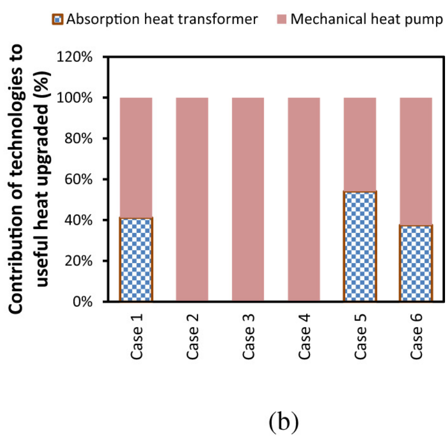


Fig. 11 – (a) Quantity of useful heat upgraded for cases 1–6 and (b) percentage contribution of technologies selected to the total useful heat upgraded.

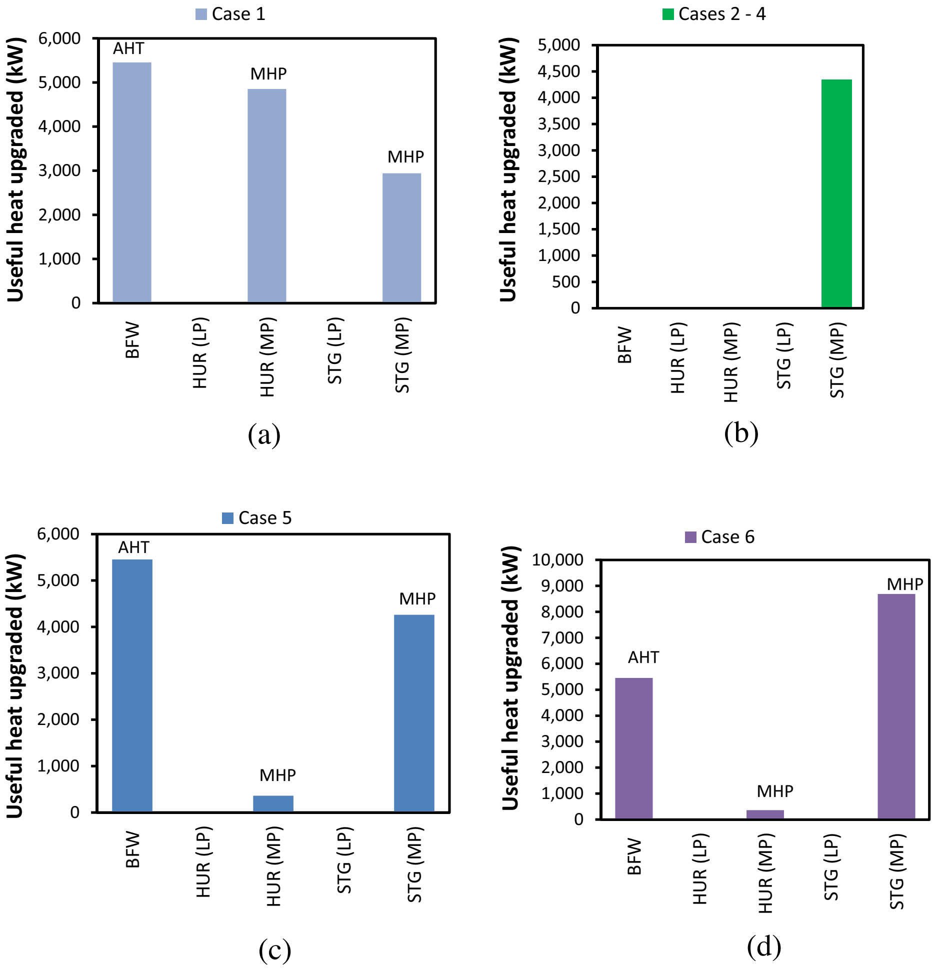


Fig. 12 – Break down of heat upgraded based on heat sinks in (a) case 1, (b) cases 2–4, (c) case 5 and (d) case 6.

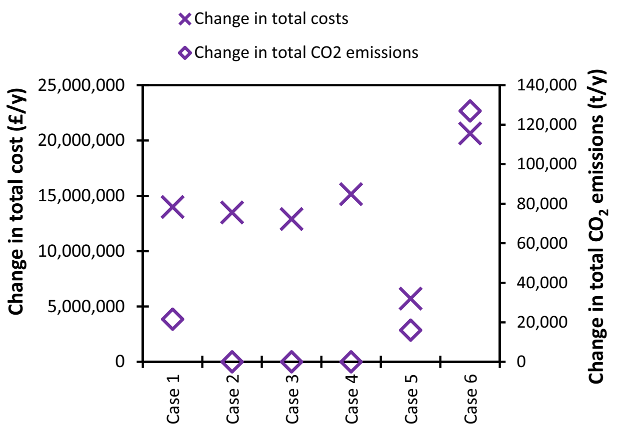


Fig. 13 – Economic benefits and reduced CO_2 emissions for all cases (with heat pump integration).

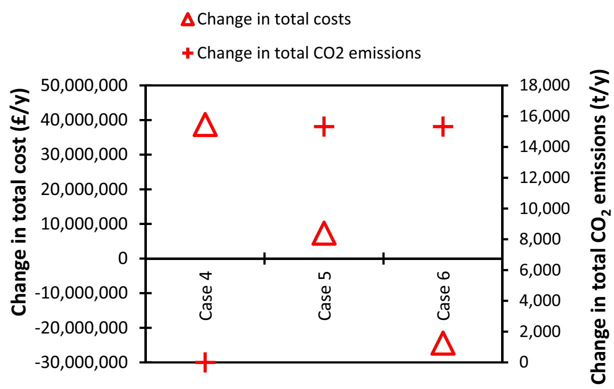


Fig. 14 – Economic benefits and reduced CO_2 emissions for all cases (without heat pump integration).

power, and the fuel cost increases as a result of higher fuel prices. The net effect is an increase in the total costs as the spark gap reduces. Fig. 14 shows the difference between the total cost and CO_2 emissions of the re-simulated base cases in Table 6 and optimized design without heat pump integration in Table 8.

In case 4 where the price of fuel is 0.71 p/kWh, operational optimization of the cogeneration system without heat pump integration reduces the total cost by 83%. However, this benefit decreases to 9% for a higher fuel price (and lower power price) in case 5 and becomes a loss when the fuel price increases to 5.68 p/kWh in case 6. The optimized case without heat pump integration becomes less economically attractive as the spark gap reduces.

In summary

- Process integration of heat upgrading technologies provides additional degrees of freedom to reduce costs and CO_2 emissions at high fuel prices and low power prices.
- Performing only operational optimization of the site utility system becomes less attractive as fuel price increases and power price reduces.
- The average decrease in total costs for the optimized design with heat pump integration is 21% compared to 0.4% for optimized design without heat pump integration.

- CO_2 emission reductions from 3–18% were obtained from integrating heat pumps into this process sites.

5. Conclusions and future work

Mature and commercialized technologies exist for waste heat upgrade. The challenge is optimal integration of these technologies in existing process sites. In this work, a mixed integer linear optimization framework was presented to address this challenge. The framework allows: (1) selection of technology options (MHP, AHP, and AHT), (2) determination of the working temperatures for the technologies, taking into account the feasible operating range of the technology working fluids, (3) selection of heat source streams for the technology options, (4) selection of sinks for heat upgraded, and (5) simultaneous optimization with the site cogeneration system to exploit sinks for upgraded heat within the system and determine their correct value. The generic mixed integer linear program can also be used to perform operational optimization of cogeneration systems.

The method was applied to the case study of a medium scale petroleum refinery. Integrating heat upgrading technologies had potential to reduce total costs by 23.1% with negligible change in the total CO_2 emissions. Performing changes to the cogeneration system without heat pump integration i.e. operational optimization had potential to reduce total costs by 55% with 18.3% increase in the total CO_2 emissions. Since the thermal demand for the site was already satisfied, majority of the benefits from operational optimization were from power export. Conversely, majority of the benefits from integrating heat upgrading technologies were from reducing fuel consumed by the site.

Sensitivity analysis was also performed to illustrate the impact of changing capital costs, fuel price and electrical power price on both schemes. Reduction in capital costs of heat pumps and increase in the fuel price increases the contribution of heat from heat upgrading technologies, the economic viability and the potential to reduce CO_2 emissions. Even at low electrical power price, integrating heat pumps is still economic. However, for operational optimization the design becomes uneconomic as fuel price increases and electrical power prices reduce. Therefore, integrating heat upgrading technologies in process sites provides additional structural and operational degrees of freedom to reduce wasted thermal energy. Future work will consider integrating other technologies like heat to power and heat to cooling systems.

Acknowledgements

The authors gratefully acknowledge the members of Process Integration Research Consortium (PIRC) for their financial support for the development of this research.

Appendix.

A.5. Steam turbine model (Aguilar et al., 2007)

Power produced calculated by a linear Willan's line approximation:

$$W_{turbine} = (n \times m) - W_{int} \tag{A.1}$$

The slope n and intercept W_{int} are calculated from:

$$n = \frac{(L+1)}{B} \times \left(\Delta h_{is} - \frac{A}{m_{max}}\right) \tag{A.2}$$

$$W_{int} = \frac{L}{B} \times ((\Delta h_{is} \times m_{max}) - A) \tag{A.3}$$

Table A1 – Values of α and β for a mechanical heat pump (Oluleye et al., 2016).

Working fluid	T_{COND} (°C)	T_{EVAP} range (°C)	α	β
Ammonia	50	10–40	0.7267	−0.4774
	60	10–50	0.7132	−0.4003
	70	15–60	0.7006	−0.3861
	80	25–70	0.6932	−0.4851
	90	25–80	0.6628	−0.3684
	100	25–90	0.6294	−0.282
	110	25–100	0.5732	−0.1195
	120	25–100	0.4971	0.0586
n-Butane	50	10–40	0.7319	−0.5154
	60	10–50	0.7259	−0.5602
	70	10–60	0.7181	−0.6077
	80	15–70	0.7081	−0.6582
	90	20–80	0.6952	−0.7107
	100	25–90	0.6781	−0.7639
	110	30–100	0.6551	−0.8149
	120	35–110	0.6217	−0.8504
	130	35–110	0.5586	−0.7767
Water	125	100–110	0.7484	−0.5518
	135	100–120	0.7482	−0.5363
	145	100–130	0.7476	−0.5177
	155	100–140	0.7468	−0.5014
	165	100–150	0.7448	−0.4729
	175	100–160	0.7448	−0.4746
	185	100–170	0.7435	−0.4639
	195	100–180	0.7418	−0.4547
	205	100–190	0.7399	−0.4474
	215	100–200	0.7376	−0.4410

Please cite this article in press as: Oluleye, G., et al., Process integration of waste heat upgrading technologies. Process Safety and Environmental Protection (2016), http://dx.doi.org/10.1016/j.psep.2016.02.003

Table A2 – Values of α and β for a water/lithium bromide absorption heat pump (Oluleye et al., 2016).

T_{GEN} (°C)	T_{EVAP} (°C)	$T_{COND} = T_{ABS}$ (°C)	α	β
90	$20 < T_{EVAP} < 30$	50	−2.5064	3.4299
100	$20 < T_{EVAP} < 30$	50	−0.7448	2.2099
	$30 < T_{EVAP} < 40$	60	−2.9497	3.7592
110	$20 < T_{EVAP} < 30$	50	−0.5081	2.0366
	$30 < T_{EVAP} < 40$	60	−0.7478	2.2099
	$40 < T_{EVAP} < 50$	70	−2.4461	3.3795
140	$40 < T_{EVAP} < 50$	80	−1.7978	2.8816

Table A3 – Values of α and β for a water/lithium bromide absorption heat transformer for $T_{COND} = 30$ °C (Oluleye et al., 2016).

T_{EVAP} (°C)	T_{ABS} (°C)	T_{GEN} (°C)	α	β
40	$60 < T_{ABS} < 90$	$50 < T_{GEN} < 80$	0.6356	−0.0549
50	$70 < T_{ABS} < 100$	$50 < T_{GEN} < 80$	0.6303	−0.0461
60	$80 < T_{ABS} < 110$	$50 < T_{GEN} < 80$	0.6270	−0.0392
70	$90 < T_{ABS} < 120$	$50 < T_{GEN} < 80$	0.6190	−0.0305
80	$100 < T_{ABS} < 130$	$50 < T_{GEN} < 80$	0.5797	−0.00704
90	$120 < T_{ABS} < 140$	$60 < T_{GEN} < 80$	0.6568	−0.0407

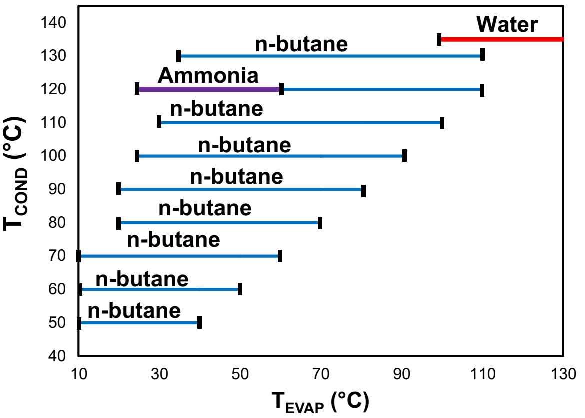


Fig. A4 – Working fluid selection for mechanical heat pump.

L is known as the intercept ratio and represents the part load performance, defined as:

$$L = \frac{W_{int}}{W_{max}} \tag{A.4}$$

Coefficients A and B represent the full-load performance of the turbine and are defined as the intercept and slope of the following regression equation:

$$W_{is,max} = A + (B \times W_{max}) \tag{A.5}$$

The term Δh_{is} in Eqs. (A.2) and (A.3) represent the isentropic enthalpy change across the turbine calculated from the pressure, temperature and the dryness fraction of the inlet and exhaust steam (Aguilar et al., 2007).

A.6. Gas turbine model (Aguilar et al., 2007)

Similar sets of equations to those for modeling steam turbines are applicable for gas turbine (gt) modeling. The power produced is calculated from the Willans' line for a gas turbine and is related to the fuel consumption *mfuel*.

$$W_{gt} = n_{gt} \cdot mfuel - W_{gt,int} \tag{A.6}$$

Slope and intercept given by:

$$n_{gt} = \frac{(L_{gt}+1)}{B_{gt}} \times \left(LHV - \frac{A_{gt}}{mfuel_{max}}\right) \tag{A.7}$$

$$W_{gt,int} = \frac{L_{gt}}{B_{gt}} \times ((LHV \times mfuel_{max}) - A_{gt}) \tag{A.8}$$

The values of the parameters L_{gt}, A_{gt} and B_{gt} are obtained by regression from manufacturer's data.

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6. 5. Introduction to Publication 7

Additional economic benefits, reductions in CO_2 emissions, increase in energy efficiency and reduction in waste heat quantity and temperature may be obtained when the site waste heat utilization systems and the site utility system are optimized simultaneously. The work in Publication 5 neglected the interconnected utility system and in Publication 6, simultaneous optimization with the site utility system was necessary to predict the true value of steam generated and hot utility saved. The benefits of a combined systems approach are explored in Publication 7.

A generic MILP model is developed for integrating all five thermodynamic cycles considered in this work and heat recovery via heat exchange. The model can be modified to explore different options to reduce and utilize waste heat. The options explored are: operational optimization of the site utility system, stand-alone design of the waste heat utilization system and combined systems design (i.e. design of the waste heat utilization system with simultaneously optimization with the site utility system). The method is applied to the case study of a chemical production site. In this case study, heat recovery within and between processing units is not maximized.

6. 6. Publication 7

Oluleye G., Smith R., Conceptual design of site waste heat utilization systems, Energy (under review)

Conceptual Design of Site Waste Heat Utilization Systems

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HIGHLIGHTS

- MILP model developed for integration of waste heat recovery technologies in process sites
- Five thermodynamic cycles considered for exploitation of industrial waste heat
- Temperature and quantity of waste heat sources considered
- Interactions with the site utility system considered
- Industrial case study presented to illustrate application of the proposed methodology

Nomenclature

ACC	Annualised capital cost (£/y)
AF	Annualisation factor
CP	Heat capacity flowrate (kW/K)
cp	Specific heat capacity flowrate (kW/kgK)
C_{fuel}	Utility system overall fuel cost (£/y)
C_{CW}	Cooling water cost (£/y)
C_{PI}	Overall cost of electrical power import (£/y)
C_{PE}	Overall revenue from electrical power export (£/y)
CC	Capital cost (£/y)
EC	Equipment cost (£/kW)
FP	Unit fuel price (£/kWh)
FEF	CO_2 produced per kW of fuel consumed (kg/kWh)
GFC	Global fuel consumption (kW)

GCO_2E	Global CO_2 emissions (t/y)
GEF	CO_2 produced per kW of electrical power generated in the grid (kg/kWh)
HP	High pressure steam (bar)
I	Set of all heat source streams
J	Set of all units producing waste heat
K	Set of all temperature intervals on a heat source stream
LHV_{fuel}	Lower heating value of fuel (kJ/kg)
L	Lower limit for technology size (kW)
ll	Set of all temperature levels for steam distribution
LP	Low pressure steam (bar)
mfuel	Mass flowrate of fuel consumed (kg/s)
mturbine	Mass flowrate of steam entering turbine (kg/s)
MC	Maintenance cost (£/y)
MP	Medium pressure steam (bar)
n	Technology life time (y)
O	Set of all end-uses for recovered energy
P	Pressure (bar)
PImp	Specific cost of imported electrical power (£/kWh)
PExp	Specific cost of exported electrical power (£/kWh)
Q	Heat rate (kW)
Qsteam	Steam generated directly from fuel combustion (kW)
QCUM	Cumulative heat duty (kW)
Qsteamgen	Already existing steam generation in the site utility system (kW)
Qsteamuse	Already existing steam consumption in the site utility system (kW)
QCOND	Latent heat of condensation (kW)
Qout	Useful heat upgraded (kW)
RF	Retrofit factor
RQ	Waste heat utilised by waste heat recovery technologies (kW)
tt	Set of all technologies combusting fuel in the site utility system
T	Temperature (°C)

U	Upper limit for technology size (kW)
W	Electrical power (kW)
X	Binary variable for existence of waste heat source streams
Y	Binary variable for the existence of technology options

Abbreviations

AbC	Absorption chiller
ABS	Absorber
AHP	Absorption heat pump
AHT	Absorption heat transformer
BFW	Boiler feed water
COND	Condenser
COP	Coefficient of performance
CW	Cooling water
DHR	Direct heat recovery
EVAP	Evaporator
FG	Fuel gas
FO	Fuel oil
GEN	Generator
HT	High temperature
HUR	Hot utility reduction
IR	Interest rate
LT	Low temperature
MILP	Mixed integer linear program
MHP	Mechanical heat pump
MT	Medium temperature
OP	Operating
ORC	Organic Rankine cycle
Perf	performance
SAT	saturation
STG	Steam generation

U	Site utility system
WHS	Waste heat source
WHUS	Waste heat utilization system

Subscripts

i	Index corresponding to the waste heat source streams
j	Index corresponding to the process units and the utility system
k	Index representing temperature intervals on a heat source stream
l	Index representing temperature levels for steam distribution
o	Index representing the end-uses of recovered energy
t	Index representing technologies combusting fuel in the site utility system

Greek letters

α, β	Regression coefficients for waste heat recovery technologies
ΔT_{MIN}	Minimum permissible temperature difference (°C)
η_t	Energy conversion efficiency of technology t (%)
μ	efficiency factor for waste heat recovery technologies
η_{power}	Grid power generation efficiency

ABSTRACT

The combination of one or more concepts to recover useful energy from industrial waste heat is defined as a waste heat utilization system. In this work a systematic methodology is presented for the design of site waste heat utilization systems. Technology options considered are organic Rankine cycles, absorption chillers, absorption heat pumps, absorption heat transformers, and mechanical heat pumps. The potential for heat recovery via heat exchange is also explored. The developed methodology allows for systematic selection and combination of heat source streams, selection of technology options and working fluids, and explores interactions with the existing site utility system. The methodology is applied to an industrial case study. Results indicate combining concepts to utilize waste heat whilst exploring interactions with the existing site utility system has potential to reduce the site operating costs by 37%, reduce global fuel consumption by 54% and 53% reduction in CO_2 emissions with a 2 year payback. The analysis also show that benefits from waste heat utilization increase when interactions with the existing site utility system are explored.

Keywords:
Waste heat utilization system; site utility system; Mixed Integer Linear Program; heat source stream selection and combination.

1. Introduction

1.1 Background

Successful integration of technologies to recover useful energy from waste heat in process sites could exploit significant amounts of currently wasted energy and thus, improve energy efficiency, reduce greenhouse gas emissions (especially CO_2), and reduce costs in the process industry. Efficiency improvement, reduction in CO_2 emissions and costs are basic factors of competitiveness, and energy security. However, due to lack of a suitable methodology for optimum integration of these technologies in existing process sites, allowing for simultaneous optimization with the site utility system, selection of heat sources, and combination of technology options to exploit the heat available, uptake of technologies by industry has been slow.

Examples of technologies recovering useful energy from waste heat include organic Rankine cycles (ORC), absorption chillers (AbC), absorption heat pumps (AHP), absorption heat transformers (AHT) and mechanical heat pumps (MHP). Organic Rankine cycles use a circulating low boiling point organic fluid, vaporized by waste heat in the evaporator, which expands to produce power (Fig. 1). In absorption chillers, waste heat provides energy to separate the working fluid pair, which is condensed, expanded in a valve, and vaporised in the evaporator thereby producing chilling (Fig. 2). Absorption heat pumps use the inverse AbC cycle to upgrade waste heat to a higher temperature (Fig. 3). Absorption heat transformers are reversed AHP, the evaporator and absorber operates at a pressure higher than the condenser and generator (Fig. 4). Mechanical heat pumps upgrade low temperature waste heat using mechanical energy (Fig. 5).

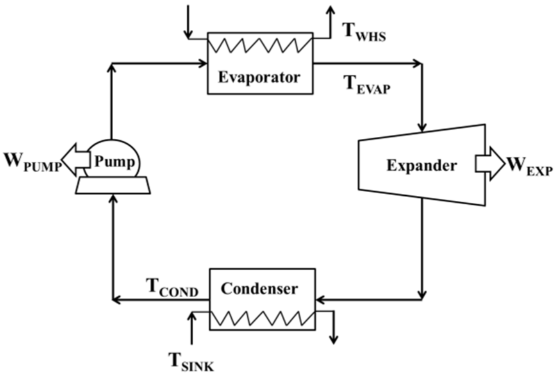


Fig. 1 Organic Rankine cycle schematic

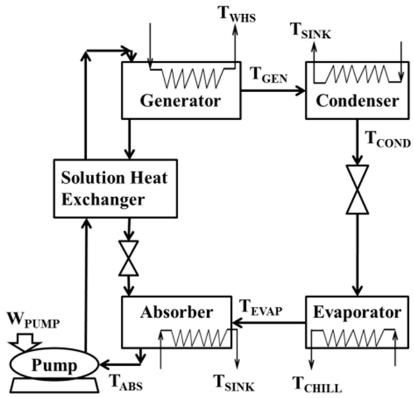


Fig. 2 Absorption chiller schematic

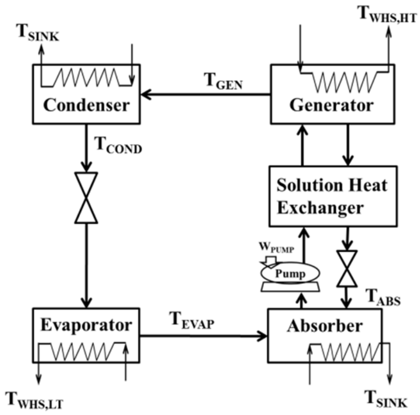


Fig. 3 Absorption heat pump schematic

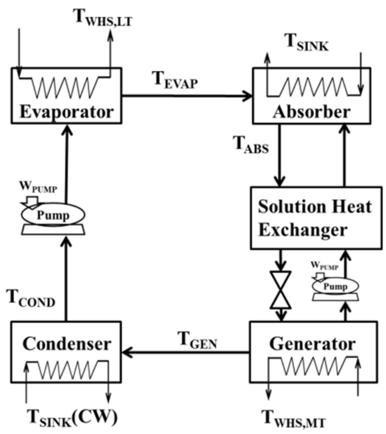


Fig. 4 Absorption heat transformer schematic

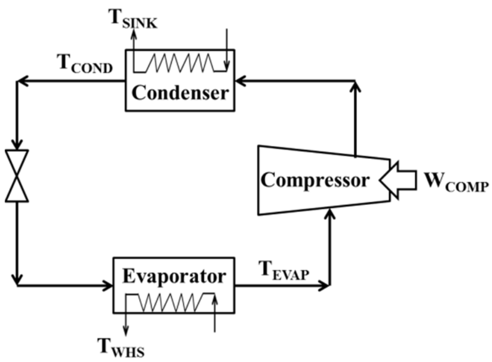


Fig. 5 Mechanical heat pump schematic

Integration of thermodynamic cycles for recovery of useful energy in form of power (ORC), heat (AHP, AHT and MHP) and chilling (AbC) from waste heat stills remains a challenge in existing process sites. In existing process sites, there are numerous streams rejecting thermal energy to cooling water and air from processing units and the site utility system. There are also numerous end-uses of recovered energy from waste heat [1]. Previous studies on waste heat recovery focused on waste heat from a single processing unit [2] and only waste heat from the utility system [3]. Even though waste heat from all processing units and the site utility system was analysed for recovery by Oluleye et al. [4], the approach was based on a graphical technique, focused on increasing the site energy efficiency; neglecting the economics (costs and benefits) and potential to reduce CO_2 emissions. Graphical techniques allow for physical understanding of the problem; however, they do not provide a framework to solve the problem systematically. Furthermore, the diverse end-uses of recovered energy and interactions with the site utility system were neglected.

Waste heat has been referred to as heat for which recovery is not viable economically [5]. It may be possible to improve the economic viability by developing a systems-oriented framework for integrating waste heat recovery technologies in process sites. A systems-oriented framework allows for systematic design of the site waste heat utilization system and simultaneous optimization with the existing site utility system.

The combination of technology options to exploit waste heat i.e. recovering multiple forms of energy could result in higher reductions in CO_2 emissions, higher increase in energy efficiency, and reduction in costs (especially when interactions with the site utility system is considered) compared to single technology options. This is possible since a technology will be applied only when it is economic to do so taking into account the quantity, temperature of heat sources and end-uses of recovered energy.

The aim of this work is to develop a generic methodology for the synthesis of site waste heat utilization systems allowing for systematic selection of one or more waste heat source streams, screening of working fluids for technology options, selection of technology options, end-uses of recovered, and simultaneous optimization with the existing site utility system. This work applies the methodology to an industrially relevant case study, to illustrate the benefits of a systems-oriented approach.

1.2 Literature review

Previous researches on waste heat utilization focus on modelling the technologies and working fluid selection. Pierobon et al. [6] proposed equation based models to determine the power produced by the ORC. However, the modelling approach is applicable to a single heat source. Quoilin et al. [7] applied detailed thermodynamic equations for every component in the cycle to determine the power produced from the ORC. However, the model was applied to compare the performance of several working fluids and the possibility of selecting heat sources was not considered. Popli et al. [3] applied the Engineering Equation Solver to predict the working states and performance of absorption chillers (AbC). Models based on external and internal steady-state enthalpy balances for each component in the AbC was developed by Kohlenbach and Ziegler [8]. Somers et al. [9] applied a simulation software to evaluate the working states and system overall efficiency of the AbC. However, the modelling approaches for the AbC cannot be applied to systematically select or combine heat sources without the need for complex iterations. Rivera [10] provided detailed thermodynamic analysis for every component in the absorption heat transformer. Mechanical heat pumps have been modelled using existing catalogue data to determine the technology basic parameters [11], and single component detailed simulation and analysis [12]. Even though these models predict the performance and useful energy recovered with a high degree of accuracy, adapting them to systematically analyse multiple heat sources and end-uses of recovered energy leads to complex iterations.

Working fluid selection for technology options has been explored in literature. Khatita et al. [13] screened working fluids for the ORC using the net power produced and volumetric flow rate as criteria. Working fluid selection for the ORC depends on the temperature of the waste heat sources; therefore there is no single winner [14]. Water/ lithium bromide is the only working fluid pair for absorption systems in industrial use [15], due to waters high enthalpy of evaporation and higher coefficient of performance compared to ammonia/ water systems. Possible working fluids for the MHP include propane, isobutene and ammonia [16]. Again the choice of working fluids for the MHP depends on the heat source temperature. The methodology proposed in this work will involve pre-screening of working fluids for the organic Rankine cycle and the mechanical heat pump based on the temperature of the waste heat sources.

Process integration of waste heat recovery technologies has been addressed by various authors. Desai and Bandyopadhyay [2] developed a graphical technique for ORC integration with a back ground process using the heat rejection profile. However, the end-uses of recovered power were not considered and waste heat available from the site utility system is neglected. Furthermore, it may be more beneficial to exploit the waste heat using other technology options. Modla and Lang [17] integrated a mechanical heat pump into a single distillation column to upgrade heat from the condenser to satisfy the reboiler hot utility demand. However, their study focused on a single heat source/end-use application. Wallin et al. [18] developed an optimisation methodology for integration of mechanical heat pumps into a processing unit, allowing for systematic selection of heat pumps. The benefits from simultaneous optimization with the site utility system were neglected. A systematic strategy accounting for the complex interactions between technology options, site processing units and the site utility system i.e. a combined systems approach has not been explored in published works. Furthermore, the waste heat sources have been taken from a single process [2]; a higher percentage in heat recovery potential is possible using multiple processing units on a site [19].

Liew et al. [19] presented a framework to determine cost-effective heat recovery options via retrofit for multiple processing units on a site. The potential to exploit waste heat rejected to cooling water and air from the site utility system was not explored. Hackl and Harvey [20] presented a holistic approach to identify opportunities for increased energy efficiency in industrial clusters. However, only waste heat from the site processing units is considered neglecting interactions with the site utility system. Furthermore, the possibility of recovering and combining diverse forms of energy and end-uses of recovered energy, depending on the temperature of the heat was not considered.

A multi-criteria decision process is involved in the design of site waste heat utilization systems; hence, optimisation tools are required due to the large number of decisions, trade-offs and degrees of freedom [21]. Becker and Maréchal [22] applied a mixed integer linear optimisation framework to identify options for heat recovery in industrial process sites. Only degrees of freedom relating to the flow of fuel and heat in the utility system, and heat transfer units were considered to minimize operating costs. Exploitation of the waste heat from the utility system (such as exhaust of combustion equipment's and heat of condensation) was not considered. Furthermore, the possibility of combining technology options to exploit the available waste heat was not explored.

Lira-Barragan et al. [23] proposed a multi-objective mixed integer non-linear problem with economic, environmental and social concerns for synthesis of a system using steam Rankine cycle, organic Rankine cycle and absorption chillers. Even though working fluid selection for the ORC and optimal system design to operate the absorption chiller was considered, interactions with the site utility system were neglected.

Viklund and Karlsson, [24] performed an energy systems analysis to determine how waste heat should be used, and the impact on CO_2 emissions. A mixed integer linear programing framework was used to synthesize the system to minimize costs [24]. The framework only considers off-site end-uses of recovered energy for district heating, district cooling and power export to the grid neglecting end-uses within the process site. Furthermore, interactions between the existing utility systems producing the waste heat are not considered making the design a stand-alone one and modelling of the technologies was done in a simplified manner i.e. using a constant performance.

Caf et al. [25] developed a framework for exploitation of waste heat from a utility system. Two waste heat sources from the flue gas and intercooler are upgraded using a mechanical heat pump. The upgraded high temperature heat was used to preheat boiler feed water. However, the site utility system was not optimized simultaneously to accurately predict the value of boiler feed water preheating and explore other end-uses of recovered energy within the utility system. Oluleye et al. [26] developed a multi-period mixed integer linear program for integrating organic Rankine cycles and absorption chillers in existing process sites. Again, interactions with the site utility system were not considered making the design a stand-alone one.

A holistic approach to integrating waste heat recovery in existing process sites could achieve higher reductions in primary fuel, CO_2 emissions and costs compared to stand-alone design; where interactions between the site processing units, utility systems and waste heat recovery technologies are neglected. This approach has not been explored in published papers.

This work proposes a novel retrofit methodology for integrating waste heat recovery technologies into existing process sites through the design of site waste heat utilization systems. To address the gaps and limitations mentioned above, systematic selection of one or more waste heat sources, selection of one or more technology options, selection of the best end-uses of recovered energy and simultaneous optimization with the site utility system are addressed in the retrofit methodology. The methodology also allows for exploring all possible ways to utilize industrial waste heat and improve the economic viability of waste heat utilization. This is crucial to increasing uptake of waste heat recovery technologies by the process industry.

2. Methodology Development

Waste thermal energy in existing process sites occurs over a wide range in temperature and quantity [4]. Diverse mature and commercialised technologies such as organic Rankine cycles, absorption chillers, and absorption heat pumps exist to recover useful energy in the form of electrical power, chilling and heat from the wasted thermal energy. There are multiple end-uses of recovered energy in process sites [28]. For example if electrical power is recovered using an ORC, the electrical power can be used to displace power import, reduce power produced from the site utility system or export electrical power to the grid.

The below issues need to be addressed in a methodological framework for design of waste heat utilization systems for existing process sites:

- Data extraction for the waste heat sources i.e. hot streams rejecting heat to cooling water and air

- Systematic selection or combination of heat source streams taking into account the temperature and quantity of thermal energy in each stream
- Data extraction for cold streams currently on hot utility in order to explore the potential for hot utility savings
- Modelling of technology options to determine the useful energy recovered
- Screening of working fluids for technology options
- Systematic selection of technology options taking into account the temperature and quantity of waste heat sources
- Simultaneously consideration for interactions with the existing site utility systems.

In this work the methodological framework addresses the above issues and allows for systematic selection of end-uses of recovered energy, and associated technology options exploiting waste heat contained in process hot streams.

The methodology for the design of site waste heat utilization systems is divided into four stages (Fig. 6). The data extraction stage is presented later in section 2.1, pre-screening in section 2.2, model formulation and optimization in section 2.3 and design evaluation in section 2.4.

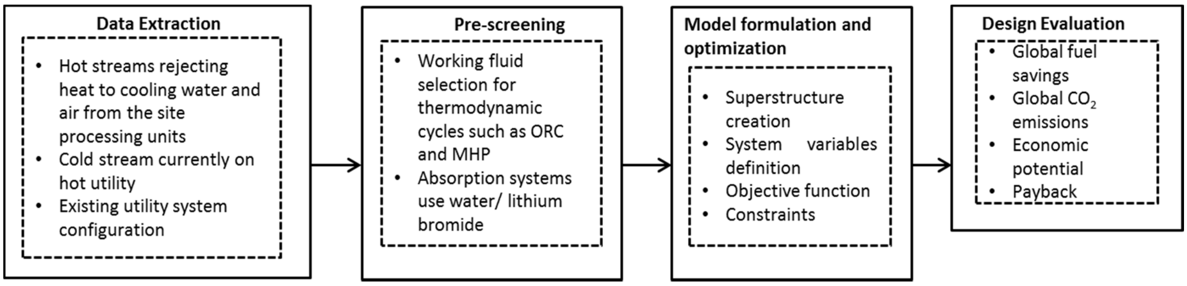


Fig. 6 Overview of conceptual design methodology for site waste heat utilization systems

2.1 Data extraction

The data extraction stage involves extracting data for the hot streams rejecting heat to cooling water and air from all processing units and the existing site utility system configuration. Data for cold streams currently on hot utility are also extracted to explore the potential for saving hot utility.

In this stage, the supply (T_{SUPPLY}) and target temperatures (T_{TARGET}), duties (Q) and heat capacity flowrates (cp) are extracted for streams rejecting heat to cooling water and air. Waste heat rejected from the site utility system includes the latent heat of condensation and the exhaust of technologies (above the acid dew point).

The hot streams need to be represented in such a way as to account for the varying quantity and temperature of heat contained. To show the temperature distribution of every hot stream, the streams are plotted on a grid diagram (as illustrated in Fig. 7). Temperature intervals *k* are then introduced on each stream *i* from processing unit *j*. the temperature intervals are selected in such a way that the combined duty of streams in any interval is greater than a minimum amount (100 kW used in this work). The minimum amount of heat is dependent on the sizes of technology options. The algorithm for extracting and representing the heat source streams is presented in Fig. 8. The algorithm allows for considering the quality and quantity of heat on each heat source stream.

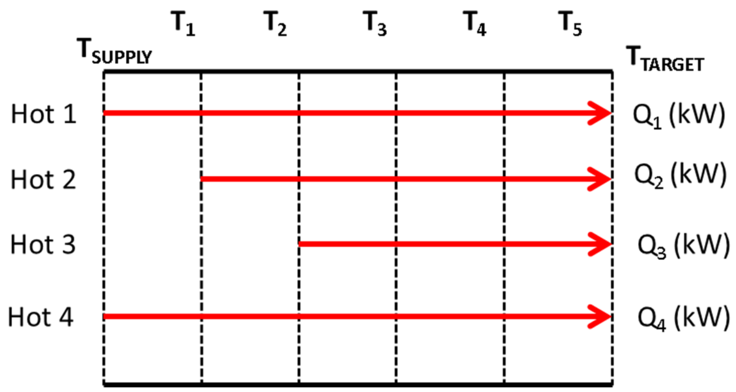


Fig. 7 Grid diagram representation for heat source streams (illustration)

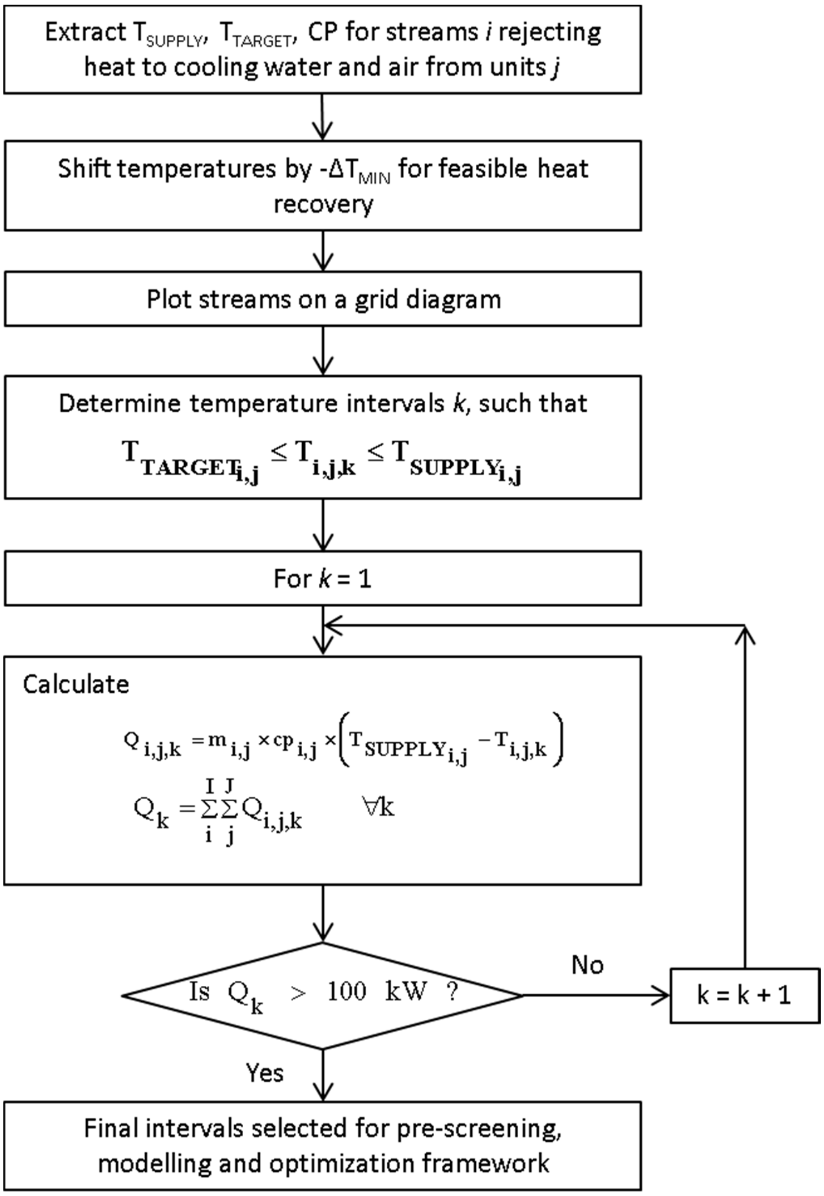


Fig. 8 Algorithm for heat source stream analysis

Data for process streams currently on hot utility are also extracted and shifted by ΔT_{MIN} for feasible heat recovery. There may be potential to reduce the hot utility required by utilizing waste heat either directly or by heat upgrade using absorption heat pumps, absorption heat transformers and mechanical heat pump. Therefore, this could serve as a sink (end-use) for recovered heat from waste heat.

To represent the waste heat sources and sinks graphically, the Total Site Profile concept [29] will be adopted. However, in this case, the profile is for an existing process site. Hot streams rejecting heat to cooling water and air represent the waste heat source profile and cold streams currently on hot utility represent the heat sink profile. The waste heat source profile (profile on the left in Fig. 9) shows graphically the temperature range and duties of all waste heat sources. The existing site sink profile (profile on the right in Fig. 9), shows the potential to reduce hot utility required by the site and establishes limits for hot utility savings. The waste heat source and sink profiles will be generated before and after waste heat utilization to show the benefits from exploiting thermal energy rejected to cooling water and air.

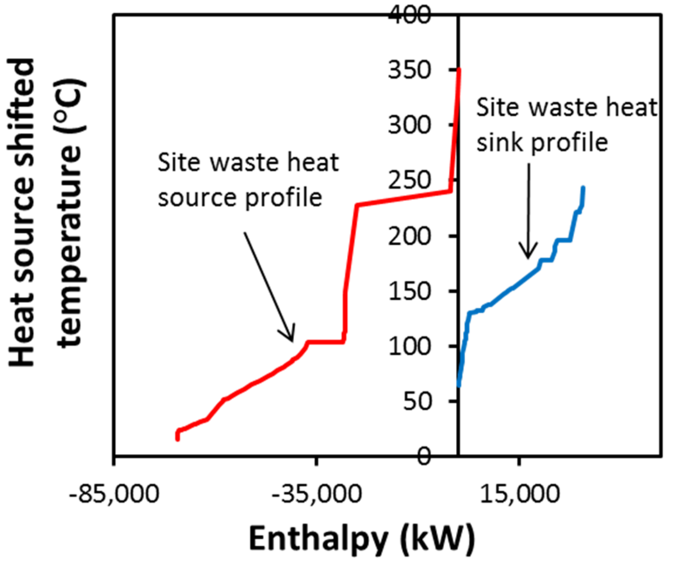
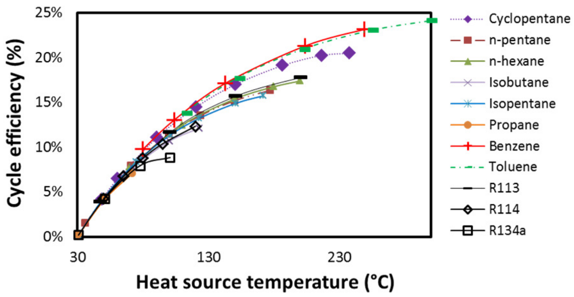


Fig. 9 Site waste heat source and sink profile

The potential for hot utility savings depends on the pressure levels for steam distribution in the existing site utility system. Therefore, the site waste heat sink profile is divided into utility levels l based on the existing steam distribution levels in the site utility system. This introduces degrees of freedom in the choice of end-uses i.e. hot utility can be saved at low, medium or high pressure steam levels.

2.2 Prescreening

While it is a common industrial practice to use water/lithium bromide absorption systems i.e. chillers, heat pumps and heat transformers [15], there is no single winner for working fluids in organic Rankine cycles (ORC) and mechanical heat pumps (MHP). Therefore, the prescreening stage involves selection of working fluids for these thermodynamic cycles. The selection of working fluids is based on the cycle's performance; net power per unit heat input for the ORC and heat upgraded per unit power input for the MHP. Fig. 10 (a) shows the pre-screening of 13 potential working fluids for an ORC, and Fig. 10 (b) shows possible selection of working fluids for mechanical heat pumps considering the system temperatures. Even though water is still applicable for higher temperature lifts (above 140°C), large compressors are required due to the high specific volumes of steam in the corresponding temperature range.



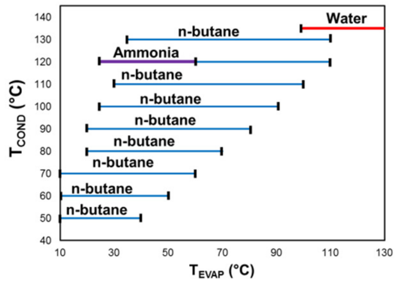


Fig. 10 Pre-screening of working fluids for: (a) organic Rankine cycles [4], (b) mechanical heat pumps

2.3 Model Formulation and Optimization

The third stage in this methodological framework is the model formulation and optimization stage. The optimization problem is formulated to allow for systematic selection and combination of waste heat source streams, technology options (including working conditions), and the use to which recovered energy (in the form of power, chilling and heat) is put. The optimization framework is also formulated to simultaneously optimize the waste heat utilization system and the site utility system.

Given waste heat source streams *i* from units j (considering both the site processing units and the existing site utility system as shown in Fig. 11) in temperature intervals *k* i.e. $Q_{i,j,k}$ (refer to section 2.1 for the methodology for heat source stream data extraction). Six technologies are considered in this work to exploit the waste heat ($Q_{i,j,k}$). Useful energy recovered from each technology can be put to use in different ways. The end use of recovered energy is referred to as what heat utilization opportunities [28]. For example, waste heat upgraded using a MHP can be used for boiler feed water (BFW) preheating, steam generation (into the site utility system) or hot utility savings for the site processing units. The demand in quantity and temperature associated with each waste heat utilization opportunity *o*, is taken into account.

To develop a systematic framework, a superset of potentially useful interconnections is created. The superset represents all possible design options for integration of waste heat utilization technologies into existing process sites. A simplified schematic is shown in Fig. 11. The superset is created for each utilization opportunity o and associated technology option receiving heat from heat source streams combined in temperature interval k. For opportunities relating to heat generation, o is dependent on the temperature levels l in the site utility system. The created superstructure allows for interactions with the site utility system, which includes changing steam flow rate for operational optimization and the possibility of including waste heat recovery technologies.

Structural and operational variables are introduced to represent the degrees of freedom. The structural variables represent selection of heat source streams and technology options. Operational variables define the operating points of the system. Definition of the variables used in this framework is provided in Section 2.3.1. Thermodynamic models to predict the useful energy recovered from organic Rankine cycles and absorption chillers in Oluleye et al [4], mechanical heat pumps, absorption heat pumps and heat transformers are applied in this work. The models for waste heat recovery technologies are presented in Section 2.3.3. Models proposed for site utility system components such as gas turbines, steam turbines and boilers in Aguilar et al. [27] are also applied. The models allow for estimation of operational load and equipment size. To represent the utility system in a linear way, the saturation temperatures and pressures of steam distribution mains are fixed [30].

By using suitable linear relationships to represent costs, energy conversion, etc., and structural variables to represent discrete choice, a mixed-integer linear model is created. Once the predictive models describing the performance of the technologies are developed and applied, the superstructure in Fig. 11 is formulated mathematically and reduced subject to an objective function and constraints. Formulation of the objective function is provided in Section 2.3.2, since the end-use of recovered energy from waste heat i.e. waste heat utilization opportunities are considered, the objective function is formulated to maximize the economic potential. The economic potential takes into account financial benefits associated with waste heat utilization opportunities (Eq. 3 in section 2.3.2). Constraints describing the feasible region of this framework are presented in section 2.3.4.

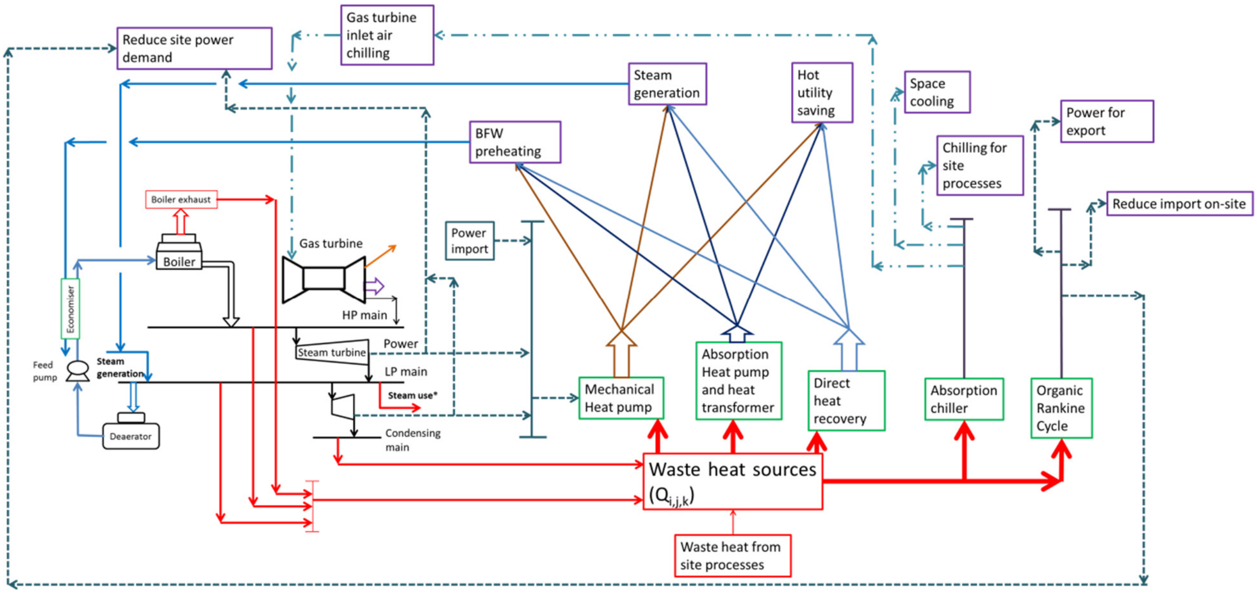


Fig. 11 Superstructure schematic for design

2.3.1 System Variables

Binary (structural) and continuous (operational) variables are introduced to represent degrees of freedom.

- Binary variables are introduced to represent existence of heat source streams *i* from units *j* in temperature interval *k*. This introduces a degree of freedom in the choice of streams.

$$X_{i,j,k} = \{0,1\} \tag{1}$$

- Binary variables are introduced for existence of technology options exploiting waste heat in temperature interval *k* to satisfy utilization opportunity *o*. when *o* is associated with steam generation and hot utility savings; *l* represents the various utility distribution temperature levels. The binary variable takes a value of 1 when a technology exists.

$$\left\{Y^{ORC}_{k,o}, Y^{AbC}_{k,o}, Y^{MHP}_{k,o(l)}, Y^{AHP}_{k,o(l)}, Y^{AHT}_{k,o(l)}, Y^{DHR}_{k,o(l)}\right\} = \{0,1\} \tag{2}$$

- Continuous variables are described below:

$W^{ORC}_{k,o}$: Net electrical power generated using combined heat sources in temperature interval *k* to satisfy opportunity *o*.

$Q^{AbC}_{k,o}$: Chilling provided from an absorption chiller driven by combined heat sources in temperature interval *k* to satisfy opportunity *o*.

$Q^{MHP}_{k,o(l)}$: Heat upgraded to satisfy opportunity *o*, from a MHP using combined heat sources in temperature interval *k*.

$Q^{AHP}_{k,o(l)}$: Heat upgraded to satisfy opportunity *o*, from an AHP driven by combined heat sources in temperature interval *k*.

$Q^{AHT}_{k,o(l)}$: Heat upgraded to satisfy opportunity *o*, from an AHT driven by combined heat sources in temperature interval *k*.

$Q^{DHR}_{k,o(l)}$: Heat generated directly from combined heat sources in temperature interval *k* to satisfy sink *o*(*l*).

$mfuel_t$: Fuel consumed in technologies for combustion in the site utility system

$mturbine_l$: Mass flow of steam into steam turbines in the site utility system

W_{Import}: Electrical power imported from the grid to satisfy site demand

W_{Export} : Electrical power exported to the grid

2.3.2 Objective function and other equations

The objective function is formulated to maximize the economic potential. The economic potential is selected to account for the financial benefits associated with utilization opportunities. For example when the heat recovered is used for boiler feed water (BFW) preheating, steam generation or hot utility reduction (as shown in Fig. 11), the operating costs of the site utility system may reduce since less fuel is required. Also when the recovered energy in form of power is exported, revenue can be generated for the site. Therefore the economic potential is defined as the utility system operating cost before heat recovery minus sum of the operating cost after heat recovery, the annualized capital cost, maintenance costs and operating cost of the waste heat utilization system.

The waste heat utilization system (WHUS) refers to all technology options that could be selected. The objective function is presented in Eq. 3.

$$\text{Maximize}: \left(OC^{U}_{before} - \left(OC^{U}_{after} + ACC_{WHUS} + MC_{WHUS} + OC_{WHUS}\right)\right) \quad (3)$$

The operating cost of the site utility system *U* is presented in Eq. 4 and the cost of fuel consumed by technologies in Eq. 5.

$$OC^{U} = C^{U}_{fuel} + C^{U}_{CW} + C^{U}_{PI} - C^{U}_{PE} \quad (4)$$

$$C^{U}_{fuel} = \sum_{t}\left(mfuel_{t} \times FP_{t}\right) \quad (5)$$

Where FP is the unit price of fuel consumed in technology *t*. The cost of cooling water accounts for cooling requirements of the utility system and processing units. Overall electrical power import cost and revenue from export are calculated as shown below:

$$C^{U}_{PI} = W_{Import} \times PImP \quad (6)$$

$$C^{U}_{PE} = W_{Export} \times PExP \quad (7)$$

PImp is the unit cost of electrical power import and PExP is the unit cost of electrical power export.

The annualized capital cost of the WHUS is calculated taking into account the equipment cost (EC) for new technology installations, the retrofit factor (RF) to account for new equipment installation and cost of retrofitting existing facilities, and the annualization factor (AF) to spread the cost over the lifetime of a technology. As shown below:

$$ACC_{WHUS} = AF \times \left(CC_{ORC} + CC_{AbC} + CC_{AHP} + CC_{AHT} + CC_{MHP} + CC_{DHR}\right) \quad (8)$$

$$CC_{ORC} = RF \times \left(EC_{ORC}\right) \quad (9)$$

Eq. (9) applies for all technologies options in the WHUS. The annualization factor is calculated as shown below:

$$AF = \frac{IR \times (1+IR)^{n}}{(1+IR)^{n-1}} \quad (10)$$

The maintenance cost of the technologies is assumed to be 2% of the equipment capital cost [27]. The operating cost for the waste heat utilization system is the sum of cooling water costs, power import costs minus revenue from power export. Majority of the electrical power imported might be for the MHP since the liquid pumping requirements of absorption systems are negligible [10]. Electrical power produced from the ORC may also be exported.

$$OC_{WHUS} = C_{CW}^{WHUS} + C_{PI}^{WHUS} - C_{PE}^{WHUS} \tag{11}$$

2.3.3 Modelling waste heat recovery technologies

The simplified explicit models of organic Rankine cycles (ORC) [4], absorption chillers (AbC) [4], mechanical heat pumps (MHP), absorption heat pumps (AHP) and absorption heat transformers (AHT) adopted in this work are provided below. The developed models show the relationship between the real i.e. actual performance and the ideal reference case of the different thermodynamic cycles considered.

For an ORC (schematic shown in Fig. 1), the relationship between the real performance in Eq. (12) and the ideal performance (Eq. (13)) is defined using the efficiency factor in Eq. (14) [4]. The efficiency factor was correlated with the ideal efficiency in Eq. (15), in order to estimate the useful power recovered, based on the system temperatures and parameters accounting for the inefficiencies in the cycle components, and working fluid non-ideal behavior. The model shows good agreement with rigorous simulation of the ORC [4].

$$\eta_{real} = \frac{W_{EXP}^{ORC} - W_{PUMP}^{ORC}}{Q_{EVAP}^{ORC}} \tag{12}$$

$$\eta_{ideal} = 1 - \frac{T_{COND}^{ORC}}{T_{EVAP}^{ORC}} \tag{13}$$

$$\eta_{real} = \mu_{ORC} \times \eta_{ideal} \tag{14}$$

$$\mu_{ORC} = (\alpha_{ORC} \times \eta_{ideal}) + \beta_{ORC} \tag{15}$$

The real COP for an absorption chiller (schematic provided in Fig. 2) is defined in Eq. (16) and the ideal COP in Eq. (17) [4]. The ratio of the real COP to the ideal COP is the efficiency factor (Eq. 18). The efficiency factor is correlated with the ideal COP in Eq. (19) [4]. The liquid pumping requirements for chillers, absorption heat pumps and heat transformers can be assumed to be negligible. The models developed shows good agreement with rigorous simulation of the AbC [4].

$$COP_{AbC,real} = \frac{Q^{AbC}_{EVAP}}{Q^{AbC}_{GEN} + W^{AbC}_{PUMP}} \tag{16}$$

$$COP_{AbC,ideal} = \left(1 - \frac{T^{AbC}_{COND}}{T^{AbC}_{GEN}}\right)\left(\frac{T^{AbC}_{EVAP}}{T^{AbC}_{COND} - T^{AbC}_{EVAP}}\right) \tag{17}$$

$$COP_{AbC,real} = \mu_{AbC} \times COP_{AbC,ideal} \tag{18}$$

$$\mu_{AbC} = \frac{\beta_{AbC}}{COP_{AbC,ideal} - \alpha_{AbC}} \tag{19}$$

The absorption heat pump real COP (schematic shown in Fig. 3) is shown in Eq. (20) and the ideal COP in Eq. (21). The efficiency factor defined in Eq. (22) is correlated with the ideal efficiency in Eq. (23); validation of the model using thermodynamic design data presented in Eisa et al. [31] as shown in Appendix B (Fig. B.1).

$$COP_{AHP,real} = \frac{Q^{AHP}_{ABS} + Q^{AHP}_{COND}}{Q^{AHP}_{GEN} + W^{AHP}_{PUMP}} \tag{20}$$

$$COP_{AHP,ideal} = 1 + \left(1 - \frac{T^{AHP}_{COND}}{T^{AHP}_{GEN}}\right)\left(\frac{T^{AHP}_{EVAP}}{T^{AHP}_{COND} - T^{AHP}_{EVAP}}\right) \tag{21}$$

$$COP_{AHP,real} = \mu_{AHP} \times COP_{AHP,ideal} \tag{22}$$

$$\mu_{AHP} = \frac{\beta_{AHP}}{COP_{AHP,ideal} - \alpha_{AHP}} \tag{23}$$

The real COP for an absorption heat transformer (Fig. 4) is provided in Eq. (24) and the ideal COP in Eq. (25). The efficiency factor is correlated with the ideal efficiency in Eq. (27); validation of the model using thermodynamic design data presented in Eisa et al. [32] is shown in Appendix B (Fig. B.2).

$$COP_{AHT,real} = \frac{Q^{AHT}_{ABS}}{Q^{AHT}_{GEN} + Q^{AHT}_{EVAP} + W^{AHT}_{PUMP}} \tag{24}$$

$$COP_{AHT,ideal} = \left(\frac{\left(T^{AHT}_{EVAP} - T^{AHT}_{COND}\right) \times T^{AHT}_{ABS}}{\left(\left(T^{AHT}_{EVAP} - T^{AHT}_{COND}\right) \times T^{AHT}_{GEN}\right) + \left(\left(T^{AHT}_{ABS} - T^{AHT}_{GEN}\right) \times T^{AHT}_{EVAP}\right)}\right) \tag{25}$$

$$COP_{AHT,real} = \mu_{AHT} \times COP_{AHT,ideal} \tag{26}$$

$$\mu_{AHT} = \frac{\beta_{AHT}}{COP_{AHP,ideal} - \alpha_{AHT}} \tag{27}$$

A mechanical heat pump (schematic provided in Fig. 5) real COP is defined using Eq. (28) and the ideal COP is Eq. (29). The ratio of the real COP to the ideal COP is defined as the efficiency factor in Eq. (30). The efficiency factor is correlated with the ideal efficiency in Eq. (31); validation of the model against rigorous simulation in Aspen HYSYS [33] is presented in Appendix B (Fig. B.3).

$$COP_{MHP,\,real} = \frac{Q^{MHP}_{COND}}{W^{MHP}_{COMP}} \tag{28}$$

$$COP_{MHP,ideal} = \frac{T^{MHP}_{COND}}{T^{MHP}_{COND} - T^{MHP}_{EVAP}} \tag{29}$$

$$COP_{MHP,\,real} = \mu_{MHP} \times COP_{MHP,\,ideal} \tag{30}$$

$$\mu_{MHP} = \alpha_{MHP} + \left(\beta_{MHP} \times \frac{T^{MHP}_{COND} - T^{MHP}_{EVAP}}{T^{MHP}_{COND}} \right) \tag{31}$$

Values of α and β for all technologies are provided in Appendix A. Temperatures in Eqs (13 – 15), (17 – 19), (21 – 23), (25 – 27) and (29 – 31) are in Kelvin (K).

The waste heat sources vaporize working fluids in the evaporators of ORC, AbC, AHP, AHT and MHP. They also drive the separation of the working fluid pair in the generators of AbC, AHP and AHT. Therefore for the technology temperatures Eq. 32 holds and for the flow of heat Eq. (33) holds.

$$T^{ORC}_{EVAP}, T^{AbC}_{EVAP}, T^{AbC}_{GEN}, T^{AHP}_{GEN}, T^{AHP}_{EVAP}, T^{AHT}_{EVAP}, T^{AHT}_{GEN}, T^{MHP}_{EVAP} \in T_k \tag{32}$$

Where T_k represents the temperature intervals (already shifted by ΔT_{MIN} to account for feasible heat recovery) on the combined heat source streams.

$$Q^{ORC}_{EVAP}, Q^{AbC}_{EVAP}, Q^{AbC}_{GEN}, Q^{AHP}_{GEN}, Q^{AHP}_{EVAP}, Q^{AHT}_{EVAP}, Q^{AHT}_{GEN}, Q^{MHP}_{EVAP} \in RQ \tag{33}$$

Where RQ represents the waste heat utilised by technology options

Useful heat upgraded from AHP, AHT and MHP can satisfy sinks for recovered energy at various temperature levels:

$$T^{AHP}_{COND}, T^{AHT}_{ABS}, T^{MHP}_{COND} \in T_{o(1)} \tag{34}$$

For feasible heat recovery ΔT_{MIN} is taken into account when determining $T^{AHP}_{COND}, T^{AHT}_{ABS}, T^{MHP}_{COND}$. The condensers of organic Rankine cycles, absorption chillers and heat transformers are designed to reject heat to cooling water. In addition to the five thermodynamic cycles considered, the potential for direct heat recovery via heat exchange (DHR) is also explored in this work.

2.3.4 System constraints

The set of equality and inequality constraints defining various limits of this modelling framework are outlined below.

1. Constraint for heat source streams:

Combining heat source streams in a temperature interval

$$QCUM_k = \sum_i \sum_j \left(Q_{i,j,k} \times X_{i,j,k} \right) \forall\ k \tag{35}$$

Heat exploited by a technology, for example an ORC.

$$RQ^{ORC}_k = \sum_o \left(Q^{ORC}_{EVAP\ k,o} \right) \forall\ k \tag{36}$$

Limit for heat exploited by a technology taking into account the cumulative heat available from T_{k-1} to T_k:

$$0 \le RQ^{ORC}_k \le \left(QCUM_k - RQ^{ORC}_{k-1} - RQ^{ORC}_{k-2} - RQ^{ORC}_{k-3} ......+ RQ^{ORC}_{k-(k-1)} \right), \quad \forall\ k \tag{37}$$

Eqs. (36 – 37) are written for all technology options.

The total waste heat exploited by all technologies in the waste heat utilization system:

$$RQ_k = \sum_o \left(RQ^{ORC}_{k,o} + RQ^{AbC}_{k,o} + RQ^{AHP}_{k,o} + RQ^{AHT}_{k,o} + RQ^{MHP}_{k,o} + RQ^{DHR}_{k,o} \right) \forall\ k \tag{38}$$

To ensure that heat utilized is available from the selected and combined heat source streams, Eq (39) is formulated:

$$QCUM_k \ge RQ_k + RQ_{k-1} + RQ_{k-2} + RQ_{k-3} ....+ RQ_{k-(k-1)}, \quad \forall\ k \tag{39}$$

2. Constraints associated with demand for end-use of recovered energy i.e. waste heat utilization opportunities [28].

For electrical power generation:

$$0 \le \sum_k \left(W^{ORC}_{k,o} \right) \le W_{Demand,o} \qquad \forall\ o \tag{40}$$

For chilling provision:

$$0 \le \sum_k \left(Q^{AbC}_{k,o} \right) \le Q_{Demand,o} \qquad \forall\ o \tag{41}$$

Where $Q_{Demand,o}$ represents chilling demand associated with opportunity *o*.

For heat generation, the recovered energy in form of heat, Qout is given as:

$$Qout_{o(l)} = \sum_k \left(Q^{AHP}_{k,o(l)} + Q^{AHT}_{k,o(l)} + Q^{MHP}_{k,o(l)} + Q^{DHR}_{k,o(l)} \right) \tag{42}$$

The recovered heat is useful for hot utility reduction (HUR), steam generation (STG) and boiler feed water preheating (BFW):

$$Qout^{HUR}_{o(l)}, Qout^{STG}_{o(l)}, Qout^{BFW}_{o(l)} \in Qout_{o(l)} \tag{43}$$

For hot utility savings, Eq. (44) is formulated to account for existing steam use,

$$0 \le Qout^{HUR}_{o(l)} \le Qsteamuse_{l} \qquad \forall\ l \tag{44}$$

For steam generation into the site utility system from waste heat:

$$0 \le Qout^{STG}_{o(l)} \tag{45}$$

The maximum limit for steam generation is determined from the capacity of the site utility system. The capacity of the site utility system is taken into account by simultaneously optimising the waste heat utilization system and the site utility system.

For boiler feed water preheating:

$$0 \le Qout^{BFW}_{o(l)} \le Q_{BFW} \tag{46}$$

Where Q_{BFW} represents the demand for boiler feed water.

3. Implicit constraints for existence of technologies within specified size limits, L represent the lower bound for technology sizes and U represents an upper bound. The upper bound is selected as a very large number.

$$W^{ORC}_{k,o} - (U_{ORC} \times Y^{ORC}_{k,o}) \le 0 \qquad \forall\ k, o \tag{47}$$

$$W^{ORC}_{k,o} - (L_{ORC} \times Y^{ORC}_{k,o}) \ge 0 \qquad \forall\ k, o \tag{48}$$

$$Q^{AbC}_{k,o} - (U_{AbC} \times Y^{AbC}_{k,o}) \le 0 \qquad \forall\ k, o \qquad (49)$$

$$Q^{AbC}_{k,o} - (L_{AbC} \times Y^{AbC}_{k,o}) \ge 0 \qquad \forall\ k, o \qquad (50)$$

$$Q^{AHP}_{k,o} - (U_{AHP} \times Y^{AHP}_{k,o(l)}) \le 0 \qquad \forall\ k, o \qquad (51)$$

$$Q^{AHP}_{k,o} - (L_{AHP} \times Y^{AHP}_{k,o(l)}) \ge 0 \qquad \forall\ k, o \qquad (52)$$

$$Q^{AHT}_{k,o} - (U_{AHT} \times Y^{AHT}_{k,o(l)}) \le 0 \qquad \forall\ k, o \qquad (53)$$

$$Q^{AHT}_{k,o} - (L_{AHT} \times Y^{AHT}_{k,o(l)}) \ge 0 \qquad \forall\ k, o \qquad (54)$$

$$Q^{MHP}_{k,o} - (U_{MHP} \times Y^{MHP}_{k,o(l)}) \le 0 \qquad \forall\ k, o \qquad (55)$$

$$Q^{MHP}_{k,o} - (L_{MHP} \times Y^{MHP}_{k,o(l)}) \ge 0 \qquad \forall\ k, o \qquad (56)$$

$$Q^{DHR}_{k,o} - (U_{DHR} \times Y^{DHR}_{k,o(l)}) \le 0 \qquad \forall\ k, o \qquad (57)$$

$$Q^{DHR}_{k,o} - (L_{DHR} \times Y^{DHR}_{k,o(l)}) \ge 0 \qquad \forall\ k, o \qquad (58)$$

4. Selection of heat source streams to be included in temperature interval k

$$X_k = \sum_i \sum_j X_{i,j,k} \qquad \forall\ k \qquad (59)$$

$$X_k - Y^{ORC}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (60)$$

$$X_k - Y^{AbC}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (61)$$

$$X_k - Y^{AHP}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (62)$$

$$X_k - Y^{AHT}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (63)$$

$$X_k - Y^{MHP}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (64)$$

$$X_k - Y^{DHR}_{k,o} \ge 0 \qquad \forall\ k, o \qquad (65)$$

5. Overall energy balance for the site utility system:

$$\left\{ \begin{array}{l} \left[\sum_t \left((mfuel_t \times LHVfuel_t) - Q^{BFW} \right) \times \eta_t \right] + \sum_l \left(Qsteamgen_l + Q^{STG}_{o(l)} \right) \\ - \sum_l \left(Qsteamuse_l + Q^{HUR}_{o(l)} \right) - \sum_l W_{turbine\ l} - \sum_l Q_{cond\ l} \end{array} \right\} = 0 \qquad (66)$$

6. Energy balance for waste heat recovery technologies.

$$W^{ORC}_{EXP} - W^{ORC}_{PUMP} - Q^{ORC}_{EVAP} + Q^{ORC}_{COND} = 0 \quad (67)$$

$$Q^{AbC}_{GEN} + W^{AbC}_{PUMP} + Q^{AbC}_{EVAP} - Q^{AbC}_{COND} - Q^{AbC}_{ABS} = 0 \quad (68)$$

$$Q^{AHP}_{GEN} + W^{AHP}_{PUMP} + Q^{AHP}_{EVAP} - Q^{AHP}_{COND} - Q^{AHP}_{ABS} = 0 \quad (69)$$

$$Q^{AHT}_{GEN} + W^{AHT}_{PUMP} + Q^{AHT}_{EVAP} - Q^{AHT}_{COND} - Q^{AHT}_{ABS} = 0 \quad (70)$$

$$Q^{MHP}_{COND} - Q^{MHPC}_{EVAP} - W^{MHP}_{COMP} = 0 \quad (71)$$

7. Mass balance per temperature region *l* (identified at the pressure levels for steam distribution in the site utility system).

$$m_{in,l} = m_{out,l} \qquad \forall\, l \quad (72)$$

8. Technology flow boundaries (on a mass basis) in the utility system

$$m_{L,t} \le m_t \le m_{U,t} \quad (73)$$

By using integer variables to represent discrete choices, a mixed-integer linear model is created. The optimisation framework is solved using Lindo's system What's Best! software [34]. The problem is solved by first providing a continuous approximation of the model, and then applying the branch-and-bound algorithm in What's Best! to identify all possible integer solutions and find an optimal integer solution.

2.4 Evaluating the design

The last stage is a post optimization step useful for evaluating different design approaches, scenarios and sensitivities to design inputs. The design in section 2.3 was formulated to maximize the economic potential defined in Eq. 3. In addition to the objective function, the design can be evaluated using the global fuel consumption before and after waste heat recovery, the global CO_2 emissions before and after waste heat recovery and the payback. Global fuel consumption (GFC) and CO_2 emissions (GCO_2E) are estimated considering: (1) fuel combustion in the site utility system, (2) fuel consumption as a result of power import, and (3) fuel displaced when power is exported. The payback is the ratio of the total investments to the profit generated.

$$GFC = \left(mfuel_t \times LHVfuel_t\right) + \left(\frac{W_{Import} - W_{Export}}{\eta_{power}}\right) \quad (74)$$

$$GCO_2E = (mfuel_t \times LHVfuel_t \times FEF_t) + ((W_{Import} - W_{Export}) \times GEF) \quad (75)$$

3. Industrial Case Study

The case study presented is for a chemical production site. Processing units for the intermediate production of high value polymers are considered. Data extracted for hot streams from the processing units and the utility system rejecting heat to cooling water and air is shown in Appendix C. This represents the available waste heat sources. Data extracted for cold streams currently on hot utility i.e. steam is also provided in Appendix C. The waste heat source profile for all waste heat source streams from the site processing units (excluding the utility system) in terms of shifted temperature and cumulative heat is shown on the negative x-axis in Fig. 12 (a). The profile on the positive x-axis in Fig. 12 (a) is for the existing cold streams on hot utility.

The existing site utility system configuration is shown in Fig. 13. It consists of two boilers burning fuel gas (FG) and fuel oil (FO). In addition to the steam distributed to the site processes from the utility system at 6bar and 35bar, the site has a 20bar steam distribution main used for internal heat generation between individual processing units. The total operating costs of the base case before heat recovery is £34,463,514/y and CO_2 emissions is 188,372 t/y. first the mathematical model developed to represent the existing site utility system is validated with the operating data provided (as shown in Table 1). The model formulated shows good agreement with the existing utility system operating data.

Waste heat available from the utility system is from the exhaust of the fuel gas boiler (2,804 kW), exhaust of the fuel oil boiler (1,487.9 kW) extracted above the acid dew point, and latent heat loss from steam condensation (6,163 kW). Including the heat loss from the utility system and placement of the utility levels is shown in Fig. 12(b). Majority of the waste heat is from the site processing units.

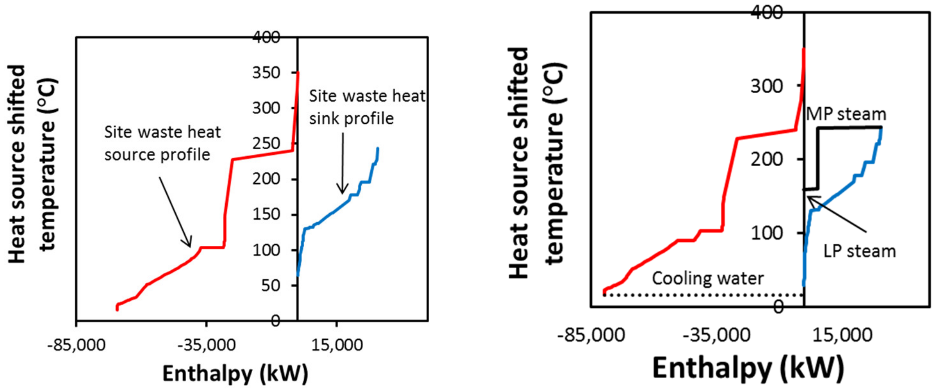


Fig. 12. Existing site waste heat source and sink profile (a) without heat rejected from the utility system, (b) with heat rejected from the utility system and placement of hot utility

The objective is to integrate waste heat recovery technologies to exploit all the available waste heat rejected to cooling water and air. The site currently imports 10,000 kW of electrical power. Identified potential utilization opportunities relate to boiler feed water preheating (after the feed pump), power generation to reduce import, power for export, steam generation into the site utility system at temperature levels indicated in the schematic of the utility system and 20bar, and reducing the steam demand by the processing units (represented by the waste heat sink profile in Fig. 12). Since there is no chilling demand, thermodynamic cycles explored include the Organic Rankine cycle, the absorption heat pump and heat transformer, the mechanical heat pump and direct heat recovery. Design assumptions are shown in Table 2 below.

An overview of the methodology is presented in Fig. 6 above. Based on the algorithm for stream analysis in Fig. 8, the number of temperature intervals T_k to analyse the streams is 23. Three temperature levels (T_l) were selected to represent the heat sinks taking into account the pressure and saturation temperature of steam distribution mains. Pre-screening of working fluids for the organic Rankine cycle and the mechanical heat pump is presented in Fig. 10 (a) and (b) respectively. While the absorption systems use water/ lithium bromide, the organic Rankine cycle operates using Benzene above 80.1°C and cyclopentane below 80.1°C. The model involves the use of 319 continuous variables and 776 binary variables; solved in less than 1 second.

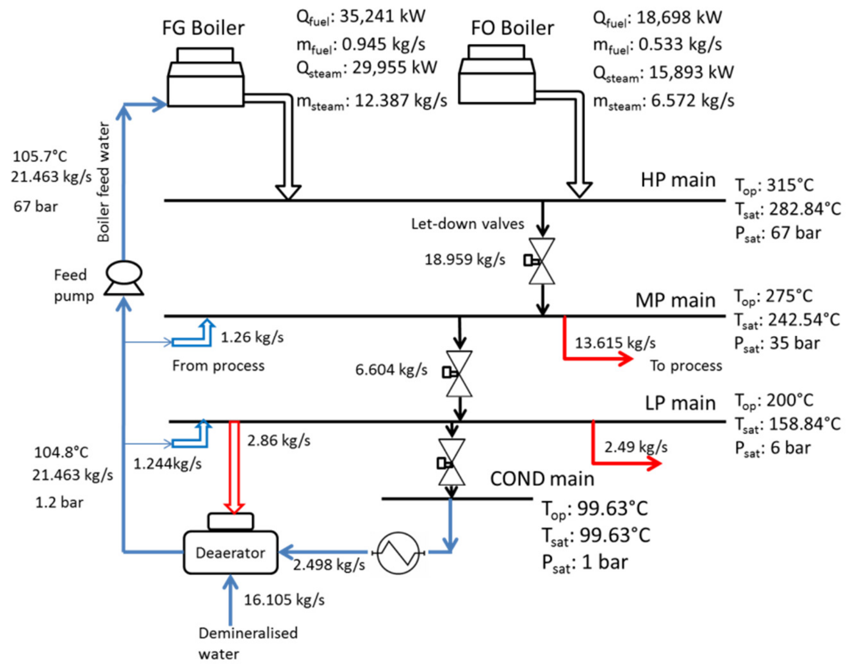


Fig. 13. Site utility system schematic (Base case)

Table 1 Site utility system model validation

Parameter	Operating Data	Model	Error
Fuel gas boiler fuel consumption	36,000 kW	35,241 kW	2%
Fuel oil boiler fuel consumption	19,100 kW	18,697 kW	2%
Total steam produced	19.528 kg/s	18.95837 kg/s	3%

Table 2 Design assumptions on prices and emissions.

Energy Prices	Emission factors [37]	Equipment costs	Others
Industrial electricity price: 13.4 p/kWh [35]	Grid emission factor: 0.485 kg/kWh	Organic Rankine cycle: 1,300 £/kW [38]	Discount rate: 15%
		Absorption chiller: 180 £/kW [3]	Operating hours: 8,600 h
			Retrofit factor: 3 [27]
Industrial fuel gas price: 4.43 p/kWh [36]	Fuel gas emission factor: 0.308 kg/kWh	Mechanical heat pump: 333 £/kW [39]	Ambient temperature 25 °C
		Absorption heat pump: 265 £/kW [40]	Technology life time: 10y
Industrial fuel oil: 5.27 p/kWh	Fuel oil	Absorption heat	

[36]	emission factor: 0.331 kg/kWh	transformer: 359 £/kW [41] Economizer: 227.5 £/m^2 [42]

There are three design approaches that have potential to reduce and utilize the available waste heat.

The design approach in Case 1 explores potential to utilize waste heat by changing only the current operating conditions of the site utility system without adding new equipment. There may be scope to improve the current operating conditions to reduce the quantity of waste heat produced. Therefore in Case 1 only operational optimization of the utility system is done. The objective function is to minimize the utility system operating costs (Eq. 4). Binary variables relating to existence of utilization technologies are 0. Relevant constraints for Case 1 are presented in Eqs 66, 72 and 73. This case is presented later in Section 3.1.

Case 2 involves the design of a stand-alone waste heat utilization system (Section 3.2). Here the site utility system fuel and steam flow is left unchanged as was previously done in literature. The objective function is to minimize the total annualized cost of the waste heat utilization system by combining Eq. 8 to Eq. 11.

Case 3 involves simultaneous design (by optimization) of the waste heat utilization and optimization of the utility system. This is presented in Section 3.3 using the objective function in Eq. 3 and all constraints are applied.

3.1 Case 1: Operational optimization of the site utility system

In Case 1, the existing utility system is optimized for minimum operating cost. The configuration of the utility system after operational optimization is presented in Fig. 14. The configuration after operational optimization shows there is scope to improve the current design by changing steam flows around the utility system. Operational optimization of the utility system results in 10.61% savings in primary fuel and 13.01% reduction in CO_2 emissions. The available waste heat reduces by 9%. Financial benefits are from £4,113,000 savings in operating costs. Since no new equipment is added, the payback for this design is zero. However, there still remains a considerable amount of heat rejected from the site processing units (Fig. 15). The dashed line on the waste heat source profile in Fig. 15 is the cumulative heat sources before operational optimization. Operational optimization of the site utility system reduces the quantity of the waste heat produced but the temperatures remain the same.

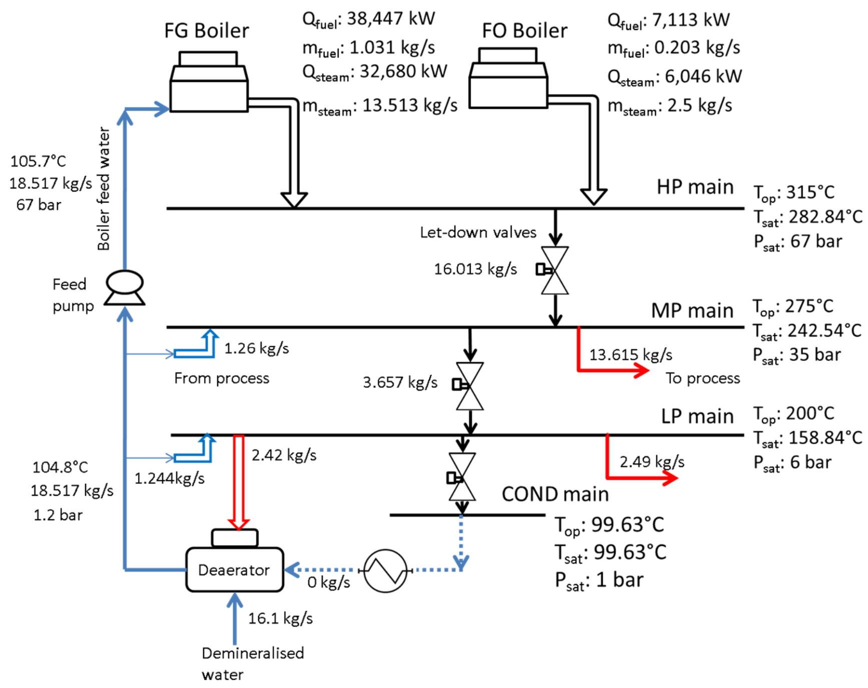


Fig. 14. Configuration of the site utility system after operational optimization

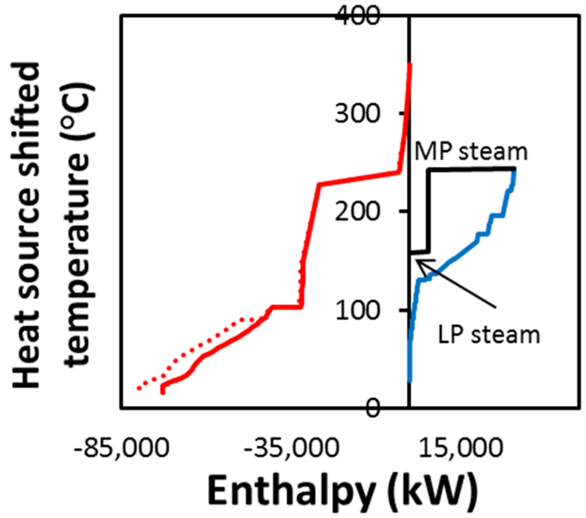


Fig. 15. Existing site waste heat source and sink profile (before and after operational optimization)

3.2 Case 2: Stand-alone design of the waste heat utilization system

Stand-alone design of the waste heat utilization system (without simultaneous optimization of the site utility system) implies that degrees of freedom relating to changing flow of fuel, and steam in the site utility system are not explored. This design involves generation of electrical power to reduce import using organic Rankine cycles.

9,272 kW of electrical power is generated requiring six organic Rankine cycles; one of them is placed in the utility system to recover power from the latent heat of condensation (Fig. 16). The remaining five exploit the heat rejected from the site processing units (Fig. 16). The non-shifted temperatures of the combined heat sources, the waste heat exploited (RQ_k) and the total heat rejected to cooling water Q_{COND} by the ORCs are also shown in Fig. 16.

This has the potential to reduce global fuel consumption by 29.36% and global CO_2 emissions by 20.53%. The payback for this design is 4 years. Comparison of Case 2 and the base case (without heat recovery) is presented in Table 3.

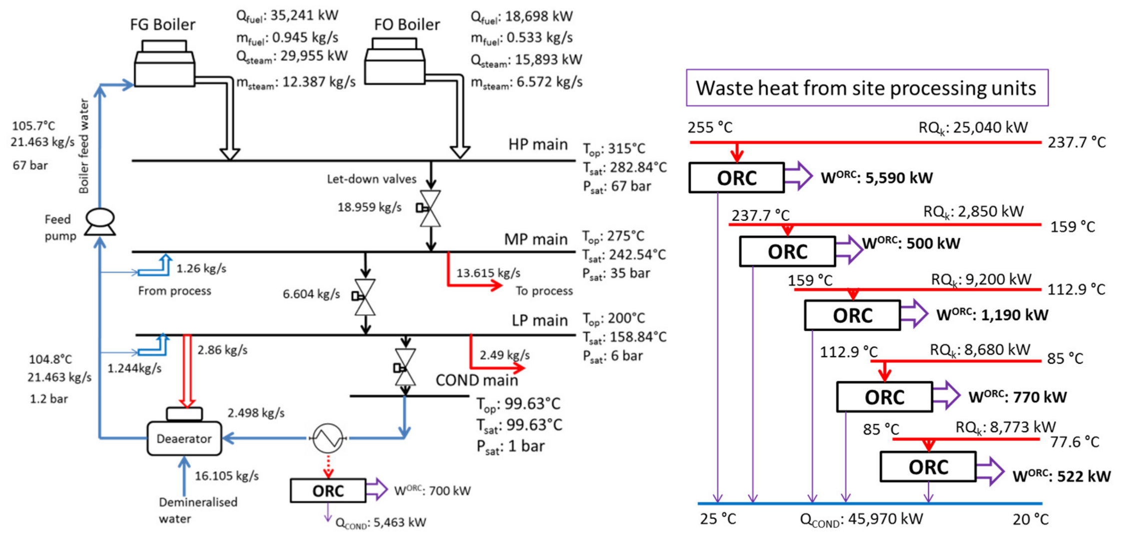


Fig. 16. Configuration of the utility system and designed waste heat utilization system (stand-alone design)

Table 3 Evaluation of results for Case 2

	Design before heat recovery	Standalone system design
Utility system fuel consumption (kW)	53,940	53,940

Global fuel consumption (kW)	78,940	55,760
Global CO_2 emissions (t/y)	188,372	149,699
Economic potential (£/y)	0	3,500,215

Eventhough the utility system fuel consumption remains the same, the global fuel consumption and CO_2 emissions reduce due to a reduction in power import. Power produced from the organic Rankine cycle displaces the need for power import from the grid. The power generated is presented in Figs. 16 and 17(a). The cost of power generation depends on the waste heat source temperature (Fig. 17(a)). This implies that the Organic Rankine cycle will only be economic when the cost of power import from the grid is greater than 11.20 p/kWh.

Stand-alone design of the waste heat utilization system has potential to reduce the quantity of available waste heat by 12% and the temperature of the residual heat sources also reduces (Fig. 17(b)). The dashed lines on the waste heat source profile (i.e. negative x-axis) in Fig. 17(b) shows the cumulative heat sources before heat recovery.

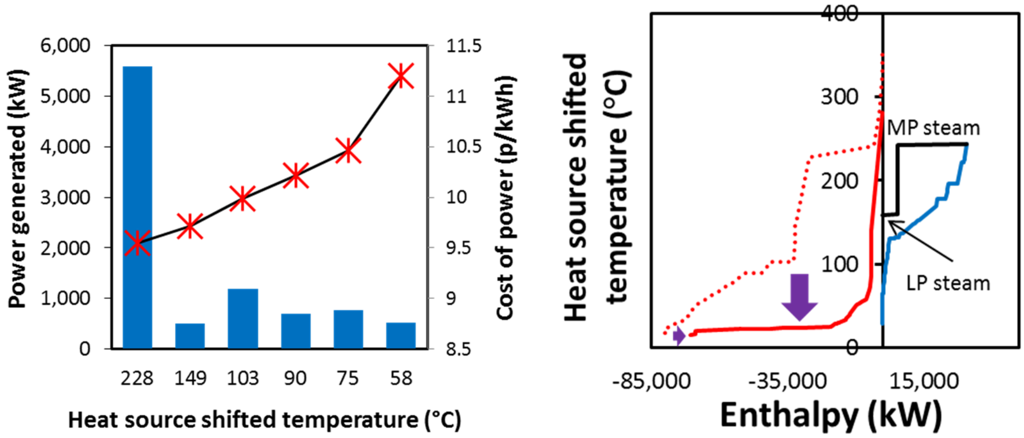


Fig. 17. (a) Analysis for power generated from waste heat, (b) Existing site waste heat source and sink profile after stand-alone waste heat utilization system design

Benefits from reduction in fuel consumption and CO_2 emissions can be calculated with an acceptable degree of accuracy. However, economic benefits are difficult to predict due to lack of accurate data on the capital cost of waste heat recovery technologies. To address this drawback, sensitivity of the results to the retrofit factor is performed as shown in Fig. 18. Stand-alone design of the waste heat utilization system becomes uneconomic (economic potential is zero) when the retrofit factor increases to 4.5.

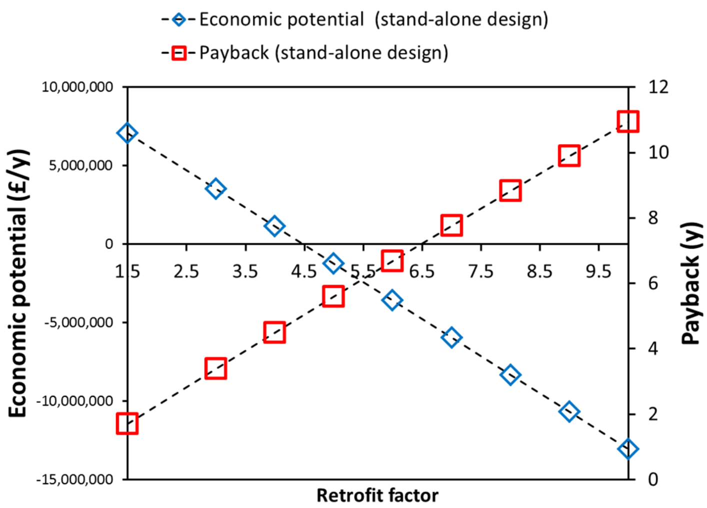


Fig. 18. Effect of the retrofit factor on the design economics (stand-alone design)

3.3 Case 3: Combined systems approach

In the combined systems approach, all technology options are included in the superstructure (Fig. 11) and the site utility system is optimized simultaneously. The final optimized design involves the generation of power using organic Rankine cycles, and heat using heat recovery via heat exchange. Integration of heat pumps for heat upgrade is uneconomic. A schematic of the site utility system and the waste heat utilization system is shown in Fig. 19.

A combined systems approach has the potential to recover 24% useful energy in the form of power and heat (i.e. steam for hot utility reduction). Furthermore, the global fuel consumption reduces by 54% and global CO_2 emissions by 53% (Table 4). The payback for this design is 2 years.

Power produced from the organic Rankine cycles reduces the need for power import on the site. The configuration of the site utility system and the designed waste heat utilization system is presented in Fig. 19. The non-shifted temperatures of the combined heat sources, the waste heat exploited (RQ_k), quantity of steam generated to reduce hot utility requirement, and the total heat rejected to cooling water Q_{COND} from the ORCs are also shown in Fig. 19. Producing electrical power from waste heat and generating steam via DHR to reduce the hot utility requirements results in a decrease in the quantity of waste heat and the temperatures of the residual heat as shown in Fig. 20. Since the heat generated reduces hot utility requirements, demand for hot utility also reduces. This is represented graphically on the site sink profile in Fig. 20. The dashed line on the positive x-axis in Fig. 20 represents the total hot utility required by the site processing units before the combined systems approach.

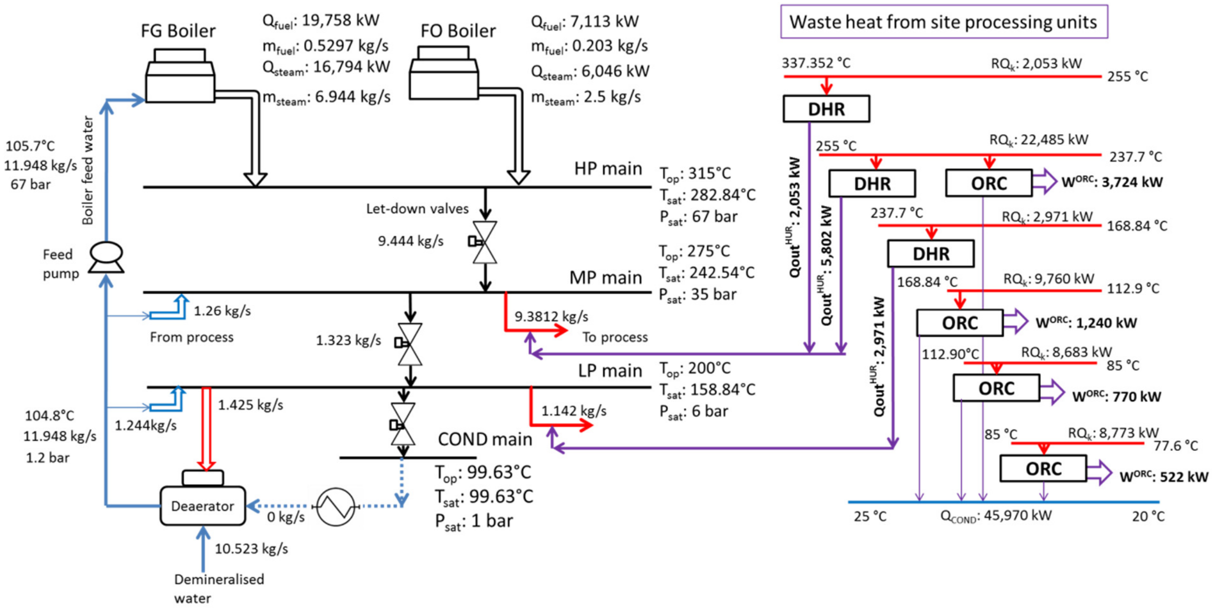


Fig. 19. Configuration of the utility system and designed waste heat utilization system (combined systems approach)

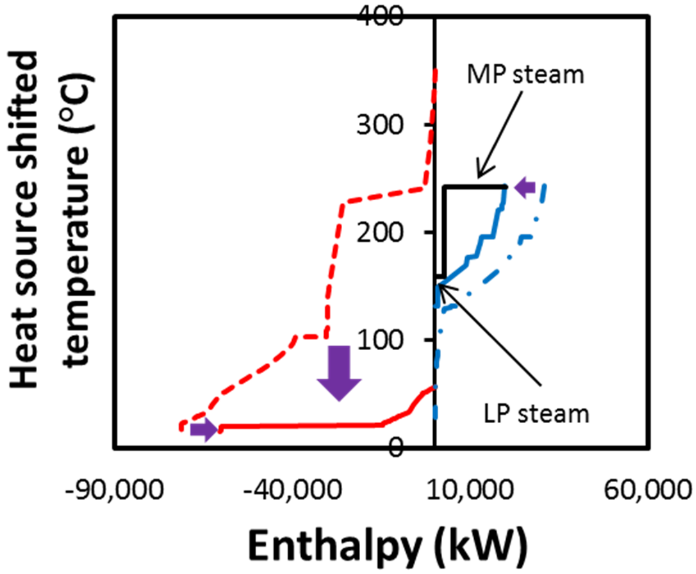


Fig. 20. Existing site waste heat source and sink profile after recovering useful energy via the combined system approach

Table 4 Evaluation of results for Case 3

	Design before heat recovery	Case 3: Combined systems approach
Utility system fuel consumption (kW)	53,940	26,871
Global fuel consumption (kW)	78,940	36,234
Global CO_2 emissions (t/y)	188,372	88,247
Economic potential (£/y)	0	12,766,800
Payback (y)	0	2

In Fig. 21, Varying the retrofit factor was done to determine the impact of inaccuracies in capital cost estimation. For the combined systems approach, when the retrofit factor increases to 4.5 the design is still economic compared to the stand-alone design (Fig. 18 above). This implies that recovering multiple forms of energy from waste heat and exploring interactions with the site utility system i.e. combining different concepts maximises production of useful energy from waste heat in process sites, and has the highest economic benefit.

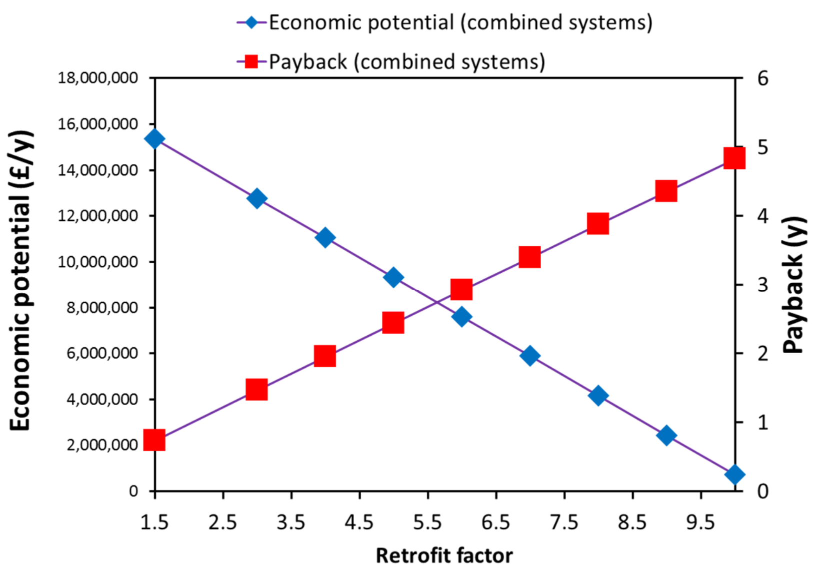


Fig. 21. Effect of the retrofit factor on the design economics (Combined systems design)

4. Case study summary

The methodological framework developed in section 2 is robust enough to explore different approaches to reduce and utilize industrial waste heat. There different approaches are explored in the case study presented in section 3: (1) operational optimisation of the existing site utility system (Case 1 in section 3.1), stand-alone design of the waste heat utilization system (Case 2 in section 3.2) and combined systems approach (Case 3 in section 3.3). The key criteria to compare between the three cases were presented in Section 2.4. A comparative analysis of all three cases is provided in Table 5.

Table 5 comparative analyses between all three cases

	Design before heat recovery	Case 1: Operational optimization of the utility system	Case 2: Stand-alone design of the waste heat utilization system	Case 3: Combined systems approach
Utility system fuel consumption (kW)	53,940	45,561	53,940	26,871
Global fuel consumption (kW)	78,940	70,561	55,760	36,234
Global CO_2 emissions (t/y)	188,372	163,866	149,699	88,247
Economic potential (£/y)	0	4,113,278	3,500,215	12,766,800
Payback (y)	0	0	4	2

Furthermore in Case 1, the quantity of waste heat reduces by 9% but temperatures remain the same (Fig. 15), in Case 2, the quantity of waste heat reduces by 12% and temperatures also reduces (Fig. 17b) and in Case 3 the quantity of waste heat reduces by 24% and temperatures also reduces (Fig. 20). The results obtained show that there are more benefits from considering interactions with the site utility system (i.e. a combined systems approach).

5. Conclusions and Future Work

In this paper, a novel methodological framework is presented for the conceptual design of site waste heat utilization systems allowing for simultaneous optimization of the site utility system. The method is divided into four stages: (1) data extraction stage for the waste heat sources and cold streams currently on hot utility, (2) pre-screening stage for selection of working fluids for the waste heat recovery technologies, (3) model formulation and optimization stage, and (4) design evaluation. The model formulation and optimization stage involves creation of a superstructure that is reduced subject to an objective function and sets of constraints. Thermodynamic cycles considered include the organic Rankine cycle, absorption chillers, absorption heat pumps, absorption heat transformers, mechanical heat pumps and potential for direct heat recovery is also explored.

The novel methodological framework was applied to an industrial relevant case study. The case study was analysed in three ways to inform management decision. Firstly, only operational optimization of the system was done to reduce the quantity of waste heat produced. This has potential to reduce costs by 12%, fuel consumption by 10.6% and CO_2 emissions by 13% with no payback required. Secondly, stand-alone design of the waste heat utilization system was performed. This has potential to reduce costs by 10%, fuel consumption by 29.36%, CO_2 emissions by 20.53% with a 4 year payback. Lastly, the framework proposed in this work was explored i.e. the combined systems approach. This has potential to reduce costs by 37%, fuel consumption by 54% and CO_2 emissions by 53% with a 2 year payback. The financial benefits and payback depends on the assumptions on costs. There are more benefits when interactions between the site processing units, designed waste heat utilization system and the existing site utility system are explored simultaneously. Waste heat recovery has potential to improve the energy security of process sites since fuel is conserved, emissions and costs are reduced.

Acknowledgement

The authors gratefully acknowledge the members of Process Integration Research Consortium (PIRC) for their financial support for the development of this research, and the financial support provided by the European Commission 7th Framework Programme: EFENIS (296003).

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APPENDIX A: Data coefficients for technology models

Table A.1. Working fluids and data coefficients for the organic Rankine cycle [4].

Working fluid	Chemical formula	$T_{critical}$ (°C)	$P_{critical}$ (MPa)	Boiling point (°C)	α_{ORC}	β_{ORC}	T_{EVAP} (°C) range
Cyclopentane	C_5H_{10}	238.4	4.257	48.78	-0.5979	0.7622	48.78 – 238
n-Pentane	C_5H_{12}	196.6	3.370	36.10	-0.7625	0.7497	36.10 – 196
n-Hexane	C_6H_{14}	234.7	3.034	68.70	-0.7402	0.7506	70 – 200
Isobutane	C_4H_{10}	134.7	3.640	−11.70	-0.9648	0.7436	30 – 134
Isopentane	C_5H_{12}	187.2	3.396	27.80	-0.7965	0.748	31 – 187
Propane	C_3H_8	96.75	4.257	-42.15	-1.3267	0.7322	31 – 95
Benzene	C_6H_6	288.9	4.894	80.10	-0.5085	0.7663	81 – 270
Toluene	C_7H_8	318.6	4.126	110.60	-0.5507	0.775	111 – 300
R113	$C_2Cl_3F_3$	214.1	3.392	47.60	-0.7006	0.7475	48 – 195
R114	ClF_2CCF_2Cl	145.9	3.261	3.57	-0.8867	0.7428	50 – 120
R134a	$C_2H_2F_4$	101	4.055	-26.13	-1.2582	0.7451	31 – 90

Table A.2 Values of α and β for a water/lithium bromide absorption heat transformer for T_{COND} = 30 °C

T_{EVAP} (°C)	T_{ABS} (°C)	T_{GEN} (°C)	α_{AHT}	β_{AHT}

40	$60 < T_{ABS} < 90$	$50 < T_{GEN} < 80$	0.6356	−0.0549
50	$70 < T_{ABS} < 100$	$50 < T_{GEN} < 80$	0.6303	−0.0461
60	$80 < T_{ABS} < 110$	$50 < T_{GEN} < 80$	0.6270	−0.0392
70	$90 < T_{ABS} < 120$	$50 < T_{GEN} < 80$	0.6190	−0.0305
80	$100 < T_{ABS} < 130$	$50 < T_{GEN} < 80$	0.5797	−0.00704
90	$120 < T_{ABS} < 140$	$60 < T_{GEN} < 80$	0.6568	−0.0407

Table A.3 Values of α and β for a water/lithium bromide absorption heat pump

T_{GEN} (°C)	T_{EVAP} (°C)	$T_{COND} = T_{ABS}$ (°C)	α_{AHP}	β_{AHP}
90	$20 < T_{EVAP} < 30$	50	−2.5064	3.4299
100	$20 < T_{EVAP} < 30$	50	−0.7448	2.2099
	$30 < T_{EVAP} < 40$	60	−2.9497	3.7592
110	$20 < T_{EVAP} < 30$	50	−0.5081	2.0366
	$30 < T_{EVAP} < 40$	60	−0.7478	2.2099
	$40 < T_{EVAP} < 50$	70	−2.4461	3.3795
140	$40 < T_{EVAP} < 50$	80	−1.7978	2.8816

Table A.4 Values of α and β for a mechanical heat pump

Working Fluid	T_{cond} (°C)	T_{evap} range (°C)	α_{MHP}	β_{MHP}
Ammonia	50	10 – 40	0.7267	-0.4774
	70	15 – 60	0.7006	-0.3861
	90	25 – 80	0.6628	-0.3684
	110	25 – 100	0.5732	-0.1195
	120	25 – 100	0.4971	0.0586
n-butane	50	10 – 40	0.7319	-0.5154
	70	10 – 60	0.7181	-0.6077
	90	20 – 80	0.6952	-0.7107
	110	30 – 100	0.6551	-0.8149
	130	35 – 110	0.5586	-0.7767
Water	125	100 – 110	0.7484	-0.5518

145	100 – 130	0.7476	-0.5177
165	100 – 150	0.7448	-0.4729
185	100 – 170	0.7435	-0.4639
205	100 – 190	0.7399	-0.4474
215	100 – 200	0.7376	-0.4410

Appendix B: Model validation for the absorption heat pump, absorption heat transformer and mechanical heat pump

In section 2.3.3 explicit models of absorption heat pumps (Eqs. 20 – 23), absorption heat transformers (Eqs. 24 – 27) and mechanical heat pumps (Eqs. 28 – 31) were applied in the methodological framework. The models were validated against thermodynamic data provided in literature and rigorous simulations in Aspen HYSYS. Comparison of the performance predicted using the models with thermodynamic design data from experiment are provided in Figs. B.1 – B.3. Thermodynamic design data from experiments are provided by Eisa et al. [31] for the absorption heat pump. The data shows the real coefficient of performance estimated from experiment. This is compared against the real COP calculated using the models in Eqs. 20 – 23, as shown in Fig. B.1. The same is done for the absorption heat transformer in Fig. B. 2. Fig. B. 3 is generated to compare between the real COP of MHP calculated from Aspen HYSYS [33] and that predicted by the explicit models in Eqs. 28 – 31.

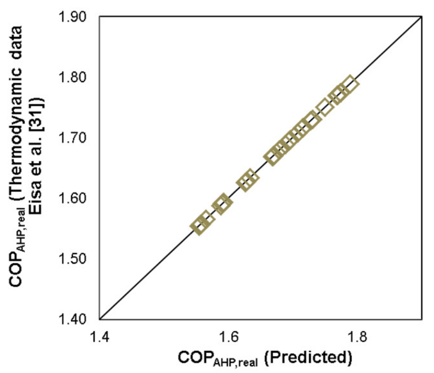

Fig. B.1 Model validation for AHP

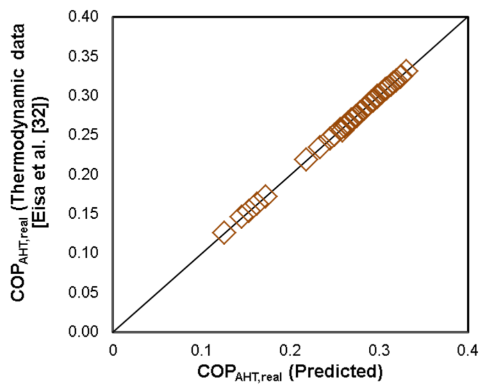

Fig. B.2 Model validation for AHT

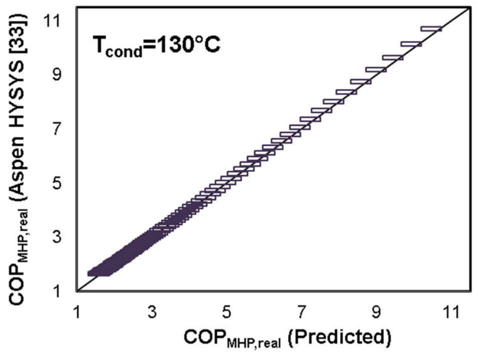

Fig. B.3 Model validation for MHP

Appendix C: Case study data

For the data in Tables C.1 and C.2 the notations are described below:

Hot 101: the first digit is the unit number, '1' for processing unit 1, '2' for processing unit 2, '3' for processing unit 3 and '4' for the site utility system. The second digit(s) represents the stream number. For example unit 1 contains 10 streams (i.e. Hot 101 – Hot 110). The same notation applies to the cold streams currently on hot utility.

Table C.1 Extracted stream data for hot streams on cold utility

Stream name	T_{SUPPLY} (°C)	T_{TARGET} (°C)	Heat duty (kW)	CP (kW/K)
Hot 101	92	70.9	339.001	16.0664
Hot 102	70.9	44.4	314.661	11.874
Hot 103	78.9	34	530	11.804
Hot 104	60.2	55.9	98	22.7907
Hot 105	101.5	34	635	9.40741
Hot 106	40.9	34	80	11.5942
Hot 107	87.5	27.7	358.5	5.99498
Hot 108	102	87.5	65	4.48276
Hot 109	100	50	562	11.24
Hot 110	43	33	5800	580
Hot 201	337.352	255	901.005	10.9409
Hot 202	250.768	237.7	22618.7	1730.85

Hot 203	360.293	255	1152	10.9409
Hot 204	108	37	1931.7	27.207
Hot 205	142	43	290	2.92929
Hot 206	38.7	25.5	45.6001	3.45455
Hot 207	130	90	13	0.325
Hot 208	253	157	2460	25.625
Hot 209	114	85	2931	101.069
Hot 210	85	61	6498	270.75
Hot 211	65	39.4	550.001	21.4844
Hot 212	113	112.9	8378.4	83784
Hot 213	91.1	40	2311	45.225
Hot 214	119	40	1510	19.1139
Hot 215	103	83	2590	129.5
Hot 216	83	37.9	234.2	5.1929
Hot 217	96.9	40	685.998	12.0562
Hot 218	100	50	80.9	1.618
Hot 219	251	159	807	8.77174
Hot 210	125	63	1830	29.5161
Hot 211	97	26.5	218	3.0922
Hot 301	97	50.6	120.3	2.59267
Hot 302	97	67.6	69.3999	2.36054
Hot 303	50.6	38.8	37	3.13559
Hot 304	74.8	31.9	820.999	19.1375
Hot 305	102	50	120	2.30769
Hot 306	33.4	26.9	18	2.76923
Hot 307	147	32	110	0.956522
Hot 308	122	30	87	0.945652
Hot 309	122	29	70	0.752688
Hot 310	123	30	67	0.72043
Hot 311	139	35	110	1.05769
Hot 312	121	32	87	0.977528
Hot 313	114	30	70	0.833333

Hot 314	117	30	67	0.770115
Hot 315	113	35	473.9	6.07564
Hot 316	35.4	28.5	46.9	6.7971
Hot 317	50	26	141.5	5.89583
Hot 401	291.249	150	2804.44	19.8546
Hot 402	291.251	150	1487.94	10.534
Hot 403	99.73	99.63	6162.93	61629.3

Table C.2 Extracted stream data for cold streams on hot utility

Stream name	T_{SUPPLY} (°C)	T_{TARGET} (°C)	Heat duty (kW)	CP (kW/K)
Cold 101	185.2	185.4	928.61	4643.05
Cold 102	270.6	291.3	67	3.23672
Cold 103	82.8	100	212.8	12.3721
Cold 104	100	101	629.1	629.1
Cold 105	87	100	42	3.23077
Cold 106	100	101	201.3	201.3
Cold 201	46	213	295	1.76647
Cold 202	43	218	320	1.82857
Cold 203	215	237	419	19.0455
Cold 204	216	237	555	26.4286
Cold 205	140	237	2153	22.1959
Cold 206	168	229	1713	28.082
Cold 207	121.9	122.1	1442.7	7213.5
Cold 208	58	105	926.7	19.717
Cold 209	142	142.2	236.2	1181
Cold 210	54	176.7	1062	8.65526
Cold 211	167.6	167.7	2700	27000
Cold 212	84	187	1593	15.466
Cold 213	125	160	11200	320
Cold 214	185.9	186.1	3250	16250

Cold 301	120	121	1779	1779
Cold 302	18.7	180	206	1.27712
Cold 303	20	21	27.1	27.1

Chapter 7: Conclusions and Future Work

7. 1. Conclusions

A considerable amount of thermal energy is wasted in the chemical process industries. This thesis presents a novel methodological framework for integrating technologies to exploit wasted thermal energy in process sites. Technologies considered are organic Rankine cycles for power generation from waste heat, absorption chillers, driven by waste heat to produce chilling, absorption heat pumps and heat transformers; thermally activated heat upgrade technologies, mechanical heat pumps to upgrade waste heat using mechanical energy and heat recovery via heat exchange. The method presented in this work presents a more accurate representation of the potential in industrial waste heat.

The main objective was to develop a systems-oriented approach for process integration of waste heat recovery technologies. The approach considered: (1) modelling of technology options, (2) comparative analysis of technologies, (3) hierarchical ordering of on-site and off-site end-uses of recovered energy, and (4) benefits from simultaneous optimization with the site utility system.

First, a comprehensive literature review was undertaken in Chapter 2 to provide the state of art in industrial waste heat utilization. Then the models of the organic Rankine cycles (ORC), absorption chillers (AbC) and absorption heat pumps (AHP) together with a graphical integration tool were presented in chapter 3 (publication 1). Models of absorption heat transformers (AHT) and mechanical heat pumps (MHP) are presented in Chapter 3 (publication 2). Publication 2 also contains a graphical tool for integrating heat pumps and a novel criterion to determine the performance of heat pumps, and to assess incorporation of heat pumps in existing process sites. A comparative analysis of technology options based on their exergy degradation was presented in Chapter 4 (publication 3). Ranking of end-uses of recovered energy taking into account economics (i.e. costs and benefits) and the potential to reduce CO_2 emissions was done in Chapter 5 (publication 4). An optimization framework for system design is presented in Chapter 6 (publication 5 – 7). In publication 5, a multi-period MILP model is presented for integrating waste heat recovery technologies; however, the opportunity for heat upgrading is not considered and simultaneous optimization with the site utility system not done. An MILP model for process integration of heat upgrading technologies (MHP, AHP and AHT) is presented in publication 6. In publication 6, simultaneous optimization with the site utility system is done to predict the true value of hot utility saved, steam generation from upgraded heat and to identify any trade-off between fuel saved from heat upgraded and power generated for export. In publication 7, a MILP model is considered for integrating the five thermodynamic cycles and heat recovery via heat exchange for waste heat exploitation in process sites. Figure 7.1 shows how all the Publications fit into the methodological framework.

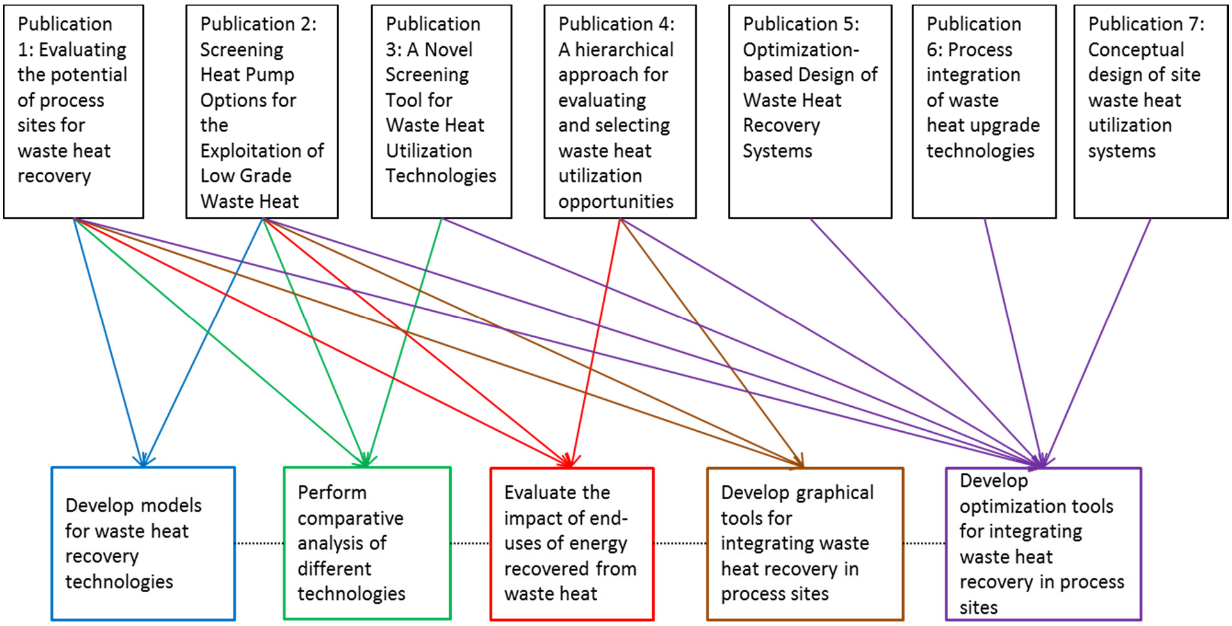

Figure 7. 1 Overview of Publications and the methodological framework

The methodological framework presented in this thesis enables the potential in industrial waste heat to be evaluated. The framework also provides the knowledge needed for engineers to determine the form of energy to recover from waste heat, end-use of recovered energy and associated technology, and design waste heat utilization systems. Such knowledge could increase the uptake of waste heat recovery by the process industries. The output of this research will also contribute to the education of future engineers in response to the needs of the fast-changing global economy.

The most important outcome of this thesis is that:

> Industrial waste heat utilization can improve the energy security of process sites and global energy security, since efficiency in the use of fuel is increased, CO_2 emissions are reduced and costs reductions are possible. A systems oriented approach to

integrating waste heat recovery in process sites yields additional savings in primary fuel, reduction in CO_2 emissions and reduction in costs.

Application of the methodological framework to two industrial case studies shows that, it is possible in the studied cases to increase efficiency and reduce CO_2 emissions. However, the economics depends on the end-uses of recovered energy, design approach, assumptions on capital and operating costs, and the acceptable payback periods in industry. The main contributions are summarized in sections 7.1.1 – 7.1.7 below.

7.1.1 Explicit models of waste heat recovery technologies

Predicting the useful energy recovered from waste heat is necessary to determine the potential in industrial waste heat. The modelling approach used in this work for the five thermodynamic cycles combined both physical models and empirically based models. Physical models based on thermodynamics identify the ideal performance of technologies. Rigorous simulations in Aspen HYSYS and from thermodynamic data in literature were used to determine the real performance. Empirical based models used to relate the real performance with the ideal performance. The analysis shows that the ratio of the real to the ideal performance is not constant; it depends on the inefficiencies in the cycle's components and the non-ideal behaviour of working fluids.

The models presented in this research show good agreement with rigorous simulation and thermodynamic design data. The models can analyse multiple heat sources and sinks for recovered energy. The models are also easy to integrate with a variety of energy systems and optimization frameworks. The advantage of these novel models is that they enable the designer to be aware of the maximum possible performance.

Screening and selection of working fluids was also performed for the ORC and MHP. Results show that dry fluids are more efficient than isentropic fluids for the ORC. In this analysis, cyclopentane and benzene have the highest efficiency. Even though benzene shows higher thermal efficiency, the condensation pressure is below atmospheric pressure. This could result in ambient air leakage into the system, thereby reducing the thermodynamic efficiency. For the MHP, n-butane had the highest coefficient of performance up to condensing temperatures of 135°C and water performed best above that temperature.

The waste heat recovery technologies considered in this work can also be driven by solar energy, geothermal energy and biomass. The models developed are useful in such applications.

7.1.2 Comparative analysis of waste heat recovery technologies based on exergy degradation

All thermodynamic cycles have an ideal performance and an actual (real) performance often calculated based on conservation of energy quantity. The ideal performance shows the maximum achievable, while the real performance accounts for inefficiencies in the cycle components, and working fluids non-ideal behaviour. However, the real performance based on conservation of energy quantity does not account for degradation of heat sources as a result of heat transfer. The real performance also assumes that heat and work are equal entities.

Adjusting the real performance to consider irreversibilities due to finite temperature heat transfer is vital to compare technologies involved in multiple energy form interactions. In this work, the deviation of the adjusted real performance from the ideal performance i.e. exergy degradation, was used to compare and rank technology options. This method of comparison is a thermodynamically sound approach since it shows the true capability of each technology, technologies are compared on the same basis, and heat and power are not assumed to be equal entities.

In this work, waste heat is defined as the residual heat after heat recovery within a process (using Pinch Analysis) or between several processing units via the site utility system (using Total Site Analysis). Even though recovery via heat exchange is easy to implement, it is still necessary to compare this with other technology options. Such comparison has not been done before.

To compare all five thermodynamic cycles and heat recovery via heat exchange, a novel screening tool was developed showing the exergy degradation versus heat source temperature. Better temperature matching can reduce irreversibilities due to heat transfer. Some useful insights deduced from applying the tool to a range of heat source temperatures (ambient to 260°C) are:

- To minimize exergy degradation in AHP, AHT, AbC, the heat source temperature to separate the refrigerant/absorbent mixture in the generators should be a minimum temperature difference hotter than the generator temperature.
- To minimize exergy degradation in MHP, the heat sink temperature should be a minimum temperature difference colder than the condenser temperature. Also, the maximum temperature lift should be 70°C.
- The exergy degradation for heat recovery via heat exchange is lowest when the difference between the heat source and sink temperatures are minimized. This finding agrees with the fundamental of PA and TSA. Based on the results, generating hot water (at 50°C) from a heat source at 200°C is not the best option, compared to using the heat to drive an AbC, generating power through an ORC, upgrading the heat to higher temperatures via a MHP or to drive an AHP for low temperature heat upgrade.
- For the range of heat source temperatures considered in the comparative analysis, heat recovery via heat exchange has the smallest exergy degradation above 93°C (assuming a minimum temperature difference between heat source and sink), absorption chillers between 70 – 93°C, organic Rankine cycles from 66 – 70°C, heat recovery via heat exchange from 50 – 66°C and mechanical heat pumps from ambient to 50°C.

Efficient utilization of waste heat is an important research field both from academic and industrial point of view. The presented screening tool can provide new technological insights in waste heat recovery and can be seen as a technical novelty.

7.1.3 Primary fuel Recovery Ratio (PRR) developed to evaluate the performance of heat upgrading technologies

Three heat pump cycles were considered in this work: MHP, AHP and AHT. The coefficient of performance (COP) has been used to evaluate the performance of heat pumps. However, the COP does not take into account the associated fuel consumption or its generation of waste heat from the high quality electrical power required by the MHP, nor does the COP take into account the impact of missed opportunities for steam generation when an AHP is used. This implies the impacts on connected systems are neglected when the COP is used as a performance indicator.

The PRR proposed in this work measures the reduction in primary fuel consumption as a result of low temperature waste heat upgrade. The PRR is a function of the COP, cogeneration efficiency, and electrical power generation efficiency. The indicator is shown to be useful for selecting a heat upgrade technology and the system temperatures. Higher savings in primary fuel were obtained using the PRR compared to the COP.

7.1.4 Hierarchical approach for evaluating waste heat utilization opportunities

This research shows that the end-use of energy recovered from waste heat determines the economics and potential to reduce CO_2 emissions. A ranking criterion measuring the economic potential associated with reduced CO_2 emissions from waste heat recovery was developed, and applied to evaluate and rank various on-site and off-site opportunities. The hierarchy depends on assumptions of capital and operating costs.

The ranking of on-site opportunities is: boiler feed water preheating (for a natural gas boiler); space heating; gas turbine compressor inlet air chilling; power to reduce import on-site; space cooling; chilling for site processes; coal boiler feed water preheating and power generation to reduce the cogeneration system fuel consumption. It was discovered that reducing the capital cost of the ORC (associated with reducing power import) makes it competitive with chilling the inlet air into a gas turbine compressor. A higher electrical power tariff also increases the ORC competitiveness. At high capital costs for all technologies, direct use of heat and gas turbine compressor inlet air chilling are still competitive, but the ORC becomes uneconomic.

The hierarchy of off-site opportunities is: hot water for export to a new neighbourhood; hot water to an existing neighbourhood and power generation for export. Heat export becomes uneconomic when investment in a district heating network is considered. Financial incentives can improve the economic viability of heat export. In countries with existing networks like Sweden, export of heat is economic (Eriksson et al. 2015). This hierarchical approach can be extended to include other end-uses not considered in this work.

7.1.5 Novel graphical tools for integrating waste heat recovery technologies

Novel graphical tools were developed for integrating ORC, AbC, AHP, AHT and MHP into process sites. First temperature enthalpy plots of the available waste heat were generated. Technologies are assigned to the temperature enthalpy plots at the ‘kinks’ and the amount of useful energy recovered is estimated using the models developed. The temperature at the kinks with the highest quantity of useful energy recovered is selected to exploit the waste heat. Graphical tools were also used to analyse the benefit from integrating multiple technologies, the impact of unlimited demand of recovered energy and finite demand.

The graphical tools show that waste heat utilization is not a homogenous problem. This implies that varying temperature and quantity of heat sources should be considered whether the heat sources are represented in a profile or as streams.

The tools can be applied in industry to evaluate the potential in industrial waste heat prior to detailed design and screen out non-viable options at the early design stage.

7.1.6 Optimization-based design of waste heat utilization systems

Benefits from industrial waste heat utilization depend on the quantity and temperature of heat sources, technology selected and associated working fluid, end-use of recovered energy and assumptions on costs. The problem is heterogeneous in nature. An optimization framework is developed to account for all these and explore different design approaches i.e. stand-alone (neglecting interactions with the site utility system) and ‘combined’ systems.

A multi-period MILP modelling framework is developed in Publication 5 for stand-alone design, considering both on-site and off-site end-uses of recovered energy. The time-dependent variations in the demand for heat export and electrical power tariff was also considered. The superstructure created represents multiple technology options and associated end-uses of recovered energy. The technology options considered are the ORC, AbC and heat exchangers for hot water generation and boiler feed water preheating. The objective was to maximize the economic potential i.e. difference between the financial benefits and total cost associated with the design. The schedule for operating each technology in the period selected was also generated.

Prior to this work, process integration of heat upgrade technologies did not consider interactions with the site utility system. Accounting for such interactions is necessary to predict the true value of hot utility saved and steam generated, capture trade-offs, allow use of energy recovered within the system and allow operational changes in the system to reduce waste heat generated.

A generic MILP model is also developed in Publication 6 for integrating the MHP, AHP and AHT into process sites incorporating the utility system. The model considers: (1) selection of streams quantity and temperature; (2) selection of end-uses of recovered energy, also accounting for varying quantity and temperature; (3) selection of technology options, (4) simultaneous optimization with the site utility system.

A superstructure containing the MHP, AHP and AHT, connected to multiple heat source streams and end-uses of recovered energy, including boiler feed water preheating, hot utility saving and steam generation into the site utility system was created. Integrating heat pumps was found to be uneconomic; therefore a sensitivity analysis was conducted by varying the capital costs and energy prices. This analysis shows that there is competition between upgrading heat to reduce fuel requirement and using the saved fuel to generate electrical power for export.

A generic conceptual design approach was developed in Publication 7 for design of site waste heat utilization systems, focusing on use of recovered energy within process sites. All five thermodynamic cycles and heat recovery via heat exchange are considered. The method is divided into four stages: (1) data extraction; (2) technology working fluid pre-screening; (3) model formulation and optimization and (4) design evaluation. In the design evaluation step, the global fuel savings, global CO_2 emissions, the economic potential and payback are measured. This step was useful to compare several approaches to reduce and utilize industrial waste heat. The approach includes operational optimization of the site utility system, stand-alone design of site waste heat utilization systems and the 'combined' systems design. Analysis shows that benefits from waste heat utilization increase when interactions with the existing utility system are exploited.

7.1.7 Application of the methodological framework to industrial case studies

Two case studies are presented in this work. The first case study is for a medium scale petroleum refinery (Fraser and Gillespie, 1992). In this case study, heat recovery within a processing unit, and the several processing units via the site utility system is already maximized. However, about 49.8% of the total energy inputs are wasted as thermal energy and 76.5% of the waste heat is from the site utility system.

The potential in industrial waste heat from this site was evaluated by integrating technologies using waste heat as the primary energy source in Publication 1. The technologies include the ORC, AbC and AHP. For the ORC, the cycle performance increases with heat source temperature; however less heat is available at high temperatures than at low temperatures.

Integrating the ORC generated 19,270 kW of electrical power from all the available waste heat. The power generated had potential to increase the site energy efficiency by 9%. Integrating the AbC increases the site energy efficiency by 13.5% for unlimited demand for chilling. Integrating an AHP for hot water generation at 80°C increased the site energy efficiency by 24% for unlimited demand for heating, and 1.2% when the demand for hot water is considered. A novel approach was introduced to explore integrating more than one technology. Integrating all three technologies to exploit waste heat increases the site energy efficiency by 33% (unlimited demand for recovered energy) and 10% (finite demand for recovered energy).

The case study shows there is potential to improve a process sites' energy efficiency by waste heat utilization, and improve availability of energy sources since fuel is saved. The case study also shows that even for process sites that have attained their maximum potential for heat recovery, waste heat utilization yields additional increases in efficiency in fuel consumption.

The same refinery case is presented in Publication 2 to explore the potential for heat upgrade. In this case, different heat sink temperatures are considered for reducing hot utility. The objective was to integrate heat pumping technology options such as MHP, AHP and AHT to upgrade waste heat to reduce hot utility requirement. The primary fuel recovery ratio is used to determine which technology to use and to select working conditions for each technology. Results show that the applying the PRR yields 9.2% additional savings in fuel compared to using the COP. Results of this case study also show that there is potential to reduce primary fuel consumption and associated CO_2 emissions from heat upgrade even when a site is pinched.

The same case is studied in publication 6, where a MILP model is developed for integrating heat upgrading technologies into process sites. The utility system was optimized simultaneously to determine the value of hot utility saved, steam generated and boiler feed water preheating. Taking into account economics, the AHT is selected for boiler feed water preheating reducing CO_2 emissions by 1.2%, AHT also selected to reduce low pressure steam required reducing CO_2 emissions by 14.6%. The MHP was selected to reduce medium pressure steam required, and to generate low pressure and medium pressure steam into the site utility system; reducing CO_2 emissions by 15.6%, 16.3% and 20.4% respectively. The economics of the design is sensitive to the difference between the electrical power price and the fuel price. When fuel is expensive relative to power, integration of heat pumps is more economic. When power is expensive relative to fuel, the utility system begins to export power to increase revenue, making waste heat upgraded uneconomic.

To assess the impact of end-uses, the ranking criterion is applied to the same case in publication 4 where finite demand for recovered energy was accounted for. When opportunities such as gas turbine compressor inlet air chilling, chilling for the site processes and boiler feed water preheating are considered, 16% useful energy is recovered, CO_2 emissions reduce by 11% and site operating costs reduces by 17%. When off-site opportunities, such as heat export to existing buildings and power export are considered, CO_2 emissions reduce by 10%, 11% useful energy is recovered and site operating costs reduce by 13%. This economic evaluation includes capital investment in the associated technologies but excludes capital investment in the heat network. Including investment makes heat export uneconomic.

The analysis also shows there are higher benefits in considering more end-uses of recovered energy; however, demand for recovered energy is a limitation.

The same refinery case is studied in publication 5, where a multi-period MILP model developed was applied. The results show that exploiting all the available waste heat for chilling provision, boiler feed water preheating, hot water for export, and electrical power export could reduce CO_2 emissions by 15.6%, operating costs by 21.5% (excluding investments in the heating network) and 22% useful energy is recovered. These economic benefits depend on assumptions of installed capital costs and operating costs. The multi-period MILP model is still applicable when assumptions change.

In summary, the refinery case study results shows that for process sites that have attained the maximum potential for heat recovery, there is still potential to improve energy security locally and globally from waste heat utilization. However, is it always thermodynamically efficient to exploit heat recovery via heat exchange first?

This question is answered through an illustration provided in Publication 3. A comparative analysis was performed based on exergy degradation. Results indicate that a minimum temperature difference minimizes exergy degradation in heat exchangers. The exergy degradation can also be minimized by better temperature matching between heat sources and the technology options, and heat sinks and technology options. For the heat source temperature range considered from ambient to 260°C, In order to minimize exergy degradation, heat recovery via heat exchange should be considered above 93°C and between 50 – 66°C, subject to a minimum temperature difference.

The second case study is for a chemical production site (found in publication 7). Three processing units for intermediate production of high value polymers are considered. Heat recovery is not maximized within and between processing units. The majority of the waste heat is from the site processing units and the utility system is a steam-only system. The model for the utility system was validated against operating data provided by the company with errors less than 3%. The MILP model developed can be modified to explore three different approaches to reduce and utilize the available waste heat: operational optimization of the site utility system, stand-alone design of the waste heat utilization system and combined systems design. Operational optimization was shown to have potential to reduce costs by 12%, fuel consumption by 10.6%, CO_2 emissions by 13% with no payback. The stand-alone design reduces costs by 10%, fuel consumption by 29.36%, CO_2 emissions by 20.53% with a payback of 4 years. The sensitivity of the economics to capital costs explored by varying the retrofit factor shows that the design no longer has an economic potential when the retrofit factor is increased from 3 to 4.5. A combined systems approach reduces operating costs by 37%, fuel consumption by 54%, CO_2 emissions by 53% with a 2 year payback period and the solutions remains economically attractive even when the retrofit factor increases. From the analysis operational optimization of site utility systems reduces the quantity of waste heat, but the temperature remains the same. Stand-alone and combined systems design approaches has potential to reduce the quantity and temperature of waste heat. The financial benefits obtained depends on assumptions of costs, the methodology can be applied when assumptions change.

In summary, the results from the case studies show that:

- There is still potential to improve the availability, acceptability and affordability of energy when heat recovery within a single processing unit and multiple processing units has been maximized.
- In process sites where heat recovery within a single processing unit and multiple processing units are not maximized, the methodological approach presented in this work can explore numerous options to exploit the residual waste heat.
- There are more benefits from a systems approach to integrating waste heat recovery in process sites.
- The economics of integrating heat pumps depends on the difference between the electrical power price and the fuel price.
- Financial benefits of integrating an ORC depend on the electricity tariff and tariff structure.

The results from applying the developed methodological framework to the case studies provide an understanding of the heterogeneous nature of waste heat recovery. Practical issues such as space available in process sites to incorporate the technologies and control issues need to be considered before implementation.

7. 2. Future work

A critical evaluation of the work presented in this thesis reveals areas that deserve further study and recommendations are also provided to advance research into integrating waste heat recovery in process sites. Further areas of research should address:

7.2.1 Waste heat source stream representation

To analyse the varying quantity and temperature of waste heat sources, temperature intervals were introduced on each stream between the supply and target temperatures. Binary variables were attached to the temperature intervals in order to produce a linear representation of streams. Future work should explore the benefits of assigning the temperatures as operational variables, making the problem an MINLP one. This could introduce additional degrees of freedom to improve benefits.

This present work only considered the supply temperature, target temperature and heat contained in streams. Future work should consider the composition and phase of heat source streams. The stream composition will affect the choice of materials for waste heat recovery technologies, and phases of streams determine the thermal conductivity and heat capacity.

7.2.2 Improved capital cost models for waste heat recovery technologies

Simple economic models are used for installed capital costs and sensitivity analyses were performed to show the impact of uncertainties. More detailed installed capital models are not used because the methodology presented in this work is intended for conceptual studies. The future work in this area is the development of economic models to show the influence of economics of scale, and impact on the type of technology components.

7.2.3 Considering other end-uses of recovered energy

The end-uses of recovered energy considered were limited to energy-related uses, for example electrical power for export, chilling and steam generation into the site utility system. Future work should consider other opportunities to exploit industrial waste heat, e.g.: (1) waste heat in desalination processes, (2) use of recovered energy for light ends recovery in refining processes and (3) use of waste heat for hydrogen production. Hydrogen is considered as a carbon neutral fuel and there are currently investments in use of hydrogen for vehicles. Also chemical, petrochemical and fertilizer industries consume hydrogen for various applications.

7.2.4 Explore benefits from revamping the utility system

The interactions with the existing site utility system were explored without revamping the system (i.e. changing the temperatures and pressure of steam distribution levels, changing the choice of technologies and fuel). A complete revamp may provide more savings but would introduce more complications. A revamp will also affect the entire site and long shut down periods may be required. Future work should aim to identify potential benefits from a revamp of the site utility system.

7.2.5 Multi-objective optimization framework for 'combined' systems design

This research has shown that there is potential in industrial waste heat to improve the energy efficiency, reduce CO_2 emissions and costs (i.e. improve energy security) in existing industrial sites. This implies that the three dimensions of energy security could be implemented in a Multi-Objective Optimization (MOO) framework which could assist in evaluation of optimal trade-offs solutions that balance several criteria. Future work should aim to explore the benefits from an MOO framework for design of waste heat recovery systems. A challenge is the increase in the computational burden and problem dimension due to the number of objectives. It is possible to reduce the problem dimension since some objectives may behave in a non-conflicting manner.

The major challenge in any MOO framework for waste heat utilization is the basis for which design inputs such as costs and emission factors are derived. The existing basis is conservation of energy quantity i.e. assuming that heat and power are equal entities and neglecting irreversibilities due to finite temperature heat transfer. This is one of the reasons why there is a considerable amount of waste heat in process sites. Therefore before applying MOO frameworks there is need to develop design inputs based on conservation of energy quantity and accounting for energy quality degradation since multiple form energy interactions occur.

7.2.6 Part-load performance of waste heat recovery technologies

The explicit thermodynamic models of waste heat recovery technologies developed in this work assume that the technologies will always operate at full loads. However, the performance of waste heat recovery technologies may vary with applied load. The future work in this area is the extension of the models to show a good description of the performance at some specified load values below 100%. This is necessary to improve the flexibility of the models to handle uncertainties in demand for recovered energy.

7.2.7 Extrapolation of results to inform government policies

The methodological framework developed in this work is able to predict the potential in industrial waste heat. Future work in this area is the application of the methodology to several industrial case studies under different scenarios. Results can be aggregated and scaled up to quantity the opportunity for waste heat recovery in process industries. This can inform policies on reducing CO_2 emissions and improving energy efficiency across the UK.

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