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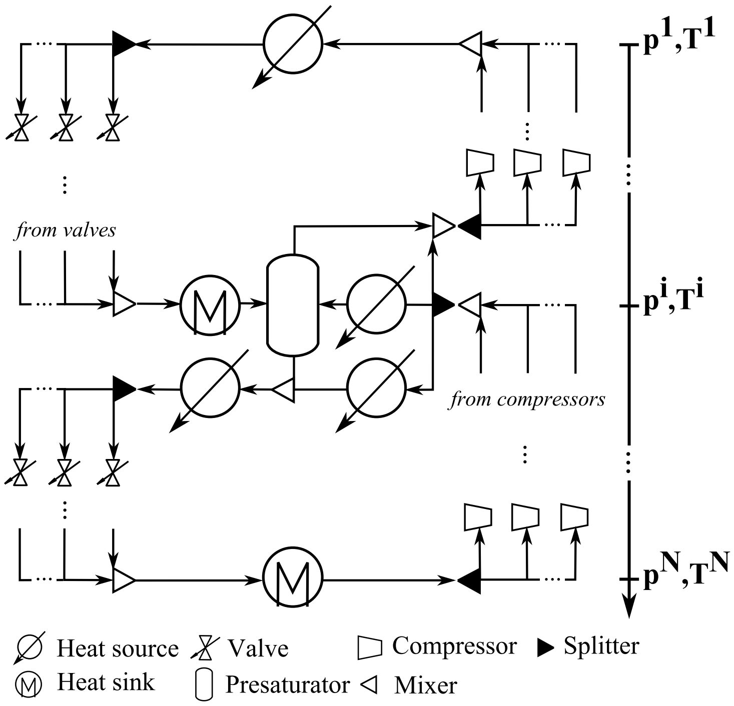
Department of the Environment, Transport, Energy and Communication DETEC

Swiss Federal Office of Energy SFOE
Energy Research

Final report dated 30/07/2020

Integrated industrial heat pump systems

Background, software development & Swiss potentials



Date: 30/07/2020
Location: Bern

Publisher:
Swiss Federal Office of Energy SFOE
Energy Research and Cleantech
CH-3003 Bern
www.bfe.admin.ch

Co-financing:
SCCER-EIP (Efficiency in Industrial Processes) – CTI

Subsidy recipient:
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SFOE contract number: SI/501487-01

Zusammenfassung

Wärmepumpen gewinnen nicht nur bei Anwendungen im Wohnbereich, sondern auch für die Verbesserung der industriellen Energieeffizienz durch die Rückgewinnung und die Verwertung von Abwärme bei höheren Temperaturen zunehmend an Bedeutung [1, 2]. Durch eine systematische Integration von Wärmepumpen können die Umweltauswirkungen industrieller Prozesse verringert werden, indem die Energieeffizienz verbessert und die Elektrifizierung erhöht werden. Dies hilft, die Ziele der Schweizer Energie-und Umweltpolitik zu erreichen.

Eine falsche Integration kann jedoch auch zu einer erhöhten Umweltbelastung führen. Obwohl die Theorie, die technische Realisierung und die wirtschaftlichen Vorteile korrekt integrierter Industrie-Wärmepumpen erfolgreich demonstriert wurden [2–4], fehlt es immer noch an Anwendungen in grossem Massstab [2–4]. Die Gründe dafür wurden in den folgenden vier Punkten [2, 5] identifiziert.

1. Die theoretischen Prinzipien sind zu wenig bekannt und es fehlen Arbeitsinstrumente, welche diese basierend auf umfassenden Datengrundlagen und Modellen umsetzen.
2. Mangelnde Sensibilisierung und Schulung von Planern und Ingenieuren
3. Fehlende Sichtbarkeit durch (viele) öffentlich verfügbare *beste* Referenzbeispiele
4. Die Potentiale und die Branchen, wo Wärmepumpen erfolgreich integriert werden können, sind nicht abgeschätzt und identifiziert.

Im vorliegenden, vom BFE unterstützten Projekt, das auch Teil des IEA HTP Annex 48 “Industrial Heat Pumps Second Phase” ist, wurden die Punkte (1), (2) und (4) behandelt. Punkt (3) wurde in einem weiteren vom BFE-unterstützten Projekt[1] bearbeitet.

Punkt (1) wurde behandelt, indem ein Überblick über theoretische Prinzipien, nützliche Methoden und vorhandene Tools für die korrekte Integration von Wärmepumpen erarbeitet wurde. Es wurde eine Reihe von Integrationsrichtlinien entwickelt, die anhand einer Fallstudie demonstriert wurden. Die Ergebnisse sind in Kapitel 2 und im Abschlussbericht des IEA HPT Annex 48 aufgeführt und wurden auf zahlreichen Konferenzen vorgestellt, womit zu Punkt (2) beigetragen wurde. Es konnte gezeigt werden, dass eine Vielzahl von Tools für unterschiedliche Fachkenntnisse zur Verfügung steht, und dass die Verwendung einfacher Prinzipien bereits wichtige Verbesserungen hinsichtlich der energetischen Effizienz und der Umweltbelastung im Vergleich zu einem "naiven" Ansatz bewirken kann.

Aus der Analyse der Tools ergab sich, dass eine weitere Entwicklung für integrierte Tools zur Konstruktion von Wärmepumpen erforderlich ist, um ihr volles Potenzial auszuschöpfen. Aus diesem Grund wurde im Rahmen dieses Projekts ein neuartiges Auslegungs-Tool für industrielle Wärmepumpen entwickelt, das in Kapitel 3 vorgestellt wird. Das Tool ermöglicht ein optimales integriertes industrielles Wärmepumpendesign unter umfassender Berücksichtigung verschiedener Wärmepumpeneigenschaften sowie der Auswahl von Kältemitteln und Kompressoren. Die Methode wurde mit Referenzfällen aus der Literatur verglichen. Unter Einbezug einer umfassenden Liste an Wärmepumpeneigenschaften wurden damit Verbesserungen zwischen 5 bis 30% im Vergleich zu den zuvor optimalen Lösungen erzielt.

Als Antwort auf Punkt (4) wurde das neu entwickelte Tool verwendet, um die Einsparpotentiale durch Wärmerückgewinnung (WR) und Wärmepumpenintegration (WPI) in verschiedenen Schweizer Industriesektoren abzuschätzen. Dies wird in Kapitel 4 beschrieben. Es wurde festgestellt, dass vor allem im Lebensmittel- und Getränkesektor eine grosse Reduktion der Treibhausgas-Emissionen erzielt werden kann. Es sind Reduktionen von 25% (konservativ: keine Extrapolation) oder 58% (optimistisch: Extrapolation) möglich. Es folgt der chemische Sektor, in dem 90% der Reduktionspotenziale, die zwischen 21% (konservativ) und 74% (optimistisch) liegen, durch Wärmerückgewinning erreichbar sind.

[1] Ein wichtiges Ziel des IEA HPT Annex 48 ist (beste Referenz-) Beispiele für die Integration von Wärmepumpen in der Industrie zu identifizieren. Ein separates BFE-Projekt (SI/501782-01) hat im Annex 48 mitgearbeitet, um diese Aufgabe für die Schweiz durchzuführen

Résumé

Les pompes à chaleur deviennent de plus en plus importantes pas seulement pour les applications domestiques, mais aussi pour améliorer l'efficacité énergétique industrielle grâce à la récupération et recyclage de la chaleur perdue à des températures élevées [1, 2]. L'intégration systématique des pompes à chaleur peut réduire l'impact environnemental des processus industriels en améliorant l'efficacité des processus et en augmentant l'électrification industrielle afin d'atteindre les objectifs de la transition énergétique suisse.

Cependant, une mauvaise intégration peut même entraîner une augmentation de la pollution de l'environnement. Bien que la théorie, la mise en œuvre technique et les avantages économiques des systèmes de pompes à chaleur industriels correctement intégrés aient été démontrés avec succès [2–4], il n'y a toujours pas d'application à grande échelle [2–4]. Les raisons ont été identifiées dans les quatre points suivants [2, 5].

1. Un besoin général de clarifier les principes théoriques et les outils disponibles ainsi que les méthodes complètes
2. Sensibilisation et formation des planificateurs et ingénieurs
3. Visibilité accrue grâce à (plus) d'exemples de référence accessibles au public
4. Besoin d'estimations du potentiel d'intégration de la pompe à chaleur pour identifier les industries les plus prometteuses pour l'application

Le projet soutenu par l'OFEN, qui a aussi participé à l'annexe 48 (phase II) du IEA sur les pompes à chaleur industrielles, traite les points (1), (2) et (4). Le point (3) fait partie d'un projet partenaire soutenu par l'OFEN[1].

Le point (1) a été traité en donnant un aperçu des principes théoriques, des méthodes utiles et des outils existants pour l'intégration correcte des pompes à chaleur. Des directives d'intégration ont été développées et démontrées à l'aide d'une étude de cas. Les résultats sont répertoriés dans le chapitre 2 et dans le rapport final de l'annexe 48 et ont été présentés lors de nombreuses conférences, qui ont été discutées au point (2). Il pourrait être démontré qu'une variété d'outils sont disponibles pour différentes connaissances spécialisées et que l'utilisation de principes simples peut déjà apporter des améliorations importantes en termes d'efficacité énergétique et de pollution de l'environnement par rapport à une approche "naïve".

L'analyse des outils a montré que de nouveaux développements d'outils intégrés pour la construction de pompes à chaleur étaient nécessaires pour atteindre leur plein potentiel. Pour cette raison, un nouvel outil de conception de pompes à chaleur industrielles a été développé dans le cadre de ce projet, qui est présenté dans le chapitre 3. L'outil développé permet une conception de pompe à chaleur industrielle intégrée de manière optimale avec une prise en compte approfondie des différentes propriétés de la pompe à chaleur ainsi que la sélection des liquides de refroidissement et des compresseurs. La méthode a été comparée sur la base des cas de référence de la littérature, où des améliorations entre 5 et 30% par rapport aux solutions précédemment optimales ont été obtenues en considérant une liste plus complète des propriétés de la pompe à chaleur.

En réponse au point (4), l'outil développé a été utilisé pour estimer le potentiel d'économies grâce à la récupération de chaleur (RC) et à l'intégration de pompes à chaleur (PC) dans les divers secteurs industriels. Ceci est décrit dans le chapitre 4. Il a été constaté que les principales économies d'émissions sont réalisables dans le secteur de l'alimentation et des boissons, où des améliorations de 25% (conservatif: pas d'extrapolation) ou 58% (optimiste: extrapolation) sont possibles. Vient ensuite le secteur chimique, dans lequel 90% du potentiel d'économies est réalisé grâce à la récupération de chaleur et se situe entre 21% (conservatif) et 74% (optimiste).

[1] Une grande partie de l'annexe 48 vise à fournir des exemples pour l'intégration des pompes à chaleur dans l'industrie adresser le point (3). Un projet OFEN distinct (SI / 501782-01) a participé à l'annexe 48 pour traiter cette tâche pour la Suisse

Summary

Heat pumping is gaining increasing attention, not only for household applications, but for improving industrial energy efficiency through waste heat recovery and valorisation at elevated temperatures [1, 2]. Through systematic heat pump integration, the environmental impact of industrial processes can be reduced by improving process efficiency and increasing electrification to meet the goals of the Swiss energy transition.

However, if integration is not performed correctly the environmental impact may actually be increased. Although the theory, technical realisation, and economic benefits of correctly integrated industrial heat pump systems have been successfully demonstrated [2–4], application on a broad scale is still lacking [5]. The reasons for marginal penetration of well-integrated systems (disregarding standard industrial refrigeration and HVAC applications) were identified in the following four points [2, 5].

1. A general need for clarification of theoretical principles and available tools together with comprehensive methods
2. Raising of awareness and training of planners and engineers
3. Proof-of-concept through (more) publicly available best reference examples
4. A need for estimates of heat pump integration potentials to identify the most promising industries for application

The underlying SFOE-supported project which also participated in the IEA HPT Annex 48 (Phase II) has addressed points (1), (2), and (4). Point (3) was addressed in a partnered SFOE project[1].

Point (1) was treated by providing an overview of the theoretical principles, useful methods and commercially available tools for correct heat pump integration. A set of integration guidelines was developed, which were demonstrated on a case study. The results are detailed in **background: theoretical principles & useful tools** (section 2) and in the IEA HPT Annex 48 final report and were further presented in numerous conferences, thereby addressing point (2). It could be demonstrated that a variety of tools are available for diverse levels of expertise and that the use of simple principles can already generate important improvements in terms of energetic efficiency and environmental impact compared to a "naive" approach.

From the analysis of tools, it resulted that further developments for integrated heat pump design tools were necessary to realise their full potential. Therefore, further addressing point (1), a novel industrial heat pump design tool was developed throughout this project which is presented in **software development: integrated design tool** (section 3). The developed tool enables optimal integrated industrial heat pump design considering heat pump features in a comprehensive manner, as well as fluid and compressor selection. The method was benchmarked on reference cases from the literature [6–8] yielding between 5 and 30% improvements compared to the previously optimal solutions by considering a more comprehensive list of heat pump features.

In response to point (4), the developed tool was used to estimate the saving potentials through heat recovery (HR) and heat pump integration in various industrial sectors, which is described in **swiss potentials** (section 4). It was found that the main carbon dioxide equivalent (CO_2-eq.) emission reduction potentials through HR and heat pump integration are achievable in the food & beverage sector, yielding improvements of 25% (conservative: no extrapolation) or 58% (optimistic: extrapolation). This is followed by the chemical sector, where 90% of the saving potentials are achieved through heat recovery (HR), reaching between 21 (conservative) and 74% (optimistic). For the entire **industrial sector**, improvements of 6%-47% could be achieved through HR, while 3%-21% additional savings could be unlocked by heat pump (HP) integration, amounting to a total of 9%-68% reduction potential in CO_2-eq. emissions. This highlights a large uncertainty related to the diversity of the industrial sector. These findings also reveal a large uncharted potential which should be explored in more detail.

[1] A large fraction of the IEA HPT Annex 48 has aimed at identifying (best reference) examples of heat pump integration in industry, thus addressing point (3). A separate SFOE project (SI/501782-01) has participated in the Annex to conduct this task for Switzerland

Highlights

- This project identified paths to reduce the environmental impact of industrial processes through correct heat pump integration
- The barriers for large-scale application were identified and several steps were undertaken to overcome these, namely:
  1. Clarification of theoretical principles
  2. A novel heat pump pre-design tool was developed
  3. With help of the developed tool, an analysis of heat pump potential in the main five Swiss industrial sectors
- The most promising **industrial sector** for heat pump integration was characterised as the food & beverage sector, yielding an overall carbon mitigation potential between 25%-58%[1] with payback times between 3 and 6 years, followed by the chemical sector with total improvements between 21-74% (mainly due to HR)
- For the entire **industrial sector** improvements in the direct carbon emissions of 6%-47% could be achieved through HR, while 3%-21% additional savings could be achieved through HP integration, amounting to a total CO_2-eq. emissions reduction potential of 9%-68%.
- The developed methods also allowed identification of the most promising compressor and refrigerant types recommended for further research: The five **compressors types** present among the best results of each process: twin screw, GFB radial, centrifugal, mono screw, and liquid ring. The four **fluid types**: R1233zd(E), R1234ze(Z), R600a, and water.

[1] *Note:* The ranges reflect the difference between the *conservative* assumption that only the investigated processes can be improved; and the *optimistic* assumption that the emission reductions of the investigated processes are representative of the entire sector.

Main findings

With an increasingly imperative need for action to reach climate goals, industry is asked to face their responsibilities and reduce their environmental impact. This project identified paths to reduce the environmental impact of industrial processes through correct heat pump integration. The barriers for widescale application were identified and several steps were undertaken to overcome these, most importantly:

(1) **Clarification of theoretical principles** for *correct* heat pump integration. Development of guidelines and overview of tools which aid during the planning phase
(2) Using the developed tools and methods, an **analysis of heat pump potentials in industrial processes** was conducted in the five most energy intensive Swiss industrial sectors, while considering also their heat recovery (HR) potential

Addressing (1), it was clarified that the benefits of industrial heat pump integration are only valid if the design follows a set energetic principles. If these principles are not respected and, thus, heat pump systems are not well integrated, the environmental impact and energetic performance of the process may actually deteriorate.
The principles refer to the coefficient of performance (COP) of the heat pump system, and to the concept of *excess* and *useful heat*. The COP of a heat pump describes the ratio of thermal energy provided (heating and/or cooling) over electricity required. If this ratio is lower than 2, the environmental impact of the process may actually increase through heat pump integration. Similarly, if the heat pump does not upgrade *excess heat* to produce *useful heat* it will be ineffective. **Pinch analysis (PA)** is a methodology developed by Linnhoff and Flower [9, 10], which allows estimation of the maximum heat recovery potential, required *useful heat*, and available *excess heat* in industrial processes. With PA, the so-called grand composite curve (GCC) can be derived, depicted in Figure 7(b) which displays the net thermodynamic requirements of the process. This allows identification of the pinch point or pinch temperature[1]. Above the pinch, the process exhibits a net heating requirement, and below, a net cooling requirement; meaning that: only heat provided to the process above the pinch temperature is classified as *useful heat*, while the heat available below the pinch is defined as *excess heat*. Following these principles, correctly placed **heat pumps (HPs)** need to be installed across the pinch, with the evaporator below and the condenser above the pinch temperature, as shown for different heat pump types in Figure 9.

The tools and methods developed in this project were used to estimate the saving potentials through heat recovery (HR) and HP integration in various Swiss industrial sectors, thus addressing point (2). Figure 38 shows that the most promising **industrial sector** for HP integration was found to be the food & beverage sector, yielding carbon mitigation potentials between 18%-42%[2] by optimised HP integration and 7%-16% by improved HR, which amounts to a total reduction potential of 25-58%, with payback times between 3 and 6 years. This is followed by the chemical sector, where most saving potentials are achieved through HR 19%-67% (HP 2%-8%), reaching a total of 22%-74% emission reduction potential (payback 2.1 years). For the entire **industrial sector**, improvements of 6%-47% could be achieved through HR, while 3%-21% additional savings could be unlocked by HP integration, amounting to a total of 9%-68% reduction potential in CO_2-eq. emissions. This highlights a large uncertainty related to the diversity of the industrial sector. These findings also reveal a large uncharted potential which should be explored in more detail. The developed methods also allowed identification of the most promising compressor and refrigerant types recommended for further research: The five **compressors types** present among the selected industrial HP integration cases were: twin screw, gaseous film bearing (GFB) radial, centrifugal, mono screw, and liquid ring. Centrifugal compressors are recommended for large HP systems whereas smaller applications included combinations of the other types. The four **fluid types** most present among the selected industrial HP integration cases were: R1233zd(E), R1234ze(Z), R600a, and water.

[1] The pinch point is marked by the impingement of the GCC on the temperature axis

The **added value** of the project lies in (1) providing a holistic methodology for consistent and optimised industrial HP integration, (2) identification of the most promising industries for HP integration in Switzerland (CH), and (3) illustrating potential benefits of heat pumping toward GWP reduction objectives for the Swiss energy transition 2050.

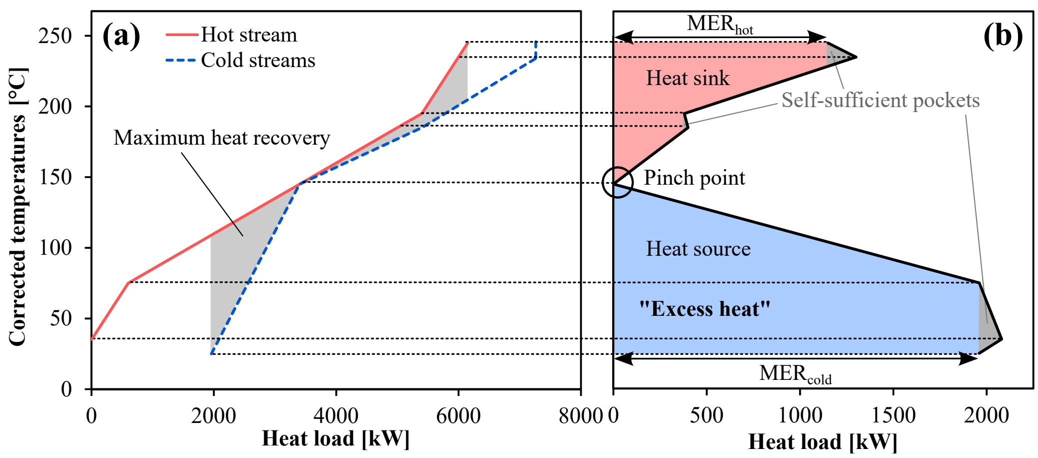

Figure 7 Temperature enthalpy diagram of (a) hot and cold composite curves (CCs), and (b) grand composite curve (GCC), reprinted from [16].

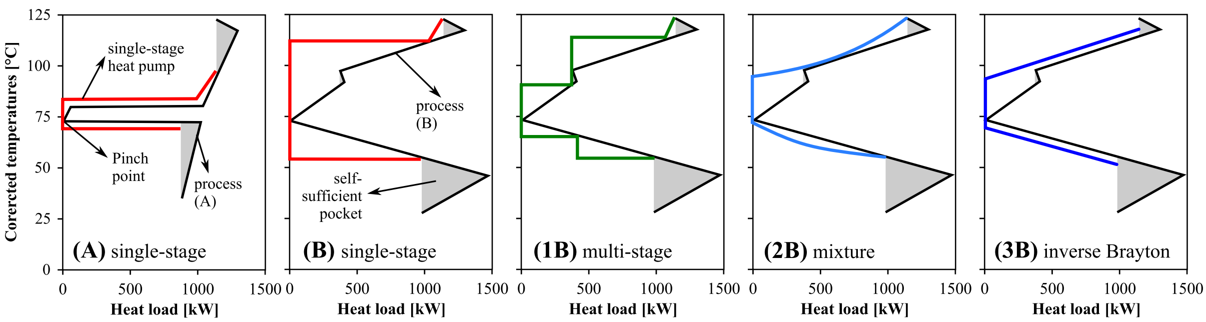

Figure 9 *Correct* heat pump integration across the pinch temperature for different process GCC; (A) single-stage HP, (B) single-stage HP, (1B) multi-stage HP, (2B) mixture HP, (3B) inverse Brayton HP.

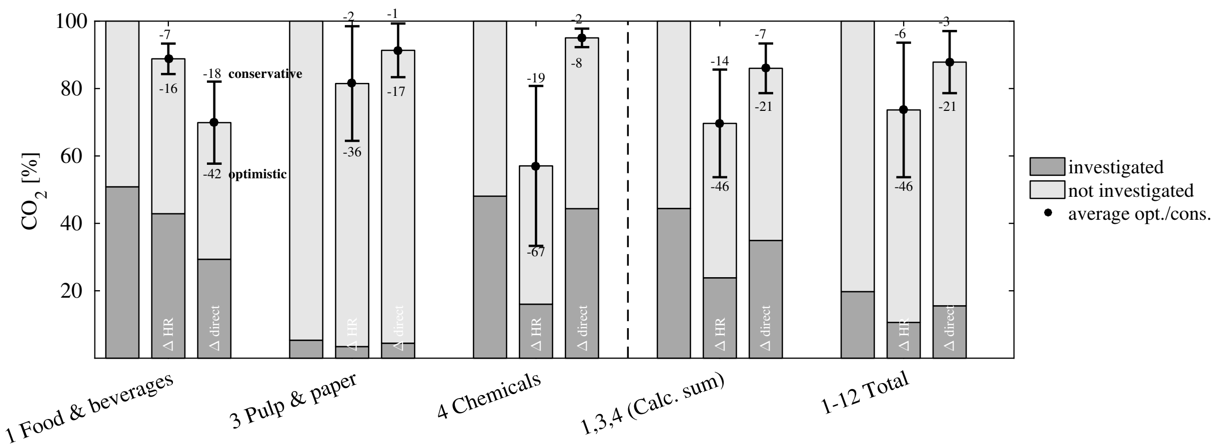

Figure 38 Sector relative CO_2-eq. emissions of (here) investigated processes and the rest, and reduction potential through heat recovery (ΔHR) and HP integration ($\Delta direct_{HP}$).

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Abbreviations

ADt	Air dried ton
AMB	Active magnetic bearing
AMPL	A Mathematical Programming Language [149]
BAU	Business as usual
BREF	European reference documents for best available techniques
capex	Annualized capital expenses
CC	Composite curve
CEPCI	Chemical Engineering Plant Cost Index [180]
CFC	Chlorofluorocarbon
CH	Switzerland
CHP	Combined heat and power
CO_2-eq.	Carbon dioxide equivalent
COP	Coefficient of performance
CPLEX	IBM ILOG CPLEX Optimization Studio [150]
EAF	Electric arch furnace
EIP	Efficiency of Industrial Processes
EL	Electricity
EO	Expert opinion
EU	European Union
FFB	Fluid film bearing
FOEN	Swiss Federal Office for the Environment
GCC	Grand composite curve
GFB	Gaseous film bearing
GUI	Graphical user interface
GWP	Global warming potential
GWP_{100}	Global warming potential for of time horizon 100 years
HC	Hydrocarbon
HCFC	Hydrochlorofluorocarbon
HEN	Heat exchanger network
HFC	Hydrofluorocarbon
HFO	Hydrofluoroolefin
HO	Hydroolefin
HP	Heat pump
HPR	Heat pumping and refrigeration
HPS	Heat pump superstructure
HPT	Heat Pumping Technologies
HR	Heat recovery
HVAC	Heating ventilation and air conditioning
ICC	Integrated composite curve
IDHL	Immediate danger to life or health [v/v]
IEA	International energy agency
IPESE	Industrial Process and Energy Systems Engineering

LP	Linear programming
MER	Minimum energy requirement
MILP	Mixed integer linear programming
MINLP	Mixed integer nonlinear programming
MOGA	Multi-objective genetic algorithm
MW	Molar weight [g/mol]
NLP	Nonlinear programming
NOGA	General classification of economic activities [97]
NR	Natural refrigerant
ODP	Ozone depletion potential
OECD	Organization for Economic Co-operation and Development
OEL	Occupational exposure limit
opex	Yearly operating expenses
ORC	Organic rankine cycle
PA	Pinch analysis
RAC	Refrigeration and air conditioning
REB	Rolling element bearing
SCCER	Swiss Competence Center for Energy Research
SEC	Specific energy consumption
SFOE	Swiss Federal Office of Energy
TAC	Total annualized costs
TEE	Thermal energy engineering
TH	Thermal energy
u-HCFC	Unsaturated hydrochlorofluorcarbon
u-HFC	Unsaturated hydrofluorocarbon

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1 Introduction: Integrated industrial heat pump systems

According to the Swiss Federal Office for the Environment (FOEN) [11], industrial processes account for 20% of Swiss carbon dioxide equivalent (CO_2-eq.) emissions, as displayed in Figure 1, with Swiss emissions totalling 47.2 Mt/year in 2017, or 5.6 t/cap. With an increasingly imperative need for actions to reach climate goals, industry is asked to face their responsibilities.

Reducing industrial emissions is most effectively achieved through energy efficiency measures, together with cleaner fuels, and a reduced demand for products by society. Assuming that the latter cannot be altered by industry alone, this study addresses the two former points.

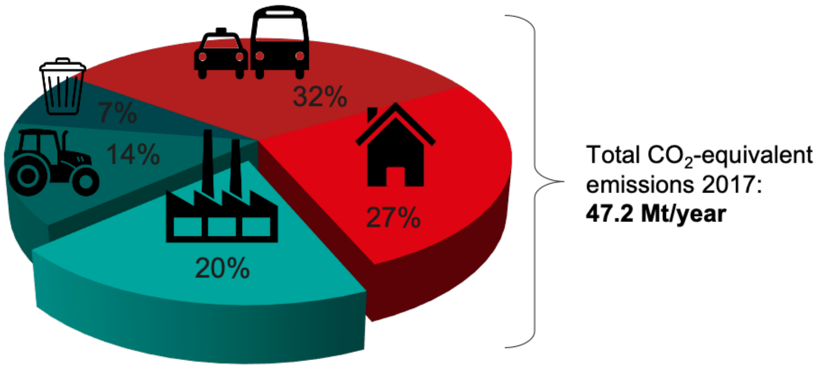


Figure 1: CO_2-eq. emissions of various sectors in CH 2017 [12]. From top (clockwise): transport, households, industry and services, agriculture, waste (incineration).

1.1 Apparent benefits

Integrated heat pump systems, as opposed to standard industrial refrigeration and HVAC applications, directly interact with processes by providing (ideally) simultaneous heating and cooling, thereby valorising excess heat. Such integrated systems provide avenues for industrial pursuit of process electrification and improved internal valorisation of excess heat, which would otherwise be rejected to the environment. Consequently, the environmental impact of industrial processes can be reduced through improved process efficiency and increased industrial electrification to meet goals of the Swiss energy transition. Electrified industry also unlocks various potentials for demand-side electricity management and flexibility, which become increasingly necessary with stochastic generation profiles of renewable electricity sources.

Figure 2 represents the various types of available heat pump technologies. This work focuses on open- and closed-cycle, mechanically driven heat pumps based on latent heat and single fluids.

A conceptual **representation of a *well* integrated industrial heat pump system** is presented in Figure 3. It shows an industrial process which requires **2 units of electricity**, **5 units of heat**, and releases **4 units of low temperature excess heat**. The electricity requirement can be satisfied by the electrical grid while the heat requirement can be provided by (3a) a burner requiring 6 units of gas; or (3b) a heat pump requiring 1 unit of electricity (to upgrade the 4 units of excess heat) **reducing the CO_2-eq. emissions by a factor of 5**[1].

[1] CO_2-eq. emission ratio in Switzerland [gas to electricity mix]: ≈ 2 according to Ecoinvent [13] (energetic basis), CO_2-eq. emissions original process: 6x2 + 2x1 = 14 units CO_2-eq., heat pump solution: 3 units, ratio = 14/3 $\approx$ 5

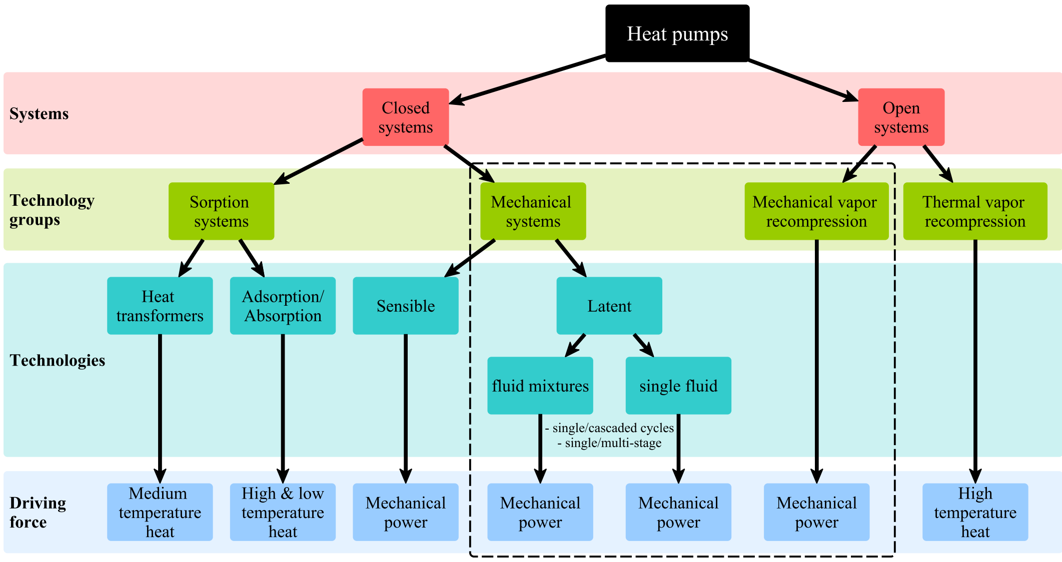
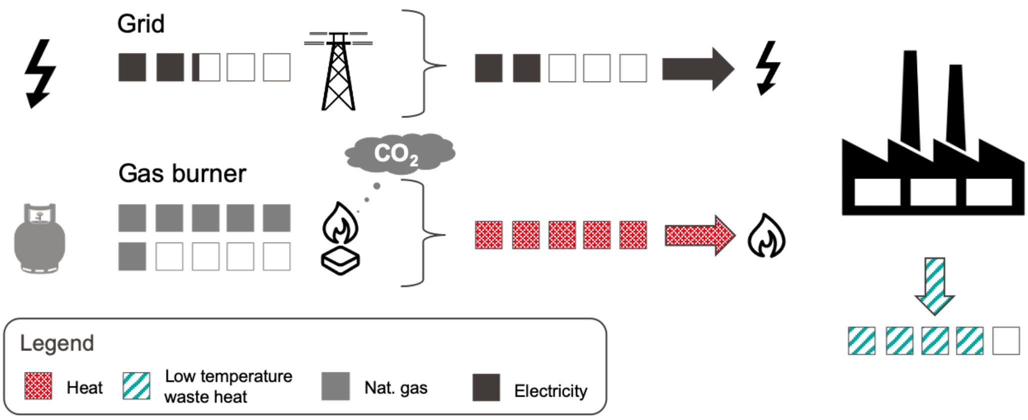
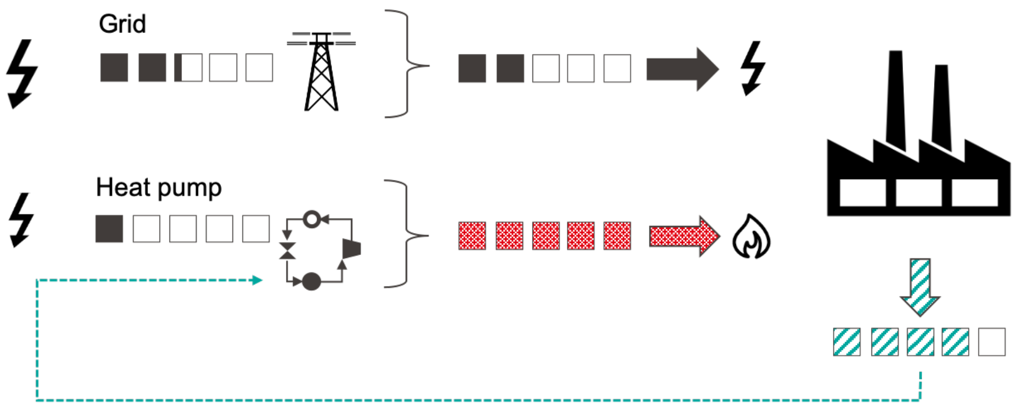


Figure 2: Heat pumping technology tree diagram, adapted from Nellissen and Wolf [14].



(a) Industrial process with standard utilities.



(b) Industrial process with *well* integrated heat pump.

Figure 3: Conceptual representation of *well* integrated industrial heat pump system.

1.2 Potential errors

As described previously, it can be concluded that integrated heat pump systems bring great environmental and energetic benefits to industrial processes. This statement is, however, only true if integration with the process follows a set of energetic principles. If these principles are not respected and, thus, heat pump systems are not well integrated, the environmental impact and energetic performance of the process may actually worsen.

The principles refer to the coefficient of performance (COP) of the heat pump system, and to the concept of *excess* and *useful heat*. The COP of a heat pump describes the ratio of thermal energy provided (heating and/or cooling) over electricity required. If this ratio is too low[1], the environmental impact of the process may actually increase through heat pump integration. Similarly, if the *excess heat* upgraded by the heat pump is not actually *excess heat*, meaning that the heat could serve the process needs instead, the heat pump integration might also be completely ineffective. And vice versa, if the heat produced by the heat pump is not actually *useful* for the process, meaning that e.g. process excess heat could satisfy this heat requirement, the heat pump might likewise not serve any purpose.

The principles behind proper heat pump integration are discussed in detail in **background: theoretical principles & useful tools** (section 2). This discussion simply highlights that despite great potential benefits, false conclusions might be drawn from insufficient investigation of heat pump integration potentials.

1.3 Barriers for broad application

Although the theory, technical realisation, and economic benefits of correctly-integrated industrial heat pump systems have been successfully demonstrated [2–4], large scale application is still lacking [5]. The reasons for the marginal penetration of well-integrated systems were identified in the following four points [2, 5].

1. A general need for clarification of theoretical principles and available tools together with comprehensive methods
2. Raising of awareness and training of planners and engineers
3. Proof-of-concept through (more) publicly available best reference examples
4. A need for estimates of heat pump integration potentials to identify the most promising industries for application

1.4 Motivation and structure of this report

The motivation for the underlying SFOE-supported project stems from the barriers identified in the previous section. The project also included participation in the IEA Technology Collaboration Program on Heat Pumping Technologies (HPT) Annex 48 (Phase II), which addressed points (1), (2), and (4). Point (3) was addressed in a partnered SFOE project[2].

Point (1) was treated by providing an overview of the theoretical principles, useful methods and commercially available tools for correct heat pump integration. A set of integration guidelines was developed, which were demonstrated on a case study. The results are detailed in **background: theoretical principles & useful tools** (section 2) and in the IEA HPT Annex 48 final report and were further presented in numerous conferences, thereby addressing point (2). It could be demonstrated that a variety of tools are available for diverse levels of expertise and that the use of simple principles can already generate important improvements in terms of energetic efficiency and environmental impact compared to a "naive" approach.

From the analysis of tools, it resulted that further developments for integrated heat pump design tools were necessary to realise their full potential. Therefore, further addressing point (1), a novel

[1] In Switzerland the COP should not be lower than 2 (for the heat pump to show better environmental impact than burning gas), see footnote 1, CO_2-eq. emission ratio [gas to electricity mix]

[2] A large fraction of the IEA HPT Annex 48 has aimed at identifying (best reference) examples of heat pump integration in industry, thus addressing point (3). A separate SFOE project (SI/501782-01) has participated in the Annex to conduct this task for Switzerland

industrial heat pump design tool was developed throughout this project which is presented in **software development: integrated design tool** (section 3). The developed tool enables optimal integrated industrial heat pump design considering heat pump features in a comprehensive manner, as well as fluid and compressor selection. The method was benchmarked on reference cases from the literature [6–8] yielding between 5 and 30% improvements compared to the previously optimal solutions by considering a more comprehensive list of heat pump features.

In response to point (4), the developed tool was used to estimate the saving potentials through heat recovery (HR) and heat pump integration in various industrial sectors, which is described in **swiss potentials** (section 4). It was found that the main CO_2-eq. emission reduction potentials through HR and heat pump integration are achievable in the food & beverage sector, yielding improvements of 25% (conservative: no extrapolation) or 58% (optimistic: extrapolation). This is followed by the chemical sector, where 90% of the saving potentials are achieved through heat recovery (HR), reaching between 21 (conservative) and 74% (optimistic). For the entire **industrial sector**, improvements of 6%-47% could be achieved through HR, while 3%-21% additional savings could be unlocked by HP integration, amounting to a total of 9%-68% reduction potential in CO_2-eq. emissions. This highlights a large uncertainty related to the diversity of the industrial sector. These findings also reveal a large uncharted potential which should be explored in more detail.

2 Background: Theoretical principles & useful tools

The total efforts undertaken for the IEA HPT Annex 48 and reported in this section are summarised in four points.

- The **theoretical principles** for systematic heat pump integration with industrial processes was efficiently summarised and presented in a concise manner (section 2.1).
- An analysis of **industrial heat pump integration tools** was conducted and an overview was provided in a single, comparative table (section 2.2).
- An easy-to-use set of **practical guidelines** for correct industrial heat pump integration was derived that can be used with or without tools and specific training (section 2.3).
- Use of existing tools and **application of guidelines along a case-study** was illustrated (section 2.4).

2.1 Theoretical principles

Figure 4 shows an onion diagram representing the hierarchical nature of the process energy conversion system as presented by Kemp [15], following the general approach to process synthesis. The main drivers of industrial processes are chemical reaction and separation steps (R, S), and are thus situated at the core for designing or optimising a process. The next step addresses internal heat recovery in the process (H) and finally, design or modification of the utility system should be considered (U). Assuming the process chemical reactor and separation systems are of state-of-the-art technologies, pinch analysis (PA) [9] addresses the final two steps in the onion diagram, providing a sound methodology to estimate the maximum heat recovery potential in a process, and the theoretical background for thermodynamically ideal placement of hot and cold utilities.

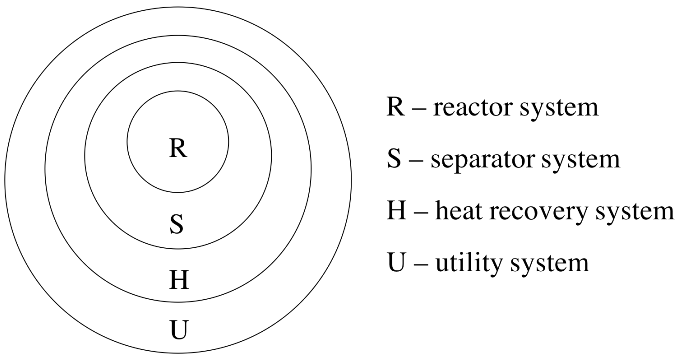


Figure 4: Onion diagram of process synthesis approach, adopted from Ref. [15], Figure 1.3.

This section is based in great parts on the *context and motivation* chapter from Wallerand [16]. It introduces PA as a methodology that, as mentioned, allows identification of the heat recovery potential in a process and the recommended utility placement based on the true thermodynamic requirements of a process. In reality, decision-making is seldom driven by thermodynamic requirements, but rather by economic, safety, and practical concerns. Hence, various additions to classic PA have been provided in research (e.g. by means of cost optimisation) [17–19] and in practical tools [20, 21].

Pinch analysis is introduced in section 2.1.1 with the main rules and conclusions for utility (in sec. 2.1.1.2) and heat pump placement (in sec. 2.1.2 & 2.1.3). This is followed by a short overview of extensions to PA accounting for practical problems (section 2.1.4), and a summary and critical review presented in section 2.1.5.

2.1.1 Heat recovery potential in a process: pinch analysis

Pinch analysis is a methodology developed in the 1970s by Linnhoff and Flower [9, 10] and extensively discussed by Kemp [15], which allows estimation of the maximum heat recovery potential of industrial processes. This requires decomposition of an industrial site into its thermodynamic requirements. The result is a set of hot (net cooling requirement) and cold (net heating requirement) thermal streams.
The second principle of thermodynamics states that heat can only flow from a source at higher temperature to a sink at lower temperature. Ensuring thermodynamic feasibility, the heat cascade[1] is derived which allows estimation of the maximum heat recovery potential of an industrial process and the temperature ranges in which external heating and cooling are required.

2.1.1.1 Minimum approach temperature ΔT_{min} An ideal heat exchanger is an adiabatic device in which a hot stream transfers heat to a cold stream at lower temperatures as depicted in Figure 5. The second law of thermodynamics dictates that a temperature gradient between the hot and the cold stream is required to provide a driving force for heat to flow.

From the principles of PA, a minimum approach temperature, ΔT_{min}, defines the point in a heat exchanger where the hot and the cold streams exhibit the smallest temperature difference. The position of ΔT_{min} depends on the inclination of the temperature-enthalpy profiles of the hot and cold streams, which are proportional to the inverse product of heat capacity and mass flowrate (mc_p). The optimal minimum temperature difference is conventionally found by optimisation which considers the balance between operating and investment cost for heat exchangers. A smaller approach temperature reduces the operating cost due to higher heat recovery while increasing investment cost related to larger heat exchange area.

In general practice, engineering estimate values of the minimum approach temperature difference are assumed and to ensure thermodynamic feasibility, the hot (cold) streams are shifted downwards (upwards) by half of this difference, resulting in what are referred to as corrected temperatures.

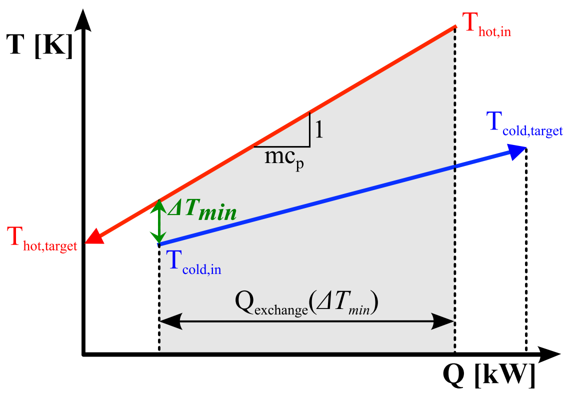


Figure 5: Temperature enthalpy profile of a counter current heat exchanger for illustration of ΔT_{min}, reprinted from [16].

2.1.1.2 Graphical representation, pinch point, and pinch rules An example of a hot composite curve generated from the process thermal requirements is illustrated in Figure 6. It is constructed by vectoral addition of all hot stream contributions in each temperature interval. The cold composite curve is constructed likewise. The hot and cold process composite curves represent the process total heating and cooling demand. The vertical overlap between the two curves marks the maximum possible heat recovery potential of the industrial process, as shown in Figure 7(a).

The GCC, depicted in Figure 7(b), is derived by subtraction of the thermal load of the cold from the hot composite curve in each temperature interval. The GCC monitors the net heating and cooling

[1] The heat cascade refers to the theoretical concept of successively transferring thermal energy from high to low temperature levels within a process.

loads and their temperature levels under the assumption of maximum heat recovery or minimum energy requirement (MER). The pinch point is marked by the impingement of the grand composite curve on the temperature axis. Above, the process exhibits a net heating requirement (heat sink), and below, a net cooling requirement (heat source). This cooling requirement can be defined as *excess heat*.

The distance from the temperature axis at the highest and lowest temperature represents the minimum hot (MER_{hot}) and cold (MER_{cold}) energy requirements, respectively.

The pinch point or pinch temperature induces four thermodynamics-based, so-called, pinch rules [9, 10]:

1. Hot utilities should only be installed at temperatures above the pinch (point),
2. Cold utilities should only be placed below the pinch (point), and
3. No heat exchange should occur across the pinch (point).
4. Self-sufficient pockets require no additional heating or cooling.

Violating any of these rules results in an increase of the utility requirements and, hence, a reduction of the process exergy efficiency. In the context of pinch analysis, "excess heat" is referred to as the heat available below the process pinch point which represents the process' net cooling demand.

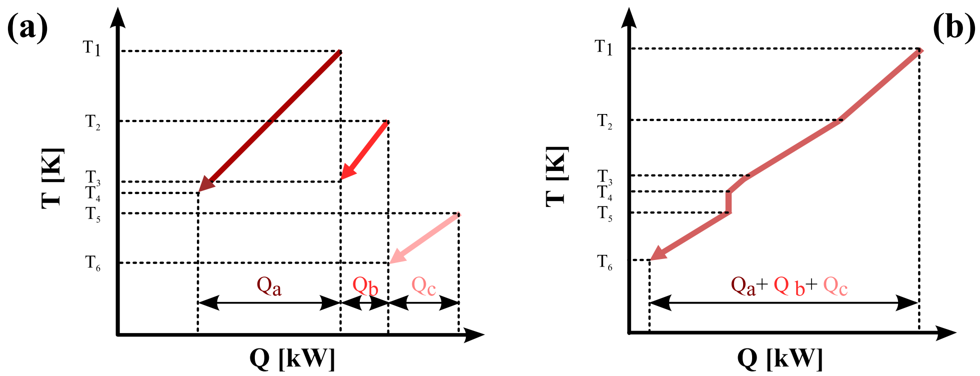


Figure 6: (a) Individual hot streams, (b) composite hot curve in the temperature enthalpy diagram [15].

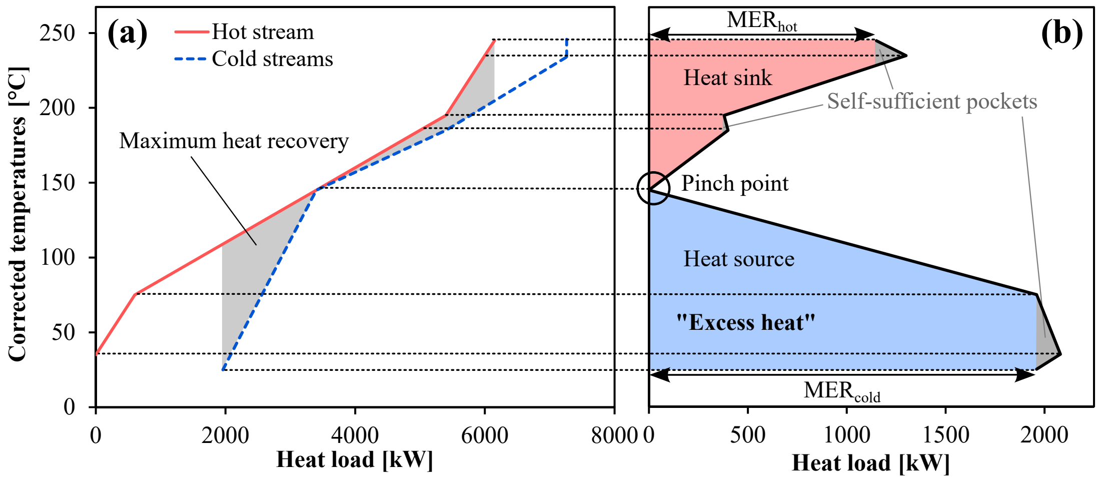


Figure 7: Temperature enthalpy diagram of (a) hot and cold composite curves (CCs), and (b) grand composite curve (GCC), reprinted from [16].

2.1.2 Energetically optimal heat pump placement

This section addresses mechanically driven heat pumps (HPs) due to their widespread application [5]; however, it should be noted that sorption systems present different and interesting integration options but are not within the scope of this work.

2.1.2.1 Heat pump rules

Rule No. 1 (necessary condition)
Townsend and Linnhoff [3] derived the theoretical foundation for optimal placement of heat pumps in an industrial process based on pinch analysis: heat pumps should always be placed across the process pinch point if energy savings are desired. In essence, energy savings through *heat pumping* are achieved by

- recovering *excess* heat from **below the pinch** (temperature)
- upgrading it through application of mechanical work, and
- supplying it back to the process **above the pinch** temperature

which is hence referred to as *excess* heat valorisation or reuse. For practitioners, it is important to recognise that heat pumping entirely above or below the pinch point violates the fundamental tenets of pinch theory.

Placed above the pinch, where the process is a pure heat sink, heat pumps act as an electric heater since any heat provided at higher temperature is compensated by an equivalent heat requirement with the only difference due to input of electricity. Below the pinch point, where the process is a pure heat source, heat pump acts as a refrigeration cycle providing a hot stream which violates the pinch rule excluding hot utility placement below the pinch which, in turn, necessitates a greater consumption of cold utility e.g. cooling water.

Rule No. 2 (sufficient condition)
Rule No. 1 generates net energy savings as long as the coefficient of performance (COP) of the heat pump and the electricity production efficiency are confined. Therefore, in order to assure energy savings, a second rule is defined in equation (1).

$$\text{COP}_{\text{real}} \times \eta_{\text{electricity production}} > 1 \tag{1}$$

Since in small and medium sized industry, electricity if often provided by the grid and the efficiency of grid electricity production is not known, CO_2-eq. equivalent emissions can be used. The adopted formulation is depicted in equation (2).

$$\text{COP}_{\text{real}} \times \frac{\text{CO}_2\text{-eq. emissions}_{\text{el grid}}}{\text{CO}_2\text{-eq. emissions}_{\text{heat production}}} > 1 \tag{2}$$

Simply stated: the product of the COP and the electricity production efficiency should be greater than unity.

Explanation
For example, if electricity is generated at 50% efficiency (e.g. combined cycle power plant), the heat pump should have a COP of at least 2 to realise net energy savings. Similarly, referring to eq. (2), **in Switzerland** the ratio of CO_2-eq. equivalent emissions from the electricity grid and heat production (with a fuel mix), is approximately below 0.5[1], requiring as well a minimum COP of 2 and higher.

[1] Electricity grid (medium voltage) global warming potential (GWP) 100a: 0.03591 [kg CO_2-eq. equivalent / MJ], combustion of: light fuel oil GWP 100a: 0.08958 [kg CO_2-eq. equivalent / MJ], heavy fuel oil GWP 100a: 0.09182 [kg CO_2-eq. equivalent / MJ], natural gas GWP 100a: 0.06922 [kg CO_2-eq. equivalent / MJ] Ecoinvent [13]

If the above-mentioned product is equal to (or less than) 1, the same amount (or more) of heat is required to drive the electricity production than the heat that is delivered by the heat pump. Such a configuration does not bring energetic benefits.

The COP for the above-mentioned rule should be calculated as the hot COP_h if only heat is supplied; and calculated as the combined COP if both heating and cooling are supplied to the process. The theoretical hot $COP_{th,h}$ (for a single-stage cycle) can be calculated by equation (3), with the hot side heat pump temperature, T_h [K], and the cold side temperature T_c [K].

$$\text{COP}_{\text{h,th}}[-] = \frac{T_h}{T_h - T_c} \tag{3}$$

While the combined theoretical COP_{th} (for a single-stage cycle) is calculated by equation (4).

$$\text{COP}_{\text{th}}[-] = \frac{T_h + T_c}{T_h - T_c} \tag{4}$$

Assuming a second-law efficiency of 55%, the real COP_{real} is calculated by equation (5).

$$\text{COP}_{\text{real}} = \text{COP}_{\text{th}} \times 0.55 \tag{5}$$

Table 1 shows three different real, hot COPs, indicating that a COP of 2 requires the same thermal power plant input as the heat pump condenser delivers. Figure 8 illustrates different COPs between 30 ℃ and various temperature lifts (ΔT). Only temperature lifts above 120K generate a real COP of 2, which illustrates that this case is not particularly common.

Table 2: Comparison compression power and required power plant thermal power for various hot COPs.

COP (hot real)	Unit	4	3	**2**
Thermal output heat pump condenser	kW	100	100	100
Compressor power	kW	25	33	50
$\eta_{\text{combined cycle}}$	-	0.5	0.5	0.5
Thermal input of electrical power plant	kW	50	67	100

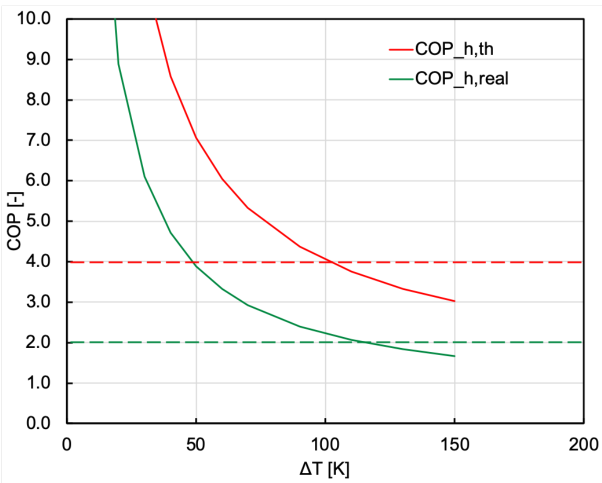


Figure 8: Theoretical and real COP of heat pump (for heating) with evaporation temperature at 30 ℃, exergy efficiency 55%.

2.1.2.2 Heat pump types and process GCC As mentioned previously, the COP has a major influence on the performance and energetic gain of the heat pump. One crucial factor which influences the efficiency of single-stage, single fluid heat pump cycles: the required temperature lift and thus the compression ratio. In the context of industrial excess heat valorization, the adequate temperature lift is directly linked to the "sharpness" of the pinch, meaning the shape of the process grand composite curve close to the pinch point.

Figure 9 shows the temperature enthalpy diagrams of processes (A) and (B). Process (A) has a sharp pinch point with a small temperature lift. While process (B) shows a smooth pinch point with heating and cooling requirements spanning over a range of temperatures. Integration of different mechanical heat pump systems are illustrated, starting from a single-stage, single fluid (inverted Rankine cycle) heat pump in Figure 9-(A) and (B). If a high temperature lift is required as illustrated in Figure 9(B), the efficiency of standard (single-stage, single fluid) heat pump cycles is drastically compromised.

Three options to overcome this issue are discussed in the literature which are depicted in Figure 9(1B-3B).

- (1B) **Multi-stage or cascaded heat pump cycles** based on latent heat release and consumption in condenser and evaporator with multi-stage compression and/or expansion [6, 22–24]
- (2B) **Zeotropic mixture cycles** based on latent heat release of mixtures where the difference in fluid boiling points is expressed in a temperature glide and liquid/ vapor composition shift during evaporation and condensation [25, 26]
- (3B) **Inverse Brayton cycle** heat pumps based on sensible heat release and consumption in the condenser and evaporator, respectively [27]

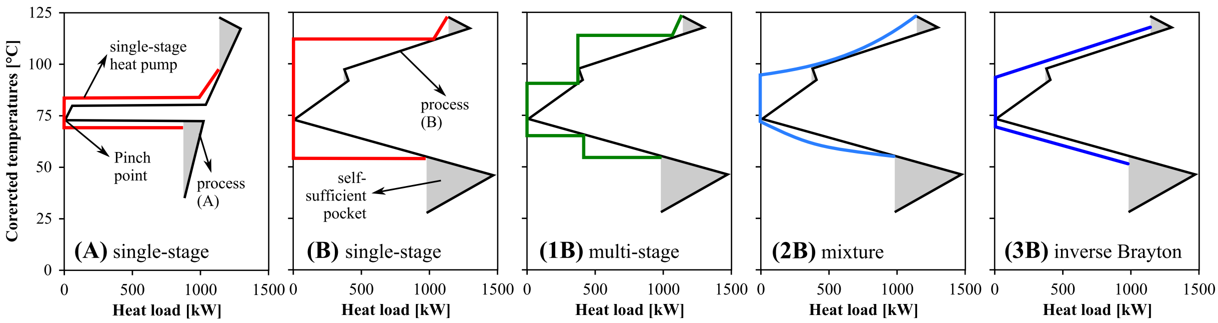


Figure 9: Heat pump integration to process GCC. (A) GCC with "sharp" pinch point & single-stage HP, (B) "smooth" pinch point & single-stage HP, (1B) "smooth" pinch point & multi-stage HP, (2B) mixture HP, (3B) inverse Brayton HP.

Single fluid (inverse Rankine) heat pumps can satisfy constant temperature thermal requirements (single-stage) as well as continuous temperature ranges with help of multi-stage cycles at a reasonable COP (above 2). In generating a temperature glide, zeotropic mixtures [25, 26] or heat pumps relying on the inverse Brayton cycle [27] may be advantageous for demands spanning wide temperature ranges, but less flexible relative to constant temperature requirements. This report focuses on mechanically driven, single fluid, multi stage (inverse Rankine) heat pumps (depicted in the first three diagrams in Figure 9-(A-B-1B)), due to their operational flexibility, wide-spread application, and the technical realisation being mostly dependent on mature technologies [5].

The discussion above highlights the variety of options which may be considered in order to satisfy the requirements of a process, which are represented by the GCC shown in Figure 9. Choosing between options can be simplified by application of optimisation algorithms and with the help of tools, which is discussed in more detail in sections 2.1.4 and 2.2, respectively.

2.1.3 Heat pump integration beyond heat pump rules

2.1.3.1 Refrigeration The rules identified above for energetically optimal placement of heat pumps are also valid for refrigeration cycles which work based on the same principle as heat pumps. Usually, however, the main focus of refrigeration is efficient cooling of the process at sub-ambient temperatures. If the process pinch point is at high temperature, it may not be reasonable to cross the pinch with the refrigeration cycle. The reason for this is discussed in Section 2.1.2, Rule No. 2.

Figure 10 (a) shows a process with a refrigeration need at -20℃ and a pinch point at 54℃. A single-stage refrigeration cycle crossing the pinch between -25℃ and 60℃ would lead to a real, combined COP of 3.7. However for simplicity, often, a standard refrigeration cycle would be selected to provide the cooling need and would be placed entirely below the pinch point (evaporation / condensation at -25 / 25℃). This means that cooling water would be required to cool the process below the pinch (but above the ambient temperature) and to cool the condensation stage of the refrigeration cycle. Applying rule no. 2, the combined COP is above 2 which indicates that heat pump integration could be beneficial. These benefits could be achieved with a single heat pump or a cascaded system as shown in Figure 10 (b). Here, in addition to the standard refrigeration cycle, a multi-stage heat pump is proposed to recover excess heat of the refrigeration cycle and process (adding evaporators at 15 and 35℃), to supply the upgraded heat above the pinch temperature (at 60℃). In this solution the cooling water consumption is drastically reduced which also indicates improved thermodynamic performance of this solution. These two examples indicate the variety of options which are possible for satisfying the process requirements shown by the GCC, and how complex a consistent analysis without adequate integration tools/methods is. Available methods and tools are discussed in sections 2.1.4 and 2.2, respectively.

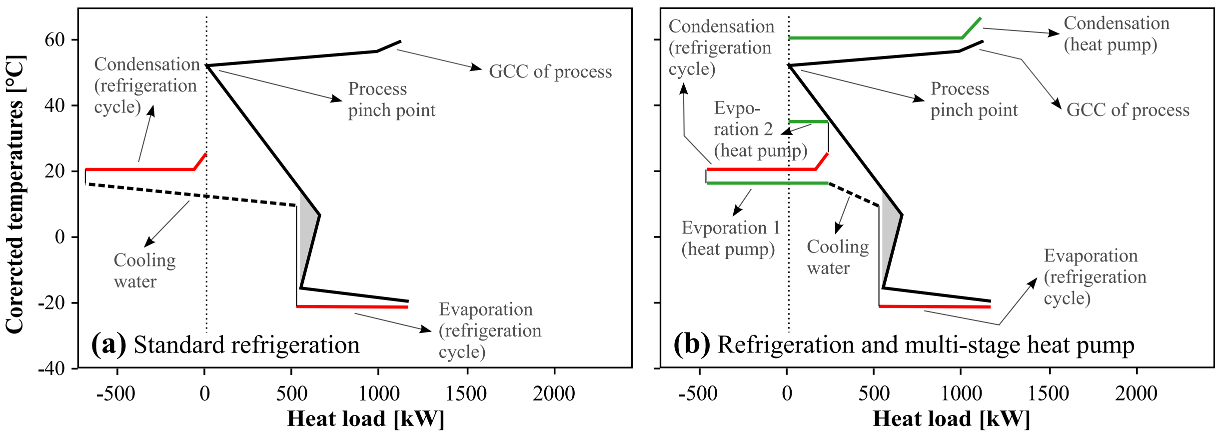


Figure 10: Refrigeration integration to process GCC with pinch point at 54℃. (a) Standard refrigeration between -25℃ and 25℃, (b) Standard refrigeration and heat pump between 15, 35℃ (evaporation) and 60℃ (condensation).

2.1.3.2 Pinch violations Some processes have intrinsic pinch violations for economic or practical reasons, which require cooling above or heating below the process pinch point. In these cases, it is important to understand the purpose of implementation to ensure that it is strictly necessary from the process perspective; however, the heat pump rules may be violated in these specific cases.

2.1.3.3 Summary The following pinch violations may create acceptable heat pump placement against the *heat pump rules*. Their validity, however, needs to be carefully considered.

- **A subambient cooling requirement below the pinch** may require a refrigeration cycle with condensation below the pinch (with heat evacuated to the environment when necessary)

- **A (pinch violating) cooling requirement above the pinch** could be satisfied by a heat pump which may bring energetic advantages compared to a pure cooling utility because it also provides process heating above the pinch; or
- **A (pinch violating) heating requirement below the pinch** may be satisfied by a heat pump, since it also provides cooling below the pinch.

While these conditions should be avoided wherever possible, some aspects of plant operation surmount energy efficiency measures and thus sub-optimal heat pump integration may be used to satisfy specific requirements where **alternatives are impossible**. The latter two cases are especially rare and should only occur in extremely restricted circumstances; however, heat pumping may yield energetic benefits compared to satisfying rule-violating requirements with alternative utilities.

2.1.4 Advanced methods for heat pump and utility integration

The above mentioned rules and methods address systematic reduction of the energetic requirements of a process. Decision-making in industry, however, is seldom based upon energetic objectives. Other drivers play a major role, including economic and environmental concerns as well as technical constraints and motivational barriers. PA, however, is the **necessary** foundation for all subsequent steps in the sense that it is the only approach which allows thorough understanding of the process and its true (thermodynamic) requirements. Considering PA during the planning phase assures that novel utilities (including heat pumps) are planned with respect to actual process needs. This ensures that even if heat recovery measures are added to the process at a later stage, these novel utilities would not be oversized or wrongly placed.

Advanced methods have been developed to consider the principles of PA as well as other drivers, including economic and environmental objectives. Optimisation in the form of mathematical programming is a widely-used technique based on systematically scanning various heat pump and utility options to identify the *best* alternative with regard to selected objective(s). Researchers have published a variety of studies presenting 'superstructure'-based optimisation algorithms. 'Superstructure' refers to a generalised model that represents all design alternatives, of which one solution is finally selected during the optimisation step. Papoulias and Grossmann [17] presented an optimisation model based on mixed integer linear programming (MILP) which allows determination of the optimal utility system for an industrial process, considering the heat cascade, to achieve minimum process energy requirement (in agreement with pinch analysis). This approach is generally referred to as utility targeting and is adopted by most researchers working on process modelling and optimisation.

In a subsequent work, Papoulias and Grossmann [18] presented the mathematical model for designing industrial heat exchanger networks (HENs), so that the minimum energy requirements found during the utility targeting could be fulfilled. More information can be found in reviews of this topic [28].

The first comprehensive methodology for optimal industrial heat pump design based on the utility targeting principles was presented by Shelton and Grossmann [6, 22] in the form of an MILP superstructure. Based on a discrete set of temperature intervals and predefined working fluids, the active presaturators, evaporators, condensers, and their sizes could be optimally determined. Further developments are summarised in [29] and later in this report (section 3) where a novel synthesis method and bi-level solution approach was presented which identifies optimal industrial heat pump configurations, considering a comprehensive list of heat pump features comparing their results to various literature cases.

2.1.5 Summary and discussion

PA is a methodology which identifies heat recovery potential within a process, and with that, the minimum heating and cooling requirements. The pinch rules help to establish recommendations for thermodynamically-beneficial placement of utilities and heat exchangers, while violating the rules results in higher energy consumption and lower efficiency of the process energy system.

With help of the pinch rules, Townsend and Linnhoff [3] derived theoretical principles for energetically favourable placement of heat pumps. Two rules were presented in this report indicating that heat pumps should cross the pinch (1) as long as the temperature lift is not too large (2), resulting in a COP which is too low to generate overall energetic benefits. Two cases were identified in which the heat pump rules may be, or even must be, violated: (1) refrigeration of subambient cooling requirements, where crossing the pinch can be circumstantially considered; (2) if the process features internal pinch violations, then heat pumping may be considered to satisfy these violations.

The theoretical framework described here is the basis for the practitioner guidelines derived in section 2.3; furthermore, most tools described in section 2.2 rely on these principles.

> The applicability and feasibility of PA and its principles is sometimes criticised due to technical and economic constraints which may render design or redesign of a process based on purely energetic targets difficult to attain. Further, it is stated that the use of PA principles requires specific proficiency which inhibits broader usage.
>
> The first aspect of criticism can be faced with the note that it remains the sole method which allows a deep insight and detailed thermodynamic understanding of processes. It offers a holistic view on the process from an energetic/thermodynamic perspective. Considering PA during planning assures that novel utilities (including heat pumps) are planned with respect to actual process needs. This ensures that even if heat recovery measures are added to the process at a later stage, these novel utilities will not be oversized or incorrectly placed. The second point can be addressed in two ways: firstly, by pointing out that there is a variety of programs and tools (discussed in section 2.2) available to aid in understanding and using the principles better; and secondly, that understanding of the underlying principles and a basic analysis can already provide a good starting point without the need for a detailed audit (as discussed in section 2.3).

2.2 Industrial heat pump integration tools

An analysis of available tools was conducted and an overview is provided in Table 2. The list of criteria as well as the identified properties of the tools were discussed with support staff of the different software packages. The list of considered tools stems from a literature review as well as the previous international energy agency (IEA) Heat Pump Annex 35 [5] Task 2 report and IEA SHC Task 49 [30]. Only tools of which online documentation could be found were considered in this analysis. Three categories were defined to classify the respective tools: **pinch analysis (PA)**, **heat pump design**, and **utility integration**. Most tools cover at least one of these categories, often several, as depicted in Figure 11.

From this overview, four groups were identified and are color-coded in Table 2.

- Heat pump (HP) design (marked in red): Tools that aid in designing and planning heat pump systems based on selected operating conditions, not considering PA.
- Pinch analysis (PA) and heat exchanger network (HEN) design (marked in blue): Tools that aid pinch analysis of an industrial process to estimate the heat recovery potential and/or aid in planning and re-designing the heat exchanger network. In these tools, the focus is placed on process heat recovery, not on utility integration.
- PA and heat pump integration (marked in turquoise): Tools which allow analysis of the heat recovery potential through PA and heat pump integration without thermodynamic property calculations.
- PA and heat pump integration with thermodynamic properties (marked in purple): Same as green, but with thermodynamic property calculations incorporated within the tool.

A set of properties for each tool is provided in Table 2. This includes the licensing, indicating whether the tools can be openly accessed, need to be purchased or are utilised in an academic setting. The targeted user type, required level of proficiency and other criteria are indicated to better identify which tools should be recommended for various interests. The ultimate goal of this analysis is to provide a concise overview of the breadth of tools available for various purposes and users.

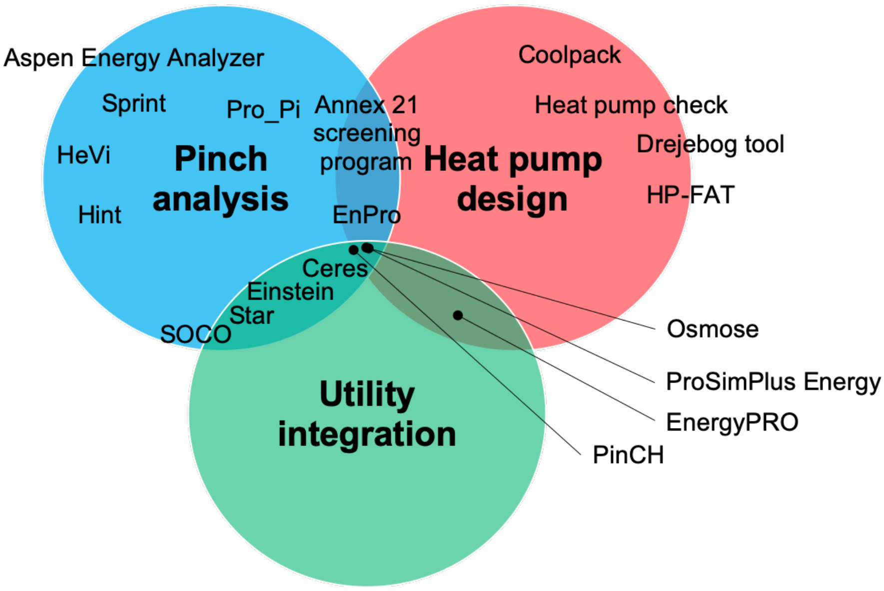


Figure 11: Categories for grouping of relevant tools.

Table 2 reveals that a variety of tools are available for diverse levels of expertise ranging from pure heat pump design to tools (such as) which allow heat pump design based in knowledge of two temperature levels to comprehensive energy audit tools (such as) which allow conducting a full energy audit including PA

The use of some of the open access tools is discussed in section 2.3, showing that a combination of certain tools can reach good results and can overcome some barriers of specific tools. Energy auditors, heating ventilation and air conditioning (HVAC) planners, and heat pump producers are encouraged to try some of the tools to gain deeper understanding of different aspects in industrial heat pump integration. Tools with a free version are especially recommended since they allow study of the matter without an initial investment.

Table 3: Overview of available heat pump and process integration tools. (Table sorted by release date.)

Name	Institution	Language	Latest release	First release	Functionalities	License	Main use	Interface	Targeted user	User prof.	Industry	Opt.	Comments	Source
Osmose	EPFL	EN	2019	2009	[pinch], [HEN], [utility], [HP multi-stage] [data]	[academic]	Research	Script	researchers, students	★★★	all	☑	(+) Optimization algorithms, (−) No graphical user interface (GUI), academic use only	[31, 32]
Sprint	UMIST	EN	2018, v2.9	v1.4	[pinch], [HEN]	[academic]	Research	GUI	students, energy auditors	★★	all	☑	(+) GUI, (−) license required, pure PA tool	[33]
Star	UMIST	EN	2018, v2.9	v1.4	[pinch], [utility], [steam]	[academic]	Research	GUI	students, energy auditors	★★	all	☑	(+) GUI, utility integration (−) license required	[33]
TOP Energy	RWTH Aachen	EN	2018, v2.8.5	-	[HP], [utility]	[proprietary]	Commercial	Flow-sheet	energy auditors, industry	★★★TEE	all	X	(+) flowsheet software, simulation (−) no PA	[34]
PinCH 3.0	HSLU	EN	2018, v3.0	2010	[pinch], [HEN], [utility], [HP]	[proprietary], [academic]	Industry, teaching	GUI	energy auditors, industry, students	★★TEE	all	(☑) rule based	(+) user friendly/GUI, 10 steps to completing PA, tutorials, documentation material & website, (−) proprietary	[35]
EnergyPRO	EMD International	EN, var.	2018, v4.5	?	[HP], [utility]	[proprietary]	Commercial	GUI	engineers	★★	(☑)	☑	(+) energy system planning with multi-period analysis, focus on district energy systems, (−) proprietary	[36]
HP FAT	Teknologisk Institut	EN	2018	2016	[HP]	[open access]	Research	GUI	Researchers, engineers	★	X	X	(+) user-friendly, simple functionality, open access, (−)	[37]
Einstein	E4-Experts GmbH	EN, various	2017, v2.5	2007, v1.0	[pinch], [HEN], [utility], [HP]	v2.4: [open access]; v2.5: +/-1.8 k€	Commercial/industrial	GUI + flowsheet	energy auditors, industry	★★TEE	all (*)	(☑) rule based	(+) integrated approach, one tool for full energy audit, transparency, open-source version, method for auditing, (−) User-friendliness of interface could be improved	[20]
EnPro	AEE INTEC, AIT, TUW	German	2017, v3.0	2017	[HP], [pinch]	[open access]	Research	Excel interface	process operators, preliminary	★TEE	all	X	(+) easy to use user interface, (−) not more than 20 process streams can be defined à limited use for industry	[38, 39]
ProSimPlus Energy	Prosim	EN	2017, v3.6.2	-	[pinch], [HEN], [utility], [HP multi-stage] [data]	[proprietary]	Commercial	GUI	energy auditors, industry	★★★TEE	all	☑	(+) flexible use, wide range of possibilities, thermodynamic property, (−) proprietary	[34]
Drejebog tool	Dansk Fjernvarme	Danish	2017	2017	[HP]	[open access]	Education	Excel interface	engineers	★	X	(☑) rule based	(+) heat pump integration for district heating, (+) [open access], (−) no PA	[40]
AspenEnergyAnalyzer	Aspen Technology Inc.	EN	2015, v34	1981	[pinch]	[proprietary]	Commercial	GUI	energy auditors, industry	★★TEE	all	☑	(+) easy to use, can be integrated to other ASPEN tools, (−) limited, mainly PA functionalities	[41]
Heat Pump Check	De Kleijn Energy Consultants	EN	2014, v2.5	-	[HP] [data]	[open access]	Education	GUI (web based)	industry	★	-	☑	(+) easy to use, generates best heat pump cycle for specific requirements	[42]
SOCO	AEE INTEC	EN	2014	2014	[pinch], [utility], [HEN]	[academic]	Research	GUI	researchers	★★★	all	?	(+) focus on multi-period PA for solar energy systems with storage, (−) heat pumping not really considered	[43]
Pro_Pi1,2	Chalmers	EN	2013	2008	[pinch], [HEN]	v1: [open access], v2: [academic]	Teaching, research	Excel interface	students	★★TEE	all	X	(+) user-friendly, teaching tool, (−) not design for utility integration, esp. not heat pumps	[44]
Ceres	C.E.S Paristech	EN	2013	2010	[pinch], [HEN], [utility], [HP] [data]	[academic]	Research	GUI	energy auditors, students	★★	all	☑	(+) GUI, optimisation, general analysis, (−) proprietary	[45]
Hint	Universidad de Valladolid	EN	2009	2009	[pinch], [HEN]	[open access]	Teaching	GUI	students	★★TEE	all	X	(+) open access teaching resource, (−) not actualised any more	[46]
HeVi	University of Aalto	EN	2008, v0.2.6	2008	[HEN]	[open access]	Research	GUI	students, researchers	★★TEE	all	X	(+) helps for visualisation of [HEN], open access, (−) not updated past 2008, no documentation	[47]
Annex 21 IHP Screening Program	Heat pump center (HPC)	EN	1997	1997	[HP] [data], [pinch]	[proprietary] 75 €	Education	GUI	HVAC engineers	★★HVAC	all	X	(+) GUI, screening, (−) Few / outdated refrigerant list, user-handled screening, unfriendly GUI, data export, outdated	[48]
CoolPack	DTU	EN	v1.5	1995	[HP multi-stage] [data]	[open access]	Research	GUI	HVAC engineers	★★HVAC	-	X	(+) tool is mainly developed for heat pump design considering various features, open access, (−) no process integration (PA) possible	[49]
SuperTarget	KBC Advanced Technology	EN	?	?	[pinch], [HEN], [utility]	Not available	Commercial	-	energy auditors (company internal)	★★★	all (**)	☑	(+) tool from founder of PA (Linnhoff and Flower), (−) only for consulting company internal use	[46]
TRIAS-Energetica	EURIMA	EN	?	?	urban planning	[open access]	Research	Concept	urban planners	★	-	-	Concept for energy-aware urban planning	[50, 51]
KWA HP screen	RVO (high temperature HP)	EN	?	?	[HP]	Not available	?	GUI	industry	★	all	X	(−) neither the tool, nor documentation can be found online	[5]

User prof. – user proficiency: ★- low to ★★★- high,
Functionalities: [pinch]: pinch analysis, [HEN]: heat exchanger network synthesis, [HP]: heat pump design ([HP multi-stage] multi-stage) with thermodynamic properties data included [data], [utility]: utility integration, [steam]: steam network
Opt – optimization algorithms.
License: [open access]: open access, [academic]: academic, [proprietary]: proprietary
HVAC: heating ventilation and air conditioning, TEE: thermal energy engineering;
(*) limitations above 400 °C
(**) focus on petrochemical

2.3 Practical guidelines

Table 3 presents the practical guidelines derived for the IEA HPT Annex 48 to achieve smart industrial heat pump integration in a step-by-step fashion. The guidelines aid in the data acquisition, analysing the status quo, process heat recovery quatification, optimisation and identification of the heat pump integration points. Each point is discussed in greater detail below with an example application in section 2.4. The relevant steps in which software tools may be useful are indicated with a tool symbol: 🔧; however, all guidelines can be applied without the use of tools.

These guidelines were inspired by other guidelines from the IEA SHC Task 49 - Integration Guideline [30] for solar process heat and the industrial heat pump technology guide [42].

Table 4: Step-by-step method for *smart* industrial heat pump integration.

Heat pump integration guidelines	
Go, no-go decision	**(1) Initial data acquisition** – Questionnaire to identify general data and clients motivation – Generic questionnaire for all industry
	(2) Preparation and decision – Analysis of questionnaire with background information on the sector – Decision: of further in-depth study?
Feasibility analysis	**(3) Company visit** – Data gathering, overview of main production processes, technical data, sketches – Identify the strategy of the company
	(4) Analysis of the status quo (🔧) – Cross-check data with available benchmarks – Data reconciliation, energy and mass balances of single sub-processes
	(5) Pinch analysis (heat recovery) 🔧 – Define hot and cold streams, use PA tool – Alternative: get public PA data – Heat recovery potential > 50%? → high unused heat recovery potential which should be harvested before HP is considered
	(6) Utility integration and heat pump design 🔧 – Pinch temperature < 160 C – Heat sink < 200 C – Temperature lift $\Delta T < 50K$ (90K)
	(7) Identify the point of integration (🔧) – Temperature levels – Heat capacity of the identified streams – Time overlap (storage?)
Final decision	**(8) Decision** – Discuss about options with company – Take educated decision
	(9) Detailed planning – Based on company's decision, detailed planning – Repeat some of the prior steps to verify energy consumption data

(1) Initial data acquisition The goal of this step is to gain a general overview of the energy bill, the process boundary conditions, and the motivation of the company management to invest in energy efficiency measures. This can be conducted with a general questionnaire, which is not specific to any industrial sector.

Here, the main data of interest are the annual energy bill, plant operating hours and the minimum/maximum temperature levels of the process. Additionally, it may be of interest to identify refrigeration requirements, maximum thermal power demands, and constant temperature requirements. These data are helpful for informing decisions that are made in the following step, based upon the progress and outlook of the project.

The temporal coincidence of heating and cooling demands, such as in continuous processes, form the basis of pinch analysis and is considered to be the case here. Pinch analysis with batch processes is an area of research with many potential strategies to account for differences in operational periods. For considering heat exchange between time steps, storage must be included. Since this discussion would detract from the core methods intended in this report, these aspects are not discussed in further detail.

(2) Preparation and decision This step aims at analysing the outcome of the questionnaire and making a decision whether a further in-depth study seems promising. This can be conducted alongside several questions:

- Is there general interest from the company to implement energy efficiency measures?
- Are there refrigeration needs?
- Is the maximum process temperatures below 300 °C? Helpful, but not necessary

The final decision needs to be made on a case-specific basis; however, the above criteria can provide additional motivation.

(3) Company visit The company visit serves for gathering technical data, gain insights to the main production processes and internal dependencies, and to receive or draw sketches of key conversion steps. These data can be further completed by conducting in-depth interviews with process operators and decision makers to identify opportunities for integration potential.

(4) Analysis of the status quo (🔧) The analysis of the status quo serves the purpose of getting a more detailed understanding of the process energy requirements. The aim is to perform a cross-check of the process data with available benchmark values, and to reconcile the data by ensuring that mass and energy balances in the system are satisfied. Data reconciliation is a data preparation and treatment technique which uses non-linear optimization to yield better estimates of uncertain measurements and provide insights where measurements are not reliable or available.

> 🔧 Most industrial systems can be treated more easily with the use of **process software tools**, such as Belsim Vali [52] or gProms [53], which supply flowsheeting interfaces and data reconciliation algorithms.

Such software are especially useful in large systems where many measurements are available and links between measurement points can easily be overlooked. These techniques require redundant measurements to effectively reconcile the data and provide statistically 'better' measurements than those read directly from instrumentation. In smaller systems, or if software is not available, data reconciliation techniques can still be applied based on engineering fundamentals of mass and energy balances combined with the appropriate mathematical formulation.

(5) Pinch analysis (heat recovery) 🔧 The best option for conducting pinch analysis is by using one of the available tools as document-ed below.

🔧 **Pinch analysis tools**: Aspen Energy Analyzer [41], Sprint [33], Hint [33], EnPro [38, 39], Pro_Pi [44] , Ceres [45], Einstein [20], Star [33], PinCH [35], Osmose [31, 32].

Most of these tools require input data in a similar form as presented in Table 5. Of the open source software, the EnPro and Einstein tools were tested. It was found that EnPro is an easy to use tool which does not require much prior training; however, it is limited in the number of streams which can be implemented. Einstein offers a wide possibility of uses, however, the application requires a higher level of knowledge and may require some training.

The outcome of such an analysis should be a set of composite curves: the hot and cold composite curves and a grand composite curve. These curves represent the process minimum energy requirements assuming maximum possible heat recovery, and can be considered as a benchmark of the process. Comparing the benchmark minimum energy requirement to the current energy bill yields the current level of heat recovery of the process. Alternative to the use of tools: If it is not possible to generate a composite curve e.g. due to a lack of data or time, there are publications which provide indications for typical profiles in various industries, which may be taken as a reference [54] to generate an approximate level of heat recovery in the process.

If the level of heat recovery is below 50%, the primary studies should initially focus on heat recovery measures instead of heat pump integration studies.

(6) Utility integration and heat pump design 🔧 After having created the GCC (or a proxy thereof) in the previous step, this step aims at identifying the correct point of integration of a heat pump and other utilities with the process. The goal is to identify the temperature levels and heat load of the heat pump and other utilities. Satisfying the pinch rules during this step assures that utility placement will still comply to thermodynamic rules and bring energetic benefits to the system in the event of future heat exchanger network redesigns toward maximum heat recovery. The indications provided in the guidelines provide support to identify whether heat pump integration is feasible.

- Pinch temperature < 160 °C?
- Heat sink < 200 °C?
- Temperature lift ΔT < 50K or 90 K?

The goal is to use the indications above and the information provided in the GCC to identify the temperature and heat load of a heat pump and other utilities. The heat pump pre-design can then be conducted with the help of one of the following tools:

🔧 **Heat pump design tools**: Coolpack (Open access) [49], Heat pump check [42], Drejebog tool [40], EnPro [38, 39], Annex Screening program [48], PinCH [35], Osmose [31, 32].

(7) Identify the point of integration (🔧) The point of integration should be identified at this step to proceed with the decision and detailed planning. Therefore, it is recommended to identify heat exchangers, or process units that fulfil the criteria identified in the previous steps. The main points to follow to are depicted below:

- Temperature level of the identified streams and suggested heat pump
- Heat capacity of the identified streams
- Time overlap (for batch processes)

There are also tools available which may be used to help in finding the adequate points of integration, which are depicted below.

Tools for heat exchanger network design to identify the ideal point of integration: Aspen Energy Analyzer [36], Sprint [33], Hint [46], EnPro [38, 39], Pro_Pi [44] , Ceres [45], Einstein [33], PinCH [35], Osmose [31, 32].

(8) Decision Many approaches using mathematical or heuristic methods to attain optimal heat pump integration provide a single solution which is suited to the process. Practically, the identifed solution might not be viable and thus providing several 'good' solutions is a preferable alternative to a single, 'optimal', solution. Providing several solutions leaves flexibility for the decision-maker to choose integration options which account for non-technical factors or to explore possibilities which might be more acceptable to different levels of an organisation. Selecting one or several solutions is required to proceed to the detailed planning phase.

(9) Detailed planning Integrating heat pumps with industrial processes requires detailed engineering work following the screening steps which had been carried out until this point. Methods applied for identifying the potential integration options are based on generalised formulae, equipment behaviour and operational characteristics and thus the calculations and design need to be refined in a final step before implementation. Technical, non-technical, economic and environmental calculations should be performed in detail to ensure the best integration of heat pumping in the process, respecting the requirements and constraints of the company which may have been difficult to incorporate at the screening stage.

2.4 Application of guidelines along a case-study

This section presents the application of existing models, tools, and theoretical principles to a real case study based on the set of guidelines presented in section 2.3. Steps marked with a tool "" may be easier to complete with aid of software tools. Some tools may also be used for the entire set of the guidelines; however, this is not specifically discussed in this section. For the sake of brevity, the full content of this section is provided in appendix A.1.

3 Software development: Integrated design tool

This section presents the advanced heat pump integration tool which was developed within the scope of this project. In the first part, the functionality of the **tool** is described from the perspective of a *user*. While the second part describes the underlying mathematical problem formulation and resolution **method**. The third part presents **results - benchmark analysis** with improved solutions to well known examples from the literature.

3.1 Tool

The software tool developed during this project is a preliminary design platform for providing optimal industrial heat pump integration considering a comprehensive list of heat pump features, fluid and compressor selection. This section aims at providing a straight-forward overview of the required **input data**, the **features considered**, and the available **output data**.
Figure 12 shows the general overview of the software inputs and outputs, which will be explained in more detail in the following subsections.

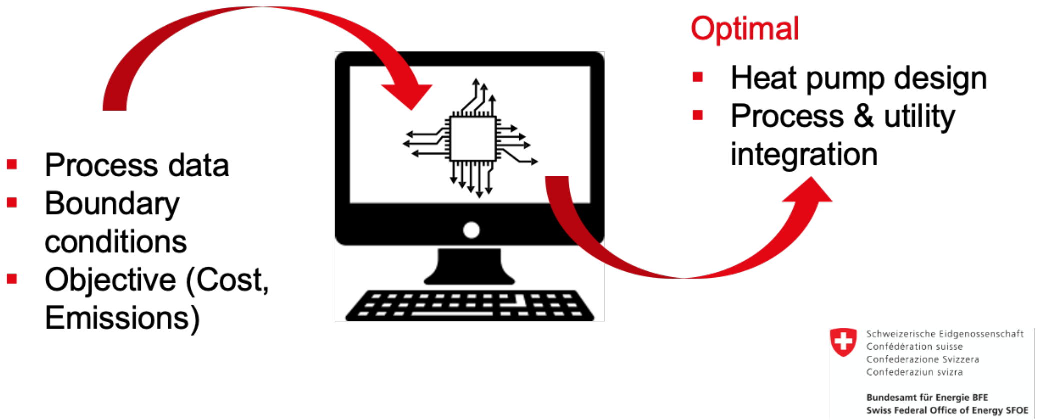


Figure 12: Software overview.

3.1.1 Input data

Three main input data sources are required. These are summarised in the list below and described in more detail in the following sections.

1. Process data
2. Boundary conditions
3. Objective (function)

3.1.1.1 Process data Industrial process data are needed to provide the basis for characterising the process where heat pump integration is to be investigated. The industrial process data need to be provided in the form of thermal heating and cooling requirements. The minimum data required are inlet and outlet temperatures (T_{in}, T_{out}) and thermal requirements (ΔH) of the process streams. The operating schedule of each thermal stream, heat capacity (c_p), minimum temperature difference inside a heat exchanger (ΔT_{min}), and the material of the stream are optional information. The above-mentioned data are summarised in the list below. Data marked in *italic* are not strictly necessary.

- Industrial process thermal streams: T_{in} [K,°C], T_{out} [K,°C], ΔH [kW], *operating schedule (batch processes)*, c_p [kJ/kg/K], ΔT_{min} [K,°C], *material (water, gas, brine, etc.)*
- Utility data: same as above, fuel consumption, efficiency, type
- Operating time / schedule

3.1.1.2 Boundary conditions The boundary conditions entail the economic situation (energy prices and expected interest rates) as well as specifications related to the heat pump system considered. Here, specific safety concerns related to certain fluids, or complexity concerns (maximum heat pump stages) could be addressed. The list of potential working fluids in the heat pump also need to be specified. These data set the boundary conditions for the optimisation algorithm and should therefore not be too restrictive for initial stages of investigation; however, overly complex or unrealistic results could be excluded in advance by adding such constraints. The above-mentioned data are summarised in the list below. Data marked in *italic* are not strictly necessary.

- Energy prices: electricity, nat. gas, oil
- *Bank interest rates*
- Heat pump specifications: safety concerns? complexity concerns (e.g. only single/two-stage cycles)? *General temperature ranges, super/sub-critical*, fluid list

3.1.1.3 Objective (function) The objective function is the target which the optimisation algorithm tries to improve. By default, it is a cost-driven optimisation which aims at minimising total annualized costs (TAC) of the system.

- Goal of the design: *cost reduction and/or emission reduction?*

3.1.2 Features considered

3.1.2.1 Fluid selection To identify relevant working fluids for HP integration in the CH industrial sector, a freely available, web-based refrigerant selection platform [55] was created for this project. It allows identification of the relevant fluids, which can then be set as input to the heat pump design software. An exemplary list of criteria is presented below:

1. GWP $\leq$ 10
2. Ozone depletion potential (ODP) $=$ 0
3. Boiling point $<$ x ℃ $\rightarrow$ above x ℃: the pressures (of all fluids still present) are above atmospheric conditions
4. Critical temperature $\geq$ y ℃ $\rightarrow$ below y ℃: all fluids (still present) are sub-critical

A screenshot of the platform can be seen in Figure 23, where the favourable properties can be selected by brushing the appropriate axes. The resulting list of fluids fulfils all selected criteria and can be exported in csv-format. For example, the criteria selected above (x = 100℃, y = - 33 ℃) yield a list of 13 fluids, consisting of 10 natural refrigerants (NRs) (including hydrocarbons (HCs)), 2 hydrofluoroolefins (HFOs), and one unsaturated hydrochlorofluorcarbon (u-HCFC).

3.1.2.2 Heat pump features The list of heat pump features considered in this software are depicted in Table 21.

3.1.2.3 Compressor types The list of considered compressors is depicted in Figure 14. Cost data and operating conditions were retrieved from manufacturer data and engineering handbooks [56] which are published in deliverable D3.

The types of compressors considered are specified in Table 4.

3.1.3 Output data

The software conducts a consistent utility targeting, considering heat pump design and integration with an industrial process. The energetic requirements of the industrial process are satisfied and the heat pump integrates optimally with the utilities in-place and/or new technologies. The heat pump design comprises a selection of equipment (flashdrums, valves, compressor types) together with their sizes and a specification of operating conditions (pressure levels, fluids, mass flow rates) for continuous and batch operations. For further reading, the publication of Wallerand et al. [29] is recommended.

group	ASHRAE	ASHRAE R-	name	lifetime	ODP	GWP100	OEL
HC	R-170	170	Ethane	12	0	5.5	1000
HC	R-290	290	Propane	12	0	3.3	1000
HC	R-600	600	Butane	12	0	4	1000
HC	R-600a	600	Isobutane	12	0	3	1000
HC	R-601	601	Pentane	12	0	4	600
HC	R-601a	601	Isopentane	12	0	4	600
HC	R-610	610	Diethyl ether	12	0	4	400
HCC	R-30	30	Dichlorome…	-1	0	8.7	100
HCFO	R-1233zd	1233	Chloro-triflu…	0.07	0	1	-1
HCFO	R-1224yd	1224	HCFO-122…	-1	0	1	-1
HFO	R-1234yf	1234	Tetrafluoro…	0.03	0	4	500
HFO	R-1234ze	1234	Tetrafluoro…	-1	0	6	800

Figure 13: Working fluid selection platform [55].

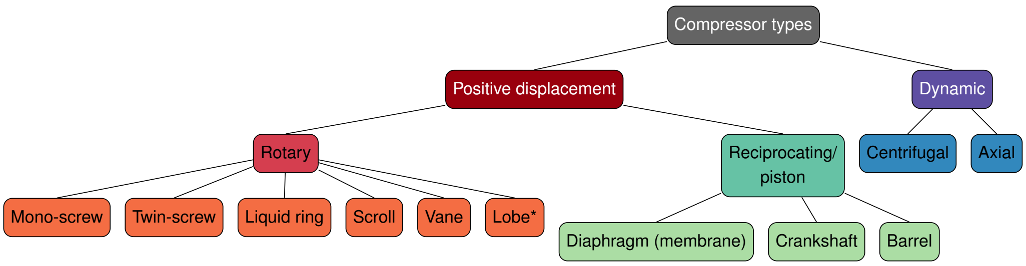


Figure 14: Tree diagram of compressor types, adapted from Wikipedia [57] with inspiration from Favrat [58]. Novel technologies are marked with asterisk (*).

Table 5: Input data to MOGA algorithm, adapted from Table 26 (1-11) and Table 27 (12).

	Type	Volume [m³/h]		Pressure [bar]		Pressure ratio [-]		Power [kW]		Effi-ciency [%]	Cost function	Stag. p. casing
		min	max	min	max	min	max	min	max	avg		
	c	$\dot{V}^{c,\min}$	$\dot{V}^{c,\max}$	$p^{c,\min}$	$p^{c,\max}$	$PR^{c,\min}$	$PR^{c,\max}$	$\dot{E}^{c,\min}$	$\dot{E}^{c,\max}$	η^c	$log(C_p)$	$n^{c,\max}$
1	Liquid ring	10	1'000	0.01	6	1	4	1	300	65	f_{c1}	2
2	Mono-screw	100	12 $\cdot 10^3$	0.1	24	3	5	20	1'000	67.5	f_{c2}	1
3	Twin-screw	300	35 $\cdot 10^3$	0.1	30	3	5	20	1'000	70	f_{c2}	1
4	Scroll	600	15 $\cdot 10^3$	0.1	25	3	8	1	35	60	f_{c2}	1
5	Vane	15	5'000	0.1	10	3	4	1	350	60	f_{c2}	1
6	Lobe	25	50 $\cdot 10^3$	0.3	2	1	2	10	1'000	70	f_{c2}	2
7	Centrifugal	2'000	288 $\cdot 10^3$	0.1	690	2.5	3	10	8'000	80	f_{c3}	9
8	Axial	9'000	850 $\cdot 10^3$	0.1	10	1.2	1.4	10	8'000	85	f_{c3}	20
9	Crankshaft	20	15 $\cdot 10^3$	0.01	4150	3	5	1	2'000	70	f_{c4}	8
10	Barell	1	800	0.01	400	3	8	1	2000	70	f_{c4}	8
11	Diaphragm	1	150	0.01	1400	1	10	1	1500	70	f_{c5}	3
12	GFB radial	1	1'300	0.34	139	1.5	6	0.2	250	78.5	f_{c5} [a]	9 [b]

[a] data not available: highest cost function taken (from diaphragm)
[b] data not available: taken from centrifugal compressors

3.2 Method

This section presents the developed methodology for the software tool presented before. The section first presents an analysis of **state-of-the-art: advanced heat pump (integration) concepts**, followed by the **objectives**, the **problem statement** and the **problem resolution: general approach**.

3.2.1 State-of-the-art: advanced heat pump (integration) concepts

Analysis of the most cited publications during the past 10 years related to the key words *waste heat recovery* shows that HPs are not considered as a primary option for waste or excess heat recovery and efficiency improvement in industry. Figure 15 illustrates the distribution of the most cited publications within the last 10 years with an average of five or more citations, totalling 158 publications. Research in the field of (industrial) waste or excess heat recovery is largely dominated by organic rankine cycle (ORC) [59, 60] and thermo-electric devices [61]. This may stem from a fully explored state-of-the-art of industrial heat pumps and integration methods; however, the marginal penetration of integrated industrial heat pump systems (apart from basic refrigeration and air-conditioning) [2, 5] contradicts this notion.

The main barriers for broad usage in industry were summarised in section 1.3. Point (1) addresses the lack of knowledge and of comprehensive heat pump integration methods to provide improvement potentials [2, 5]. This subsection aims at bridging the knowledge gap by summarising the comprehensive literature review of available heat pump synthesis methods depicted in subsection B.1. The focus was placed on multi-stage (single fluid) heat pump cycles using latent heat. These systems rely on the most widely used technologies [5] and were therefore selected for further analysis.

For these systems, a distinction was made between **methodology-based studies**, which provide mathematical or conceptual synthesis strategies for heat pump systems, and **application-based studies** which present analytical synthesis or experimental analysis of novel heat pump features and advanced cycles.

Typically, methodology-based studies propose advanced heat pump synthesis methods considering process integration techniques using standard components available on the market. Application-based studies are focused on resolving technical challenges with novel components and cycle configurations. Ideally, there should be synergies between the two approaches to succeed in advancing heat pump systems and integration concepts. This can be achieved by considering novel components from application-

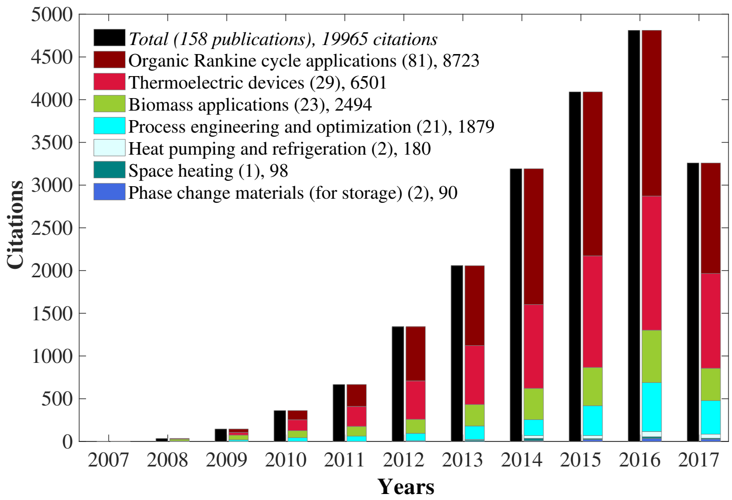


Figure 15: Web of science [62], key words: *waste heat recovery*, top cited papers of last 10 years ($\geq$ 5 citations/year), accessed 11.08.2017.

driven research in synthesis methodologies, or by providing experimental proof for theoretical results from synthesis methodologies.

3.2.1.1 Application-based studies From application-based studies discussed in appendix B.1.2, five elements were identified as potential features for improved heat pump performance.

1. Multi-stage compression, where latent heat is released or consumed at multiple pressure levels [63, 64]
2. Multi-stage expansion, same principle as above, except that different pressure levels are reached with valves instead of compressors. [65, 66]
3. (Multi-stage) ejection, same principle as above except that ejectors are used to partially substitute compressors [67, 68]
4. Cascaded cycles, use of several separated cycles which can interact through heat exchange [69–72]
5. Gas-cooling with heat exchange, by recovering heat from superheated vapor at the compressor outlet, a multi-temperature profile is generated [73, 74]

3.2.1.2 Methodology-based studies Studies presenting conceptual and mathematical methods for optimal heat pump design and integration with industrial processes were presented in appendix B.1.1 and can be summarised as follows:

1. Conceptual methods provide important insight to problems but cannot assess solution optimality. The advantage is, however, that technical infeasibilities and practical constraints can be considered without facing computational problems.
2. Mathematical methods may experience convergence issues for large-scale problems due to increasing complexity. Therefore, many studies considered a reduced solution space.
3. Technical constraints for realistic solutions are not considered.
4. Few studies provide a combination of conceptual and mathematical approaches, which leverage the advantages of both methods, e.g. through introduction of technical constraints, or multi-solution generation.
5. There is a lack of methods addressing optimal design of industrial heat pumps considering a comprehensive range of heat pump features and fluid selection.
6. Compressor type selection has not been treated in the literature.

3.2.2 Objectives

The literature review presented in the previous (section 3.2.1) provides extensive evidence for the need of continuing and thorough research in the field of methods for integration of industrial heat pumps. The purpose of this section was to overcome the above-mentioned shortcomings in state-of-the-art approaches. This project has aimed at addressing points (2)-(6).

This was achieved by development of a novel HPS synthesis method which is solved using mathematical programming for optimal design and integration of industrial heat pump systems. The approach was integrated in a software tool to enable different applications. A multi-objective decomposition solution strategy allowed convergence for large problems and provides multiple solutions for expert judgement adapted to the diverse criteria relevant in industry. The developed methods integrate innovative concepts of industrial heat pumps considering progress in working fluids, heat exchange, multi-stage systems, and compression technologies using optimisation methods and process integration techniques.

3.2.3 Problem statement

Given

- industrial process thermal and material demands
- set of candidate utility technologies, including potential heat pumps with operating ranges

Determine

- optimal utility system design
- optimal design of the heat pump system including:
  - specification of technologies
  - features
  - working fluid
  - operating conditions (temperatures, pressures, etc.)

This method aims at providing a utility target and preliminary design of the heat pump system as the basis for detailed design considering dynamic behavior in a subsequent step (not treated here).

3.2.4 Problem resolution: general approach

A flowsheet and a temperature entropy diagram of the novel heat pump superstructure (HPS) are depicted in Figure 16. It illustrates the various potential pathways and features considered in the superstructure. Some features are represented in sample cycles.

The superstructure is equipped with a condenser and evaporator at the highest and lowest pressure levels, respectively. The intermediate levels additionally contain a presaturator, a post-compression gascooler, a subcooling heat exchanger, and a superheater. Compressors and valves are made available between all pressure levels. Superheated vapor exiting the compressor can be de-superheated in a heat exchanger (gas-cooler) and condensed (represented by one heat exchanger), and/or sent to a presaturator which saturates the fluid and separates it into its phases. Two-phase flow leaving the expansion valves can be evaporated (and potentially superheated by mixing or heat exchange) and then compressed or mixed with condensate with options of inter-cooling and/or subcooling before expansion.

The statement above corresponds to a non-convex mixed integer nonlinear programming (MINLP) problem. The integer variables relate to activation of different technology options while nonlinearities mainly arise from capital cost correlations and the intrinsic nonlinearity of thermodynamic property correlations. Therefore, a decomposition strategy [75] is applied as presented in Figure 17 which incorporates the nonlinearities at the master level solving the linear problem at the slave level. The variables present in the nonlinear constraints are set at the master level and thus act as parameters for the slave optimisation. At the slave level, the linear problem is solved and the decision variables contained in the linear constraints and the linear objective function are transferred to a post-computational analysis where the nonlinear capital cost correlations and objectives are calculated. Based on the objective function values,

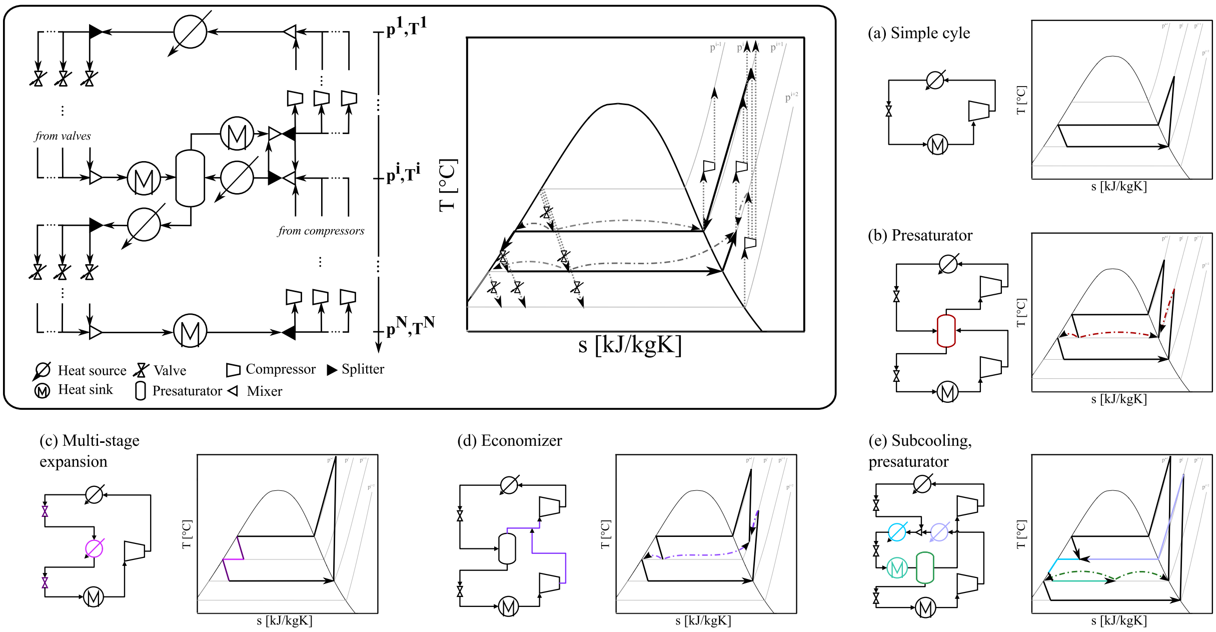


Figure 16: Flowsheet and temperature-entropy diagram of the HPS with sample cycles.

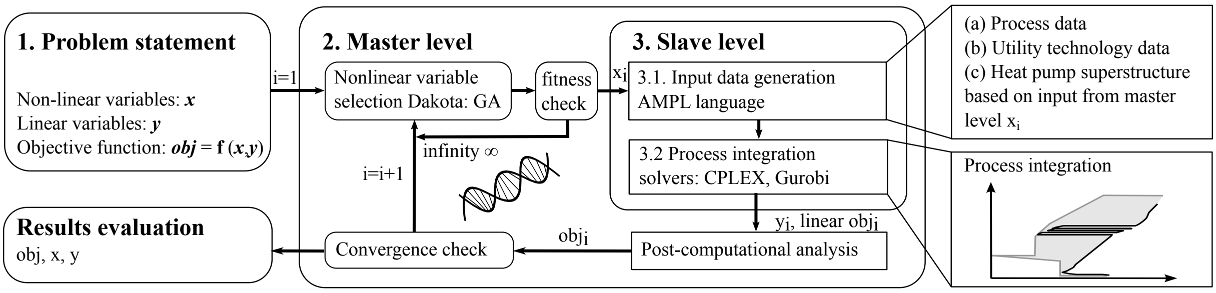


Figure 17: Flowchart of decomposition strategy solving MINLP superstructure implemented in Lua OSMOSE platform [31, 75].

a convergence check is performed and a new iteration is initiated at the master level.

The main assumptions considered in the heat pump superstructure are:

- the thermodynamic behavior is at steady-state
- heat losses and pressure drops in piping and the components are negligible
- the outlet of a condenser is either saturated or subcooled
- the outlet of an evaporator is either saturated or superheated
- isenthalpic expansion in the valves
- the minimum approach temperature difference is fixed for every stream (and follows the indications from the literature cases)

More details about the problem formulation and solution strategy can be found in appendix B.2.

3.2.5 Fluid selection

A theoretical background, working fluid review and state-of-the-art analysis of fluid selection algorithms is presented in appendix B.3.

3.2.5.1 Screening step The first step includes a screening step. Thereby, the preliminary set of working fluids is identified using heuristics based on thermodynamic, physical and environmental criteria. Therefore, an interactive parallel coordinate visualization tool [76, 77] was developed, which is used to easily filter the potential fluid candidates for ORC and heat pumping and refrigeration (HPR) applications. Based on the desired properties, the list of fluids can be exported and further treated in the second step.

3.2.5.2 Optimization step Presuming fluid selection from known fluids, there are two options for conducting a fluid selection in the presented method.

(a) the list of candidate fluids is added to the **slave level**, in which every unit (condenser, evaporator, compressors, etc.) is reproduced as many times as there are fluids; the fluids are then activated using binary variables connected to the existence of each unit (y^w), or

(b) an integer variable referencing the fluid is added to the **master level**

The advantage of selection at the slave level, (a), is that cascaded cycles with different fluids can be designed and convergence of the decomposition strategy is reached after fewer iterations (due to fewer variables at the master level). The disadvantage is that the slave problem size increases proportionally with the number of fluids which impacts the MILP resolution time significantly. Both options were applied in this study depending on the respective problem statement (which will be indicated).

3.2.6 Compressor type selection

A theoretical background, large data collection of compressor types and full methodology is presented in appendix B.4.

Two methods for adding equipment selection to the previously-established methodology are proposed and tested in this work. They are presented in deliverable D3 and are summarised below. In the figure, the modified elements are highlighted in colour and the mathematical background is discussed in more detail in the following two subsections.

(a) Selection at **master level**. In this approach, one or several variables at the master level decide which type(s) of compressors are considered at the slave level. In this way, equipment sizing and selection at the slave level is performed with a pre-selected subgroup of possible compressor types and their respective operating ranges (pressure ratio, volume flow rate, absolute pressure, power, stages per casing) and performance data (isentropic efficiency). The best compressor types, working fluid and temperature levels are hence identified throughout the propagation of the multi-objective genetic algorithm (MOGA).

(b) Selection at **slave level**. Using this approach, all possible compressor types are added to the slave level with their respective operating ranges and performance data. Selection is then achieved through binary variables associated with each compressor at the slave level. The best compressor types are, therefore, identified in each run of the slave level, while the working fluid, temperature levels and other variables present in the nonlinear constraints are selected throughout the propagation of the MOGA at the master level.

The types of compressors considered are specified in Table 4.

3.3 Results - benchmark analysis

The **method** presented in the previous section (3.2) aims at providing a screening tool for heat pump pre-design and component pre-selection. The **results - benchmark analysis** stemming from the optimisation, which are presented in this section, serve as starting point for subsequent detailed design.

To benchmark the generic HPS computational framework were applied to the three literature cases. The selected cases were each treated in several publications.

(a) Case *E2* was selected because it was treated in two consecutive studies by Shelton and Grossmann [6, 22] and due to its heating and cooling requirements which span over a continuous temperature range as shown in Figure 41(a). This case provides exploration potential of a multi-temperature, multi-stage heat pump system which crosses the pinch located at -8 °C.

(b) An *ethylene plant* separation train [78] discussed by Colmenares and Seider [8] was chosen due to the refrigeration needs at extremely low temperatures (-115 °C) as shown in Figure 41(b). The pinch point is located at approximately 130 °C, which leaves little room for a heat pump crossing the pinch. Vaidyaraman and Maranas [23] discussed a slightly modified version of the same problem (different ΔT_{min}) with higher total cost, which is not treated here.

(c) A *Cold Tray* distillation sequence presented by Colmenares and Seider [7] and later studied by Swaney [79] was selected to revisit the original solution which disregarded an obvious improvement of heat pumping across the process pinch (≈ 60 °C). Figure 41(c) shows the process temperature enthalpy profile indicating the process thermal demands and pinch point. Swaney [79] considered a solution with heat pumping across the process pinch for this case study, however with modified input data (isentropic compressor efficiency of 0.8) and is, therefore, not considered here.

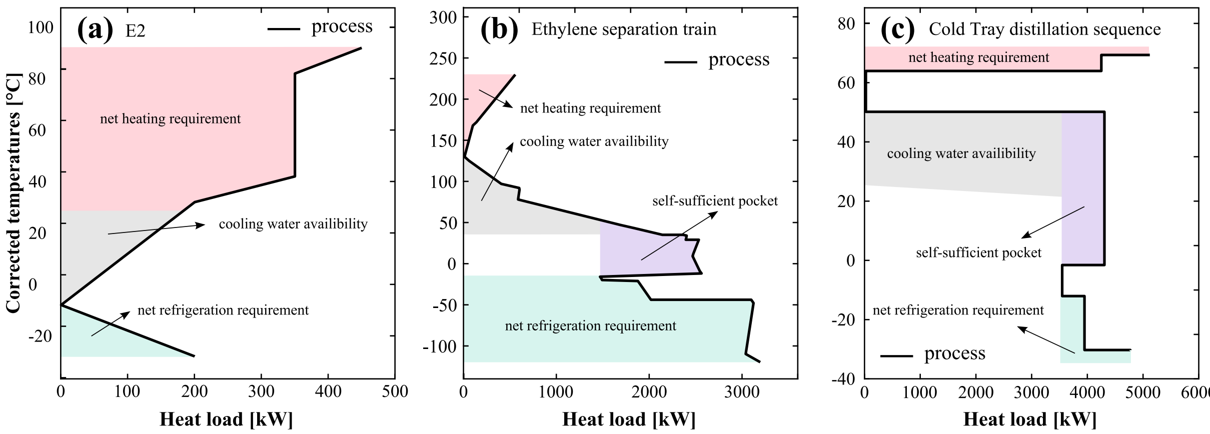


Figure 18: Grand composite curves (temperature enthalpy profiles) from process thermal streams of three benchmark cases, reproduced from (a) Shelton and Grossmann [6], (b) Lincoff et al. [78], (c) Colmenares and Seider [7], respectively.

Multi-objective optimization was carried out with regard to the two competing objectives being the yearly operating expenses (opex) and annualized capital expenses (capex). The saturation temperature levels and sub-cooling temperature differences (only in case *E2*) were the variables at the master level. Due to the more or less constant temperature requirements in the *Ethylene* and *Cold Tray* case studies, liquid subcooling and gas-cooling were not considered here. However, for these two cases, fluid selection was considered following the data from the literature [7, 8]. To investigate the potential for cascaded cycles, the set of candidate fluids was added at the slave level. The three cases are discussed in the next paragraphs.

3.3.1 General approach

The content of this section, section 3.3.2 and the **method** section is based on the following publication [29]:

A.S. Wallerand, M. Kermani, I. Kantor, and F. Maréchal, Optimal heat pump integration in industrial processes, ISSN 0306-2619. doi: 10.1016/j.apenergy.2018.02.114

For more detailed information, please refer to this publication.

3.3.1.1 Problem E2 - Shelton and Grossmann [6] The multi-objective results in Figure 19(a) exhibit a pattern of diagonal lines with interstitial gaps. These lines can be explained by the differing numbers of compressors. A trade-off is constituted between a reduction of opex by multi-stage compression, and an increase in capex related to a higher number of compressors with their associated variable and fixed investment costs. The number of compressors for solutions in the non-dominated frontier between opex and capex ranges from three to six. Minimum total annualized costs (TAC) was achieved with four compressors in contrast to the six suggested in the Reference. One additional advantage of this multi-objective optimisation approach is also that sub-optimal solutions with lower system complexity can be identified. The best solution with three compressors e.g. bears similar TAC ($\leq +1\%$) as the overall minimum cost solution with four compressors and may therefore be a better solution from the practical perspective. One advantage of the HPS is that it allows for a comprehensive analysis of heat pump features and operating conditions. The proposed minimum TAC solution consists of a heat pump with inter-cooling, subcooling, and gas-cooling heat exchangers as depicted in Figure 19(b) which contribute to achieving similar performance (in terms of opex) at reduced compressor fixed costs capex compared to the Reference. This leads to a potential overall 5% reduction in TAC as displayed in Table 5.

As indicated in Table 5, two other cases from the literature were treated leading to improvements in the TAC of around 30%.

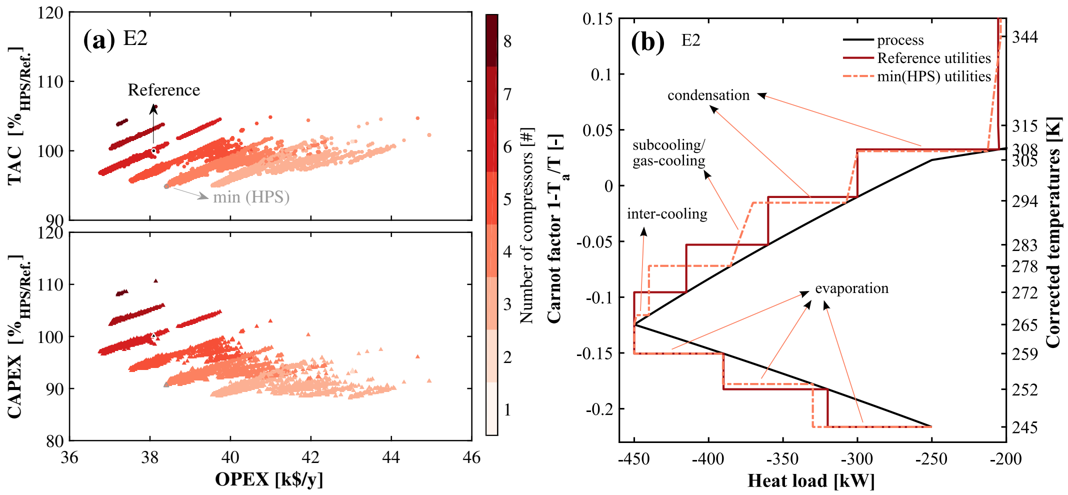


Figure 19: *E2 [6]*. (a) Multi-objective results, (b) integrated composite curves (Carnot factor enthalpy profiles) of Reference and min(HPS). Termination: 100k iterations (961 generations); last 50'000 iterations displayed.

3.3.1.2 Summary The HPS can represent a wide range of heat pump features and cycle architectures, while at the same time providing improved solutions (5-30%) to literature optimal cases with very different characteristics. This is attributed to a wider range of heat pump features considered and variable temperature level selection. As demonstrated, the level of complexity, variety of heat pump features considered, and technical constraints added depends on the choice of the user, which makes the superstructure flexible to handle. The solution strategy allows to generate a set of non-dominated solutions which enable the user to perform further analysis, thereby gaining deeper insight to the problem, and to apply other selection criteria. The literature cases discussed in this section serve for benchmarking

Table 6: Optimisation results. Data shown as *Reference* was generated with HPS based on the respective literature input data.

		E2 *[6]*		***Ethylene*** *[8]*		***Cold Tray*** *[7]*	
		Reference	min(HPS)	Reference	min(HPS)	Reference	min(HPS)
Opex							
Cooling water	$/y	0	0	25,020	23,150	29,930	4,810
Steam	$/y	10,460	10,370	0	0	287,090	39,310
Electricity	$/y	27,620	28,040	327,580	223,340	96,370	189,900
Capex							
No. of compressors	#	6	4	5	5	3	5
Compressors	$/y	54,710	49,630	230,810	159,140	56,380	109,220
TAC	$/y	92,790	88,050	583,410	405,630	469,770	343,230
Improvement	%	0	5.1%	0%	30.5%	0%	26.9%
$COP_{refrigeration}$	-	4.4	4.3	1.8	2.6	5.3	5.8

the underlying approach, however, important criteria are neglected, such as HEN costs, compressor isentropic efficiencies, ”real” utilities, and technical constraints thus generating ”theoretical” solutions.

3.3.2 Fluid selection

For the fluid selection, case *E2* [6] from the literature was treated further. A generic compressor with isentropic efficiency of 70% and a maximum compression ratio of 8 [bar/bar] was assumed.

3.3.2.1 Screening The choice of fluids considered for a heat pump integration to case *E2* was based on the following criteria.

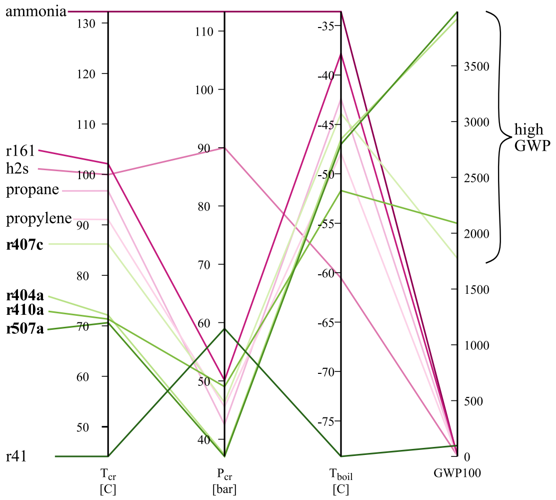
- critical temperature ($T_{crit} \geq 40$ ℃)
- the boiling point ($T_{boil} \leq -33$ ℃)
- global warming potential (GWP $\leq 4{\times}10^3$)

The fluid investment cost was not considered in this analysis. The working fluid selection platform developed for this project [55] was used to facilitate the fluid screening step which led to ten relevant fluids.

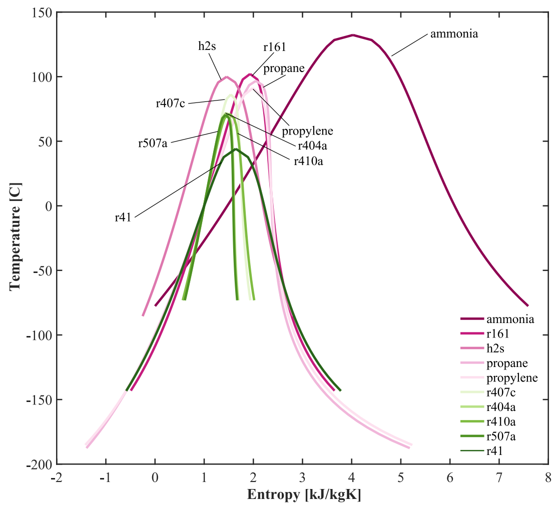
Figure 20 shows the fluid list and some of their properties generated with the tool. The GWP of most selected hydrofluorocarbons (HFCs) (r407c, r404a, r410a, r507a) is above 1500 [80] compared to hydrogen sulfide and natural refrigerants (ammonia (r717), propane (r290), propylene (r1270)) with GWP of below 10 [80, 81] and lower-impact HFCs such as r161 (12 [82]) and r41 (97 [83]). It has to be noted that some of these fluids are also the most recurring fluids currently used as depicted in the **fluid selection** appendix (app. B.3). The screening also considered several HFOs fluids, namely r1233zd, r1234yf, r1234ze(e/z), but the low temperature refrigeration requirement excluded their choice.

3.3.2.2 Optimisation The heat pump system for case *E2* was optimised with respect to opex and capex, since these are the industrial main drivers, and the safety and environmental concerns were addressed in the screening step.

Both fluid selection methods described in section 3.2.5 were applied and compared during this analysis. To ensure reasonable propagation of the optimisation algorithm (performed by a MOGA) during fluid selection at the slave level, a time limit of 600 seconds was imposed for the MILP solver. If the limit is reached, the solver returns the best integer solution at that point even if it is above the specified optimality gap. Nevertheless, a total of 25,000 MOGA iterations required higher computational time than 100,000 iterations with master level fluid selection.

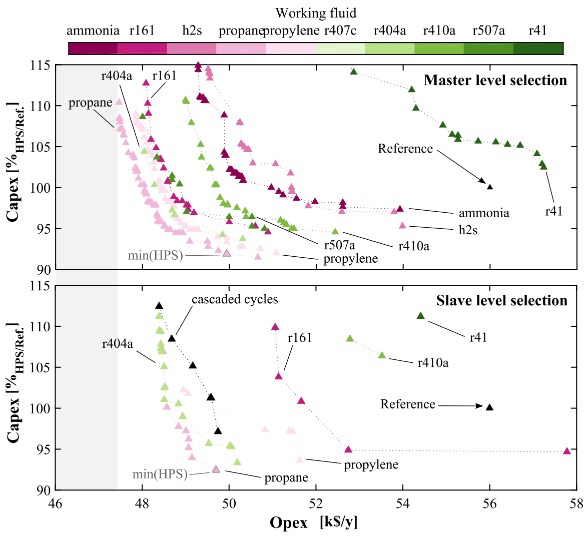


(a) Relevant data of selected fluids. Parallel coordinates selection platform [55, 77] (thermodynamic properties: CoolProp [84] GWP data: [80–83]).

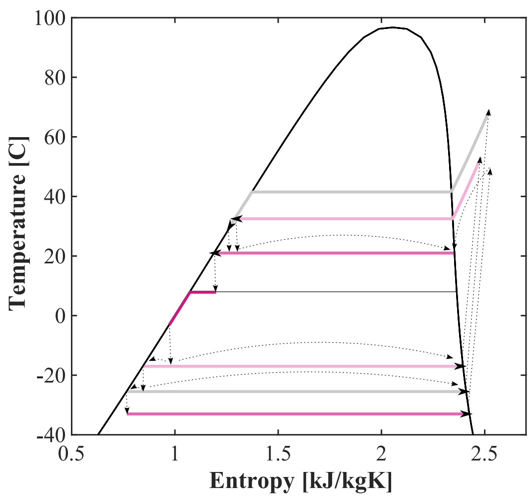


(b) Vapor-liquid saturation curves of selected fluids in temperature entropy diagram.

Figure 20: Set of selected fluids considered during multi-objective optimisation.



(a) Top: Selection at master level; 100k iterations, 211k sec. Bottom: Selection at slave level; 25k iterations, 890k sec.



(b) Temperature entropy diagram of the minimum TAC solution.

Figure 21: (a) Multi-objective optimisation results. In black: multi-fluid solution. R407c is not present, due to a Coolprop [84] problem with this fluid, (b) Temperature entropy diagram of the minimum cost heat pump solution.

Figure 21a shows the optimisation results of the different fluids generated over all MOGA iterations by both fluid selection methods. The non-dominated frontiers between opex and capex are the best solutions for each fluid in one of the two objectives. The results from the slave level selection (after intense computational effort) are dominated by the frontier of the master level selection, and it is thus concluded that if not necessary (e.g. for studying cascaded cycles) this method should be avoided. In the master level selection, propane dominates the other fluids over the entire range of solutions. This outcome was reproduced multiple times by rerunning MOGA with different seeds. Since the MOGA algorithm is aimed at improving the global non-dominated frontier, the frontier of propane yields a good approximation of the global Pareto curve for this case. The closest competitors to propane were: propylene, r161, r404a, r410a, and r507a. Ammonia and hydrogen sulfide generated higher-cost solutions, still strongly outperforming r41. All solutions (except r41) outperform the solution presented by the reference case updated with equivalent input data.

3.3.2.3 Summary The previous section presented the newly integrated fluid selection feature to a mathematical approach for optimal design and integration of industrial heat pump systems. The fluid selection is handled in a two-step approach. The first step aims at screening the full set of fluids in order to identify the most promising candidates with respect to some of the relevant criteria. During the second step, an optimisation algorithm is performed identifying the optimal heat pump design and integration, including the working fluid and operating conditions.

The method was tested on a reference case from the literature [6]. The screening step determined 10 fluids most of which were HFCs and NRs (about 50/50). The lowest cost solutions were achieved with propane over r40a, r161, r507a, hydrogen sulfide, and ammonia. The total cost with respect to the reference were improved by about 10%, which is attributed to the impact a comprehensive approach including rigorous fluid selection methods. The dominance of propane could be explained by its favorable thermodynamic properties, which may in future work be used to derive novel fluids based on those desired properties. It could further be shown that in a particular industrial process with optimised heat pump design, different performance can be achieved with consistent working fluids as compared to the typical conditions (standard single-stage HP). In this case, propane yields the highest performance, while ammonia is in the lower midfield, unlike the results generated from simple COP calculations.

3.3.3 Compressor selection

For the compressor selection the test case *E2* [6] was used to compare the results to the generic compressor type assumed in the previous section.

Figure 57 shows the non-dominated frontiers of the original and the two compressor selection algorithms. It can be seen that the master level compressor selection in Figure 57b and slave level algorithm in Figure 57c show a similar shape as the original algorithm in Figure 57a. On all frontiers, only propane is selected as the working fluid. With all three approaches, gas-cooling is only activated for the lowest opex solutions. All three algorithms have propane in their lowest TAC point with three compressor stages and subcooling. It is interesting to note that the slave and master level selection reach almost the same minimum TAC point and non-dominated frontier as the original work, though with lower opex. The master level selection reaches this solution for the same number of runs in shorter time. However, it was not investigated whether the slave level selection algorithm would have reached that frontier after fewer iterations. Therefore, it is only concluded that both selection algorithms work well and either of them or any combination should achieve good solutions, though performance of one approach may be slightly better depending on the application at hand.

Two conclusions can be drawn from this analysis: Firstly, the minimum TAC point exhibits similar features in all three approaches, which means that the generic compressor used in the *simplified* original method must have similarities to one of the compressor types in the advanced methods; therefore, conclusions drawn from the *simplified* original method still hold. Secondly, the two equipment selection algorithms show similar performance in terms of non-dominated frontiers and computational effort which is why both and any combination of them are recommended for further use, depending on the application.

It can be noted that, in both the master and slave level equipment selection, one compressor type is principally present, namely the **GFB radial** compressor described in appendix B.4. This compressor type was developed at the Swiss Federal Institute of Technology and promises superior properties for the case study at hand. It is noted, that this is not the compressor type with the highest isentropic efficiency; therefore, other properties should also be studied. Axial and centrifugal compressors, for example, offer higher isentropic efficiencies; however, they are limited to applications with high volumentric flowrates and low pressure ratios. It could be shown that pressure ratios between 1.5 and 6 are present in the non-dominated solutions. This explains the preference of the GFB radial compressor over the two standard dynamic machines by the selection algorithm. This conclusion is further reinforced by observing the minimum and maximum volumetric flowrates which indicate ranges between 10 and 350 m^3/h, well outside the boundaries of the dynamic compressors listed here. The pressure ranges indicate that none of the compressors exceed their higher limit. In fact, they do not exceed 15 bar absolute pressure, thereby staying below the ranges of $\geq$ 400 bar for reciprocating compressors.

Master level selection was also tested for three compressor types at the slave level to evaluate mixed compressor type heat pumps. However, due to the superior fit of GFB radial compressors, the optimisation yielded the same results. Since GFB radial compressors are novel and not yet widely available on the market, no cost function was available. The highest cost function of commercially-available compressors f_{c5} (diaphragm compressors) was, therefore, assumed for this compressor type. There is, however, a significant uncertainty related to this assumption which should be explored in future work.

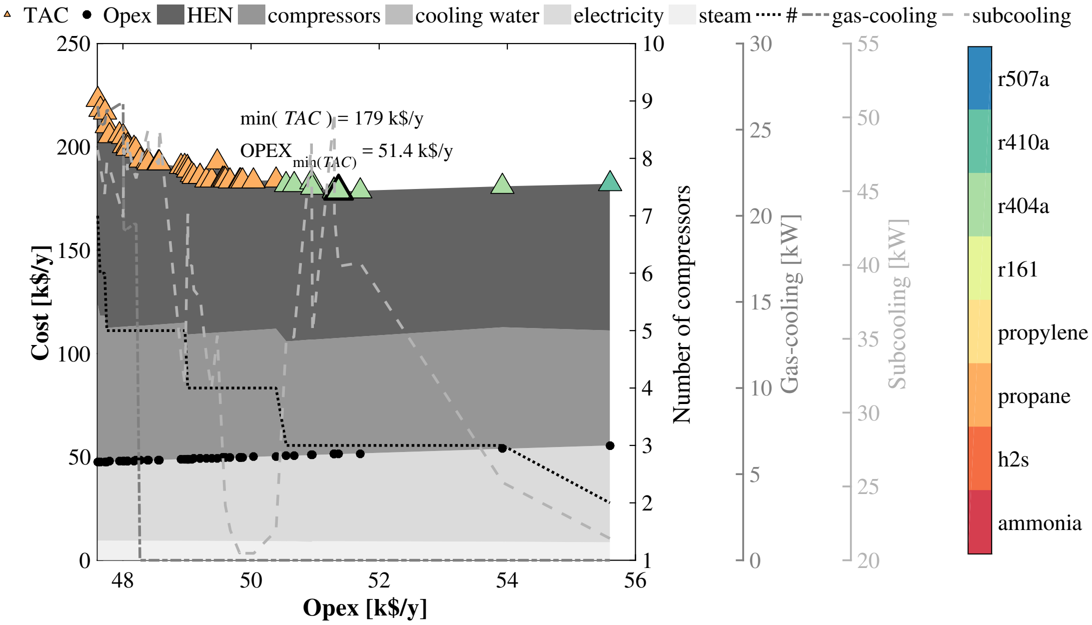


Figure 22: Non-dominated frontier of *Master level selection* without GFB radial compressors (one type at slave level).

To analyse the outcome of the approach independent from this uncertainty, two optimisation runs with master level selection were carried out without considering the GFB radial compressors. The two optimisation runs contained one run with a single compressor type and one run with three compressor types present at the slave level. The results were similar and hence only one compressor type at the slave level is discussed further. Figure 22 shows the non-dominated frontier of this run. As can be observed in Figure 22, the lowest total cost solution has a different working fluid than the results of the compressor type selection with GFB radial compressors discussed previously (propane). This indicates that fluid and compressor selection influence each other, and should be considered simultaneously. It can further be seen that (if GFB radial are neglected) diaphragm compressors are the favored compressor type for this case study. Diaphragm compressors exhibit similar properties to the GFB radial compressor, allowing slightly higher compression ratios and lower maximum volumetric flowrates. Investigating the maximum compression ratio and volumetric flowrates of the non-dominated solutions shows that the limit of both properties is often reached, indicating that these two properties (similar to the GFB radial) have a decisive impact in compressor selection. It can be observed that higher opex, lower capex solutions exhibit lower pressure ratios with a different working fluid. This indicates again that compressor type selection and fluid selection are largely intertwined. This also explains why higher pressures (up to 25 bar) were reached during this optimisation, which is again associated with the different fluid types present in the solutions.

3.3.3.1 Summary An additional level of detail has been added to the methodology presented in the two previous sections 3.2.4 and 3.2.5 which aims at further exploring the chance to provide detailed directions for experimentalists and equipment manufacturers. The aim was to consider various compressor types and their impact on system performance. Two compressor selection methods were considered as presented in section 3.2.6.

It was found that compared to the original algorithm, the computational effort was not increased by adding both compressor selection methods to the methodology. In all three approaches, the minimum TAC point exhibited similar features (propane, three compression stages, subcooling), which means that the generic compressor used in the *simplified* original method must have similarities to one of the compressor types in the advanced methods and, therefore, conclusions drawn from the *simplified* original method still hold.

However, depending on the available compressor types, the equipment selection had a strong effect on the choice of fluids in the non-dominated frontier and should, therefore, be considered when searching for solutions. The two equipment selection algorithms show similar performance in terms of non-dominated frontiers and computational effort which is why both and any combination of them are recommended for further use depending on the application at hand.

Novel gaseous film bearing (GFB) radial compressors developed at the Swiss Federal Institute of Technology and positive displacement compressors (mainly diaphragm) were favoured over rotary and standard dynamic compressors for the case study at hand which is accompanied by high compression ratios and low volumetric flowrates. Such conclusions are limited to the investigated case study and cannot be considered general recommendations but rather shows the strength of the approach to identify the most appropriate compressor, working fluid, and design options in each case.

4 Swiss potentials

In this section, the methods and tools developed throughout this project are used to estimate the saving potentials through heat pump integration in various industrial sectors. This allows impact quantification of heat pumping toward the CH energy transition, and role of compressor types and fluids in various industrial sectors. Firstly, the adopted **method** is presented, followed by the **status quo** of the CH energy system. And finally, the **swiss potentials** describe the CO_2-eq. mitigation potential of heat pumping in the various processes and sectors studied.

4.1 Method

4.1.1 Keywords and assumptions

The list of key words and key assumptions and their meaning for calculation of energy saving potentials is discussed below.

- **BAU**: The business as usual (BAU) energy consumption is based on current consumption values documented e.g. in the BREFs, which is indicated for each investigated process.
- **Reference plant** here refers to the current consumption data of industry and is used as a reference for the estimation of relative saving potentials.
- Two energy saving scenarios were investigated for each of the considered processes with respect to the reference plant.
  - **ΔHR**: In this scenario, HR is considered in the process and, thereby, allowing derivation of the minimum thermodynamic energy requirements.
  - **Δdirect$_{HP}$**: In addition to the HR, saving potentials through optimal HP integration were analysed. HP can reduce the hot utility consumption at the cost of increasing the electricity requirements.
- Expert opinion (EO): For each of the investigated processes an indicator for the feasibility of the realisation of the calculated potentials was introduced. This qualitative indicator relies on an expert opinion to judge safety constraints, heat transfer restrictions, and the maturity of required equipment.
  - ★☆☆: Technically very challenging realisation (due to safety, technical maturity) (factor 0.2)
  - ★★☆: Technically feasible, but with challenges to face (factor 0.5)
  - ★★★: Technically possible, even economically feasible (factor 0.8)
- Extrapolation to sector: as the processes modelled in this study do not cover the entirety of their respective industrial sectors in terms of energy consumption, three saving scenarios were developed at the sector level. In the results section, the optimistic and conservative scenario are presented in Figure 38 and Table 16.
  - **Optimistic**: Assumption that the weighted average of saving potentials of the modelled processes can be extrapolated to the entire sector.
  - **Technical**: Based on the optimistic potential, though reduced accounting for the expert opinion (EO). *This scenario is not specifically reported.*
  - **Conservative**: Assuming that within the sector the **Technical** savings potentials can be realized only for the processes investigated in this report. All other processes in the sector are assumed to have zero saving potential.

- This work focuses on thermodynamic and technical potentials achievable through heat recovery (HR) and heat pump (HP) Upgrading existing equipment apart from HP equipment (e.g. to higher efficiency, or modern technology) was not taken into account. The calculated energy requirements are therefore linked to the current process operation with current equipment (pumps, mills, compressors, etc.). Analysis of electrical (and thermal) saving potentials linked to upgrading of equipment as performed, for example, by Zuberi and Patel [85] was, hence, not considered.

4.1.2 Screening energy saving potentials: solution generation

4.1.2.1 ΔHR The ΔHR saving potential was derived based on the thermal profile (GCC) of the process. It was reported with respect to the business as usual (BAU).

4.1.2.2 Δdirect To derive the Δdirect energy saving potentials, a screening step was introduced using the MILP sub-process from section 3.2.4 [29] and not the full approach. For each process thermal profile, 1,000 samples were created with various combinations of compressor types (max. two different from a choice of 12 different as presented in section 3.2.6) and fluid types (max. two different from a choice of 14 fluids). In each run of the MILP, the TAC were minimised. Subsequently, the solution which minimises both the CO_2-eq.-equivalent emissions and TAC (selection reported in each case separately) was identified. Relative improvements were computed with respect to the BAU.

4.2 Status quo

Assessing the current status of the Swiss industrial energy consumption data is necessary for two reasons: It (1) serves the purpose of identifying which processes are the largest energy consumers and emission generators in each sector and their relative fraction and (2) forms the basis for extrapolating the understanding consumption in each sector to identify relevant industry for assessing energy saving potentials.

An extensive literature study was performed to identify the current BAU energy consumption data of various processes in the six most energy intensive industrial sectors. Energy consumption was determined based on the product specific energy consumption (SEC) and estimated Swiss production rates. The SEC data was mainly based on the European reference documents for best available techniquess (BREFs) documents, while the annual the production rates were based on information available from Swiss trade associations. The results of the *status quo* analysis of industrial energy requirements are presented in Table 6. Detailed descriptions of these data with extensive references are provided in appendix C.2.

The Swiss industrial sectors considered here are: food & beverage, pulp & paper, chemical, cement, steel and non-ferrous metals. These industries account for 82% of thermal and 56% of electrical consumption in Swiss industry. Using annual production volumes and the SEC, the total annual energy consumption of each investigated process and its relative impact in the sector is estimated. This allows identification of the relevant processes, which is further discussed in the following sections. The details of each sector are briefly introduced in the following section to aid comprehension of the work performed and results.

4.2.1 Sectoral energy consumption

4.2.1.1 Food & beverage The food & beverage sector is responsible for approximately 15% of the Swiss industrial electricity and thermal energy consumption. The sector is extremely diverse and thus difficult to represent completely. Several representative processes were identified which consume approximately 74% and 54% of the thermal and electrical energy of the sector, respectively. The most impacting processes in Switzerland were identified as: the dairy industry, sugar production, chocolate-making, fresh bread, tobacco, and meat production. Heat pump integration in the food & beverage sector is generally favourable due to low pinch temperatures and often have existing refrigeration systems which can be integrated with a proposed heat pump system. The processes in this sector typically include water-based fluids below 100 °C. The main obstacles for HP integration in the food & beverage

Table 7: Swiss current industrial process energy consumption and comparison to sector totals, sorted by SFOE no. and thermal energy requirements.

Sector / process specifications				CH annual consumption				Annual production	SEC		Pinch temperature
									Public BAU[00]		
Sector	SFOE No.	Process	NOGA	Electricity (EL)		Thermal energy (TH)		2018*	EL	TH	
				TJ/y	(% Total SFOE)	TJ/y	(% Total SFOE)	t/y	MJ/t	MJ/t	°C
Food & beverage	1	Dairy	10.1501, 3,.52	2,435[01]	(31.7%[02])	1,878[01]	(21.3%[02])	1,962,115[10]	1,241[11]	957[11]	60[86]
	1	Cheese	10.1502	555[01]	(7.2%[02])	880[01]	(10%[02])	191,321[10]	2,900[11]	4,600[11]	40 [86]
	1	Sugar	10.81	126[01]	(1.6%[02])	793[01]	(9.0%[02])	267,000[12]	577[13]	3,622[13]	70 [87]
	1	Chocolate	10.82.01	457[01]	(6.0%[02])	588[01]	(6.7%[02])	141,282[14]	3,237[15]	4,160[15]	25[16]
	1	Fresh bread	10.71.11	7[01]	(0.1%[02])	543[01]	(6.2%[02])	114,264[17]	60[18]	4,750[18]	25[19]
	1	Beer	11.05.1	138[01]	(1.8%[02])	435[01]	(4.9%[02])	365,941[1a]	378[1b]	1,188[1b]	15[88]
	1	Meat	10.7	192[01]	(2.5%[02])	276[01]	(3.1%[02])	360,651[1f]	533[1g]	764[1g]	25[1h]
	1	Tobacco	12.00	181[01]	(2.4%[02])	181[01]	(2.1%[02])	34.6 [Gcig][1c]	5,239,800 [MJ/Gcig][1d]	5,239,800 [MJ/Gcig][1d]	65[1e]
	1	Total (calc.)[03]	10, 11, 12	4,092	(53.4%[02])	5,573	(63.2%[02])				
	1	**Total (SFOE)**[04]	10, 11, 12	7,669	(14.9%[05])	8,813	(15.0%[05])				
Pulp & paper	3	Pulping (sulphite)	17.11	126[01]	(2.4%[02])	432[01]	(7.7%[02])	53,942[30]	2,340[31]	8,000[31]	75[89]
	3	Pulping (thermomechanical)	17.11	685[01]	(13.1%[02])	12[01]	(0.2%[02])	80,914[30]	8,460[32]	150[32]	N/A
	3	Packaging paper	17.12	621[01]	(11.9%[02])	1,802[01]	(32.2%[02])	345,239[33]	1,800[34]	5,220[34]	25[90]
	3	Paper	17.12	2,886[01]	(55.3%[02])	3,263[01]	(58.3%[02])	697,116[33]	4,140[35]	4,680[35]	25[90]
	3	Total (calc.)[03]	17.1	4,318	(94.2%[02])	5,508	(117.1%[02])				
	3	**Total (SFOE)**[04]	17, 18	4,585	(8.9%[05])	4,930	(8.4%[05])				
Chemicals	4	Refining	19.2, 20	555[01]	(6%[02])	10,319[01]	(60.4%[02])	3,626,640[40]	153[41]	2,845[41]	120[91]
	4	Total (calc.)[03]	19.2, 20	555[01]	(6%[02])	10,319[01]	(60.4%[02])				
	4	**Total(SFOE)**[04]	19, 20, 21	9,297	(18.0%[05])	17,084	(29.1%[05])				
Cement	5	Dry process	23.51	1,429[01]	(87.6%[02])	11,442[01]	(98.4%[02])	3,687,966[50]	388[51]	3,102[51]	1,000[92]
	5	Total (calc.)[03]	23.51	1,429[01]	(87.6%[02])	11,442[01]	(98.4%[02])				
	5	**Total (SFOE)**[04]	23.32, 23.51, 23.52	1,632	(3.2%[05])	11,631	(19.8%[05])				
Steel	7	EAF	24.10	3,610[01]	(85.8%[02])	3,654[01]	(95%[02])	1,400,000[70]	2,578[71]	2,610[72]	25[93]
	7	Total (calc.)[03]	24.10	3,610[01]	(85.8%[02])	3,654[01]	(95%[02])				
	7	**Total (SFOE)**[04]	24.10,.20, .31-34,.51-52	4,207	(8.1%[05])	3,847	(6.6%[05])				
Non-ferrous metals	8	Aluminum (2nd)	24.42	107[01]	(8.4%[02])	904[01]	(59.6%[02])	237,900[80]	450[81]	3,800[81]	650[82]
	8	Total (calc.)[03]	24.42	107[01]	(8.4%[02])	904[01]	(59.6%[02])				
	8	**Total (SFOE)**[04]	24.41-.46	1,272	(2.5%[05])	1,518	(2.6%[05])				
Sector total	1,3-5, 7,8	Total (calc.)[06]	10,11,17, 19, 20,23, 24	14,141	(48%)	38,355	(79%)				
	1,3-5, 7,8	Total (SFOE)[07]	10-12, 17-23,24	28,662	(56%)	47,823	(82%)				
	1-12	**Total (SFOE)**[08]	10-33	**51,626**	(100%)	**58,615**	(100%)				

* if not indicated elsewise

00 **Public Business as usual (BAU)**: [MJ/ton product] Based public data from current consumption e.g. in the BREFs, which is indicated in each case.

01 *Calculated value* from the flow rate and BAU.

02 *Calculated* percentage of *SFOE sector total*[04].

03 *Calculated sector total* from investigated processes.

04 *SFOE sector total* 2018 energy consumption data from Swiss Federal Office of Energy (SFOE) [94].

05 *Calculated* percentage of *SFOE industry total*[09].

06 *Calculated* values and percentage of the processes covered in this table.

07 *Calculated* values and percentage of the sector totals (SFOE) covered in this table.

08 *SFOE industry total* energy consumption data from SFOE [94].

sector are safety, contamination regulations, and batch operations (such as in breweries) which require storage between batches.

Selected processes for HP integration For the reasons mentioned previously, heat pump integration is studied extensively in the food & beverage sector. The five most energy intensive processes (except bread-making) are therefore studied in more detail in the **swiss potentials** section: dairy, cheese, sugar, chocolate, and brewing. Making fresh bread relies on very specific ovens and heat transfer between a heat pump and the dough is qualified as "challenging" and is therefore disregarded for HP integration.

4.2.1.2 Pulp & paper In Switzerland, there are two main processes for making pulp, the sulphite process and mechanical processes [95]. The production volumes reveal, however, that the most dominant energy consumer in the CH pulp & paper industry is paper-making, since most producers use recycled paper as raw material [96]. This is also in agreement with the energy consumption data, which are dominated by the paper-making process, accounting for 90% and 70% of the thermal and electrical energy of the sector, respectively. The calculated estimate of the individual processes slightly exceeds that of the SFOE total and may be linked to the production volumes which date back to 2014 (more recent data were not available), while the SFOE data are from 2018 [94].

Selected processes for HP integration Heat pump integration is primarily interesting in the sulphite pulping process, exhibiting a moderate pinch temperature. The thermo-mechanical process principally consumes electricity, while paper-making is largely a heat sink [90].

4.2.1.3 Chemicals Though an extremely diverse sector, the chemical industry is classified here into refining and production of fine chemicals. The *refinery* category comprises products derived from crude oil such as gasoline, diesel, liquefied petroleum gas, etc. Organic fine chemicals include pharmaceuticals and vitamins, crop protection, dyes, etc. Due to product diversity and limited public data from organic fine chemicals and dominance (60%) of refineries in terms of thermal requirements, the latter were the only process considered in this sector. Potential for improvements in Swiss refining could be realised by integration with other processes such as biomass-derived fuel synthesis; however, these potentials are not explored in the context of this report.

Selected processes for HP integration The refining process has comparably low pinch temperature (120 ℃) which motivates analysis of HP integration potentials.

4.2.1.4 Cement In Europe, the dry cement process is the most common. In Switzerland, it is the only process used for making cement. The specific energy consumption, together with the estimated CH production volume, accounts for 100% of the value reported by the SFOE.

Selected processes for HP integration The highly integrated nature of clinker production, where the hot utility cannot be extricated from the process, led to the conclusion that heat integration is difficult to realise in the cement process. The high pinch temperature further renders heat pump integration uninteresting, which leaves room for further analysis with heat recovery/conversion technologies such as ORC.

4.2.1.5 Steel, non-ferrous metals The metals sector is categorized by the SFOE in two groups: ferrous metals and non-ferrous metals. The total calculated energy consumption based on the assumed specific energy consumption and production volumes accounts for 86% (thermal) of the steel sector consumption reported by the SFOE, which is sufficiently precise using generalized data. In Switzerland, steel production from scrap is the only process in operation and thus analysis and improvements which can be realised in the blast furnace/basic oxygen furnace route were not considered. This limited the analysis compared to other publications in the field of steel sector energy consumption.

For the non-ferrous sector, secondary aluminum production was used as the sector representative, being the largest consumer. It accounts for approximately 60% (thermal) of the sector SFOE total, missing noble metal, lead, zinc, tin, and copper production (general classification of economic activities [97] (NOGA)).

Selected processes for HP integration For both ferrous and non-ferrous metals, HP integration is less interesting since either the pinch temperature is too high (aluminum production), or heat transfer between solid (steel) and liquid (HP) is considered challenging. Therefore, HP applications in these sectors were not pursued.

4.2.2 Sectoral CO_2-eq. equivalent emissions

To assess the impact of HP integration on the CH energy transition, the CO_2-eq.-equivalent emissions of the individual processes and sectors must be quantified. An analysis of the fuel types in various sectors was therefore conducted based on the data from the Bundesamt für Energie BFE [94] which included: light/heavy fuel oil, coal, natural gas, district heating, and industrial waste incineration (refineries, pulp & paper, and cement). With emission factors from Ecoinvent [13], the sector-specific emission factors could be derived, and therefore the sector-specific equivalent CO_2-eq. emissions for energy resources. The emissions of the entire industrial sector (1-12 Total) were compared to results from the FOEN [11], which result in 4.69 M t CO_2-eq.-eq/y. The emissions reported by the FOEN neglect emissions related to industrial waste incineration, do not specify whether emissions related electricity consumption are considered, and show differences in the the sectors included in the calculations. Comparison between the two values is therefore impossible but are similar in many respects. Analysing the sectors discussed previously (Table 6), shows that these account for 71% of total industrial emissions, highlighting their impact in the CH energy transition.

Table 8: CH industrial sector annual CO_2-eq. emissions and according factors (scaled by energetic requirements of sector), based on data from Ecoinvent [13], Bundesamt für Energie BFE [94].

Sector	**EL** [kg CO_2-eq. / MJ]	**TH** [kg CO_2-eq. / MJ]	**Total emissions** [Mio. t CO_2-eq./y]	
1 Food & beverages	0.0359	0.0727	0.916	14.9 %
3 Pulp & paper	0.0359	0.0252	0.289	4.7 %
4 Chemicals	0.0359	0.0667	1.473	24.0 %
5 Cement	0.0359	0.0881	1.084	17.7 %
7 Steel	0.0359	0.0764	0.445	7.2 %
8 Non-ferrous	0.0359	0.0700	0.152	2.5 %
1,3-5,7,8 (Calc. sum)	0.0359	0.0696	4.359	71.0 %
1-12 Total	0.0359	0.0731	6.138	100.0 %

Emission factors from Ecoinvent [13]:
Electricity GWP 100a: 0.03591 [kg CO_2-eq. equivalent / MJ]
Light fuel oil GWP 100a: 0.08958 [kg CO_2-eq. equivalent / MJ], Heavy fuel oil GWP 100a: 0.09182 [kg CO_2-eq. equivalent / MJ], natural gas GWP 100a: 0.06922 [kg CO_2-eq. equivalent / MJ], Coal GWP 100a: 0.13568 [kg CO_2-eq. equivalent / MJ]
Biogenic carbon in **pulp and paper** GWP 100a: 0.00000 [kg CO_2-eq. equivalent / MJ], scrap burning in **cement** GWP 100a: 0.06648 [kg CO_2-eq. equivalent / MJ], **refinery** waste burning GWP 100a: 0.07784 [kg CO_2-eq. equivalent / MJ]
District heating (Swiss municipal waste incineration) GWP 100a: 0.00024 [kg CO_2-eq. equivalent / MJ]

4.3 Results

4.3.1 Input data

4.3.1.1 Fluid selection To identify relevant fluids for HP integration in the CH industrial sector, a web-based refrigerant selection tool [55] (created for this project) was used with the following criteria:

1. GWP $\leq$ 10
2. ODP $=$ 0
3. Boiling point $<$ 100 ℃
4. Critical temperature $\geq$ -33℃

A screenshot of the tool can be seen in Figure 23, where the favourable properties can be selected by brushing the relevant axes. The resulting fluid list is reported in Table 8 including some fluid characteristics. It contains 13 fluids, 10 NRs (including HCs), 2 HFOs, and one u-HCFC. The list of fluids is in agreement with the results from appendix B.3.4, highlighting the importance of natural refrigerants, HFOs, and u-HFCs in industrial HP systems.

Figure 23: Working fluid selection platform [55].

4.3.1.2 Cost data A set of the following general assumptions was used for the results presented below.

- natural gas price: 0.0735 CHF/kWh
- electricity price: 0.1221 CHF/kWh
- operating time: 8000h/y
- investment annualization factor: 0.08
- investment maintenance fraction: 0.05
- compressor cost functions: appendix B.4.4, HEN cost functions: Taal et al. [98], Cost of a shell/tube heat exchanger with mixed materials (carbon steel-stainless steel)

4.3.2 Sectoral energy and emission saving potentials

To quantify the emissions mitigation potential of HP integration in various industrial sectors, sector representative thermal profiles as described by Kantor et al. [54] were identified and HP integration was studied using such profiles. This section contains the detailed analysis of each representative process thermal profile selected in the **status quo** section and their potential for HP integration. The subsequent subsection presents the **summary and impact** of this analysis.

4.3.2.1 Food & beverage In the food & beverage sector, the following five processes including their thermal profiles were analysed in detail for HP integration: dairy [16, 54], cheese [86], sugar [87], chocolate [99], and brewing [88]. The detailed results are presented in the subsequent discussion.

Table 9: Fluids considered in the analysis for the in the Swiss energy transition.

Sub-stance group	ASHRAE	Name	ODP	GWP_{100}	OEL	Toxi-city	Flamma-bility	IDHL	MW	Boiling temp. [°C]	Critical temp. [°C]	Crit. pressure [bar]
u-HCFC	R1233zd(E)	Chloro-trifluoropropene	0	1	-1	1	1	-1	130.5	19	166.5	36.2
HFO	R1234ze(Z), (E)	Tetrafluoro-propene	0	6	800	1	1.5	16000	114	-19	150.1	35.3
HFO	R1234yf	Tetrafluoro-propene	0	4	500	1	1.5	16000	114	-29.4	94.7	33.82
HO	R1270	Propene (Propylene)	0	1.8	500	1	3	1000	42.1	-47.6	92.42	46.65
HC	R601a	Isopentane	0	4	600	1	3	1000	72.1	27.7	187.78	33.78
HC	R601	Pentane	0	4	600	1	3	1000	72.1	36.1	196.56	33.58
HC	R600a	Isobutane	0	3	1000	1	3	4000	58.1	-11.7	134.7	36.4
HC	R600	Butane	0	4	1000	1	3	4000	58.1	0	152.01	37.96
HC	R290	Propane	0	3.3	1000	1	3	5300	44.1	-42.1	96.7	42.48
HC	R170	Ethane	0	5.5	1000	1	3	7000	30.07	-88.6	32.18	48.72
NR	R744	Carbon dioxide	0	1	5000	1	1	40000	44	-78	31.04	73.8
NR	R718	Water/ Steam	0	0.2	-1	1	1	-1	18.02	100	373.95	220.6
NR	R717	Ammonia	0	0	25	2	1.5	320	17.03	-33.34	132.4	112.8

u-HCFC unsaturated hydrochlorofluorcarbons (u-HCFCs), HFO hydrofluoroolefins (HFOs), NR natural refrigerants (NRs) (inclduing HCs)

Dairy The process representative for the Swiss dairy industry which was considered here has been discussed extensively by Wallerand [16] and Kantor et al. [54]. The process thermal profile was scaled according to Swiss production volumes. During fresh dairy production, raw milk is initially centrifuged to produce cream and skimmed milk. Fresh dairy products are created from cream, such as butter, while others are manufactured from skimmed milk, such as milk powder/concentrated milk, ultra-high temperature (UHT) milk, and most types of yogurt and desserts. The main conversion steps involve heating (pasteurisation), mixing, homogenisation, and refrigeration.

For this representative thermal profile of a typical Swiss dairy process, a set of heat pump integration scenarios is investigated. To this end, as presented in section 4.1.2, a sample of compressor types and fluid combinations is selected, with the goal of minimising the TAC. The results of this *screening step* are presented below.

Figure 24 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq.. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler, a refrigeration cycle, and cooling water. It can be seen that no predominant fluid or compressor type is present in the lowest-cost solutions. Among the lowest TAC solutions (highlighted in the inset), more than half of the solutions contain two compressor types, indicating that combined types may have advantages due to larger ranges of operating conditions. Among those solutions, that with the lowest CO_2-eq. emissions was selected for further analysis.

In Figure 25, the ICC of the process with utility integration of the selected and a reference case are depicted. It is shown that the heat pump completely encloses the process, obviating the existence of the boiler. This is achieved through four compressors between 33 and 177 kW, as shown in Table 9, reducing the CO_2-eq. emissions compared to the reference plant by approximately 57%. The selected types are: **twin screw** and **GFB radial**, with **isobutane**, a HC, as working fluid. It should be noted that isobutane is a dry fluid, which is why 5K preheating before compression is considered. A payback time of 3.1 years is achieved with this solution and the overall COP (fraction between total condenser thermal power and total compression power) is slightly increased.

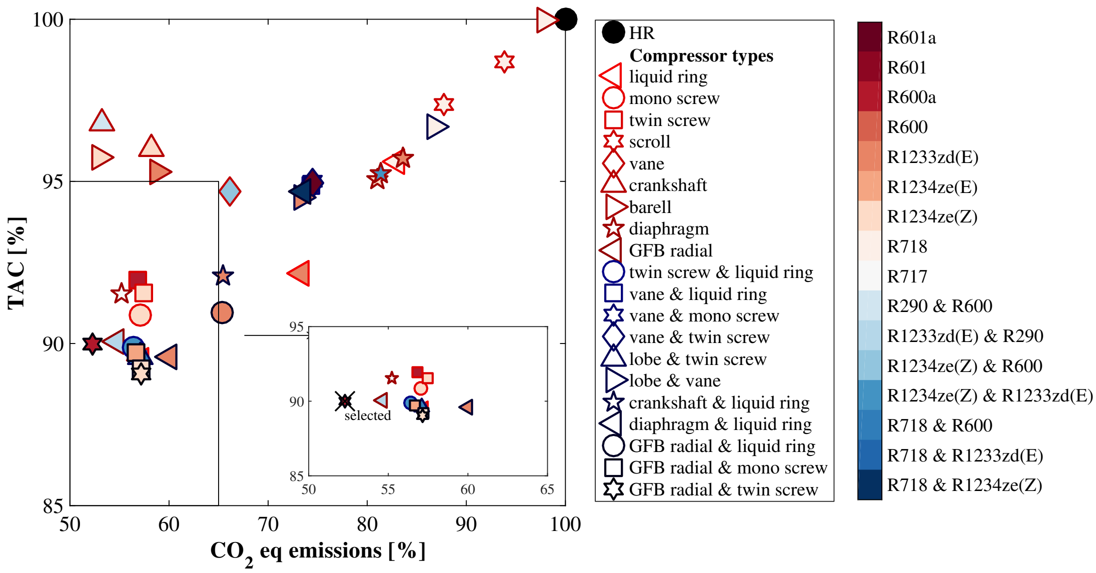


Figure 24: Results of *screening step* presented in section 4.1.2 for dairy process.

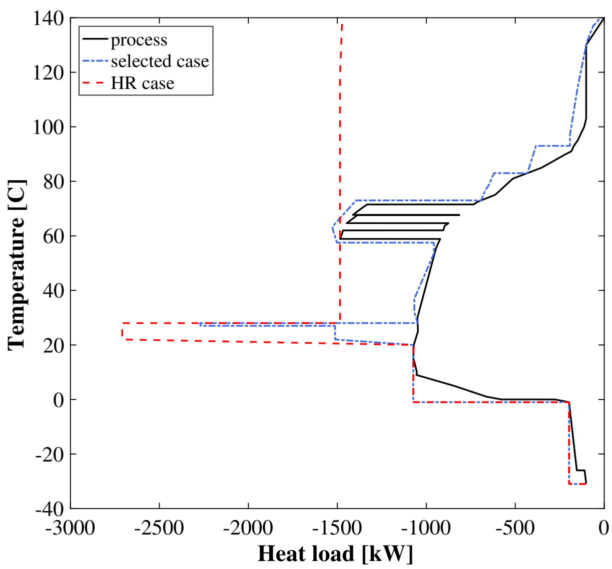


Figure 25: ICC of dairy process [16] with utility integration of selected and reference case.

Table 10: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for daries.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	147,737		328,539	
$Capex_{HEN}$	CHF/y	-	-	147,737		114,680	
$Capex_{HP}$	CHF/y	-	-	0		213,859	
Opex Total (8000 h)	CHF/y	18,374,488	3,990,663	3,594,955	(-9.9 $\%_{Ref.}$)	2,906,407	(-19.2 $\%_{HR}$, -27.2 $\%_{Ref.}$)
TAC Total	CHF/y	18,374,488	3,990,663	3,742,692	(-6.2 $\%_{Ref.}$)	3,234,947	(-10.0 $\%_{HR}$, -18.9 $\%_{Ref.}$)
Payback period (8000 h)	y			2.5		3.1	
(3000 h)	y			5.5		6.6	
Energetic data							
Size	kg/s	10					
Thermal energy (TH)	kW	9,570	2,078	1,485	(-28.5 $\%_{Ref.}$)	0	(-100.0 $\%_{HR}$, -100.0 $\%_{Ref.}$)
	kJ/kg	957.0	207.8	148.5		0.0	
Electricity (EL)	kW	12,410	2,695[C]	2,687[C]		2,975[C]	(10.7 $\%_{HR}$, 10.4 $\%_{Ref.}$)
	kJ/kg	1241.0	269.5	268.7		297.5	
Waste heat	kJ/kg	-	-	163.6		44.0	
	℃	-	-				
CO_2-eq. emissions	kg/t	114.1	24.8	20.4	(-17.5 $\%_{Ref.}$)	10.7	(-47.7 $\%_{HR}$, -56.9 $\%_{Ref.}$)
Expert opinion (EO)				0.8 (★★★)		0.8 (★★★)	
Heat pump properties							
Compressor number[HP]	#			0		4	
Compressor types[HP]	#			-		GFB radial & twin screw	
Compressor fluids[HP]	#			-		R600a	
Compressor sizes[HP]	kW			-		55/ 177/ 24/ 33	
Compressor sizes[REF]	kW			22/ 231		22/ 231	
$COP^{overall}$ (tot. cond./ tot. power)	-			4.82		4.90	(1.6 %)
COP each comp.	-			4.82		4.82/ 4.96	

* Reference plant data from Becker [86] (Table B.3) ratio reference plant to HR thermal 6164/4404, electricity 443/429.

C Electricity consumption of ref. plant (original data) refers to refrigeration needs only. Therefore the electricity consumption of the reference plant, HR and $\Delta direct_{HPS}$ were increased by public BAU (without refrigeration) $\Delta Ref_{EL} = BAU_{EL} \cdot Ref_{TH} / BAU_{TH} - Ref, refrigerat._{EL}$

Cheese Data for cheese-making was adopted from Becker [86]. During both cheese and fresh dairy production, raw milk is initially centrifuged to produce cream and skimmed milk. In cheese production, rennet is combined with milk to initiate curdling. The resulting curds may further be merged with cream, followed by forming, refining and packaging. The generated whey is dried and exported as a co-product.

The results of the HP *screening* for the cheese representative thermal profile are presented below.

Figure 26 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler, a refrigeration cycle, and cooling water. It can be seen that no predominant fluid or compressor type is present in the lowest cost solutions. As reported for the fresh dairy process, among the lowest TAC solutions (highlighted in the inset), more than half of the solutions contain two compressor types, indicating that combined types may have advantages due to the larger range of operating conditions. Among those solutions, that with the lowest TAC was selected for further analysis.

In Figure 27, the ICC of the process with utility integration of the selected and a reference case are depicted. It can be seen that for the selected case, the heat pump is capable of providing utilities for approximately half of the process, drastically reducing the boiler consumption and reducing the CO_2-eq. emissions compared to the reference plant by approximately 35%. This is achieved through four compressors between 23 and 557 kW, as shown in Table 10.

The selected types are: **twin screw** and **GFB radial**, with **R1234ze(Z)**, a HFO, as working fluid. A payback time of 2.4 years can be achieved with this solution and the overall COP is slightly decreased, since a heat pump system with a temperature lift of up to 60K is installed in addition to the refrigeration cycle with a temperature lift of 20K.

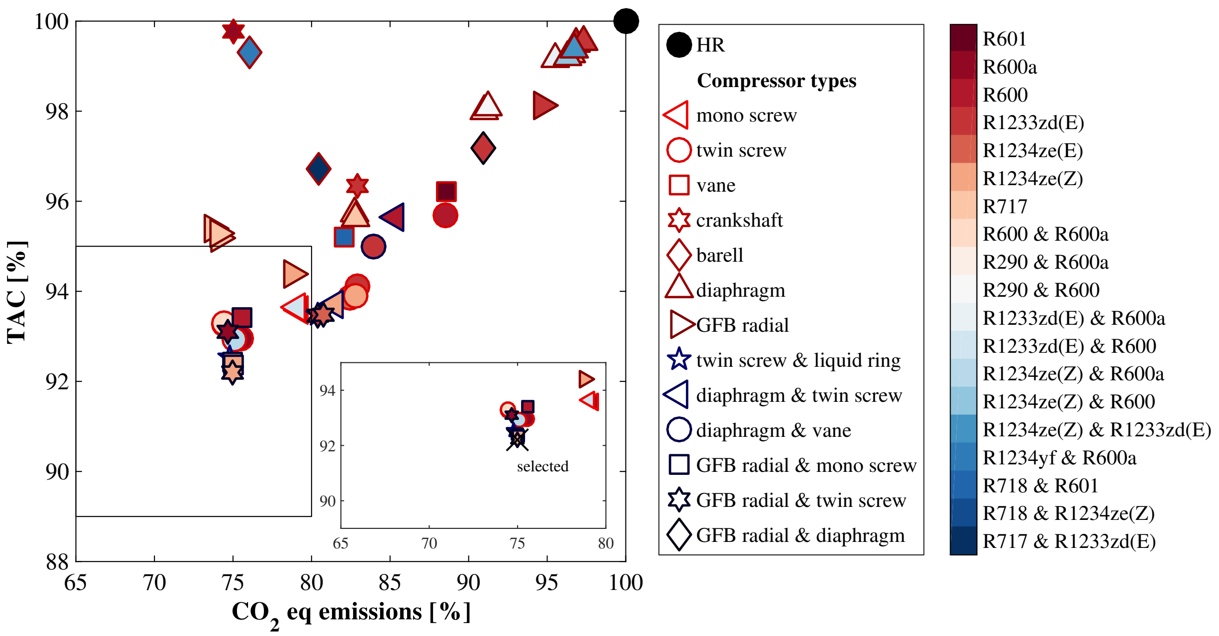


Figure 26: Results of *screening step* presented in section 4.1.2 for cheese making process.

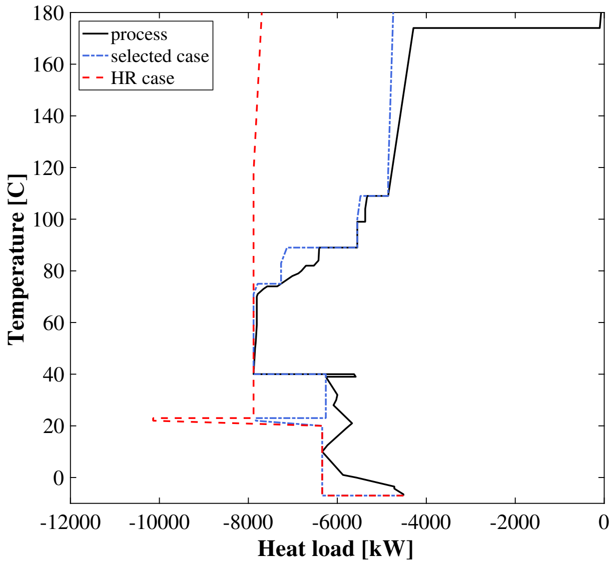


Figure 27: ICC of cheese making process [86] with utility integration of selected and reference case.

Table 11: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for cheese making.

	Unit	**Public BAU**	**Ref. plant***	**ΔHR**		**$\Delta direct_{HP}$**	
Cost data							
Capex Total	CHF/y	-	-	130,859		441,328	
$Capex_{HEN}$	CHF/y	-	-	130,859		66,621	
$Capex_{HP}$	CHF/y	-	-	0		374,707	
Opex Total (8000 h)	CHF/y	5,838,053	11,904,298	10,666,074	(-10.4 $\%_{Ref.}$)	9,391,753	(-11.9 $\%_{HR}$, -21.1 $\%_{Ref.}$)
TAC Total	CHF/y	5,838,053	11,904,298	10,796,933	(-9.3 $\%_{Ref.}$)	9,833,080	(-7.8 $\%_{HR}$, -17.4 $\%_{Ref.}$)
Payback period (8000 h)	y			0.8		2.4	
(3000 h)	y			2.0		5.2	
Energetic data							
Size	kg/s			1			
Thermal energy (TH)	kW	4,600	9,380	7,884	(-16.0 $\%_{Ref.}$)	4,858	(-38.4 $\%_{HR}$, -48.2 $\%_{Ref.}$)
	kJ/kg	4600.0	9379.8	7883.6		4857.6	
Electricity (EL)	kW	2,900	5,913^C	5,646^C	(-5%)	6,366^C	(12.7 $\%_{HR}$, 7.7 $\%_{Ref.}$)
	kJ/kg	2900.0	5913.4	5646.5		6365.8	
Waste heat	kJ/kg	-	-	3801.1		1494.5	
	℃	-	-				
CO_2-eq. emissions	kg/t	438.6	894.3	775.9	(-13.2 $\%_{Ref.}$)	581.7	(-25.0 $\%_{HR}$, -34.9 $\%_{Ref.}$)
Expert opinion (EO)				0.8 (★★★)		0.8 (★★★)	
Heat pump properties							
Compressor number^HP	#			0		4	
Compressor types^HP	#			-		GFB radial & twin screw	
Compressor fluids^HP	#			-		R1234ze(Z)	
Compressor sizes^HP	kW			-		23/ 49/ 90/ 557	
Compressor sizes^REF	kW			237/ 195		237/ 195	
$COP^{overall}$ (tot. cond./ tot. power)	-			5.23		4.49	(-14.1 %)
COP each comp.	-			5.23		5.23/ 4.05	

* Reference plant data from Becker [86] thermal 2895*0.9 kWh/kg, electricity 194 kWh/kg.

C Electricity consumption of ref. plant (original data) refers to refrigeration needs only. Therefore the electricity consumption of the reference plant, HR and $\Delta direct_{HPS}$ were increased by public BAU (without refrigeration) $\Delta Ref_{EL} = BAU_{EL} \cdot Ref_{TH} / BAU_{TH} - Ref, refrigerat._{EL}$

Sugar The sugar process was modelled after Morandin et al. [87], using case 1 with improved multi-stage evaporation to match the BREF BAU numbers for sugar production. It consists of four main steps being: (1) extraction; (2) juice treatment; (3) multi-effect evaporation; and (4) boiling, centrifuging & drying. Morandin et al. [87] describes sugar production from cane instead of beets, which is the feedstock used in Switzerland. It was assumed that the main energy-consuming steps (multi-effect evaporation, boiling, and drying) are similar and therefore the process data are still relevant. For a typical Swiss sugar factory, seasonal production based on the harvesting season is assumed, which is why the operating time appears as 3000 hours/y instead of 8000.

The results of HP *screening* for the sugar representative thermal profile are presented in Figure 28.

Figure 28 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler and cooling water. The solutions show that the trade-off between lower CO_2-eq. emissions and higher TAC identified for other processes is not present here. This indicates that HP integration is very favourable in the sugar production process which mainly relies on phase-changes in a small temperature range (≤50 ℃). The difference between solutions are the fluid and compressor type combinations and the associated cost and emissions, of which **centrifugal** compressors with **water** as working fluid are the most favourable for both criteria. The *second best solution* is achieved with two heat pumps relying on **water and R1233zd(E)**, a u-HCFC, with both **centrifugal and mono-screw** compressors.

In Figure 29, the ICCs of the process with utility integration of the selected and a reference case are depicted. It can be seen that for the selected case, the heat pump encloses the process entirely, reducing the natural gas consumption by 100%. This is achieved through four compressors between 2,490 and 3,180 kW, as shown in Table 11. This solution achieves approximately 86% CO_2-eq. equivalent emission reductions compared to the reference plant. The reduced operating time yields a longer payback time of 4.4 years compared to the previous processes. A COP of 5.68 can be achieved for the HP through multi-stage compression and intercooling. Centrifugal compressors are selected due to their large power range, which are, however constrained by the volumetric flowrate. This also provides an explanation for the necessity of two compressors for each stage.

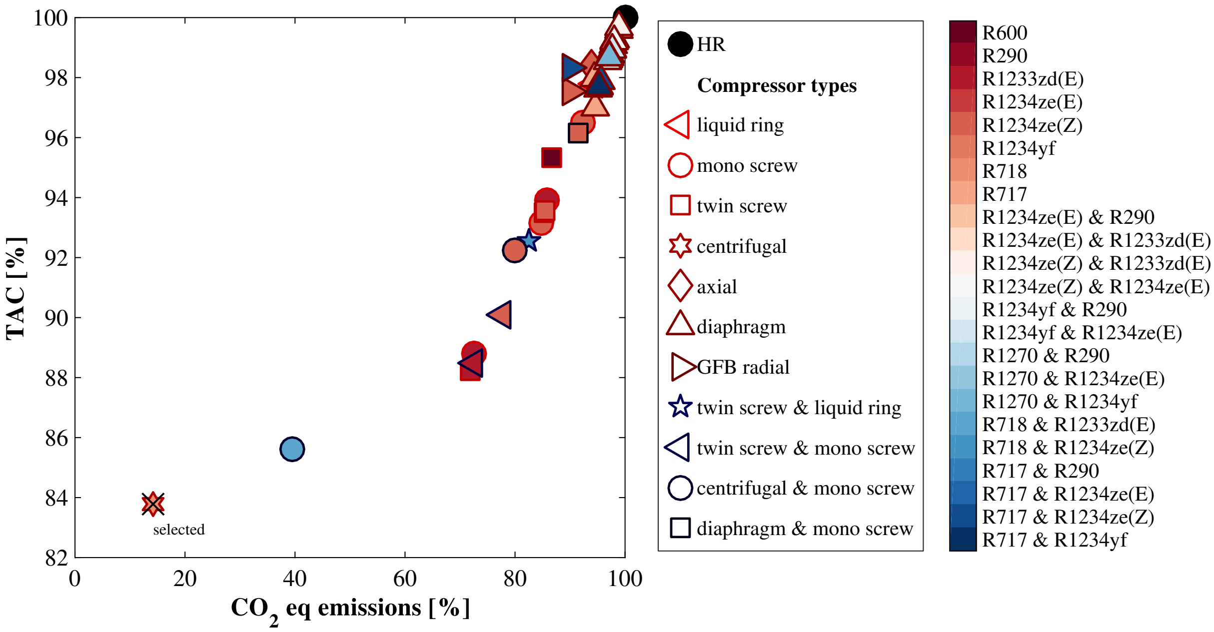


Figure 28: Results of *screening step* presented in section 4.1.2 for sugar making process.

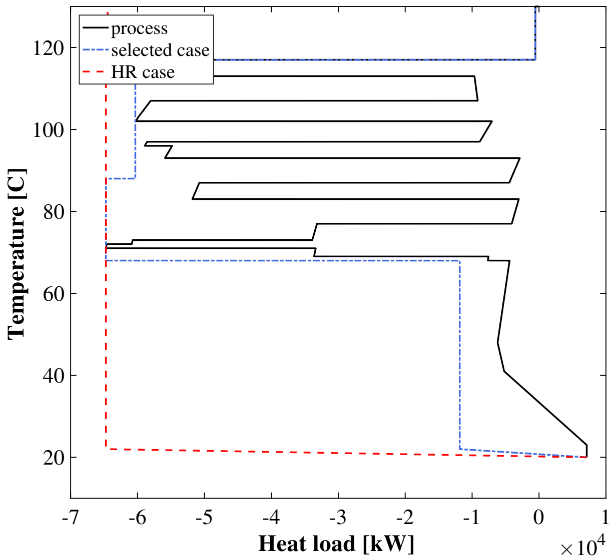


Figure 29: ICC of sugar making process [87] (case 1) with utility integration of selected and reference cases.

Table 12: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for sugar production.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	1,248,913		8,584,753	
$Capex_{HEN}$	CHF/y	-	-	1,248,913		712,333	
$Capex_{HP}$	CHF/y	-	-	0		7,872,420	
Opex Total (3000 h)	CHF/y	14,508,425	18,501,683	18,501,437	(-0.0 $\%_{Ref.}$)	6,917,291	(-62.6 $\%_{HR}$, -62.6 $\%_{Ref.}$)
TAC Total	CHF/y	14,508,425	18,501,683	19,750,350	(6.7 $\%_{Ref.}$)	15,502,044	(-16.2 $\%_{HR}$, -16.2 $\%_{Ref.}$)
Payback period (3000 h)	y			20.0		4.4	
(3000 h)	y			20.0		4.4	
Energetic data							
Size	kg/s			13			
Thermal energy (TH)	kW	47,827	64,726	64,726	(-0.0 $\%_{Ref.}$)	557	(-99.1 $\%_{HR}$, -99.1 $\%_{Ref.}$)
	kJ/kg	3622.0	4901.8	4901.8		42.2	
Electricity (EL)	kW	7,619	7,218	7,217	(-0.0 $\%_{Ref.}$)	18,512	(156.5 $\%_{\Delta HR}$, 156.5 $\%_{Ref.}$)
	kJ/kg	577.0	546.6	546.6		1401.9	
Waste heat	kJ/kg	-	-	5441.9		1437.7	
	°C	-	-				
CO_2-eq. emissions	kg/t	284.0	376.0	376.0	(-0.0 $\%_{Ref.}$)	53.4	(-85.8 $\%_{HR}$, -85.8 $\%_{Ref.}$)
Expert opinion (EO)				1 (★★★)		1 (★★★)	
Heat pump properties							
Compressor number^{HP}	#			0		4	
Compressor types^{HP}	#			-		centrifugal	
Compressor fluids^{HP}	#			-		R718	
Compressor sizes^{HP}	kW			-		2916/ 3182/ 2711/ 2485	
Compressor sizes^{REF}	kW						
$COP^{overall}$ (tot. cond./ tot. power)	-			NaN		5.68	(NaN %)
COP each comp.	-					5.68/ 5.68	

* Reference plant data from Morandin et al. [87] is not explicitly reported, therefore assumption: same consumption as HR case, since very close to public BAU data.

Chocolate The process representative for the Swiss chocolate industry was taken from the work of Muller et al. [99] and internal communication with Nestlé. It is interesting to note that in this case, the HR case and reference plant show similar energy consumption data, indicating that the plant is well-integrated (see Table 12). Due to limited knowledge of typical Swiss chocolate processes, the thermal requirements were not scaled according to Swiss production volumes. However, the thermal requirements agree with expectations, requiring a significant heat load near 35 ℃ for chocolate melting, and some higher temperature heat requirements for the binder and nut roasting.

Figure 30 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler, a refrigeration cycle, and cooling water. It can be seen that twin screw, mono screw and diaphragm compressors are present in the lowest cost solutions. The lowest CO_2-eq. emissions solution, which was selected for further analysis, however, contains two compressor types: **GFB radial** and **twin screw** compressors, reducing emissions compared to the reference plant by approximately 55%. This may indicate again that combined types may have advantages due to larger ranges of operating conditions.

In Figure 31, the ICC of the process with utility integration of the selected and a reference case are depicted. It can be seen that for the selected case, the heat pump completely encloses the process, obviating the need for a boiler. This is achieved through two compressors between 84 and 124 kW, as shown in Table 12. The selected working fluid is **R1234ze(Z)**, a HFO, of which the critical pressure and temperature are 35.3 bar and 150.1 ℃, respectively. The staged twin screw - GFB radial compressors reach 44.7 bar, confirming that the last stage is at supercritical conditions, as indicated on the ICC. A payback time of 4.3 years is achievable, though higher than some other studied processes. The overall COP is significantly reduced due to a COP in the HPS of 2.4. This indicates that lower efficiency in the HP also leads to less profitable solutions, as expected.

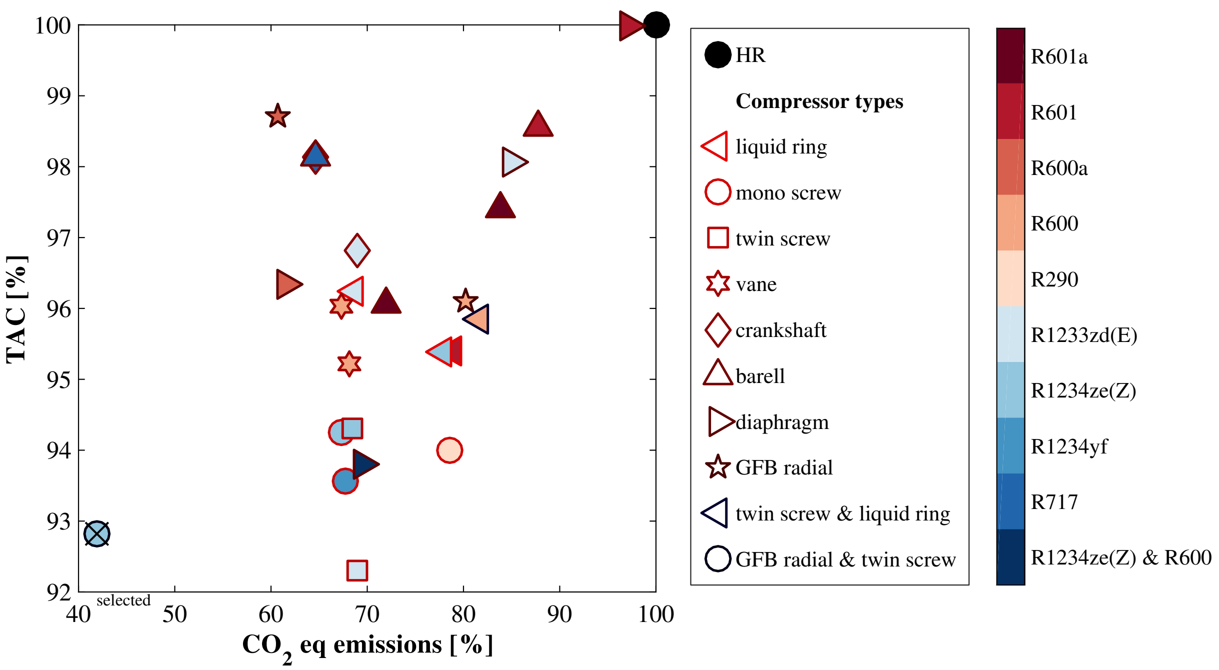


Figure 30: Results of *screening step* presented in section 4.1.2 for chocolate process.

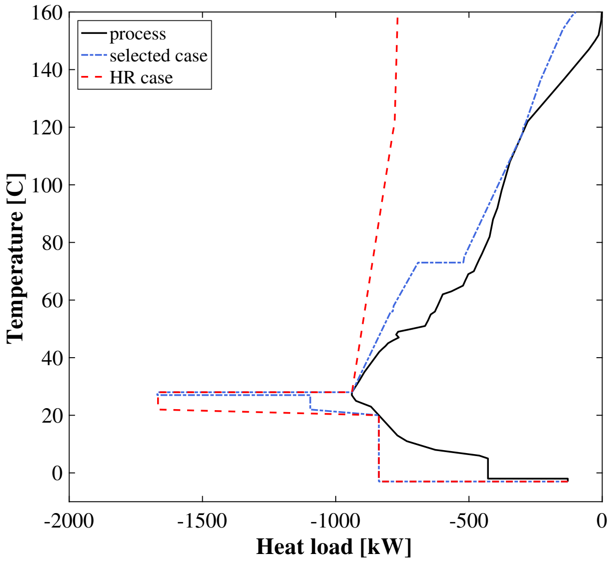


Figure 31: ICC of chocolate process [99] with utility integration of selected and reference case.

Table 13: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for chocolate production.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	205,128		214,608	
$Capex_{HEN}$	CHF/y	-	-	205,128		55,468	
$Capex_{HP}$	CHF/y	-	-	0		159,139	
Opex Total (8000 h)	CHF/y	3,062,379	1,090,973	1,270,114	(16.4 $\%_{Ref.}$)	964,329	(-24.1 $\%_{HR}$, -11.6 $\%_{Ref.}$)
TAC Total	CHF/y	3,062,379	1,090,973	1,475,242	(35.2 $\%_{Ref.}$)	1,178,937	(-7.2 $\%_{HR}$, 8.1 $\%_{Ref.}$)
Payback period (8000 h)	y			*nonsense*		4.3	
(3000 h)	y			*nonsense*		8.4	
Energetic data							
Size	kg/s			1			
Thermal energy (TH)	kW	2,167	772	780	(1.0 $\%_{Ref.}$)	0	(-100.0 $\%_{HR}$, -100.0 $\%_{Ref.}$)
	kJ/kg	4160.0	1482.0	1497.3		0.0	
Electricity (EL)	kW	1,686	601[C]	779[C]		987[C]	(26.8 $\%_{HR}$, 64.4 $\%_{Ref.}$)
	kJ/kg	3237.0	1153.2	1495.1		1895.5	
Waste heat	kJ/kg	-	-	1591.1		494.2	
	℃	-	-				
CO_2-eq. emissions	kg/t	418.7	149.2	162.5	(9.0 $\%_{Ref.}$)	68.1	(-58.1 $\%_{HR}$, -54.4 $\%_{Ref.}$)
Expert opinion (EO)				0.8 (★★★)		0.8 (★★★)	
Heat pump properties							
Compressor number[HP]	#			0		2	
Compressor types[HP]	#			-		GFB radial & twin screw	
Compressor fluids[HP]	#			-		R1234ze(Z)	
Compressor sizes[HP]	kW			-		124/ 84	
Compressor sizes[REF]	kW		*unknown*	178		178	
$COP^{overall}$ (tot. cond./ tot. power)	-			4.98		3.57	(-28.3 %)
COP each comp.	-			4.98		4.98/ 2.37	

* Reference plant data from Muller et al. [100] (internal communication with plant) thermal 6175 MWh/y, 15,000 t/y, electricity not known and therefore adopted from BAU
C The electricity consumption of the reference plant, HR and $\Delta direct_{HPS}$ were increased by public BAU $\Delta Ref_{EL} = BAU_{EL} \cdot Ref_{TH} / BAU_{TH}$

Brewing The process representative for the Swiss brewery industry was taken from Klemeš [88]. Due to limited knowledge of typical Swiss brewery processes and the assumption that most brewery processes are similar and beer type specifications are negligible, the thermal requirements were not scaled according to Swiss production volumes. It should be noted that the brewing process is usually operated in batches. Therefore, time averaging (as indicated by [15]) of thermal requirements was applied. This can be technically achieved by installation of storage tanks or sufficiently large production sites in which several batch phases occur at shifted time intervals. The brewery and bottling processes can be split into hot and cold portions[1].

Figure 32 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler, a refrigeration cycle, and cooling water. It can be seen that combined compressor types, including: mono screw & liquid ring, diaphragm & liquid ring, and GFB radial & lobe compressors are present in the lowest cost solutions highlighted in the inset. This may indicate again that combined types may have advantages due to larger operating condition ranges. The solution with lowest TAC was selected for further analysis since the emission reductions of the other points are negligible compared to the increase in TAC. The selected point contains two compressor types: **mono screw** and **liquid ring** compressors.

In Figure 33, the ICC of the process with utility integration of the selected and a reference case are depicted. It is observed that for the selected case, the heat pump completely encloses the process, obviating the need for the boiler. This is achieved through three compressors between 22 and 91 kW, as shown in Table 13. The selected working fluid is **R1233zd(E)**, a u-HCFC. This solution achieves an 85% reduction in CO_2-eq. emissions compared to the reference plant. A payback time of 4.6 years is achievable, though higher than some other studied processes. The overall COP is significantly reduced due to a COP in the HPS of 2.5. This might lead to the conclusion that lower efficiency in the HP also leads to less profitable solutions; however, the closest solution to the minimum TAC has much higher COP with no improvement in the payback time. A trade-off between the HEN cost and COP related opex is suggested by this result, and appear to be balanced in this case. The commonality between the brewing and chocolate processes are evidenced here by comparatively small process sizes and large temperature lifts.

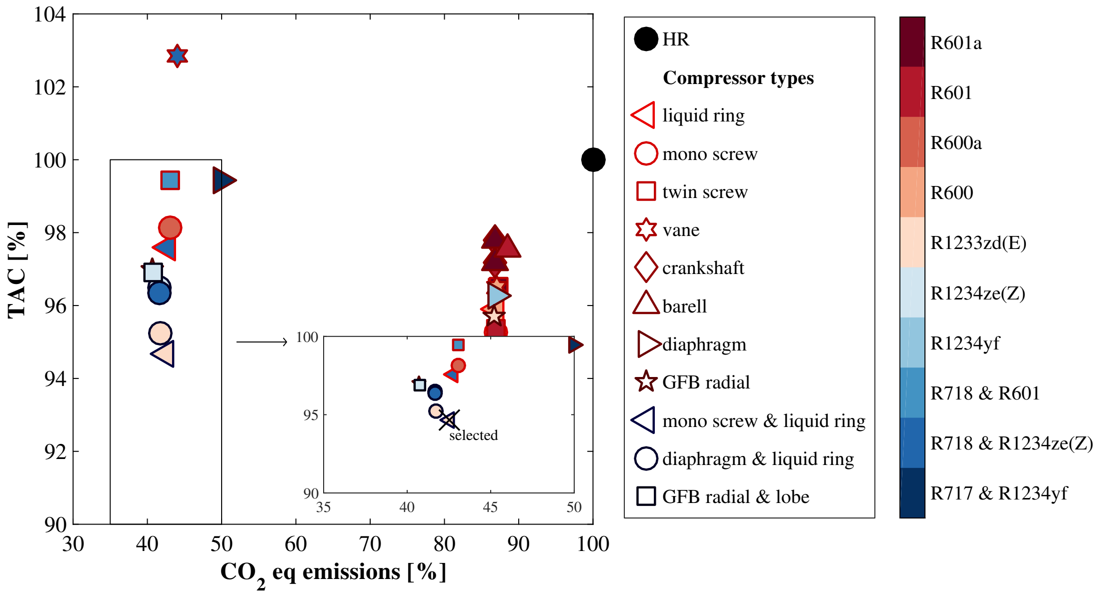


Figure 32: Results of *screening step* presented in section 4.1.2 for brewery process.

[1] During the hot batch, the raw ingredients are mixed, heated, filtered, boiled, and centrifuged, to separate the trub from the wort. On the cold side, fermentation occurs at approximately 10 °C, followed by filtering, dilution, and pasteurisation which requires heating and rapid cooling. The glass bottles are cleaned in several phases before the bottles are filled and packaged.

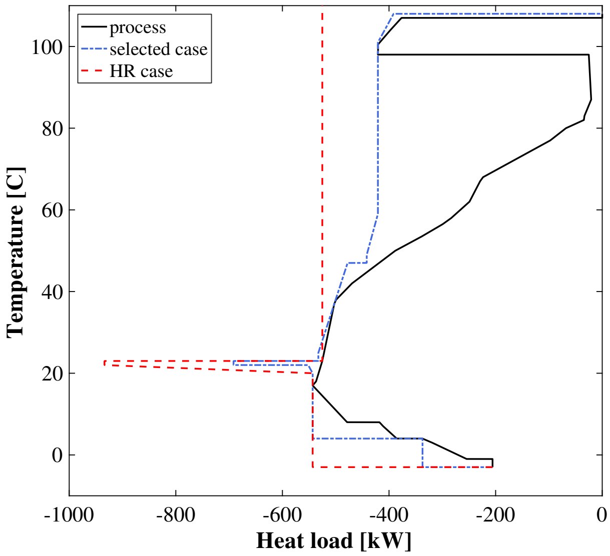


Figure 33: ICC of brewery process [88] with utility integration of selected and reference case.

Table 14: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for beer making.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	94,070		157,179	
$Capex_{HEN}$	CHF/y	-	-	94,070		30,348	
$Capex_{HP}$	CHF/y	-	-	0		126,831	
Opex Total (8000 h)	CHF/y	2,481,679	1,868,614	868,305	(-53.5 $\%_{Ref.}$)	664,919	(-23.4 $\%_{HR}$, -64.4 $\%_{Ref.}$)
TAC Total	CHF/y	2,481,679	1,868,614	962,375	(-48.5 $\%_{Ref.}$)	822,098	(-5.3 $\%_{HR}$, -56.0 $\%_{Ref.}$)
Payback period (8000 h)	y			0.7		4.6	
(3000 h)	y			1.8		8.8	
Energetic data							
Size	kg/s			2			
Thermal energy (TH)	kW	2,574	1,938	525	(-72.9 $\%_{Ref.}$)	0	(-100.0 $\%_{HR}$, -100.0 $\%_{Ref.}$)
	kJ/kg	1188.0	894.5	242.4		0.0	
Electricity (EL)	kW	819	617^{C}	538^{C}	(-12.8%)	681^{C}	(26.6 $\%_{HR}$, 10.4 $\%_{Ref.}$)
	kJ/kg	378.0	284.6	248.2		314.2	
Waste heat	kJ/kg	-	-	180.3		3.9	
	℃	-	-				
CO_2-eq. emissions	kg/t	99.9	75.3	26.5	(-64.7 $\%_{Ref.}$)	11.3	(-57.5 $\%_{HR}$, -85.0 $\%_{Ref.}$)
Expert opinion (EO)				0.8 (★★★)		0.8 (★★★)	
Heat pump properties							
Compressor number^{HP}	#			0		3	
Compressor types^{HP}	#			-		mono screw & liquid ring	
Compressor fluids^{HP}	#			-		R1233zd(E)	
Compressor sizes^{HP}	kW			-		22/ 73/ 91	
Compressor sizes^{REF}	kW			71		28	
$COP^{overall}$ (tot. cond./ tot. power)	-			5.74		2.90	(-49.5 %)
COP each comp.	-			5.74		5.74/ 2.48	

* Reference plant data from Klemeš [88] (Table 27.3) thermal requirement 17,062 kW, electricity 1,322 kW, flow rate 19.0739 kg/s of beer.
C Electricity consumption of ref. plant (original data) refers to refrigeration needs only. Therefore the electricity consumption of the reference plant, HR and $\Delta direct_{HPS}$ were increased by public BAU (without refrigeration) $\Delta Ref_{EL} = BAU_{EL} \cdot Ref_{TH} / BAU_{TH} - Ref, refrigerat._{EL}$

4.3.2.2 Pulp & paper In Switzerland, there are two main processes for making pulp, the sulphite process and mechanical processes [95]. Because Switzerland does not employ the kraft pulp process, the profile for Swiss pulp production differs slightly compared to that from other countries and is thus specific to the Swiss context. The thermo-mechanical process consumes very little heat and is thus not considered here, while paper-making is neglected because it is principally a heat sink and therefore not interesting for industrial HP integration.

Sulphite pulping The process representative for the sulphite process was taken from Perin-Levasseur [89]. The pulping process starts with steaming and screening the wood chips to be prepared for cooking. The wood chips are then sent to a high-pressure cooking vessel (i.e. digester) where cellulosic fibers are separated from the chips. Chemical treatment is used to facilitate component separation. The fresh chemical mixture is termed ‘white liquor’, and ‘black liquor’ results from the previous cooking step. Spent liquor (i.e. black liquor) is separated from the fibers in the washing section and proceeds through a recovery process for reuse, conventionally being incinerated for process heat.

Figure 34 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler and cooling water. It can be seen that no predominant fluid or compressor type is present in the lowest cost solutions. Among the lowest TAC solutions (highlighted in the inset), less than half of the solutions contain two compressor types. Among those solutions, the one with lowest TAC was selected for further analysis.

In Figure 35, the ICC of the process with utility integration of the selected and a reference case are depicted. It can be seen that for the selected case, the heat pump largely encloses the process curve, therefore reducing the boiler consumption by 83% compared to the reference plant. This is achieved using four compressors between 5 and 180 kW, as shown in Table 14. This leads to overall emission reductions of up to 50%.

The selected compressor types are: **mono screw** (both above 150 kW) and **diaphragm** (both around 5 kW), with **R1234ze(Z)**, a HFO, as working fluid. A payback time of 1.8 years and a COP of 4.8 can be achieved with this solution, which would likely result in excess black liquor which could valorised in other ways.

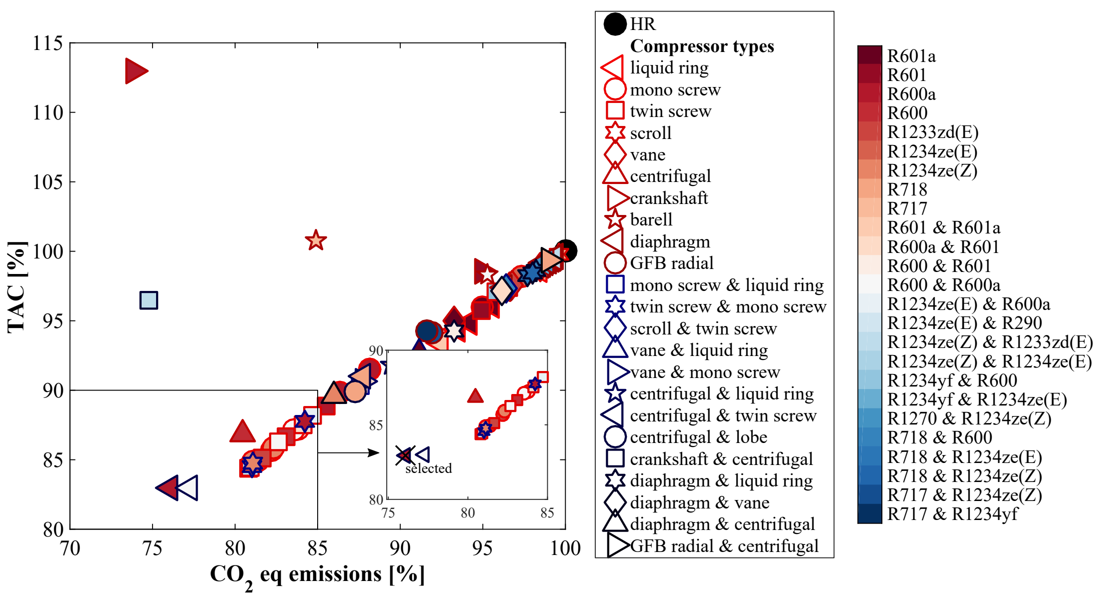


Figure 34: Results of *screening step* presented in section 4.1.2 for sulphite pulping process.

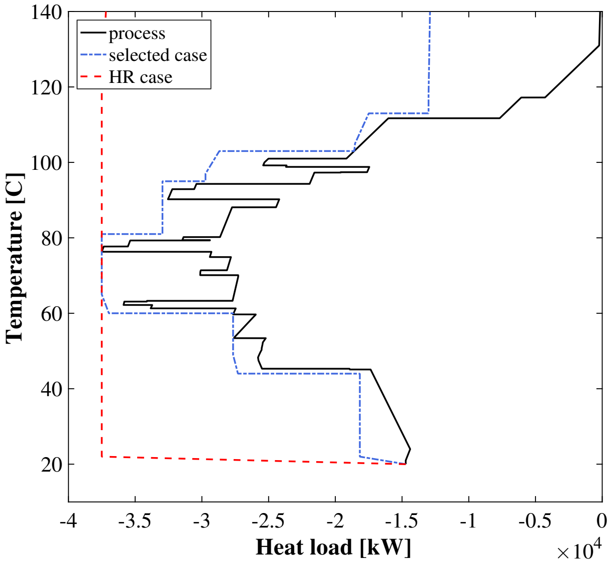


Figure 35: ICC of sulphite pulping process [89] with utility integration of selected and reference case.

Table 15: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for sulphite pulping.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	380,134		2,795,453	
$Capex_{HEN}$	CHF/y	-	-	380,134		271,959	
$Capex_{HP}$	CHF/y	-	-	0		2,523,494	
Opex Total (8000 h)	CHF/y	34,397,909	72,770,135	47,948,540	(-34.1 $\%_{Ref.}$)	36,978,553	(-22.9 $\%_{\Delta HR}$, -49.2 $\%_{Ref.}$)
TAC Total	CHF/y	34,397,909	72,770,135	48,328,674	(-33.6 $\%_{Ref.}$)	39,774,006	(-17.0 $\%_{\Delta HR}$, -45.3 $\%_{Ref.}$)
Payback period (8000 h)	y			0.1		1.8	
(3000 h)	y			0.3		4.1	
Energetic data							
Size	kg/s			5			
Thermal energy (TH)	kW	36,631	75,496	37,504	(-50.3 $\%_{Ref.}$)	13,014	(-65.3 $\%_{\Delta HR}$, -82.8 $\%_{Ref.}$)
	kJ/kg	8000.0	16488.1	8190.7		2842.3	
Electricity (EL)	kW	10,714	24,003	24,003^B	(0.0 $\%_{Ref.}$)	29,152^B	(21.5 $\%_{\Delta HR}$, 21.5 $\%_{Ref.}$)
	kJ/kg	2340.0	5242.2	5242.2		6366.7	
Waste heat	kJ/kg	-	-	4974.8		751.1	
	°C	-	-				
CO_2-eq. emissions	kg/t	285.6	603.7	394.6	(-34.6 $\%_{Ref.}$)	300.2	(-23.9 $\%_{\Delta HR}$, -50.3 $\%_{Ref.}$)
Expert opinion (EO)				0.8 (★★★)		0.8 (★★★)	
Heat pump properties							
Compressor number^HP	#			0		4	
Compressor types^HP	#			-		centrifugal & twin screw	
Compressor fluids^HP	#			-		R600a	
Compressor sizes^HP	kW			-		1000/ 2308/ 1000/ 842	
Compressor sizes^REF	kW						
$COP^{overall}$ (tot. cond./ tot. power)	-			NaN		4.76	(NaN %)
COP each comp.	-					3.55/ 5.05	

* Reference plant data from Perin-Levasseur [89], electricity 210,265,847 kWh (Table 3.1), product flow rate 144,398 t/y (Table 3.1), thermal consumption 75,496 kW (Table 3.5)
B electricity consumption for HR and $\Delta direct_{HPS}$ case was adopted from reference plant data, since no more information are available.

4.3.2.3 Chemicals Though an incredibly diverse sector, the chemical industry can be classified into refinery products and organic fine chemicals. The *refinery* category comprises products derived from crude oil such as gasoline, diesel, liquefied petroleum gas, etc. Organic fine chemicals include pharmaceuticals and vitamins, crop protection, dyes, etc. Due to the diversity of production, limited public data of organic fine chemicals and dominance of refineries in terms of thermal requirements (60%), they are the only process considered in this sector.

Oil refinery The process representative for a refinery was adapted from [91] which represents the main processes in a typical refinery. Each sub-process in the refinery performs a specific separation or conversion function to yield a single, or specific, mixture of hydrocarbon compounds. The first sub-process, crude oil distillation, is the most important and energy-consuming part of the refinery. This is followed by the hydro-treating catalytic cracking, and vacuum distillation. Typical refinery sites employ combined heat and power (CHP) units to co-generate heat and electricity. Typical plants are often around 100 MW of thermal demand.

Figure 36 shows the best results for each compressor type (combination) plotted with respect to their CO_2-eq. emissions and TAC. The results are reported relative to the reference solution with an industrial boiler and cooling water. It can be seen that combined compressor types, including: GFB radial & mono screw, diaphragm & mono screw, and centrifugal & twin screw are present in the lowest cost solutions highlighted in the inset. This may indicate again that combined types may have advantages due to larger ranges of operating conditions. The solution with lowest CO_2-eq. emissions was selected for further analysis since the TAC was insignificantly higher than the minimum TAC point. The selected point contains two compressor types: **twin screw** and **centrifugal** compressors.

In Figure 37, the ICC of the process with utility integration of the selected and a reference case are depicted. Comparing to Table 15, the highest energy saving solution is achieved by heat recovery (HR). For the selected HPS case, the heat pump encloses a small fraction of the process, reducing the natural gas consumption by an additional 29%, leading to overall CO_2-eq. emission reductions of approximately 75% compared to the reference plant. This is achieved through four compressors between 1,000 and 2,240 kW, as shown in Table 15. The selected working fluid is **R1233zd(E)**, a u-HCFC. A payback time of 2.1 years and a COP of 4.4 can be achieved with this solution.

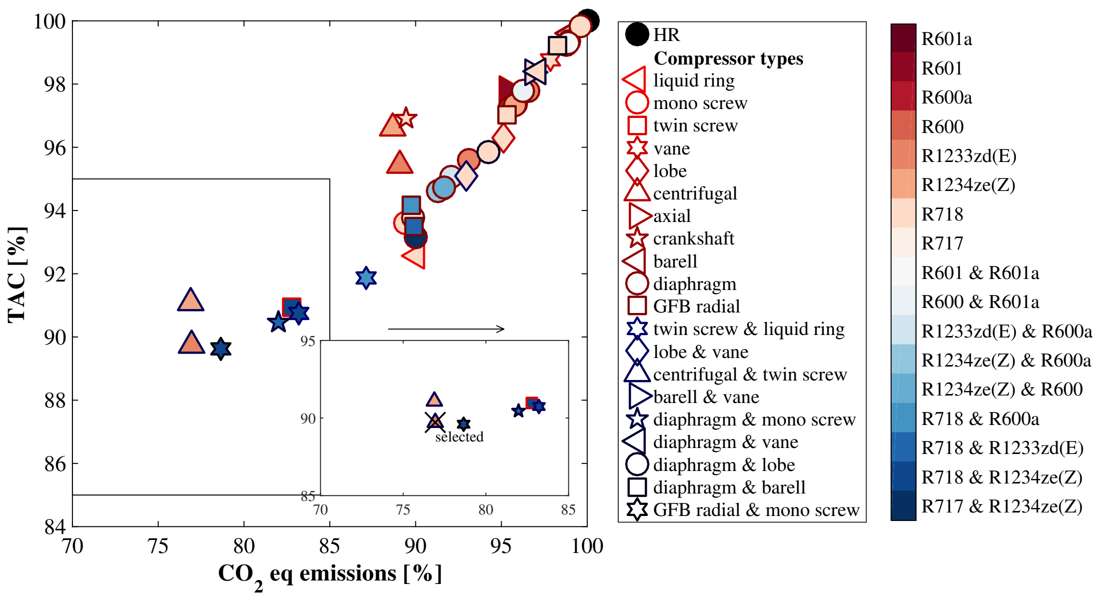


Figure 36: Results of *screening step* presented in section 4.1.2 for refinery process.

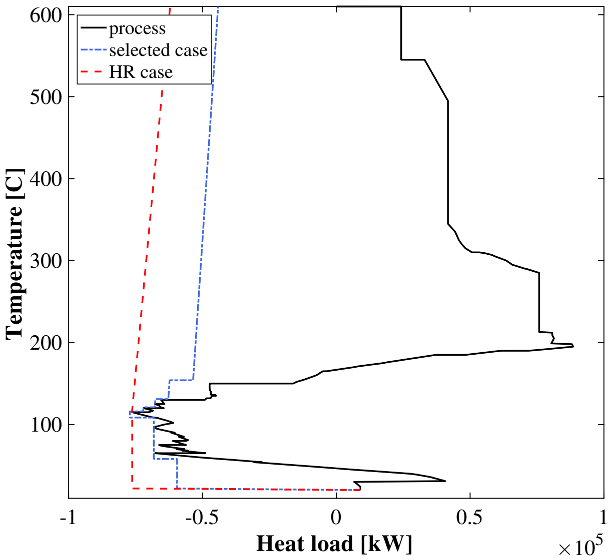


Figure 37: ICC of refinery process [91] with utility integration of selected and reference case.

Table 16: Comparison between BAU, ref. plant, ΔHR and $\Delta direct_{HP}$ case for refineries.

	Unit	Public BAU	Ref. plant*	ΔHR		$\Delta direct_{HP}$	
Cost data							
Capex Total	CHF/y	-	-	1,216,363		2,848,575	
$Capex_{HEN}$	CHF/y	-	-	1,216,363		339,648	
$Capex_{HP}$	CHF/y	-	-	0		2,508,927	
Opex Total (8000 h)	CHF/y	173,707,893	171,490,732	62,582,239	(-63.5 $\%_{Ref.}$)	53,313,760	(-14.8 $\%_{HR}$, -68.9 $\%_{Ref.}$)
TAC Total	CHF/y	173,707,893	171,490,732	63,798,602	(-62.8 $\%_{Ref.}$)	56,162,335	(-10.3 $\%_{HR}$, -67.3 $\%_{Ref.}$)
Payback period (8000 h)	y			0.1		2.1	
(3000 h)	y			0.2		4.8	
Energetic data							
Size	kg/s	86					
Thermal energy (TH)	kW	246,093	242,951	76,255	(-68.6 $\%_{Ref.}$)	54,234	(-28.9 $\%_{HR}$, -77.7 $\%_{Ref.}$)
	kJ/kg	2845.0	2808.7	881.6		627.0	
Electricity (EL)	kW	13,235	13,066	13,066[B]		18,305[B]	(40.1 $\%_{HR}$, 40.1 $\%_{Ref.}$)
	kJ/kg	153.0	151.0	151.0		211.6	
Waste heat	kJ/kg	-	-	985.9		791.9	
	°C	-	-				
CO_2-eq. emissions	kg/t	195.3	192.8	64.2	(-66.7 $\%_{Ref.}$)	49.4	(-23.1 $\%_{HR}$, -74.4 $\%_{Ref.}$)
Expert opinion (EO)				0.6 (★★☆)		0.6 (★★☆)	
Heat pump properties							
Compressor number[HP]	#			0		4	
Compressor types[HP]	#			-		centrifugal & twin screw	
Compressor fluids[HP]	#			-		R1233zd(E)	
Compressor sizes[HP]	kW			-		2240/ 1000/ 1000/ 1000	
Compressor sizes[REF]	kW						
$COP^{overall}$ (tot. cond./ tot. power)	-			NaN		4.37	(NaN %)
COP each comp.	-					4.37	

* Reference plant data from Bungener et al. [91], ratio reference plant to HR thermal 99.4/31.2, electricity scaled based on BAU
B electricity consumption for HR and $\Delta direct_{HPS}$ case was adopted from reference plant data, since no more information are available.

4.3.3 Summary and impact

Figure 38 shows the sector relative CO_2-eq. emissions of the investigated processes in this report and their reduction potentials. Two saving potentials were investigated for each industrial process:

1. **ΔHR**: optimised internal heat recovery (HR) in the process
2. **Δdirect**: integration of optimised (multi-stage) heat pump (HP). (This is categorised as a *direct* efficiency improvement measure.)

Both saving potentials were derived for each of the investigated processes by application of the *screening* tool and methods developed in this project and presented in section 3.

The data behind Figure 38 are reported in Table 16. Detailed explanation of the approach used for extrapolating from process thermal profile reduction potentials to the entire sector can be found in section 4.1.1.

As expected from analysis of the Pinch temperatures in 4.2, it can be seen that the main CO_2-eq. emission reduction potentials are achievable in the food & beverage sector, yielding carbon mitigation potentials between 18%-42%[1] by optimised HP integration and 7%-16% by improved HR, which amounts to a total reduction potential of 25-58%, with payback times between 3 and 6 years. This is

[1] *Note:* The range reflects the difference between the *conservative* assumption (only the investigated processes can be improved); and the *optimistic* assumption (the emission reductions of the investigated processes are representative of the entire sector).

followed by the chemical sector, where most saving potentials are achieved through HR 19%-67% (HP 2%-8%), reaching a total of 22%-74% emission reduction potential (payback 2.1 years). In the pulp & paper sector, only the sulphite pulping process was investigated, which leaves a large uncertainty for the saving potentials of the entire sector, due to the large share of paper-making processes in that sector in Switzerland. Potentials for CO_2-eq. emission savings through heat pump integration vary between 52% and 2% for optimistic and conservative cases. For the entire **industrial sector**, improvements of 6%-47% could be achieved through HR, while 3%-21% additional savings could be unlocked by HP integration, amounting to a total of 9%-68% reduction potential in CO_2-eq. emissions. This highlights a large uncertainty related to the diversity of the industrial sector. These findings also reveal a large uncharted potential which should be explored in more detail.

As reported in Table 16, most HP scenarios contain mixed compressor types. This indicates an advantage of combined types due to larger ranges of operating conditions, and with that, a coverage of more heat pump features. This can also be seen in terms of additional integration possibilities, corresponding to a larger solution space.

The six compressors types present among the selected industrial HP integration cases, together with their integration occurrence (and respective process size specification), are shown below:

- twin screw, 5# (small-medium processes, ≤MW range)
- GFB radial, 3# (small-medium processes, ≤MW range)
- centrifugal, 3# (medium, large processes,MW to 100 MW range)
- mono screw, 1# (small-medium processes, ≤MW range)
- liquid ring, 1# (small processes, <MW range)

No staged heat pump cycles with two different fluids were among the selected solutions. The four fluid types most present among the selected industrial HP integration cases are shown below with their respective occurrence: R1233zd(E), 2 ; R1234ze(Z), 2 ; R600a, 2 ; water, 1.

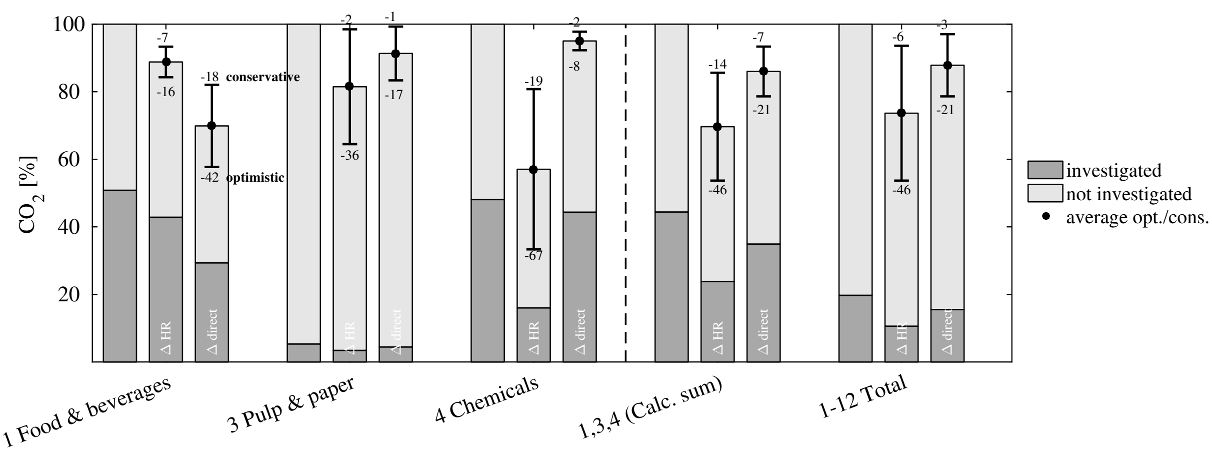


Figure 38: Sector relative CO_2-eq. emissions of (here) investigated processes and the rest, and reduction potential through heat recovery (ΔHR) and HP integration ($\Delta direct_{HP}$).

Table 17: Total reduction potential summary.

Process		**Electricity (EL)**		**Thermal energy (TH)**		**EO**	**CO_2-eq. eq. emissions**			
		MJ/y	Δ	MJ/y	Δ		Mio t/y	Δ	ΔOpt.	ΔCons.
1 Food & beverages		7,669		8,813		0.83	0.92			
	ΔHR		-0.3 %, -0.7 %		-11.3 %, -21.7 %				-15.7 %	-6.7 %
	Δdirect		10.8 %, 22.3 %		-35.4 %, -68.2 %				-42.3 %	-17.9 %
Dairy	ΔHR	.52,435	0.0 %	.51,878	-28.5 %	.50.8	.50.224	-17.4 %	.7GFB radial & twin screw	R600a
	Δdirect		10.4 %		-71.5 %			-39.5 %		
Sugar	ΔHR	.5126	0.0 %	.5793	0.0 %	.51.0	.50.062	0.0 %	.7GFB radial & twin screw	R1234ze(Z)
	Δdirect		156.5 %		-99.1 %			-80.5 %		
Cheese	ΔHR	.5555	-4.7 %	.5880	-16.0 %	.50.8	.50.084	-13.3 %	.5centrifugal	water
	Δdirect		12.4 %		-32.2 %			-21.6 %		
Chocolate	ΔHR	.5457	0.0 %	.5588	0.0 %	.50.8	.50.059	0.0 %	.7GFB radial & twin screw	R1234ze(Z)
	Δdirect		64.4 %		-100.0 %			-54.4 %		
Beer	ΔHR	.5138	0.0 %	.5435	-72.9 %	.50.8	.50.037	-63.0 %	.7liquid ring & mono screw	R1233zd(E)
	Δdirect		10.4 %		-27.1 %			-22.0 %		
3 Pulp & paper		4,585		4,930		0.80	0.29			
	ΔHR		0.0 %, 0.0 %		-4.4 %, -50.3 %				-35.5 %	-1.5 %
	Δdirect		0.6 %, 21.5 %		-2.8 %, -32.5 %				-16.6 %	-0.7 %
Pulping (sulphite)	ΔHR	.5126	0.0 %	.5432	-50.3 %	.50.8	.50.015	-35.5 %	.7centrifugal & twin screw	R600a
	Δdirect		21.5 %		-32.5 %			-16.6 %		
4 Chemicals		9,297		17,084		0.60	1.47			
	ΔHR		0.0 %, 0.0 %		-41.4 %, -68.6 %				-66.7 %	-19.2 %
	Δdirect		2.4 %, 40.1 %		-5.5 %, -9.1 %				-7.7 %	-2.2 %
Refining	ΔHR	.5555	0.0 %	.510,319	-68.6 %	.50.6	.50.708	-66.7 %	.7centrifugal & twin screw	R1233zd(E)
	Δdirect		40.1 %		-9.1 %			-7.7 %		
1,3,4 (Calc. sum)		21,551		30,827		0.70	2.68			
	ΔHR		-0.1 %, -0.6 %		-26.9 %, -54.1 %				-46.3 %	-14.4 %
	Δdirect		5.0 %, 24.5 %		-13.6 %, -27.4 %				-21.4 %	-6.6 %
1-12 Total		51,626		58,615		0.70	6.02			
	ΔHR		-0.1 %, -0.6 %		-14.1 %, -54.1 %				-46.3 %	-6.4 %
	Δdirect		2.1 %, 24.5 %		-7.2 %, -27.4 %				-21.4 %	-2.9 %

5 Conclusions

The scientific value of the work completed in the context of this project is very high, providing a comprehensive method for optimal heat pump integration considering many features, fluids and compressor technologies. This work provides the best current reference for such techniques with the intention of encouraging broad applications of industrial heat pumps by showing the best potentials for heat pump integration for industrial processes. Additionally, representative processes for energy-intensive industries were evaluated with this technique to show the potential within each sector of Swiss industry, providing a reference for potential energy savings which can serve as benchmarks and targets for energy efficiency improvements. Shortcomings of the work are related to the level of detail which can be included in such methods, as in-depth design and costing cannot be included in such screening approaches. Despite this, the detail provided by this approach is beyond the state-of-the-art methods and provides valuable insight for detailed design at a later stage.

Given the high quality of this work and scientific contribution to the field (published in renowned journals [55, 101]), the aspirations of this work are to encourage broad applications of industrial heat pumps; however, economic restrictions and technical constraints remain the most difficult obstacle. Heat pump systems and detailed design and engineering often yield cost-prohibitive projects when applying typical industrial economic targets (with payback times below three years).

- This project identified paths to reduce the environmental impact of industrial processes through correct heat pump integration
- The barriers for large-scale application were identified and several steps were undertaken to overcome these, namely:
  1. Clarification of theoretical principles for effective integration. Development of guidelines and overview of tools which aid during the planning phase
  2. A novel heat pump pre-design tool was developed considering a comprehensive list of heat pump features, compressor and fluid selection
  3. With help of the developed tool, an analysis of heat pump potential in industrial processes was conducted in the five Swiss most energy intensive industrial sectors; while considering also their heat recovery (HR) potential
- The most promising **industrial sector** for heat pump integration was characterised as the food & beverage sector, yielding carbon mitigation potentials between 18%-42%[1] by optimised heat pump (HP) integration and 7%-16% by improved heat recovery (HR), which amounts to a total reduction potential of 25-58%, with payback times between 3 and 6 years. This is followed by the chemical sector, where most saving potentials are achieved through HR 19%-67% (HP 2%-8%), reaching a total of 22%-74% emission reduction potential (payback 2.1 years).
- For the entire **industrial sector**, improvements of 6%-47% could be achieved through HR, while 3%-21% additional savings could be unlocked by HP integration, amounting to a total of 9%-68% reduction potential in carbon dioxide equivalent (CO_2-eq.) emissions. This highlights a large uncertainty related to the diversity of the industrial sector. These findings also reveal a large uncharted potential which should be explored in more detail.
- The developed methods also allowed identification of the most promising compressor and refrigerant types recommended for further research: The five **compressors types** present among the selected industrial HP integration cases were: twin screw, gaseous film bearing (GFB) radial, centrifugal, mono screw, and liquid ring. The four **fluid types** most present among the selected industrial HP integration cases were: R1233zd(E), R1234ze(Z), R600a, and water.
- The **added value** of the project lies in (1) providing a holistic methodology for consistent and optimised industrial heat pump integration, (2) identification of the most promising industries for heat pump integration in Switzerland (CH), and (3) illustrating potential benefits of heat pumping toward GWP reduction objectives for the Swiss energy transition 2050.

6 Outlook and next steps

There remain many interesting areas for research and application within the domain of industrial process efficiency, and the developments packaged within this project contribute an exceptional piece toward a comprehensive approach for industrial energy efficiency improvements. As mentioned at several points in publications and project-related deliverables, integration between HPs and other technologies must be considered to provide the best solutions for improving industrial energy efficiency, reducing environmental impact, improving Swiss industrial competitiveness and contributing toward the Swiss energy

[1] *Note:* The range reflects the difference between the *conservative* assumption (only the investigated processes can be improved); and the *optimistic* assumption (the emission reductions of the investigated processes are representative of the entire sector).

transition. One key research aspect which must follow this work is considering competing and complementary technologies together with heat pumps, enabling further improvements in cost and emissions beyond the heat pumping potential described throughout this work. This also includes expanding the tool to incorporate more heat pump types, namely: mixtures and ad/absorption systems. Another step is commercialisation of the tool.

Additionally, time-dependent impacts of electricity consumption and the role and potential of digitalisation in industrial processes should be explored to better understand temporal aspects of operation. Influences of and by industry in electrical (and thermal) grids and impacts related to electricity consumption are especially pertinent in the context of heat pumping due to increased electrical demands for such systems. Additional research should be conducted to explore influences from these areas and to consider relationships between heat pumps and other technologies, considering temporal aspects of batch operations and implied storage requirements related to process optimisation for time-dependent benefits.

Relationships, complementarity and competition between industrial and residential heat pumping to provide more efficient heating, cooling, storage and electricity supply for the residential sector encourages circular economy concepts and may provide economy-of-scale manufacturing benefits for widespread adoption of heat pumps on multiple scales. Such an approach may partially allay the economic barriers posed by practical implementation and should be explored more thoroughly. Additionally, the role of third-party utility providers could be considered to propose new business models for heat pump implementation, considering excess heat supplied by industries and required within the residential sector.

A final recommendation for future work is that legislative, regulatory and economic mechanisms should be explored to identify which aspects would encourage broad implementation of industrial heat pumps, as instances of installation are significantly lower than their proven potential would suggest.

7 National and international cooperation

7.1 National cooperation

The Industrial Process and Energy Systems Engineering (IPESE) group has participated actively in work package 1 of the CTI managed project Swiss Competence Center for Energy Research (SCCER)-Efficiency of Industrial Processes (EIP). During the past three years, the work related to the underlying Swiss Federal Office of Energy (SFOE) project was presented in the context of three SCCER-EIP network meetings and site visits with positive feedback.

While the focus of this work concentrates on considering only mature technologies and their applications in industry, additional benefits were gained by incorporating the possibilities of novel technologies in the superstructure. Collaboration with the Laboratory for Applied Mechanical Design (LAMD) at EPFL-Neuchâtel and major partner of SCCER-EIP WP2 has been leveraged for assessing the possibility of utilizing novel compressor technologies as could be shown in section 4.

7.2 International cooperation

The IPESE group participated in the IEA HPT Annex 48 regarding industrial heat pumping on behalf of Switzerland. Members of the IPESE group participated in six international meetings presenting the work developed in this BFE-project. Our efforts were presented to an international community, highlighting the methods developed and the necessity of their application. In the presentations, the structure and content of the project were discussed in detail. The work was received with positive feedback, indicating a great need of the international community for clear dissemination of principles and methods to accurately integrate industrial heat pumps. Valuable exchanges and cooperation with other partners in IEA HPT Annex 48 improved the quality, dissemination and data used within this project. Expert opinion brought valuable insights to the developments of the project. A large database of successful heat pump implementation projects is a major output of the IEA HPT Annex 48 work and will be beneficial to showcase exemplary projects and provide real data for further methodological developments and implementation actions. The efforts of IPESE were appreciated by the operating agent of the Annex as a valuable contribution toward methodological developments for indutrial heat pump integration. These contributions are included in the final Annex 48 report, which is under preparation.

The work was further presented at two international conferences with excellent feedback. An additional international collaboration with the University of Singapore was recently initiated to incorporate the superstructure approach to design optimal air conditioning systems in tropical climates.

8 Publications

Six peer-reviewed articles were published in the context of this project. Their details can be found in the list below. To this date, the last two deliverables (D3, D4) are not yet published, but in preparation or already submitted (as marked below). Table 17 presents the full list of publications within the context of this project.

Table 18: Publications associated to this project.

Citat.	Bibliography entry	Description
[102]	Anna S. Wallerand, Ivan Kantor, Maziar Kermani, Stefano Moret, and François Maréchal. Energy saving potentials in the main industrial sectors. in perparation, Frontiers in Energy Research, 2020	**Journal article** summarising the energy saving potentials in the main Swiss industrial sectors through HP and HR derived throughout this project and in collaboration with SCCER EIP Phase II (see section 4)
[103]	Anna S. Wallerand, Ivan Kantor, and François Maréchal. Compressor type selection for industrial heat pump systems. In Proceedings of ECOS 2020, volume 33, Osaka, Japan, July 2020. Osaka Prefecture University Graduate School of Engineering	**Conference proceedings** describing the methodology and results of the compressor selection algorithm developed for this project (see sections 3.2.6 & 3.3.3)
[104]	Anna Sophia Wallerand, Ivan Daniel Kantor, and François Maréchal. Bottom-up method for potential estimation of energy saving measures. Computer Aided Chemical Engineering, 46:1597–1602, 2019. doi: 10.1016/B978-0-12-818634-3.50267-8. URL http://infoscience.epfl.ch/record/268665. Publisher: Elsevier	**Book chapter** presenting an optimization approach which allows to create energy saving scenarios for various environmental and economic boundary conditions (e.g. for different countries)
[16]	Anna Sophia Wallerand. Integration of solar energy with industrial processes. 2018. doi: 10.5075/epfl-thesis-8635. URL https://infoscience.epfl.ch/record/256107	**Docotral thesis** describing the heat pump superstructure (HPS) approach and its integration with solar energy use in the industry
[54]	Ivan Kantor, Anna S. Wallerand, Maziar Kermani, Hür Bütün, Allessio Santecchia, Raphaël Norbert, Sahar Salame, Hélène Cervo, Sebastian Arias, Franz Wolf, Greet van Eetvelde, and François Maréchal. Thermal profile construction for energy-intensive industrial sectors. In Proceedings of ECOS 2018, Portugal, June 2018	**Conference proceedings** presenting sector thermal profiles used for this project and exemplary heat pump integration with the HPS approach (see section 4)
[29]	Anna S. Wallerand, Maziar Kermani, Ivan Kantor, and François Maréchal. Optimal heat pump integration in industrial processes. Applied Energy, 219:68–92, June 2018. ISSN 0306-2619. doi: 10.1016/j.apenergy.2018.02.114. URL https://www.sciencedirect.com/science/article/pii/S0306261918302393	**Journal publication** describing the HPS approach, the fluid selection and the benchmark analysis (see section 3.2)
[101]	Anna S. Wallerand, Maziar Kermani, Régis Voillat, Ivan Kantor, and François Maréchal. Optimal design of solar-assisted industrial processes considering heat pumping: Case study of a dairy. Renewable Energy, 128:565–585, December 2018. ISSN 0960-1481. doi: 10.1016/j.renene.2017.07.027. URL http://www.sciencedirect.com/science/article/pii/S0960148117306390	**Journal publication** describing the HPS approach and its integration with solar energy use in the industry
[105]	Anna S. Wallerand, Maziar Kermani, Ivan D. Kantor, and François Maréchal. General superstructure synthesis and bi-level solution strategy for industrial heat pumping. In Antonio Espuña, Moisès Graells, and Luis Puigjaner, editors, 27th European Symposium on Computer Aided Process Engineering, volume 40 of Computer Aided Chemical Engineering, pages 1159 – 1164. Elsevier, 2017. doi: 10.1016/B978-0-444-63965-3.50195-1. URL http://www.sciencedirect.com/science/article/pii/B9780444639653501951	**Book chapter** describing the original HPS approach (see section 3.2)

9 Acknowledgements

This study was carried out within the framework of the international energy agency (IEA) HPT Annex 48 project (HPT, Phase 2), which was funded by the Swiss Federal Office of Energy (SFOE) within the project “Integrated industrial heat pump systems” (Vertragsnummer: SI/501487-01). This research project is also part of the Swiss Competence Center for Energy Research (SCCER) EIP (www.sccer-eip.ch) of the Swiss Innovation Agency Innosuisse.

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A Background

A.1 Application of guidelines along a case-study

(1) Initial data acquisition The data acquired from the dairy plant is depicted in Table 18. It highlights that the maximum temperatures do not exceed 100 °C, which indicates a great potential for heat pump integration. The operating time indicates quasi non-stop operation of the process apart from short maintenance breaks.

Table 19: Dairy plant data acquisition.

Vector	Data	Unit
Products	Pasteurised milk, yogurt, cream	
Production rate	10	kg/s
Annual operating time	8'000	h
Energy prices	0.081	€/kWh nat. gas
	0.1	€/kWh electricity
Energy resource consumption	2'333	kW nat. gas
	167	kW electricity (refrigeration)
Boiler efficiency	90	%
Energy bill	1'512'000	€/y gas
	133'600	€/y electricity
	5.7	€/t total
Refrigeration requirement	500	kW
Operating temperature ranges	0	°C (min)
	100	°C (max)
Constant temperature requirements (chemical reactions, evaporation, condensation)	multi-stage evaporation, around 60 °C	

(2) Preparation and decision The operating time is relatively high, representing non-stop operation. The low operating temperatures, multi-effect evaporation system and company interest to improve site energy efficiency bring motivation to continue the analysis in a more thorough manner.

(3) Company visit The company visit revealed that heat recovery is already performed to a high degree in the dairy plant. The two main production steps identified were the raw milk pasteurisation and centrifugation (process A) to produce pasteurised milk and cream and the concentrated milk production (process B). The main data can be found on the flowsheet sketches in Figure 39 and Figure 40.

Raw milk enters the pasteurisation unit (process A), in which it is heated and then centrifuged to separate high fat content cream from low fat content milk. The pasteurised milk from process A is partially sold and partially processed further to produce desserts and concentrated milk in a multi-effect evaporation system.

(4) Analysis of the status quo (🔧) Crosscheck. The process overall specific energy consumption was derived to be 233 kJ/kg (gas) and 17 kJ/kg (electricity). Cross-checking that data with available benchmarks from reference data from the European Union [106] (Table 3.59), displayed in Table 19, reveals that the electricity consumption is below the reference consumption. This was attributed to the fact that the company only reported the electricity consumption from the refrigeration cycles. The specific gas consumption is also at the lower end of the spectrum considering that the plant produces not only pasteurised milk and cream, but also yogurt and concentrated milk.

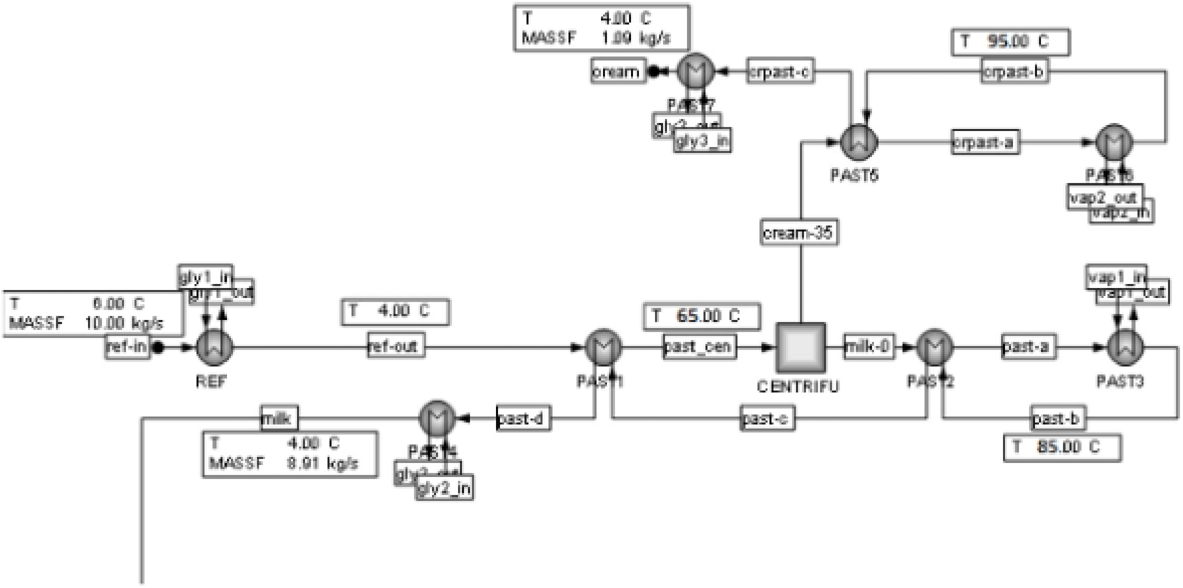


Figure 39: Process A. Pasteurisation section with centrifugation for cream and milk separation.

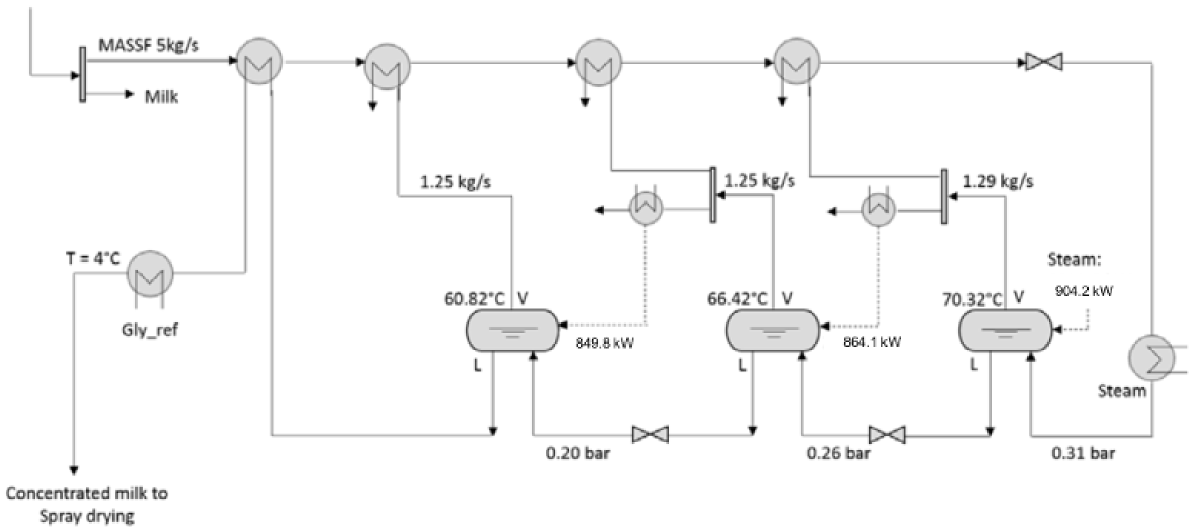


Figure 40: Process B. Concentrated milk production with multi-effect evaporation system.

Table 20: Average consumption values in EU dairies ([106], Table 3.59)

		Milk	Yogurt, others	Cheese	Milk powder	Whey
Fuel	GJ/t	0.18	1.5	4.6	3	20
Electricity	GJ/t	0.15	2.5	2.9	0.1	3.3

Overall, the energy consumption data is in the range of common benchmark values. In order to analyse the current energy system at more detail, energy and mass balances of the dairy plant were generated. This included generation of a table with heating and cooling requirements needed by the process, depicted in Table 20.

Table 21: Hot and cold streams of the dairy process, reprinted from [16], from Becker [86].

Unit	Name	T_{in} [℃]	T_{out} [℃]	$\Delta\dot{Q}$ [kW]	$\Delta T_{min}/2$ [℃]	Remarks
Regrigeration	ref	6.0	4.0	-76.0	2.0	refrigeration inlet milk
Pasteurization	pasto1a	4.0	66.0	2356.0	2.0	preheating
	pasto2a	66.0	86.0	676.4	2.0	pasteurization milk
	pasto3a	86.0	4.0	-2773.2	2.0	refrigeration milk
	pasto4a	66.0	98.0	119.7	2.0	pasteurization cream
	pasto5a	98.0	4.0	-351.6	2.0	refrigeration cream
Concentration	eva1	4.0	70.3	504.0	2.0	preheating
	eva2	70.3	70.3	904.2	1.2	evaporation 1.effect
	eva3	66.4	66.4	864.1	1.2	evaporation 2.effect
	eva4	60.8	60.8	849.8	1.2	evaporation 3.effect
	eva5	60.8	4.0	-151.5	2.0	refrigeration concentrated milk
	eva6	68.9	68.9	-904.2	1.2	condensation 1.effect
	eva7	65.9	65.9	-864.1	1.2	condensation 2.effect
	eva9	68.9	15.0	-87.8	2.0	condensation 3.effect
Condensates cooling	eva10	65.9	15.0	-80.8	2.0	cooling condensates 1.effect
	eva8	60.1	60.1	-849.8	1.2	cooling condensates 2.effect
	eva11	60.1	15.0	-69.7	2.0	cooling condensates 3.effect
Yoghurt production	yog1	4.0	94.0	1026.0	2.0	heating
	yog2	94.0	10.0	-957.6	2.0	cooling
Desert production	des1	4.0	90.0	817.0	2.0	heating
	des2	90.0	70.0	-190.0	2.0	cooling
Hot water	hw	15.0	55.0	167.2	2.0	hot water prodcution
Cleaning in place	CIP1a	58.7	70.0	188.6	2.0	maintain temperature CIP1
	CIP1b	65.0	15.0	-104.5	2.0	recuperation waste heat CIP1
	CIP2a	67.5	80.0	209.5	2.0	maintain temperature CIP2
	CIP2b	75.0	15.0	-125.4	2.0	recuperation waste heat CIP2
Fridge	frig	5.0	5.0	-300.0	2.0	maintain storage temperature

Since redundant measurements were not available, data reconciliation could not be performed in this case. The process heating and cooling requirements were modelled based on relatively few measurements, such as the mass flowrates and temperature levels, though only available at several point in the process. The data table was generated based on the following information. The first process step is **pasteurisation and centrifugation** of the raw milk. This requires heating to 66 ℃ and centrifugation (consuming electricity), which results in separation of milk and cream. Milk is then further heated to 86℃, while the cream is heated to 98℃, resulting in pasteurised milk and cream which are cooled again to 4℃. The heating and cooling requirements of the individual process steps (referred to as process streams) are estimated based on the specific heat capacity and temperature levels. The specific heat capacity of (raw) milk was approximated to be 3.8 kJ/kgK, and that of cream to be 3.4 kJ/kgK. The streams are depicted in Table 20.

Pasteurised milk can be further converted to various products. Fabrication of **yogurt and dessert** requires addition of further ingredients and various heating, storing and cooling steps. In agreement with process operators, both were modelled by assuming heating and cooling requirements between 4 and $\approx$ 90℃. The dessert is packaged at 70℃, during which the temperature is assumed to drop to 20℃. For all conversion processes mentioned above, milk properties are assumed with a specific heat capacity of

3.8 kJ/kgK.

Concentrated milk is produced in a three-stage evaporation process, at sub-atmospheric pressures between 0.7 and 0.25 bar. Water thermodynamic properties were assumed for partial evaporation. The vapor is assumed to be captured and subsequently condensed and cooled to ambient conditions to harvest the latent and sensible heat. Products were always modelled to reach operating conditions (4 °C) after the conversion steps before being placed in the storage unit. The storage unit cooling requirements were modelled at constant temperature and based on data provided by the process operators. The cleaning in place system requires make-up water at 80 °C.

(5) Pinch analysis (heat recovery) 🔧 The dairy process hot and cold composite curves (CC) and grand composite curve (GCC) are presented in Figure 41. The pinch point temperature is observed to be 59 °C and the minimum heat requirement is approximately 1.6 MW. Compared to 2.1 MW from the current energy bill yields the current level of heat recovery to be approximately 75%. This is a promising result, indicating that the dairy process is already at a sufficient level of heat recovery.

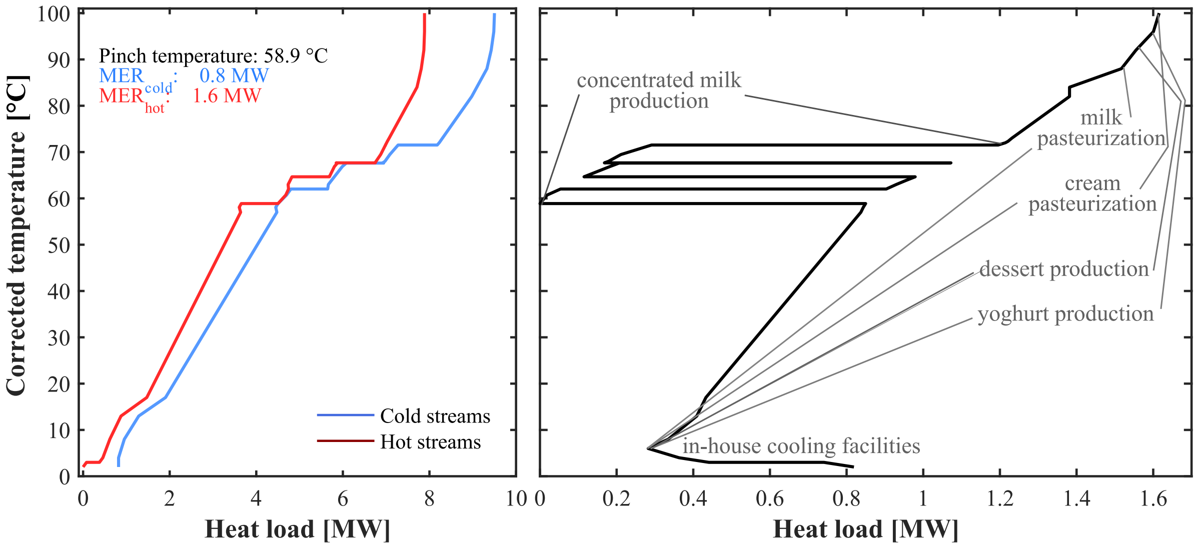


Figure 41: (Left) hot and cold composite curves, (right) grand composite curve of dairy process, reprinted from Ref. [16] for raw milk inlet of 10 kg/s.

(6) Utility integration & heat pump design 🔧 *Pinch analysis* Figure 42 shows the dairy plant grand composite curve (GCC). The pinch point is created by the multi-stage concentrated milk production unit. A self-sufficient pocket is visible below this region which indicates that the outlet vapour from the third evaporation effect should be partially used for preheating liquid milk. This is currently done in the existing plant, as highlighted in Figure 43.

Pinch rules Applying the pinch rules (1 and 2) to the case study requires heating above 59 °C and cooling below this temperature. The pinch temperature is below 160 °C, the heat sink is below 200 °C, and the temperature lift between heat sink and source is below 50K, which satisfies all conditions described in subsection 2.3, suggesting favourable conditions for installation of a heat pump across the pinch. A heat pump across the pinch point temperature, framing the concentrated milk production between 55 °C and 75 °C, is suggested.

However, there is a self-sufficient pocket, which indicates (according to pinch rule 4) that no additional heating or cooling is required within this region, so a heat pump could only be applied in the region outside the self-sufficient pocket, as shown in Figure 44(a). This analysis, however, excludes the view on the full utility system. The dairy plant also requires refrigeration at 0 °C. The condenser of this refrigeration cycle could be used to provide the heat that the steam currently supplies. This would allow for increasing the size of the heat pump across the process pinch point as indicated in Figure 44(b).

This analysis also points to two important conclusions: (1) It is important to always look at the entire utility system, especially considering the refrigeration cycles, to conduct a proper analysis. (2) Pinch analysis (PA) helps to identify saving potentials that generate true benefits. If the marked heat exchanger (in Figure 43), was not already present in the plant, this link might have been easily missed in an analysis without pinch analysis (PA), and a heat pump may have been installed which would not have generated any real benefit.

A.1.0.1 Heat pump design The heat pump check tool from the de kleijn consultants [42], was tested for the design of the heat pump system across the process pinch point temperature and the results are presented in Figure 45. The tool suggests an ammonia based heat pump between 58 ℃ and 75 ℃ with a COP of 13.5 and a payback period of 1.6 years. Other tools could be used for the heat pump design, but are not illustrated here. Another option would be consideration of direct mechanical vapour re-compression of the steam from the third effect evaporator. These results indicate high economic potential, and support a case to proceed with the analysis.

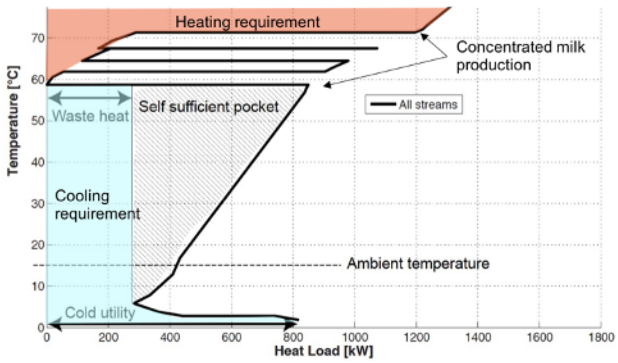


Figure 42: Dairy plant grand composite curve (GCC), reprinted from Becker [86].

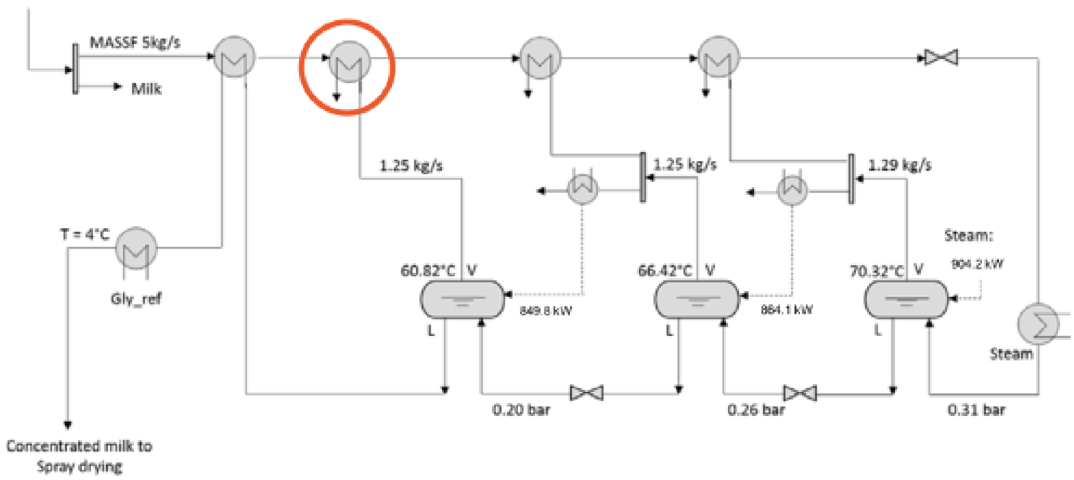


Figure 43: Concentrated milk production, reprinted from Becker [86].

(7) Identify the point of integration (🔧) In the dairy plant, the point of integration has basically been identified during the previous step, indicating that the steam from the last effect of evaporation should be recovered to partially heat an ammonia heat pump which then can be used to produce steam for

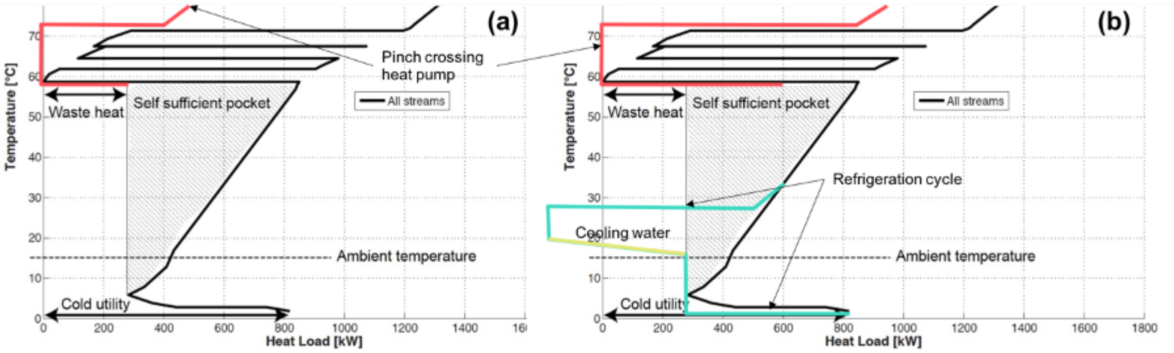


Figure 44: Dairy plant grand composite curve (GCC), from Becker [86], with (a) heat pump, (b) heat pump and refrigeration cycle integration.

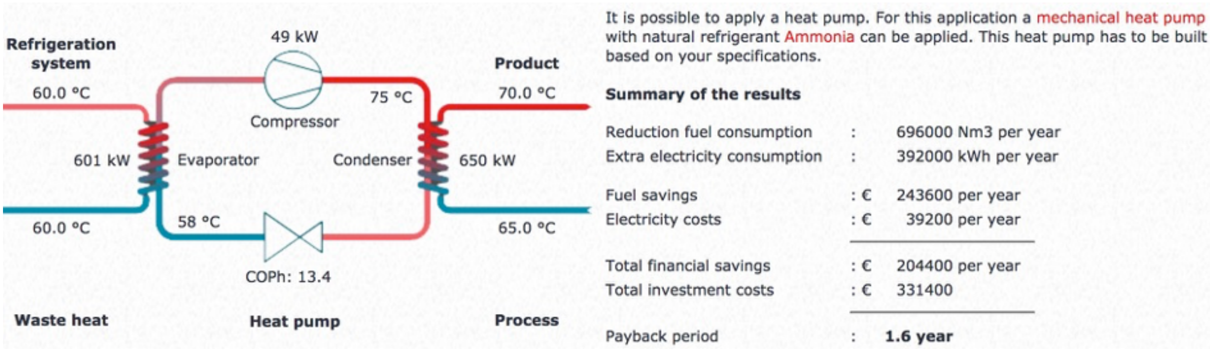


Figure 45: Results of heat pump check tool [42], with 8000 operating hours, 10 ct€/kWh electricity cost, and 35 ct€/m3 gas cost.

the highest effect. The other option would be direct mechanical re-compression of this vapour. The temperature levels, heat capacity and time overlap are verified in this case, if it is assured that the refrigeration cycle then provides heating to the liquid milk at lower temperature levels.

(8) Decision In the case study, two potential heat pumping options are shown in Figure 44 though other solutions undoubtedly exist. With many solutions, a decision-maker would be required to filter the options based on their own criteria, given insights into the relevant key performance indicators of each. With only two solutions, deciding between the two or to evaluate both options in more detail are viable strategies. Due to preferential elements inherent to individuals or industry, no additional guidance can be given for the remainder of the procedure.

(9) Detailed planning The level of detail to implement the solution for the case study would need to be explored here. This analysis has not been completed and thus the exploration of the case study cannot be taken beyond this point.

B Integrated design tool

B.1 State-of-the-art

A literature review of the state-of-the-art of advanced heat pump integration concepts and synthesis methods was conducted. Methodology-based studies concerning single-fluid heat pump systems based on the inverse Rankine cycle are presented in subsubsection B.1.1 and application-based studies are described in subsubsection B.1.2. Novel heat pump systems that are not captured by the "classical" terminology are illustrated in paragraph B.4.3.2.

B.1.1 Methodology based studies

Mathematical approaches, as opposed to conceptual approaches, typically make use of superstructure optimization which relies on mathematical principles. Large scale problems may induce convergence issues due to the problem complexity. Conceptual approaches are based on expert judgment, heuristic rules, and/or graphical methods which do not guarantee optimality of the final result. The advantage is, however, that technical infeasibilities and practical constraints can be considered in this insight-based scheme. The convergence of the resolution strategy is independent from the problem size. Mathematical and conceptual approaches are described in section B.1.1.1 and section B.1.1.2, respectively.

B.1.1.1 Mathematical approaches Optimizing multi-temperature industrial refrigeration and heat pump systems aims at reaching the cost or energy-optimal configuration of equipment (compressors, evaporators, etc), their sizes, operating conditions (pressure and temperature levels), and working fluids. The nature of the problem structure is a mixed integer non-linear programming (MINLP) problem. These nonlinearities have diverse causes: cost correlations, nonlinearities related to non-isothermal mixing of vapor after compression stages, and most importantly the intrinsic non-linear relation between the pressure ratio and compression work. Most approaches in literature incorporate concepts of pinch analysis and utility targeting based on heat cascading. In this work, and in most previous studies, pressure levels are used equivalently to temperature levels. These temperatures refer to the saturation temperatures at the respective pressure levels.

The above-mentioned MINLP problem has traditionally been solved either by relaxing the integer constraints or simplifying the nonlinearities to formulate a nonlinear (NLP) or mixed-integer linear (MILP) problem. Optimization of MINLP superstructures has also been addressed in more recent literature with higher computational complexity.

Mixed Integer Linear Programming (MILP). The first comprehensive methodology for optimal industrial heat pump design based on utility targeting [19] was presented by Shelton and Grossmann [22] in the form of an MILP superstructure. Based on a discrete set of temperature intervals and predefined working fluids, the active presaturators, evaporators, condensers, and their sizes were determined. The property and performance calculations were based on a shortcut method presented by the same authors in a previous study [107]. In a next step, they aborted integers and the solutions were strategically enumerated decreasing the resolution time and the degrees of freedom [6]. The disadvantage of the approach was that compression across active temperature levels was no longer permitted.

Swaney [79] proposed a linear programming (LP) procedure for heat engine and heat pump integration in industrial processes which is complementary to heat exchanger network (HEN) synthesis techniques. By definition of an extended transportation array [108] the optimal heat flow patterns were derived using basic economic criteria. The working fluids and pressure levels (temperature intervals) were selected in advance and thermodynamic properties were estimated based on simple correlations.

Vaidyaraman and Maranas [23] extended the MILP superstructure proposed by Shelton and Grossmann [22] to incorporate economizers and working fluid selection. The fluids were grouped into blocks based on their operating temperature levels. The set of interesting fluids and temperature intervals was added to the superstructure and selected using integer variables. The temperatures were discretized using 1 K intervals, thus increasing the computational burden for this approach.

Maréchal and Kalitventzeff [109] proposed a methodology for identification of working fluids, heat pump cycle configuration and selection of the best compression technologies. This relied on (a) a technology database, (b) an optimal MILP insertion model, and (c) an expert system selecting adequate temperature intervals and working fluids.

Holiastos and Manousiouthakis [110] introduced a linear algorithm for minimum utility (hot, cold and electrical) operating cost targeting. The temperature intervals were predefined and fluid selection was not discussed.

Oluleye et al. [111] optimized heat engine, mechanical and absorption heat pump and transformer design in industrial processes. The problem was formulated as an MILP with 10K temperature discretization. The thermodynamic properties were derived from Aspen HYSYS with simplified heat pump cycle properties based on fitting functions of the coefficient of performance (COP).

Nonlinear Programming (NLP). A non-linear programming (NLP) approach was proposed by Colmenares and Seider [7]. Various simple (one-stage compression) heat pump cycles (and engines) were sized for a set of fluids during the optimization. Superposition of the simple cycles allowed generation of multi-temperature systems. Temperature intervals were pre-set and based on lumped heat cascade intervals to reduce the problem size. The nonlinearities stemmed from non-linear cost correlations. In a later publication [8], a second step was added which contained a continuous temperature level selection, though still considering simple heat pump cycles.

Bagajewicz and Barbaro [112] presented a non-linear targeting procedure based on analytical principles that generated optimal cost savings and temperature levels for heat pumping similar to the enumeration scheme proposed by Shelton and Grossmann [6] in total site integration. Their algorithm explored all heat pump combinations across each of the pinches $P_{i,j}$ and analytically solved for the best temperature levels of simple heat pump cycles. As such, the method does not require fixed temperature intervals which can be seen as an advantage. The thermodynamic properties were based on simple correlations and heat pump features were simplified.

Mixed Integer Nonlinear Programming (MINLP) Hasan et al. [113] derived an MINLP model to optimize the pressure levels and refrigerant flow rates in a retrofit problem given a fixed set of refrigeration cycles, compressors and working fluids (including mixtures) in an LNG plant. In this way, optimal operation of a fixed design was derived without consideration of PA tools.

Zhang and Xu [114] presented an general methodology for energy-optimal synthesis of cascaded heat pump cycles. The exergy embedded MINLP model accounts for non-isothermal mixing of vapor after compression, sub-cooling and fluid switching. The temperature levels were selected during the optimization by using integer variables based on the process target temperatures in the retrofit problem.

Helen Becker [86, 115] proposed a bi-level decomposition strategy [75], in which a master non-linear optimization (genetic algorithm) determined the pressure levels and fluid, while the slave MILP optimization determined component sizing. This approach allows compressor type and fluid selection from a database created in a flow-sheeting software [52]. The database contained single-stage compression heat pump cycles for 10 fluids.

Kamalinejad et al. [116] introduced a two-step MINLP approach. In the first step, a simplified heat pump structure was optimized neglecting several features such as presaturators or desuperheaters, and multi-stage cycles. The pressure levels and partition temperatures were determined in this way and used as input to the second step which solved the full model with more heat pump features.

Summary A multitude of mathematical linear and non-linear integer programming methods have been proposed to determine optimal design of industrial heat pumps. Due to the convoluted nature of the problem, computational cost grows drastically with model complexity and with a wider variable solution space. Two major strategies to overcome this issue have been identified in the literature:

(A) reducing the variable set (e.g. by discretising the temperature/pressure levels) reduces the solution space to be explored

(B) simplifying the heat pump model (e.g. using simplified property calculations, or predefined heat pump cycles) reduces the resolution complexity

B.1.1.2 Conceptual approaches As early as 1974, Barnés and King [117] proposed a method based on a set of heuristic rules with a set of potential multi-stage heat pump candidates which were selected using dynamic programming (making this a hybrid approach). Later Cheng and Mah [118] extended this analysis by adding expert judgment inside their modeling tool.

Townsend and Linnhoff [3] derived the theoretical foundation for optimal placement of heat engines and heat pumps in the context of PA, as mentioned previously. With this work, they justified why heat pumps should be placed across the pinch and heat engines should be placed either entirely above or entirely below the pinch from a thermodynamic point of view.

Ranade [119] discussed heat pumping in the context of total site analysis. This approach derived a theoretical maximum possible economic temperature lift based on electricity savings, heating and cooling demand reduction. As such, he illustrated the balance between cost reduction due to heat exchanger area reduction from higher temperature lifts against an increase in investment and operating cost of the compressors.

Linnhoff and Dhole [120] extended pinch analysis to include shaftwork targeting. Considering the heat exchanger network design and exergy analysis, they provided "good estimates" for shaftwork targets in a graphical manner for subambient processes.

Kauf [121] proposed a method for the optimal temperature lift of supercritical CO_2 heat pumps based on thermodynamic principles by mapping the COP for a wide pressure range.

Aspelund et al. [122] presented an exergy-based extended pinch analysis that accounted for the mechanical exergy of the stream (i.e. pressure) in addition to the thermal exergy. They used these data together with a methodology containing a set of heuristic rules to minimize the irreversibilities related to fulfilling the energy requirements of energy intensive cryogenic processes. In this way, they showed large improvements in the exergy efficiency of the LNG process by taking advantage of the pressure change of all involved streams and appropriate connections with compressors, expanders and heat exchangers.

Oluleye et al. [123] presented a screening method for optimal integration of mechanical and absorption heat pumps and heat transformers for process heat recovery. The thermodynamic modeling was based on fitted efficiency curves dependent on the temperature lift for various fluids.

B.1.2 Application based studies

Chua et al. [2] and most recently Arpagaus et al. [24] presented comprehensive literature reviews on the advances in mechanically driven (multi-temperature) heat pump systems. The most recurring features relevant for large-scale modeling of industrial heat pumps are discussed below. A summary is presented in Table 21. The features include multi-stage compression and expansion, ejectors, cascaded cycles, gas-cooling, subcooling, economizers, and presaturators. Other developments, which impose different system architectures (desiccant cooling [2]) or more refined equipment modeling (scroll and oil-free compressors [2, 24, 124, 125]) are not discussed in this work.

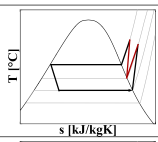
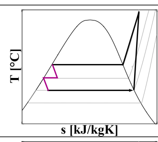
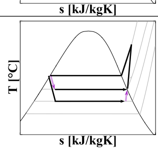
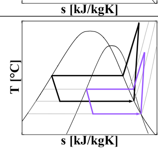
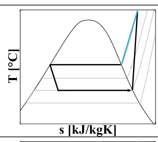
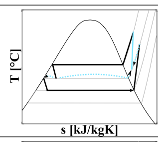
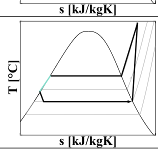
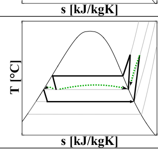
B.1.2.1 Multi-stage compression Multi-stage compression describes systems that contain a compressor with multiple stages or multiple compressors in series, such that latent heat is released or consumed at multiple pressure levels. Research on multi-stage compression is primarily focused on the design of multi-stage compressors and direct vapor injection to the compression chamber at intermediate pressure levels [63, 64]. In comparison, installation of multiple compressors in series simplifies the control of the system but induces the practical issues of lubrication management. Both options allow inter-cooling of the superheated vapour to improve the COP [24]. They also state that the popularity of CO_2 as refrigerant in transcritical cycles is constantly growing due to its environmental friendliness, non-flammability, and non-toxicity. Stoecker [126] presented the classical supermarket refrigeration which is based on a two-stage heat pump cycle with two compressors, two evaporators and one condenser. A flash drum ensures that the inlet of the second compressor is at saturated conditions.

B.1.2.2 Multi-stage expansion Multi-stage expansion systems rely on similar principles as multi- compression cycles, but instead of multiple compressors, multiple expansion valves are installed which reduces the technical complexity. Two main approaches were distinguished. Visek et al. [65] presented a two-stage heat pump cycle, in which the medium or low pressure level are alternatively used (at different times) with the same compressor operating with different compression ratios. Tamura et al. [66] presented a transcritical CO_2-based two-stage cycle, in which the refrigerant is intermediately cooled at medium pressure before expanding to the lowest stage, which resulted in superior cycle performance.

B.1.2.3 Ejectors Ejectors are devices which allow compression of a low pressure fluid through the expansion of a high pressure fluid based on the principle of suction. In this way, the potential contained in the high pressure motive stream can be partly recovered in the low pressure suction stream. In two-stage cycles, one way of making use of this principle is to expand (in a valve) from the high pressure level to the medium pressure level and then partially evaporate the working fluid. The phases are then separated in a flash drum and the liquid phase is expanded to the low pressure, where it is evaporated. The vapor phase is inserted as motive stream in an ejector while the low pressure vapor acts as suction stream. After passing through the ejector, the two gases are mixed. The result of this operation is a vapor at intermediate pressure between the medium and low level which can be fed into the simple one-stage compressor instead of solving the practical difficulties of direct vapor injection to the compressor at medium pressures. Integration of the ejector in this case necessarily excludes installation of a two-stage compressor while, nevertheless, reducing the compression work. Elakdhar et al. [67] presented this concept for household refrigeration applications. Another approach was presented by Oshitani et al. [68], and patented by the Denso corporation (Japan) [127, 128]. Here, the medium pressure level of a two-stage refrigeration cycle for cooling boxes is reached by expansion of the liquid outlet of the high pressure condenser inside an ejector. This ejector enables the vapor outlet of the low pressure evaporator to reach the same medium pressure level. After mixing and full evaporation at medium pressure, a compressor is only required between medium and high pressure level, significantly improving the system COP. The two presented examples contain only one ejector per cycle, which can obviously be expanded with several ejectors between different pressure levels [24], but since there is no conceptual difference between one and many ejectors, it is not further discussed here.

B.1.2.4 Cascaded cycles Cascaded cycles consist of several separated heat pumps which can interact through heat exchange and have two main advantages: they allow refrigeration or heat pumping over wider temperature ranges due to the possibility of switching working fluid. This application also offers the possibility for using parallel compressors on the same rack without additional difficulties of oil man-

Table 22: Heat pump features considered in this work as identified by Chua et al. [2], Arpagaus et al. [24].

Feature	Description		Feature	Description	
(A) Multi-stage compression [24, 63, 64, 126]	Provide higher COP through intermediate vapor cooling while imposing challenges for direct vapor injection (multi-stage compressor) or lubrification management (multiple single-stage compressors)		(B) Multi-stage expansion (inter-cooling) [65, 66]	Offers lower technical complexity and higher performance through cooling at intermediate pressure level (with aid of several expansion valves for a single-stage compressor)	
(C) Ejectors [24, 65, 67, 127, 128]	Allow compression of a low pressure fluid through the expansion of a high pressure fluid (principle of suction) at low maintenance and capital expenses. *Ejectors were not considered in this work, but are mentioned due to their promising characteristics*		(D) Cascaded cycles [69]	Enable coverage of wider temperatures ranges due to the possibility of working fluids switching with applications in natural gas liquefaction or other cryogenic processes, or waste heat recovery with a strong temperature lift	
(E) Gas-cooling [129]	Allows to recover heat from the superheated vapor at the compressor outlet (e.g. in a separate heat exchanger), and therefore generates a multi-temperature profile at a single pressure level at higher capital expenses		(F) Economizer [129]	Permits to preheat the saturated vapor before entering a compressor by mixing with superheated vapor at the same pressure level	
(G) Subcooling [65, 69, 126]	Subcooling before expansion improves the performance of heat pumps, however, possibly at the cost of additional heat exchanger installation		(H) Presaturators (flash-drums) [67, 126, 129]	Enable to saturate superheated vapor and to remove flash gas between expansion stages which improves the coefficient of performance in multiple ways	

agement. The main applications are (natural) gas liquefaction processes [26, 130] which are cryogenic with temperatures far below ambient; or waste heat recovery with a large temperature lift [69]. Kondou and Koyoma [69] e.g. presented a theoretical study of two cascaded cycles for waste heat recovery at 80 °C which can be upgraded until 160 °C. The heat pumps were based on a R1234ze (one-stage) and R365mfc (two-stages), achieving an overall COP of 4.7. Various other cycles were proposed [70–72], but will not be discussed in further detail.

B.1.2.5 Gas-cooling with heat exchange Gas-cooling allows heat recovery from the superheated vapor at the compressor outlet (in a separate heat exchanger) and therefore generates a multi-temperature profile at a single pressure level. Gas cooling with separate heat exchangers is only useful if several heat sinks require different temperature levels. This feature permits supplying heat at two temperature levels by installing only one compressor. The additional cost of the heat exchangers may be justified if enough sensible heat is contained in the superheated vapor which is related to the steepness of the isobars and the level of superheating. Two examples of transcritical CO_2 cycles were presented with separated gas-coolers [74, 129], while Blanco et al. [131] presented a gas-cooler in the sub-ambient regime with R410a.

B.1.3 Novel heat pump (integration) concepts

Vaidyaraman and Maranas [25] introduced a methodology based on NLP which optimized multi-stage and cascaded mixed refrigerant cycles. Sub-cooling and the internal temperature difference in the heat exchangers were neglected in the otherwise comprehensive work.

Nogal et al. [26] presented an optimization procedure of cascaded (up to two) multi-stage mixed refrigerant cycles using mathematical programming. Thereby the discrete variables were found with aid of a genetic algorithm which was followed by an NLP model to search the continuous solution space. The approach was validated on a literature LNG case.

Khan and Lee [130] used particle swarm optimization to determine the overall compression ratio and refrigerant mixture composition of a four-stage refrigeration cycle for LNG production. The cycle structure is not very flexible, not accounting for presaturators or different pressure ratios in the 4 compressors. Khan et al. [132] further presented a conceptual optimization approach for the composition of refrigerant mixtures for refrigeration in the LNG industry which was based on, among others, the fluid boiling point differentials.

Liu et al. [133] presented a graphical method for optimizing work exchange networks. It was distinguished between indirect and direct work exchangers being either expansion and compressions connected through mounting on the same shaft (former) or connected through an ejector (latter).

Fu and Gundersen [27] presented a novel sensible heat pump based on the reverse Brayton cycle (as opposed to the reversed Rankine cycle). They showed that for high temperature lifts and non-"sharp" pinches, a sensible heat pump operated with an ideal gas a working fluid had higher COPs than a single-stage latent heat pump. The COP was calculated using Carnot equations based on the temperature lift.

Table 23: Literature summary of advanced heat pump (integration) concepts.

Authors	Year	Focus	Methodolog.		Applicat.		PA	Property	Temp.	Lvl.	Objective	Cycle features								Fld.	Case studies
			Conc.	Math.	Anal.	Exp.		calc.	discret.			(A)	(B)	(C)	(D)	(E)	(F)	(G)	(H)		
This project	2017-2019	HP	TC, EO	MINLP			✔	CP	0.5 K	3	TAC, CO_2-eq.	✔	✔		✔	✔	✔	✔	✔	S	**[7, 8, 22], Dairy & cheese [86]**, chocolate [99], brewery [88], sulphite pulp [89], refinery [91]
Zhang et al. [134]	2016	AHP		MINLP				-	contin.	1	TAC				✔					G	Industrial cluster
Oluleye et al. [123]	2016	HP/AHP/ HE/AHT	TP				✔	HYSYS	10 K	2	Fuel				✔					S	Petroleum refinery
Oluleye et al. [111]	2016	HP/AHP/ HE/AHT		MILP			✔	HYSYS	10 K	2	TAC				✔					S	Petroleum refinery
Fu and Gundersen [27]	2016	HP			✔		✔	simple	contin.	1	Exergy									G	Test cases
Kamalinejad et al. [116]	2015	HP		MINLP			✔	RP	contin.	3	TAC	✔			✔	✔	✔	✔	✔	S	LNG plant
Visek et al. [65]	2014	HP				✔		-	fixed	-	-		✔	✔				✔		S	Household refrig.
Kondou and Koyama [69]	2014	HP			✔			RP 9.1	fixed	3	-	✔			✔			✔		S	Water heating
Liu et al. [133]	2014	HP	TP				✔	-	fixed	3	-	✔	✔		✔					S	Ammonia plant
Khan and Lee [130]	2013	HP		NLP			✔	PR	contin.	3	Power	4(**)								M	LNG plant
Hackl and Harvey [135]	2013	HP	TP				✔	simple	fixed	1	-				✔					G	Industrial cluster
Becker et al. [86, 115]	2012	HP		MINLP			✔	Belsim	contin.	2	Opex, Capex				✔	✔		✔		S	Dairy plant
Zhang and Xu [114]	2011	HP	TC	MINLP			✔	-	fixed	3	Exergy	✔			✔	✔	✔	✔	✔	S	Ethylene plant
Hasan et al. [113]	2009	HP		MINLP				simple	contin.	3	Power	✔			✔				✔	S/M	LNG plant
Oshitani et al. [68]	2008	HP			✔	✔		-	fixed	-	-		✔	✔				✔		S	Car cooling, coolbox
Nogal et al. [26]	2008	HP		MINLP			✔	HYSIS	contin.	3	Capex/power	✔	✔		✔				✔	M	LNG plant
Aspelund et al. [122]	2007	HP	TP					HYSIS, SRK	fixed	3	Exergy	✔	✔		✔				✔	S	LNG plant
Elakdhar et al. [67]	2007	HP			✔			RP 8.0	fixed	3	-		✔	✔					✔	S	Household refrig.
Tamura et al. [66]	2005	HP				✔		-	fixed	-	-		✔							S	Car air-condition.
Bagajewicz and Barbaro [112]	2003	HP		NLP			✔	simple	contin.	1	Opex				✔					G	Test cases
Holiastos and Manousiouthakis [110]	2002	HE/HP		LP			✔	simple	fixed	1	TAC				✔					G	Crude pre-heat train
Kanoğlu [70]	2002	HP			✔			[136]	contin.	2	-				✔					S	LNG plant
Vaidyaraman and Maranas [25]	2002	HP		NLP			✔	SRK	contin.	3	Power		✔		✔				✔	M	-
Maréchal and Kalitventzeff [109]	2001	HP	TC	MILP			✔	Belsim	fixed	3	Exergy	✔			✔				✔	S	Olefin plant [137]
Vaidyaraman and Maranas [23]	1999	HP		MILP			✔	[138]	1- 8 K	3	TAC	✔			✔		✔		✔	S	**Ethylene plant [8]**
Kauf [121]	1999	HP	TP					-	contin.	2	COP									S	-
Stoecker [126]	1998	HP			✔			-	fixed	3	-	✔						✔	✔	S	Supermarket refrig.
Nekså et al. [129]	1998	HP				✔		-	fixed	-	-					✔	✔	✔	✔	S	Water heating
Wallin and Berntsson [139]	1993	HP/AHP/ AHT	TEP				✔	generic	fixed	1	TAC									G	-
Linnhoff and Dhole [120]	1992	HP	TP				✔	simple	fixed	3	Power	✔			✔				✔	S	Ethylene plant
Swaney [79]	1989	HE/HP		LP			✔	simple	fixed	3	TAC	✔			✔				✔	S	**Cold tray distill. [7]**
Colmenares and Seider [8]	1989	HE/HP		NLP			✔	PR	contin.	2	TAC				✔					S	**Ethylene plant [78]**
Ranade [119]	1988	HP	EP				✔	simple	contin.	1	TAC									G	None
Colmenares and Seider [7]	1987	HE/HP		NLP			✔	PR	fixed	2	TAC				✔					S	**Cold tray distill.**
Shelton and Grossmann [6]	1986	HP		MILP			✔	[107]	10 K	3	TAC	✔			✔				✔	S	Test cases, **E2 [22]**
Shelton and Grossmann [22]	1986	HP		LP			✔	[107]	1 K	3	TAC	✔			✔				✔	S	Test cases, **E2**
Townsend and Linnhoff [3]	1983	HE/HP	TP				✔	Tabl.	fixed	2	Exergy									S	Industrial case study
Cheng and Mah [118]	1980	HP	HR					SRK	contin.	3	TAC	✔			✔	✔	✔	✔	✔	S	Ethylene plant [117]
Barnés and King [117]	1974	HP	HR	MIP				SRK	contin.	3	TAC	✔			✔	✔	✔	✔	✔	S	Ethylene plant

(*) This work
(**) Fixed four stages in optimization study
Focus: HP - compression heat pumps, HE - heat engines, AHP - absorption heat pumps, AHT - absorption heat transformers
Methodology based studies: Conceptual: EO - expert opinion (EO), TP - Thermodynamic principles, TC - Technical constraints, EP - Economic principles, HR - Heuristic rules, TEP - Thermoeconomic principles; Mathematical: MINLP - Mixed Integer Nonlinear Programming, MILP - Mixed Integer Linear Programming, LP - Linear Programming, NLP - Nonlinear programming, MIP - Mixed Integer Programming
PA: Pinch analysis [140]
Property calculation: CP - Coolprop [84], RP - Refprop [141], SRK - Soave-Redlich-Kwong [142] equation of state, HYSYS - Aspen HYSYS software [143], simple - simplified estimations, PR - Peng-Robinson [144], Belsim - Belsim Vali software [52]
Lvl.: Level of detail in modeling: 1 - general modeling based on thermodynamic estimations for a generic fluid, 2 - modeling of simplified (single-stage) cycles for specific fluids, 3- full detail modeling of (multi-stage) heat pumps with advanced features for different fluids
Objective: TAC - total annualized costs (TAC), CO_2-eq. - CO_2-eq. equivalent emissions (min), Fuel - primary fuel consumption (min), Exergy - exergy losses (min), Opex - operating expenses (min), Capex - capital expenses (min), Power - compression power (max)
Cycle features: (A) Multi-stage compression, (B) multi-stage expansion, (C) ejectors, (D) cascaded cycles, (E) gas cooling, (F) Economizer (preheating before compression), (G) sub-cooling, (H) presaturators
Fld.: Fluid: S - single component fluid, M - fluid mixture, G - generic fluid

B.2 Problem resolution

B.2.1 Master level

At the master level, a black box optimisation is performed where the variables present in the nonlinear constraints are the decision variables. These are mainly the heat pump saturation temperature levels (T_i), the fluid (d), the subcooling, gas cooling, and compressor preheating temperature differences ($\Delta T_{i,SC}$, $\Delta T_{i,DSH}$, $\Delta T_{i,PRE}$), and all thermodynamic properties derived from these. An additional variable is introduced in order to vary the weight (ξ) of the two components in the objective function at the slave level. The properties are retrieved from the open-source database CoolProp [84]. The variables and objective functions at the master level are presented at detail by Wallerand et al. [29]. Black-box multi-objective nonlinear optimisation is performed by Dakota [145] using a multi-objective genetic algorithm (MOGA) [146] which allows analysis of a wide solution space.

B.2.2 Objective function

Different objective functions are of interest when optimising industrial heat pumps such as the exergy efficiency, coefficient of performance (COP), environmental impact, or cost. Based on requirements from industry, the objectives of the multi-objective optimisation were based on economic criteria, i.e. annualized capital expenses (capex) and yearly operating expenses (opex) as shown in Equation 6.

$$\min_{T_i,\Delta T_{i,DSH},\Delta T_{i,SC},\Delta T_{i,PRE},d,\xi} \{C^{opex}, C^{capex}\} \tag{6}$$

The capex (C^{capex}) consists of the investment costs of all technologies w and the heat exchanger network (HEN) cost estimation. The HEN area is estimated as suggested by Townsend and Linnhoff [15, 147] based on vertical intervals in the composite curves. HEN design based on mathematical principles, as well as optimisation of the minimum approach temperature (ΔT_{min}) was not performed in this work, but could be added to the solution strategy.

B.2.3 Link to slave level

The utility and heat pump technology sizing is performed at the slave level. The results from the slave optimisation serve as input to calculate the master level objective functions. These are the maximum size (f^w) and existence (y^w) of each technology w influencing the equipment investment and heat exchanger network cost estimation.

B.2.4 Slave level

The HPS is embedded in the utility targeting problem of Maréchal and Kalitventzeff [148] where the optimal utility system for an industrial process is found based on the thermal and material needs considering maximum heat recovery. This means that all elements of the heat pump, namely condensers, evaporators, compressors, presaturators (flash-drums) and gas-coolers, are present as utility technologies in the targeting approach. The main variables at the slave level are the size and existence of each utility technology, including all heat pump elements. The size of each technology is decided by optimisation based on the objective function while remaining subject to physical and thermodynamic laws. To ensure mass and energy conservation within the heat pump, additional constraints are added at all saturated liquid, vapor, and superheated vapor points. Since the saturation temperature and respective pressure levels as well as the subcooling and superheated properties are set at the master level, component sizing is linearly dependent on the state properties. Therefore, the problem can be described as a multi-period Mixed Integer Linear Programming (MILP) problem which is solved using commercial software based on AMPL [149] with CPLEX [150].

B.2.5 Objective function

The MILP problem is solved with commercial solvers [149, 150] based on branch and cut methods for a single objective function. Investigation of a wide solution space regarding both objectives from the master level leaves two options for consideration.

(a) Constraining one objective with a variable controlled from the master level and minimizing the second objective or

(b) Defining a weighted sum of the two objectives (wC^{TAC}) where the weighting factor (ξ) is controlled at the master level.

Since alternative (a) generates more infeasible solutions and therefore leads to longer solution times, option (b) was selected and is expressed in Equation 7.

$$\min_{f_p^w, f^w, y_p^w, y^w} \left\{wC^{TAC}\right\} \tag{7}$$

B.2.6 Heat cascade

The mixed integer linear programming (MILP) slave model is subject to heat cascade constraints [148] which ensure heat transfer feasibility for maximum heat recovery.

B.2.7 Mass and energy balances

All material and non-thermal energy requirements are described by a set of constraints. These equality constraints ensure that material/energy consumption and conversion are balanced within the system boundaries or compensated with help of the grid (utilities) which factors into the operating cost.

B.2.8 Variables

The variables present at the slave level are the existence (y_p^w) and sizing (f_p^w) of each of the utility technologies w during each period p and the maximum size considering the entire operating range. Based on the objective function and thermodynamic input parameters selected at the master level, optimal sizes and operating conditions of all utilities including the heat pump technologies are derived within the optimisation.

B.2.9 Heat pump specific constraints

The general heat pump parameters such as the reference heat load of the evaporator and condenser and the reference electricity consumption of the compressors are presented in deliverable D1 and Wallerand et al. [29]. These enter into the targeting constraints and are sized based on the process thermal requirements minimizing the objective function. Enforcing energy and mass conservation within the HPS requires additional constraints to be introduced.

Mass and energy conservation are introduced at three different points on each pressure level, namely: the superheated vapor point after compression, the de-superheated or saturated vapor point before compression or condensation, and the saturated or subcooled liquid point after condensation or before evaporation. Since these points are fixed at the master level, all equations can be formulated with purely linear dependencies. Mass balances at all three points ensure that the working fluid mass flow rate is conserved throughout the heat pump system. Energy balance equations ensure that mixing (e.g. of two compressor outlets at the same pressure level) do not violate the energy conservation law. Superheated vapor mass and energy balances are introduced to study the effect of sensible heat recovery from the vapor (gas-cooling). This can either be achieved by installation of a separate heat exchanger (gas-cooler) or by accounting for sensible heat release in the condenser unit. Both options are separately modeled in this superstructure but does not have a major impact on the heat exchanger network cost estimation (since gas cooling in both cases imposes higher investment). The de-superheating temperature difference ($\Delta T_{i,DSH}$) selected at the master level can be understood as the temperature from which sensible heat release is considered. This temperature difference does not influence the energy balance but by manipulating the inlet temperature of the de-superheating, HEN solutions which require stream splitting can be avoided, which has an influence on the heat cascade. If it is set to zero, gas-cooling is neglected and the sensible heat contained in the superheated vapor is considered as if it was available only at saturation temperature levels.

Apart from energy and mass conservation, technical constraints can be considered as introduced subsequently (and in more detail in deliverable D1 and Wallerand et al. [29]): The maximum number of stages of a heat pump cycle consisting of one fluid can be restricted. Compressors with compression ratios or with pressure levels outside the bounds cannot be activated. A minimum size for heat exchangers is introduced in the form of a soft constraint (by giving it a fixed investment cost).

B.3 Fluid selection

B.3.1 Working fluid properties and historical context

Selection and development of suitable working fluids has been a key challenge in the evolution of efficient and reliable heat pumping and refrigeration (HPR) systems [151]. As shown in Figure 46, the first fluids used in the history of HPR were so-called natural refrigerants (NRs). The name stems from their natural occurrence in Earth's bio-chemical processes. The most common natural refrigerants include a variety of hydrocarbons (HCs) (such as ethane, propane, propylene, iso-butanes, etc.), ammonia, carbon dioxide equivalent (CO_2-eq.), and steam/water [152].

The environmental impact of releasing NRs into the atmosphere (due to leakage) is negligibly small, as is illustrated in Table 23, where the environmental impact refers to their global warming potential (GWP) and ozone depletion potential (ODP). Many NRs possess, however, unfavorable qualities related to their safety and handling especially in large industrial applications: Most HCs are flammable which may lead to explosions, while ammonia is highly toxic which may lead to corrosion and contamination, and CO_2-eq. needs to be operated at high pressures which may also pose safety risks.

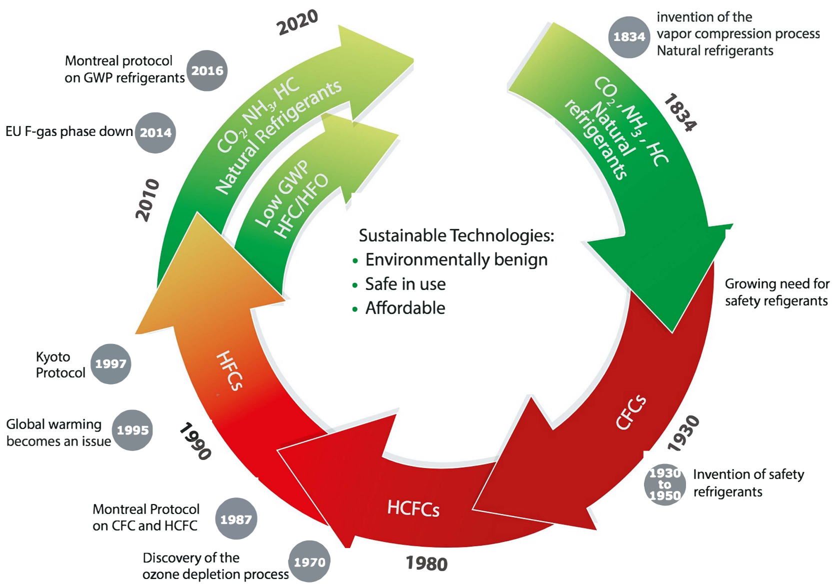


Figure 46: Historical cycle of heat pump working fluids, reprinted from Danfoss [153].

In the 1930s, a growing need for safety in heat pump and refrigeration applications led to the development of synthetic working fluids, the first ones are referred to as chlorofluorocarbons (CFCs) based on their elementary composition: chlorine, fluorine and carbon. This was followed by development of hydrochlorofluorocarbons (HCFCs). This evolution was a major step towards affordable, efficient, and

Table 24: Properties of natural refrigerants (NRs), adapted from Bentley [152].

	HFC (R134a)	**HC** (propane R290)	CO_2 (R744)	**Ammonia** (R717)	**Water**
Refrigerant type	synthetic	natural			
ODP	0				
GWP (100 y)	1430	3	1	0	0
Flammability	None	High	None	Low	None
Toxicity	Low (no identified toxicity at concentrations <400 ppm)			Toxic (<400 ppm)	None
Typical operating pressure range	0.6-6.7 bar	10-50 bar	10-50 bar	2.9-13.5 bar	0.2-5 bar
Component challenge		Flammability	High pressure	Corrosion	Low pressures
Pressure switch solution		Explosion proof sealing	Heavy duty design	Hard anodized	Special sealing

Table 25: Heat pump working fluid groups overview, adapted from Green cooling inititative [154].

Substance group	**Abbre-viation**	**ODP**	**GWP, IPCC 2007**	**Examples**
(Saturated) chlorofluorocarbons	CFC	0.6-1	4750-14,400	R11,R12
(Saturated) hydrochlorofluorocarbons	HCFC	0.02-0.11	77-2310	R22,R141b
(Saturated) hydrofluorocarbons	HFC	-	124-14,800	R32, R134a
UNSATURATED HYDROCHLOROFLUORCARBONs	u-HCFC	<0.001	0-10	R1233zd
HYDROFLUOROOLEFINs/ Unsaturated hydrofluorocarbon	HFO/ u-HFC	-	<1-12	R1234yf, R1234ze, R1234yz
NATURAL REFRIGERANTs (including hydrocarbons)	NR (incl. HC)	-	0-3	R744 (CO_2), R717 (ammonia), R290 (propane - HC)

safe working fluids in HPR applications [152]. However, at a high price: the GWP and ODP of these fluids are distinctly higher than those of NRs.

Note: The GWP is measured in tonnes of CO_2-eq. normalized with the reference value of CO_2-eq.. This means that CO_2-eq. has a GWP of 1, propane has 3, while some CFCs have more than 14,000.

General ranges of those indicators are provided in Table 24, which depicts an overview of the main working fluid groups.

With growing awareness of ozone depletion, the Montreal protocol (1987) was introduced, which aimed at a phase-out of ozone depleting gases, including CFCs and HCFC. This provided the motivation for development of hydrofluorocarbons (HFCs), which do not contain the ozone depleting chlorine and with that have a negligible ODP.

The Kyoto protocol (1997) and later the F-gas resolution (2014) of the European Union (EU) both addressing global warming (the latter in particular aimed at phasing out fluorinated gases, mainly HFCs), further underlined the need for environmentally friendly working fluids for HPR applications. The next generation of working fluids aimed therefore at reduced GWP, starting from unsaturated hydrochlorofluorcarbons (u-HCFCs), and hydrofluoroolefins (HFOs), and finally leading to a reconsideration of NRs. Previous challenges concerning NRs were addressed with improved component development and higher safety precautions. With the reintroduction of NRs, the historical circle of heat pump working fluid development as depicted in Figure 46 is closed.

Note: Not every substance which has ever been used in heat pumping and refrigeration (HPR) applications is treated here. This section focuses on the main groups that are currently used and developed.

Based on the lessons learned from this historical overview, three criteria were identified that currently play a major role in selection of HPR working fluids for industrial applications.

1. **Environmental impact.** With international resolutions in place, consideration of the GWP and ODP of working fluids has become a mandatory concern and can no longer be disregarded.
2. **Safety.** Safety is a high priority in industrial processes where large quantities are required. Especially in sterile environments (food, pharmaceutical/fine chemical), the risk of contamination and corrosion is taken very seriously.
3. **Cost.** Even though this criterion has not been specifically mentioned before, economic concerns are a main driver behind most industrial activity. This applies not only to the annualized capital expenses (capex) for purchasing the working fluids, but also to the cycle **efficiency** and the related yearly operating expenses (opex) of the system.

B.3.2 Current status

Figure 47a depicts the current consumption share of working fluids (and their GWP) in refrigeration and air conditioning (RAC) applications in the EU (27). Figure 47b shows the working fluid use and respective GWP of 75 industrial HPR projects commissioned in the past 20 years in Japan, which was obtained due to the collaboration in the IEA Heat pump Annex. From both figures, it can be seen that in agreement with the Montreal protocol ozone depleting CFCs are no longer used, and even HCFCs gases with the exception of r22 in Europe are barely consumed.

The most common working fluids in RAC in the EU are HFCs, namely: r134a, r404a, and r410a, whose GWP ranges between 1,000 and 5,000. The impact of the Kyoto protocol (the F-gas resolution was in 2014) may be underestimated, since the data from 2010 reflect consumption of all installations, including outdated systems. However, even though recent numbers suggest that the use of CO_2-eq. in European supermarket refrigeration has tripled over the past three years [155], a major shift away from HFCs is still to be expected.

In Japanese industrial projects from the past 20 years (data acquired from the international partners in the IEA HPT Annex 48), the most common refrigerants are r410a, CO_2-eq., r134a, and r245fa. There is an overlap between many of these fluids (all HFC) linked to common practice for many years and with that, the price and thermodynamic properties of these fluids. In Japan, however, CO_2-eq. has additionally been widely installed, which may be linked to a governmental strategy aimed towards the use of natural refrigerants in heating ventilation and air conditioning (HVAC) applications and the deregulation of high pressure systems (only in 2017) [156–158].

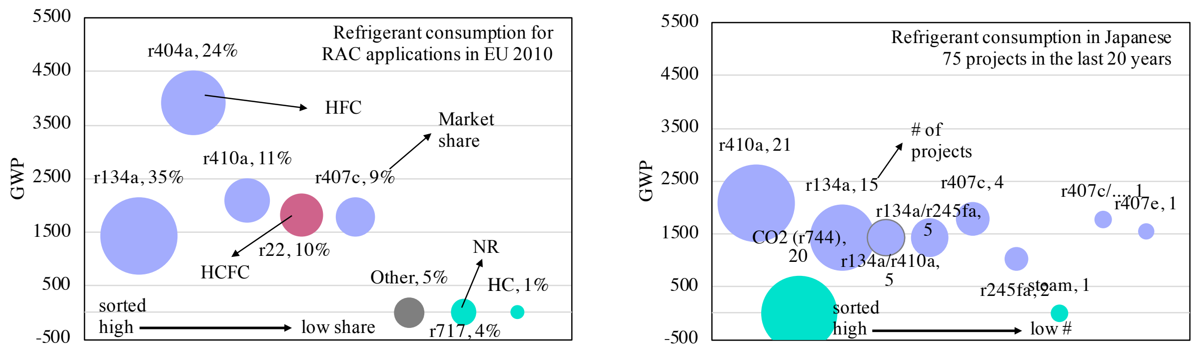
B.3.3 Future outlook

Especially with the introduction of the F-gas resolution, a phase out of high-GWP HFCs is unavoidable in the European Union. Whether this will promote u-HCFCs, HFOs, or NRs will depend on the cost, availability, and field of application of the fluids.

As shown in the previous section, political (de-)regulation and incentives have an influence on the market development. This was illustrated by the Japanese political actions to support NRs. Some experts suggest that 'institutional' barriers prevent wider use of HFOs [159].

What can be observed from the literature on industrial HPR applications, depicted in Table 22, is summarized in Figure 49. All fluids studied for integration in the various publications were enumerated, leading to an overwhelming majority of NRs. This may be linked to a lack of available data for HFOs and others due to their relative novelty, or that their thermodynamic properties do not match with industrial requirements.

This observation is in agreement with Figure 50, which suggests that industrial refrigeration will in future be dominated by natural refrigerants (CO_2-eq. and ammonia), some HFOs, and even fewer HCs;



(a) EU-27 refrigerant consumption in RAC (2010), data from Ref. [159].

(b) 75 Japanese industrial heat pump projects (2017), data from partnerst from the IEA HPT Annex 48 [160].

Figure 47: Working fluid use in different regions, sorted in descending order of market share.

and industrial heat pumps by ammonia and fewer HFOs [153]. The future application of HFO is mainly identified in commercial and residential heat pumping and air conditioning.

Figure 48 illustrates the GWP, ODP, and coefficient of performance (COP) under typical chiller conditions of widely used and new generation working fluids. This can give a good overview; however, caution should be practiced with this type of approach to identify the most promising new generation of working fluids especially for industrial applications, since the operating ranges are vastly dispersed, and additional heat pump features (multi-stage compression, sub-cooling which may not be used in residential applications) may have a different influence on the performance of different fluids.

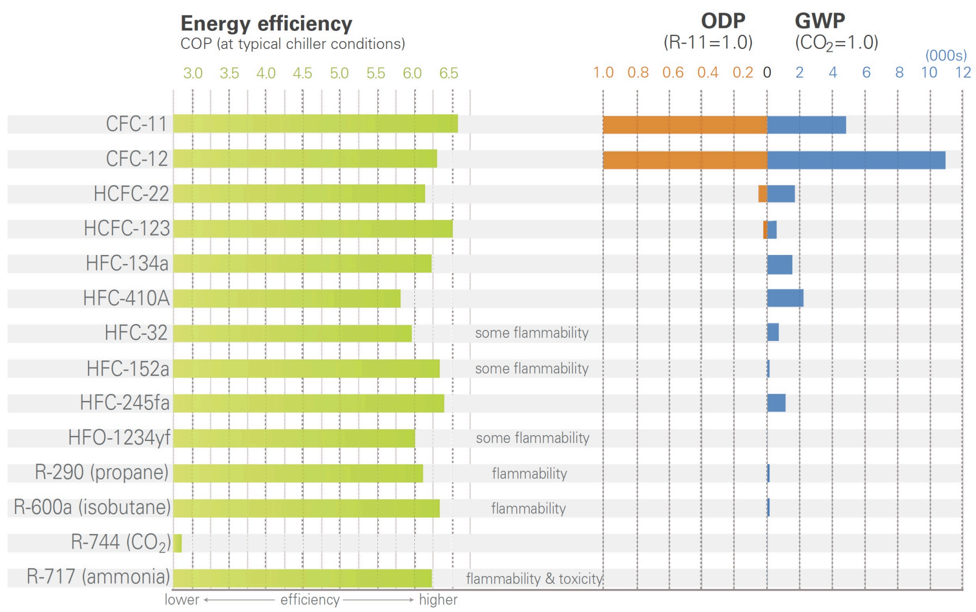


Figure 48: Widely used working fluids and their performance, reprinted from Ref. [161].

B.3.4 State-of-the-art

The previous section served as a general introduction to working fluid groups, properties, trends, and common selection criteria.

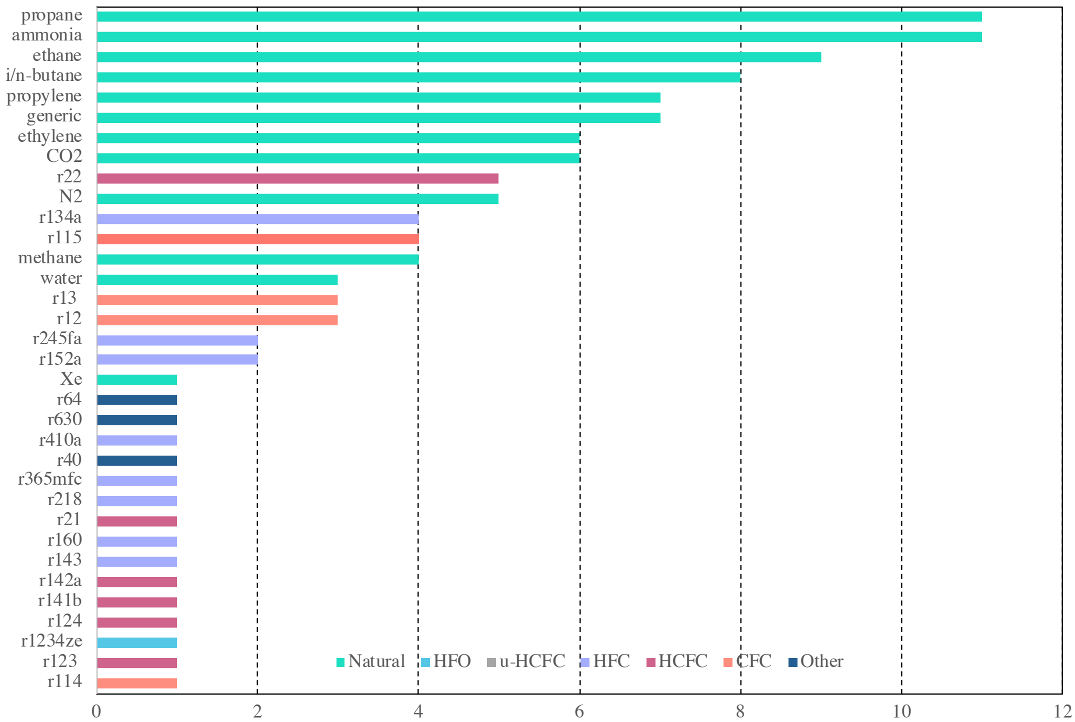


Figure 49: Working fluid use in all literature studies presented in Table 22 [3, 6–8, 22, 23, 25–27, 65–67, 69, 70, 79, 86, 110, 112–114, 116–123, 126–130, 133–135, 137, 139, 162].

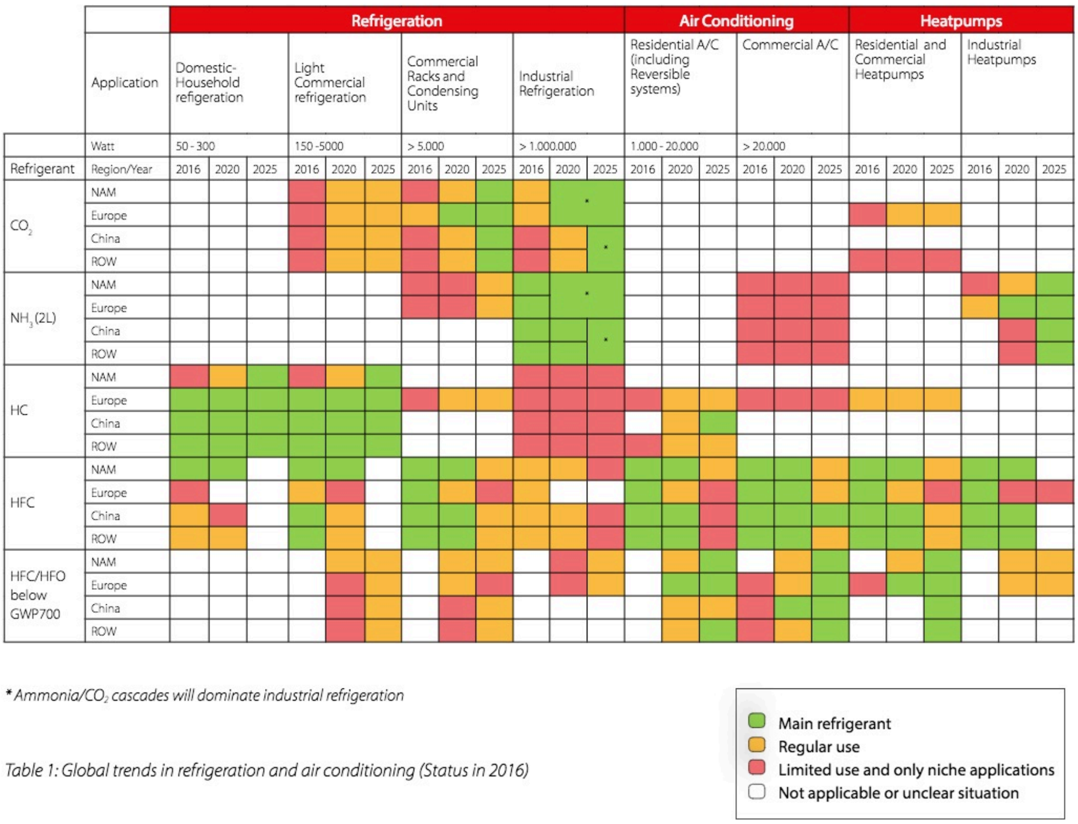


Figure 50: Current and prospected refrigerant and working fluid use in various fields and regions, reprinted from Ref. [153].

This section is oriented at summarizing approaches in the literature for working fluid selection during heat pumping and refrigeration (HPR) design and integration into industrial processes. As mentioned before, an appropriate fluid must fulfill physical, chemical, thermodynamic, environmental, and safety requirements while also satisfying case-specific and technical requirements. The literature studies considered for this analysis are depicted in Table 22. The focus has been placed on studies which address heat pump design and integration into industrial processes with mathematical approaches.

It has to be distinguished between fluid selection from existing fluids or derivation of new refrigerant types.

The latter has recently been made more achievable by the derivation of the group contribution method [163] allowing for molecular design of fluids with target properties. This method was already applied for organic rankine cycles (ORCs) [164–166]; however, not for heat pumping. One main challenge is to identify which are the desired properties.

The former has been addressed in the literature in three different ways:

- Some authors have compared working fluids based on thermodynamic principles, such as Oluleye et al. [162], Cheng and Mah [118], and Liu et al. [133], in a brute force manner.
- While others rely on mathematical programming to derive the optimal mass flow rates or composition from preselected fluids with help of continuous variables, including Nogal et al. [26], Hasan et al. [113], Zhang and Xu [114], Kamalinejad et al. [116], Khan et al. [132], Dinh et al. [167], and Vaidyaraman and Maranas [25].
- Few researchers have integrated fluid selection into their mathematical programming approaches in the form of integer, binary, or continuous variables such as Becker [86], Oluleye et al. [111],Colmenares and Seider [8], Vaidyaraman and Maranas [23], Maréchal and Kalitventzeff [148], or Colmenares and Seider [7]. The candidate fluids were principally selected based on fluid critical properties and triple point, in order to identify the fluids with the two-phase region in the required temperature ranges.

B.3.5 Summary and gaps

The discussion of studies addressing working fluid selection during industrial heat pumping and refrigeration (HPR) design and integration is summarized as follows.

1. Fluid selection either concerns existing or new working fluids.
2. Fluid selection from existing fluids has been rigorously performed with aid of integer and continuous variables with mathematical approaches. However, not in combination with design and integration of a comprehensive list of heat pump features and estimation of the heat exchanger network (HEN) costs, while considering multiple selection criteria.
3. Fluid selection concerning new working fluids and mixtures has not been addressed in the context of industrial heat pumping.

B.3.6 Goal of Task 2

The goal of this task is to explore the breadth of working fluids available for heat pumping applications and to include them in the heat pump synthesis methodology described in Task 1. The first part of the goal was addressed in the introduction section, while the second part is addressed in the **software development: integrated design tool** section thereby closing the gap mentioned in point no (2) of the summary and gaps.

Preliminary versions of this heat pump synthesis method [168, 169] were generalized and extended to incorporate fluid selection, HEN cost estimation, and technical constraints.

If time allows, the task also includes consideration of fluid mixtures addressing point (3), since the most promising options for successful implementation of heat pump systems may depend on a combination of fluid properties instead of pure fluids. This part has not been addressed yet, but may in the next months be still considered due to the high interest in the field.

B.4 Compressor selection

This section summarises the efforts which have been undertaken in order to get a consistent overview of compressor types, operating ranges, performance data and purchase cost expectations. This section is divided into four parts which aim at providing a **Compressor type overview** before describing their **Property classes** (including the casing type, etc.), **Operating conditions** and the respective **Costs**.

B.4.1 Compressor type overview

Before deep-diving into the details of compressor operating features, a general overview needs to be conducted. Figure 14 shows a tree diagram of compressor types which can be divided into two subgroups: *dynamic* and *positive displacement*. The dynamic type compressors are further distinguished between axial and centrifugal depending on the flow direction with respect to the axis of rotation. Positive displacement compressors can be subdivided into rotary and reciprocating (or piston type) compressors. Rotary compressors achieve positive displacement in a constant manner through rotation of e.g. helical screws which force the gas into a smaller volume. Reciprocating compressors generally rely on pistons with valves to achieve compression in batches. Through multiple pistons quasi-constant operation can be attained. In the following sections, the compressor types are described at a higher level of detail.

B.4.1.1 Rotary

Screw Screw compressors use (single/multiple) rotating positive-displacement helical screws. With this motion, they force the gas into a smaller space. Screw compressors are commercially available with oil, water, and gas lubrification.

Liquid ring In a liquid-ring compressor, a vaned impeller which is located eccentrically within a cylindrical casing generates compression through rotation and by centrifugal acceleration, a moving cylindrical ring is formed against the inside of the casing. The working fluid is trapped in the compression chambers formed by the impeller vanes and the liquid ring. The discharged, compressed gas may be wet which can be solved with vapor–liquid separator.

Scroll Scroll compressor make use of two interleaved spiral-like vanes to achieve compression often by fixing one and letting the other orbit around the fixed one. This Scroll compressors operate more smoothly, quietly, and reliably than other types of compressors [57].

Vane Vane compressors rely on a rotor with blades which rotates eccentrically in a cylindrical (or more complex shape) casing. Through the eccentric rotation and the contact of the blades with the casing, a series of decreasing size volumes is created, thus achieving compression.

Lobe Lobe compressors rely on two opposite direction rotating lobes which force the working fluid to travel between the lobe rotors and the casing, while being prevented from returning through their middle through their meshing.

B.4.1.2 Reciprocating

Diaphragm Diaphragm compressors or membrane compressors achieve pressure rise through movement of a flexible membrane, instead of an intake element. The movement of the membrane originates from a crankshaft mechanism. An advantage is that only the membrane and the compressor box come in contact with the gas being compressed.

Crankshaft A crankshaft or piston compressor is the standard type reciprocating compressor in which pistons operating in a cylinder with valves driven by a crankshaft achieve high pressure compression.

Barrel Barrel compressors are multi-staged reciprocating compressors which are operated in a barrel-type casing.

B.4.1.3 Dynamic

Centrifugal Centrifugal compressors, sometimes called radial compressors, are turbomachinery equipment which achieve continuous compression through acceleration by a rotor and deceleration by a diffuser. The flow leaves the casing in a 90 degree angle compared to the rotation axis. High volumetric flow rates and velocities close to the speed of sound can be achieved.

Axial Axial compressors are turbomachinery equipment in which the working fluid flows parallel to the axis of rotation. The fluid passes alternatingly through stator and rotor elements which exert a torque on the fluid, thereby achieving compression.

B.4.2 Property classes

Different kinds of property classes are discussed in the following section which are not linked to the compressor type. These additional properties can be associated with any compressor type and depend on other criteria, such as safety and maintenance concerns.

B.4.2.1 Sealing A property which is independent from the compressor type is the type of sealing of the compressor circuit towards the environment. Three types are available, as described below.

1. **Open** Open compressor units are the most common types, which need an external engine unit to provide motion.
2. **Hermetic** Hermetic compressors are isolated from the environment. The casing seals the compressor and engine units airtight from the outside.
3. **Semi-hermetic** Semi-hermetic compressors are sealed together with the engine during operation inside a casing, which can be opened for maintenance and inspection.

The pros and cons of the respective seals are presented in Table 25. In HVAC, hermetic or semi-hermetic systems are usually chosen, when contamination of the environment would be a too high risk to take, due to toxic working fluids in urban environment or sensitive processes, such as in the food and beverage sector.

> These information are used in the methodology section in combination with the fluid selection. Open type sealings are preferred, if the fluids are non-explosive, while closed type sealings are used if the fluids are flammable or explosive.

B.4.2.2 Compressor bearings and lubrication Bearings are an integral part of compressor systems and are an important element with respect to their lifetime and operation. HPR applications typically employ rolling element bearings (REBs) (i.e. with scroll, screw, piston compressors) and fluid film bearings (FFBs) (i.e. scroll). Schiffmann et al. [170] identified three types of relevant bearings for high-speed compressors:

1. **Rolling element bearings (REBs)** support a wide range of rotational speeds and are largely standardised which allows for quicker design and acquisition. According to [170], REBs are inherently stable as they do not have cross-coupled stiffness. Rotational speed is correlated to the system lifetime due to potentially excessive inertial forces generated by the rolling elements. These bearings typically use hydrocarbon lubricants which bears the risk of oil migration into the cycle and pollution of the heat exchangers leading to efficiency losses [170].

Table 26: Pros and cons of seal types.

	Hermetic	Open
Pros	+ protection from contamination (both ways) + longer lifespan of individual components (until maintenance) + lower running costs	+ lower overall cost + maintenance possible + longer overall lifetime of overall system, due to replacement of components
Cons	− increased noise and vibration − no maintenance possible, not extremely high lifetime	− higher level of contamination (both ways) − higher need for maintenance due to leakage and contamination

2. **Active magnetic bearings (AMBs)** use a current passing through electromagnets to levitate the rotor and thus do not require lubricants and can also be operated under vacuum conditions. For safety purposes, however, backup bearings are essential in the event of power-failure, whereas other bearing types are typically fail-safe. This factor, among others, increases the compressor cost relative to other types. Schiffmann et al. [170] noted that the ratio of space to rotor diameter increases decreasing compressor size which reduces the interest of these bearings for small applications [170].

3. **Fluid film bearings (FFBs)** rely on gaseous or liquid lubricants depending on the desired application. Noted advantages of gaseous film bearings (GFBs) (based on gas-lubrification) are cleanliness and avoidance of contamination issues (since the working fluid can usually be used as lubricant) which augments the cycle performance. Gas-lubrication provides further benefits at the expense of load capacity but can also be operated for a wider range of temperatures due to relatively stable physical properties compared to liquid lubricants. Schiffmann et al. [170] additionally noted that auxiliary systems which are required for externally-pressurised bearings are not needed for dynamic fluid film bearings for which the load capacity is generated directly by the rotation of the shaft. [170].

Active magnetic bearings (AMBs) are omitted for HPR applications, due to high cost. One interesting development, however, discussed by Schiffmann et al. [170] are GFBs, which is a sub-category of FFBs as introduced above. This lubrication system has the advantage of avoiding contamination and the ability to operate at high temperatures without impacting efficiency, if dynamic fluid film bearings are considered. Collaboration has been initiated to include a novel compressor type with dynamic GFBs developed at the laboratory of Schiffmann et al. [170] in the developed methodology.

The goal is to add a dynamic GFB type compressor to Table 27 and as an input to the optimisation platform presented in the Software development: Integrated design tool section.

B.4.3 Operating conditions

B.4.3.1 Market available compressor types The compressor operating conditions and properties which are discussed in this section are specific for each compressor type. They include: volumetric flowrate, pressure ratio, isentropic efficiency, minimum/maximum pressure, performance and physical properties in different conditions (corrosive gases, high temperature operation, sealing types, etc.).

Table 26 shows a summary of operating data of the standard compressor types presented in the previous section (B.4.1) and currently available on the market. The data which have been collected are mainly based on four sources [56, 58, 86, 171] where, if different values were proposed, the more conservative estimates were adopted. Figure 51 shows a summary of the so-called operating envelopes of all compressor types showing their volumetric flowrate and operating pressure ranges.

> These data serve (together with the cost data from section B.4.4) as one of the main resources for the equipment selection methodology presented in the Software development: Integrated design tool section.

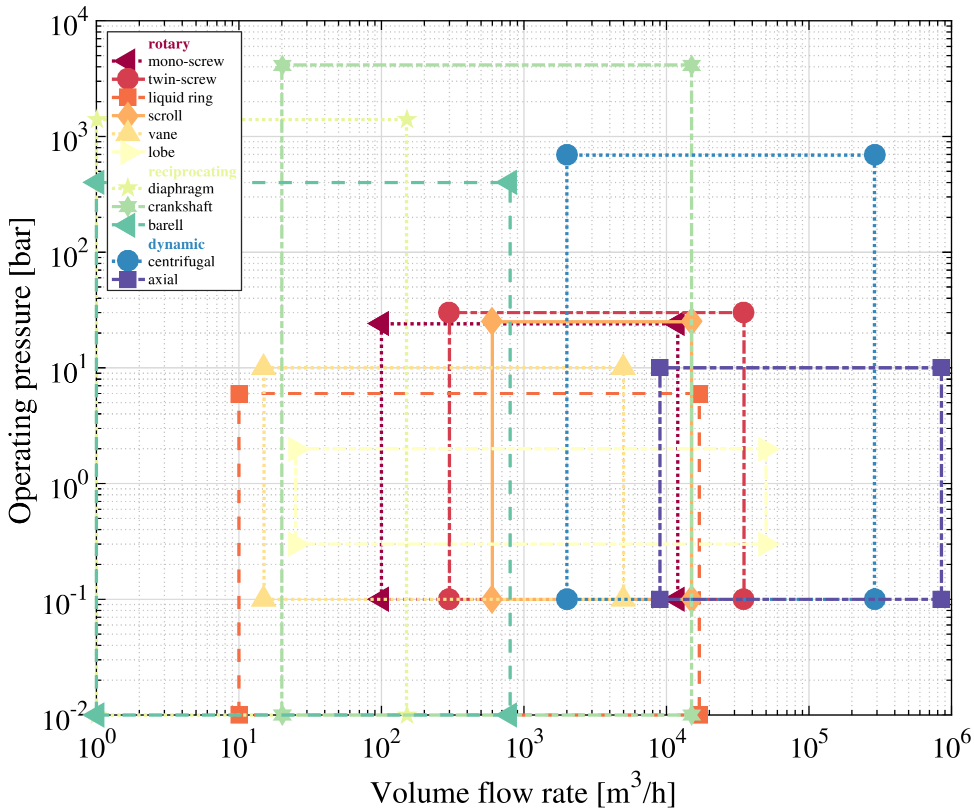


Figure 51: Operating envelope of market-available compressor types, data retrieved from Table 26.

Table 27: Operating conditions and properties of market available compressor types.

Technology	Volume flow rate [m³/h]		Pressure ratio per stage [-]		Stgs. per cas. [-]	Isentr. efficiency[a] [%]		Pressure (staged) [bar]		Power [kW]		F_{BM} [-]		Temp. [°C]	Properties					Throt-tle	Sealing type	Cooling type	Oil contact w. refr.	Source
	min	max	min	max	max	min	max	min	max	min	max	CS	SS	max	I	II	III	IV	V					
Rotary																								
Mono-screw	100	12'000	3	5	1	65 (50[v])	70	0.1	24	20	1'000	2.2	5.5	300	D	D	C	A	B	✖	liquid inj.	internal/ external	✔	[56, 58, 86, 171]
Twin-screw	300	35'000	3	5	1	60	80	0.1	30	20[m]	1'000[m]	2.2[m]	5.5[m]	300[m]	D[m]	D[m]	C[m]	A[m]	B[m]	✖	liq. inj. or not	internal /external	✔ / ✖	[56, 58, 86]
Liquid ring	10	17'000	-	4	2	50	80	0.01	6	≤ 10	300	2.2	5.5	-[d]	C	D	A	A	B	-	-	-	-	[56]
Scroll	600	15'000	3	8	-	60		-	25	1 [?]	≥ 35 [?]	2.2[m]	5.5[m]		-	-	-	-	-	(✔)	liq. inj.	internal	✔	[58, 86]
Vane	15	5'000	3	4	1	40	80	0.1	10	≤10	350	2.2	5.5	200	E	D	B	A	C	(✔)	vanes	internal	✔	[56, 171]
Lobe	25	50'000	-	2[c]	2	60	80	0.3	2	10	1'000	2.2	5.5	300	E	D	D	A	C	-	-	-	-	[56, 171]
Reciprocating/ piston																								
Diaphragm	0	150	-	10	3	60	80	0.01	1'400	≤10	1'500	2.9	4.0	320	A	D	B	A	B	✔	mem-brane	external	✖	[56, 58, 171]
Crankshaft/ piston	20	15'000	3	5[c]	8	60	80	0.01	4'150	≤10	2'000	2.9	7.3	200	D	E	C	A	C	✔	segm./ fittings	external	✔	[56, 58, 86, 171]
Barrel	0	800	3[s]	8[s]	8[s]	60[s]	80[s]	0.01	400	≤10[s]	2'000[s]	2.9[s]	7.3[s]	200[s]	D[s]	E[s]	C[s]	A[s]	C[s]	✔	segmen-tation	external	✔	[56, 58, 86, 171]
Dynamic																								
Centrifugal/ radial	2'000	288'000	2.5	3[c]	9	75	85	0.1	690	10	8'000	2.5	6.3	200	C	D	E	D	C	✖	-	-	-	[56, 86, 171]
Axial	9'000	850'000	1.2	1.4	20	80	90	0.1	10	10	8'000	2.5	6.3	200	E	D	E	D	C	✖	-	-	-	[56, 86, 171]

The preferred references were Ulrich [56] (Table 4.9 and Figure 5.30) and PIP REEC001 [171] (Table 1a). If data was available in one or both of these references, usually, the most conservative numbers were adopted for efficiencies and the largest numbers for operating ranges. If these two references did not provide the required data, then the other sources were accessed. From Becker [86] Table 4.1 was accessed, from Favrat [58] Figure 38a.

[a] Positive displacement machines: Maximum efficiencies are only achieved at the design pressure ratio, the efficiency drops with increasing pressure ratio, even if the volume ratio is adapted.

[c] compression ratios greater than 8 are possible with small machines in vacuum operation [56].

[d] limited by vapour pressure of working fluid.

[m] adopted from mono-screw data.

[v] vacuum operation.

[s] adopted from crankshaft/piston.

F_{BM} bare module factor, CS - carbon steel, SS - stainless steel.

Properties: I - corrosive gases, II - high temperature operation, III - two-phase fluids, IV - variable pressure service, V - variable capacity service.

Grades: A - excellent, no limitations, B - modest limitations, C - special units available at higher cost, D - limited, E - severely limited, ■ - unacceptable.

B.4.3.2 Novel compressor types As introduced in Section B.4.2.2 bearings and lubrication are key elements for long-lasting, and efficient compression equipment. Recent research in the domain of oil-free compression has drawn wide attention for refrigeration applications [172] to achieve higher efficiencies by avoiding heat exchanger contamination. Two promising technologies are highlighted here, which have been developed at the Swiss Federal Institute of Technology in Lausanne (EPFL): *gas-lubricated turbo-compressors* and *oil-free scroll compressors (operated with REB)*. First experimental results of a gas-lubricated, twin-staged, radial turbo-compressor [173] and a design method for heat pump applications [174] have been constantly extended throughout the last decade. Recently, Schiffmann et al. [172] showed that such compressors can be scaled up to 250 kW which enters into the required range for applications in industrial processes.

Oil-free scroll compressors, such as those developed by Mendoza et al. [175], have extended beyond the research phase to industrial production, such as those produced by Air Squared [176]. Commercially-available equipment remains below industrial requirements; however, there are numerous medical applications of oil-free scroll compressors which benefit from quiet operation without lubricant contamination for drug or fluid delivery applications. The transportation industry, encompassing truck transportation, aerospace and personal transportation have also found numerous applications of oil-free scroll compressors for specific purposes, including those for novel fuel cell transportation options.

Table 28: Operating conditions and properties of novel compressor types.

Technology	Volumetric flowrate [m³/h]		Pressure ratio per stage [-]		Stgs. per cas. [-]	Isentr. efficiency [%]		Pressure (staged) [bar]		Power [kW]		Temp. [°C]	Source
	min	max	min	max	max	min	max	min	max	min	max		
Rotary													
Oil-free scroll[a]	0.36	111	2.5	4	-	5*	53*	0.99	13	0.05	13	62[b]	[175, 176]
Dynamic													
Gas-lubricated radial[c]	1[d]	1300[e]	1.5	6	-	72	85	0.34	139	0.2	250	180	[172, 177]

* isothermal efficiencies
[a] Values for this compressor type are based on laboratory prototypes by **?**] and manufacturer data by Air Squared [176] and therefore ranges may not correspond or encompass the entirety of possible operations.
[b] higher temperatures could be reached but were limited in experimental work [**?**] by injecting water.
[c] values for this compressor type are principally based on Schiffmann et al. [172] with the flowrate range specified in Mounier [177], therefore, some ranges may not correspond.
[d] calculated from the minimum mass flowrate (20 gs^{-1}) in Mounier [177] with the highest fluid density calculated from the selection of fluids in Schiffmann et al. [172] under pressurized inlet conditions
[e] calculated from the maximum flowrate (400 gs^{-1}) in Mounier [177] with the lower fluid density calculated from the selection of fluids in [172]

B.4.4 Costs

For gathering cost data of all compressor types, two approaches have been adopted. Firstly, an extensive investigation of producer purchase prices has been conducted, which is presented in section B.4.4.1. Secondly, these data were compared to literature data from handbooks and commonly known publications in Section B.4.4.2 and conclusions are drawn for proceeding with this work.

B.4.4.1 Producer data An extensive analysis of purchase prices from various producers (namely Bitzer, DMW Copeland, Danfoss, Frascold, Tecumseh) distributed by ECR Belgium [178] has been conducted, the results of which are shown in a logarithmic plot in Figure 52 based on the electric power consumption (Figure 52a) and the volumetric flowrate (Figure 52b). To obtain the power consumption for the closed systems, the current and voltage data were used to obtain the rated power consumption.

Cost functions Generic cost functions are the most useful input for the methodology presented by Wallerand et al. [29] and the newly-developed method in the **software development: integrated design tool** section. Therefore, the data were regressed with the most common cost function for industrial equipment from Turton et al. [179], as documented in Equation 8, which describes the purchase cost, C_p [€], as a function of property, P, which is typically rated power consumption [kW] in the case of compressors.

$$log(C_p) = K_1 + K_2 \cdot log(P) + K_3 \cdot (log(P))^2 \tag{8}$$

If the cost function does not describe data from the current year, then the purchase cost needs to updated as shown in Equation 9 for inflation with an adequate index, for which it is recommended to use the Chemical Engineering Plant Cost Index [180] (CEPCI) [180].

$$C_{p,\text{ current year}} = C_{p,\text{ ref year}} \cdot \frac{\text{CEPCI}_{\text{current year}}}{\text{CEPCI}_{\text{ref year}}} \tag{9}$$

The installed cost, or bare module cost, C_{BM}, which accounts for labour, piping, and transport is then derived based on Equation 10, where F_{BM} is the bare module factor which approximates these additional costs.

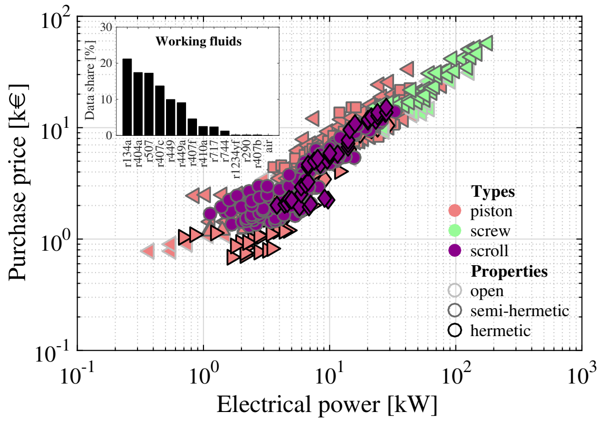
$$C_{BM} = F_{BM} \cdot C_{p,\text{ current year}} \tag{10}$$

Data regression Data of three different compressor types from ECR Belgium [178], namely piston, screw, and scroll, was regressed based on Equation 8. The results of this are displayed in Figures 53 and 54. The data are widely spread which generated an expected and acceptable error in the data regression. Nonetheless, comparing the fitted functions with each other and generic functions from the literature (Colmenares and Seider [7], Becker [86], Turton et al. [179])[1], revealed a similar order of magnitude in all functions, as shown in Figure 54b. Despite the similarity between cost functions, a higher granularity is desired for methods developed later in this work, which is necessary to distinguish among different technologies. Therefore, the literature review was extended as reported in Section B.4.4.2.

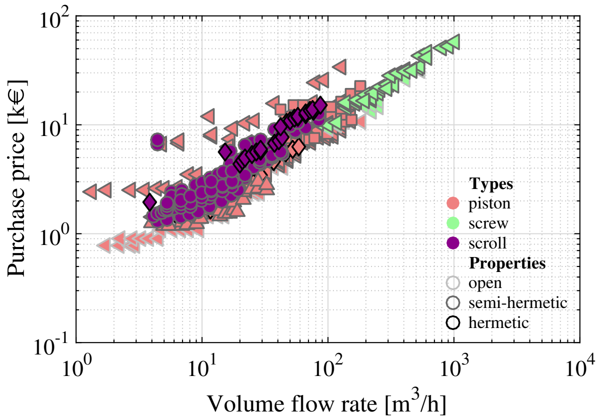
B.4.4.2 Literature data Additional literature was consulted to gain more knowledge of differences in compressor cost functions. The handbook of Ulrich [56] provided increased granularity compared to previous data as reported in Figure 55. Not only were cost data of different compressor types reported, but different drive types (and sealings) were also included. Comparing the previous data to the data of Ulrich [56] revealed that Ulrich's cost estimates are consistently higher for compression power ranges below 100 kW. Since conservative values were favored for this work and Ulrich provided the best granularity, those cost functions were assumed for further analysis. Table 28 shows the fitted cost coefficients from the updated (CEPCI) function plots reported in Ulrich [56]. With those, the installed cost of all compressor types reported in Table 26 can be derived based on Equations 8-10.

> The data from Table 26, Table 27 and Table 28 serve as major inputs for the equipment selection methodology presented in the Software development: Integrated design tool section.

[1]Some literature functions are reported as installed cost. In that case, the purchase price was estimated with an assumed bare module factor F_{BM} of 4, as reported in the figure.

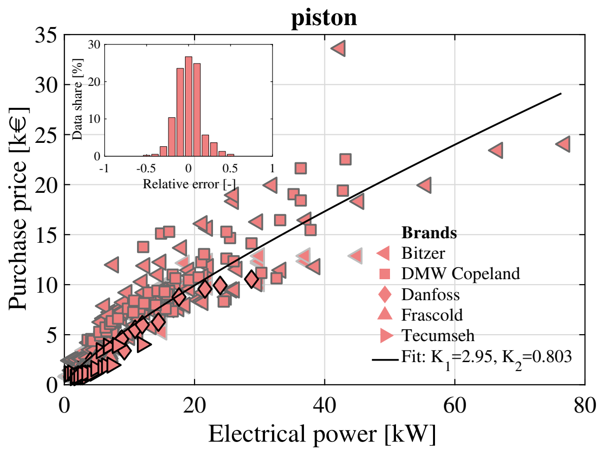


(a) Purchase cost versus max. fluid power.

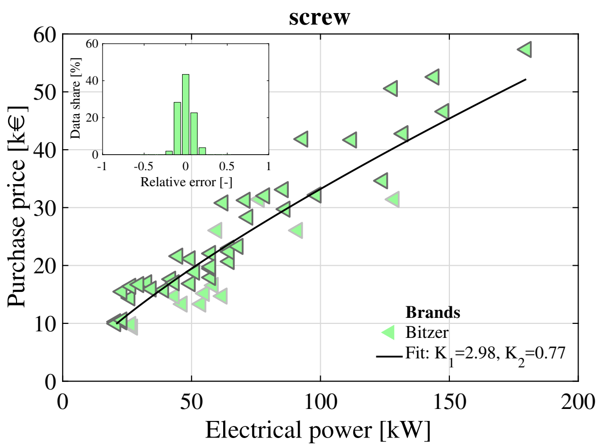


(b) Purchase cost versus max. working fluid volume flow rate.

Figure 52: Producer compressor database sorted by types, properties and fluids [178] (€ 2016).

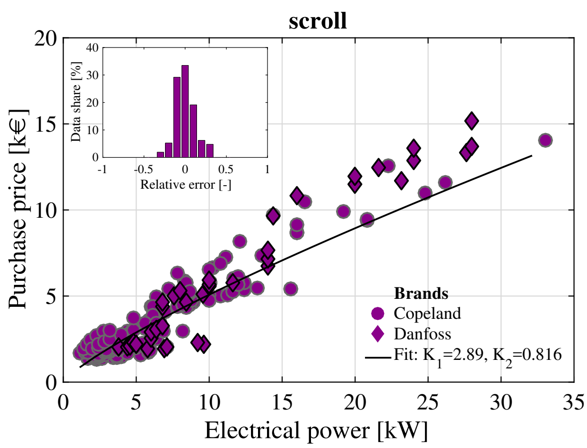


(a) Piston compressor data [178] and cost fitting function.

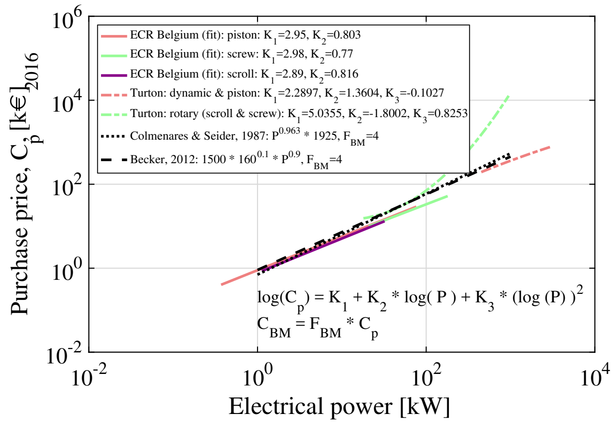


(b) Screw compressor data [178] and cost fitting function.

Figure 53: Compressor types and cost fitting functions.



(a) Scroll compressor data [178] and cost fitting function.



(b) Data fit functions compared to literature functions [8, 86, 179], updated to €$_{2016}$ with CEPCI and assumed F_{BM}.

Figure 54: Compressor types and cost functions.

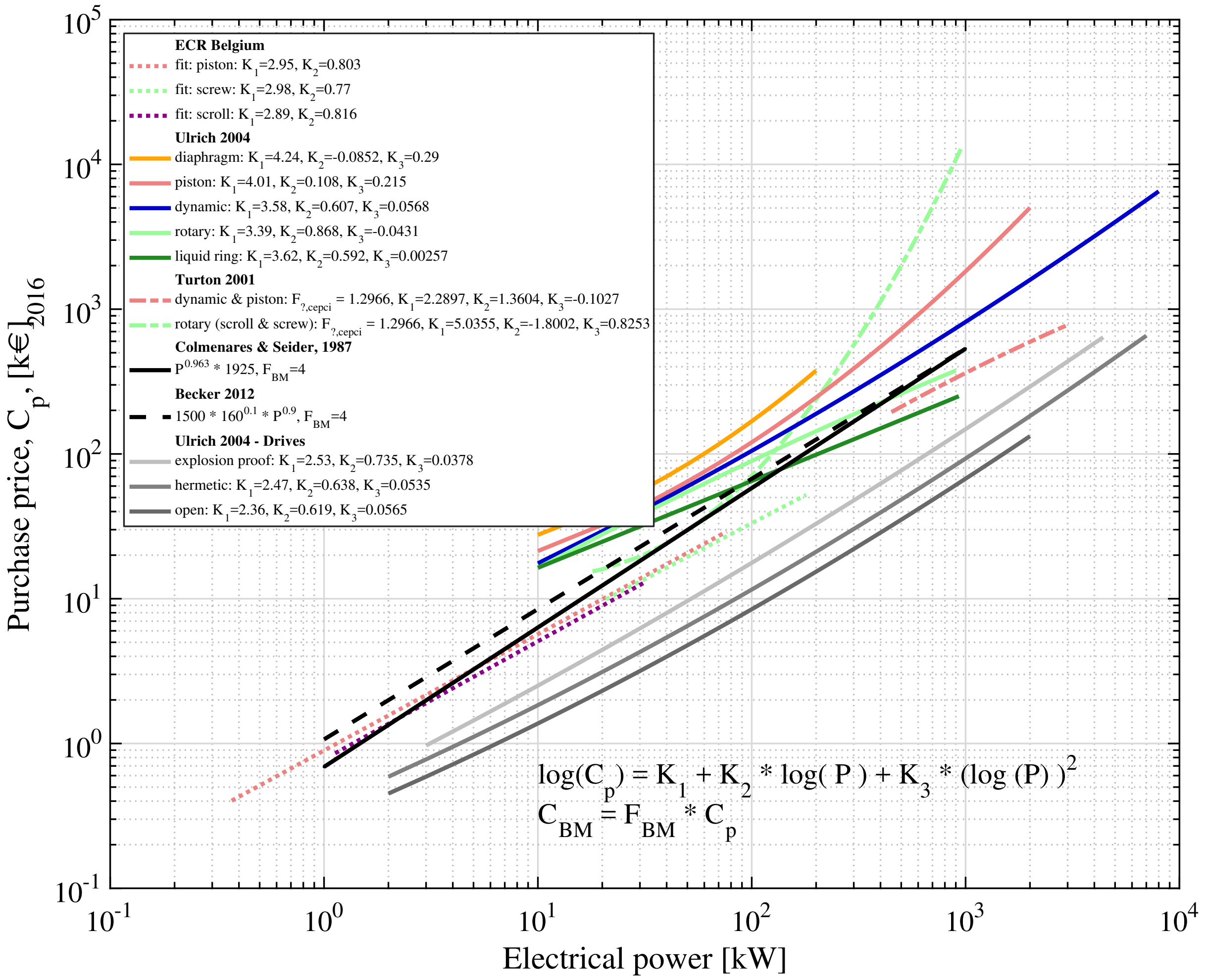


Figure 55: Compressor cost functions to be used in Equation 8-10, based on data or cost functions from ECR Belgium [178], Ulrich [56], Turton et al. [179], Colmenares and Seider [7], Becker [86].

Table 29: Fitted cost coefficients on the data of Ulrich [56], to be used in Equation 8-10, in € [2016].

Name	**Function**	K_1	K_2	K_3	F_{BM}	Associated compressor types
Compressors						
Diaphragm	f_{c5}	4.24	-0.0852	0.29	4.0	diaphragm
Piston	f_{c4}	4.01	0.108	0.215	7.3	crankshaft, barell
Dynamic	f_{c3}	3.58	0.607	0.0568	6.3	centrifugal, axial
Rotary	f_{c2}	3.39	0.868	-0.0431	5.5	mono-screw, twin-screw, scroll, vane, lobe
Liquid ring	f_{c1}	3.62	0.592	0.00257	5.5	liquid ring
Drives						
Explosion proof	f_{d2}	2.53	0.73	0.0378	1.5	Fluids with flammability ≥ 2
Open	f_{d1}	2.36	0.619	0.0565	1.5	Fluids with flammability <2

B.4.5 Methodology

The content of this section and the **compressor selection: benchmarking results** section are based on *unpublished* work which will be further elaborated in the following publication:

A.S. Wallerand, I. Kantor, M. Kermani, and F. Maréchal, Compressor type selection for industrial heat pump systems, ECOS 2020 [103]

The approach derived to identify the optimal industrial heat pump design, including fluid selection, sizing and placement of a comprehensive list of features has been introduced in previous reports (Deliverable D1 and D2) and by Wallerand et al. [29]. For the detailed structure and workflow, please refer to the preceding publications. The approach can be summarised as a bi-level optimization approach where the variables present in the non-linear constraints are selected and fixed at the higher (master) level. These fixed variables are communicated as parameters to the remaining mixed integer linear programming (MILP) model which is solved at the slave level. The results are returned to the master level, which initiates a new iteration of the multi-objective genetic algorithm (MOGA).

Two methods for adding equipment selection to the previously-established methodology are proposed and tested in this work. They are presented in Figure 56 and are summarised below. In the figure, the modified elements are highlighted in colour and the mathematical background is discussed in more detail in the following two sections.

(a) Selection at **master level**. In this approach, one or several variables at the master level decide which type(s) of compressors are considered at the slave level. In this way, equipment sizing and selection at the slave level is performed with a pre-selected subgroup of possible compressor types and their respective operating ranges (pressure ratio, volume flow rate, absolute pressure, power, stages per casing) and performance data (isentropic efficiency). The best compressor types, working fluid and temperature levels are hence identified throughout the propagation of the MOGA.

(b) Selection at **slave level**. Using this approach, all possible compressor types are added to the slave level with their respective operating ranges and performance data. Selection is then achieved through binary variables associated with each compressor at the slave level. The best compressor types are, therefore, identified in each run of the slave level, while the working fluid, temperature levels and other variables present in the nonlinear constraints are selected throughout the propagation of the MOGA at the master level.

The slave level selection adds more integer variables in the problem, which may affect the computational performance of the algorithm, while the master level selection may have the disadvantage of creating more infeasible solutions in the beginning of the MOGA propagation due to fewer choices of the MILP at the slave level.

B.4.5.1 Assumptions The method presented here provides a screening tool for heat pump pre-design and component pre-selection, including important insights for a subsequent detailed design step, which cannot be replaced by this method. The main assumptions considered in the underlying methodology are depicted below.

- **Constant isentropic efficiency** of each compressor type (independent of fluid, compression ratio, control, etc.)
- **Compressors can work with any fluid** within the operating envelope
- part-load behaviour/performance changes are not considered
- Heat losses and pressure drops are negligible
- Complete condensation/evaporation
- Valves involve isenthalpic expansion

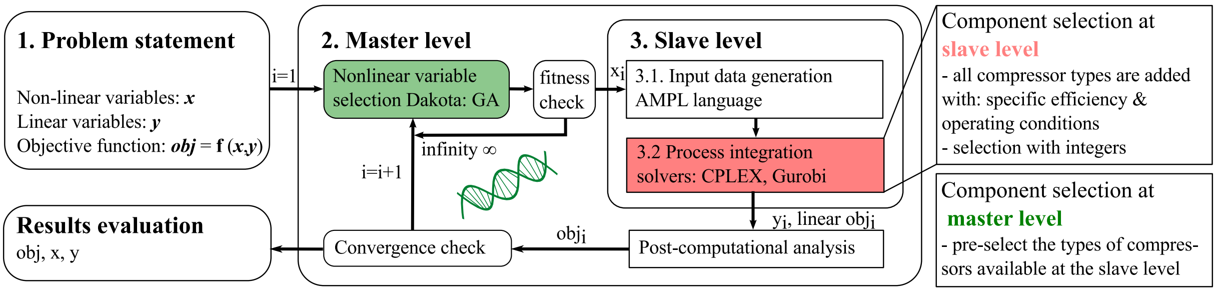


Figure 56: Two proposed methods for equipment selection, figure adopted and updated from Wallerand et al. [29].

B.4.5.2 Master level selection The master level selection is similar to the slave level selection, except that the set of compressor types is pre-selected at the master level and therefore a reduced set of compressor types is present at the slave level. All further details of the compressor selection and sizing are described in the slave algorithm.

B.4.5.3 Slave level selection In the slave level compressor selection approach, each compressor type is added to the MILP between each pressure level i and j. A set of constraints ensures that the respective operating ranges (pressure ratio, volume flow rate, absolute pressure, power, stages per casing) of the various compressor types are kept.

The performance data (isentropic efficiency, linearized cost functions) of the various compressors are individually added. Selection is then achieved through binary variables associated with each compressor at the slave level. Since an MILP is solved at the slave level, the compressor cost functions need to be linearized during this step (see paragraph B.4.5.4 and Wallerand et al. [29] for more information).

The set of additional constraints is presented below. The sets, variables, and parameters used in the equations are described in detail in Table 29. This approach currently only considers *hard* constraints such as the ones presented below. *Soft* constraints, such as the impact of corrosive working fluids on the compressor selection, are not currently considered.

Parameters and constraints *Existence of a technology* The entire set of constraints of the underlying MILP is lengthily described in Wallerand et al. [29]. The main variables associated with each utility technology w are its existence (y^w) and size (f^w). The related constraints which present these variables in relation to each other are presented in Equation 11.

$$\begin{aligned} f^w - f^w_p &\geq 0 && \forall w \in \mathbf{W}, p \in \mathbf{P} \\ y^w - y^w_p &\geq 0 && \forall w \in \mathbf{W}, p \in \mathbf{P} \\ \mathsf{f}^{w,\min} \cdot y^w_p \leq f^w_p &\leq \mathsf{f}^{w,\max} \cdot y^w_p && \forall w \in \mathbf{W}, p \in \mathbf{P} \end{aligned} \tag{11}$$

Absolute pressure and ratio range Equation 12 ensures that each compressor type c between pressure levels i and j of heat pump g is only activated if the minimum and maximum pressure levels and the pressure ratio do not exceed its operating conditions.

$$y^{\,g,i\rightarrow j,c} \leq \min\left\{\frac{\mathsf{p}^{g,i}}{\mathsf{p}^{c,\min}}, \frac{\mathsf{p}^{c,\max}}{\mathsf{p}^{g,j}}, \frac{\mathsf{p}^{g,j}/\mathsf{p}^{g,i}}{\mathsf{PR}^{c,\min}}, \frac{\mathsf{PR}^{c,\max}}{\mathsf{p}^{g,j}/\mathsf{p}^{g,i}}\right\} \quad \forall g \in \mathbf{G}, c \in \mathbf{COMP} \tag{12}$$

Volumetric flowrate and power Equation 13 ensures that each compressor type c between pressure levels i and j of heat pump g is always sized so that it is larger or equal to the minimum volume flow rate and rated power as specified for the type in Table 26. While Equation 14 ensures that each compressor type c does not exceed flow and power limitations.

$$\mathsf{f}^{\,g,i\to j,c,\min} = \max\left\{\frac{\dot{\mathsf{V}}^{c,\min}}{\dot{\mathsf{V}}^{g,j}}, \frac{\dot{\mathsf{E}}^{c,\min}}{\dot{\mathsf{E}}^{g,i\to j,c}}\right\} \quad \forall g \in \mathbf{G}, c \in \mathbf{COMP} \tag{13}$$

$$\mathsf{f}^{\,g,i\to j,c,\max} = \min\left\{\frac{\dot{\mathsf{V}}^{c,\max}}{\dot{\mathsf{V}}^{g,i}}, \frac{\dot{\mathsf{E}}^{c,\max}}{\dot{\mathsf{E}}^{g,i\to j,c}}\right\} \quad \forall g \in \mathbf{G}, c \in \mathbf{COMP} \tag{14}$$

Number of staged compressors Equation 15 ensures that the maximum number of compressor stages per casing of each compressor type c (as indicated in Table 26) is not surpassed. This equation does not control the overall number of compressors, but rather the number of compressors of a single type c.

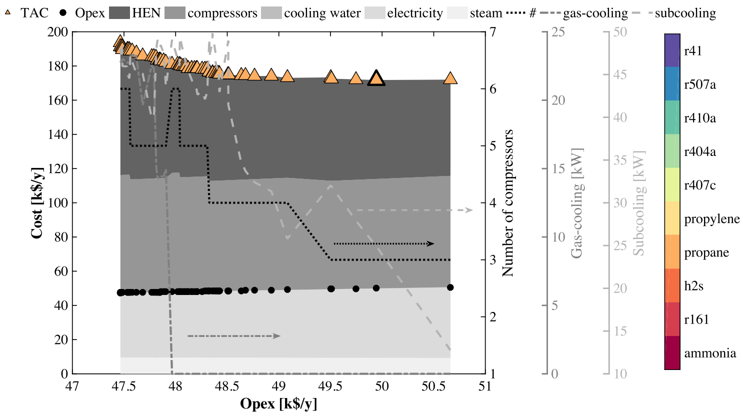
$$\sum_{i=2}^{\mathsf{n_l}} \sum_{j=1}^{i-1} y^{g,i\to j,c} \le \mathsf{n}^{c,\max} \quad \forall g \in \mathbf{G} \tag{15}$$

Table 30: Sets, variables, and parameters relevant for compressor selection at the *slave level*.

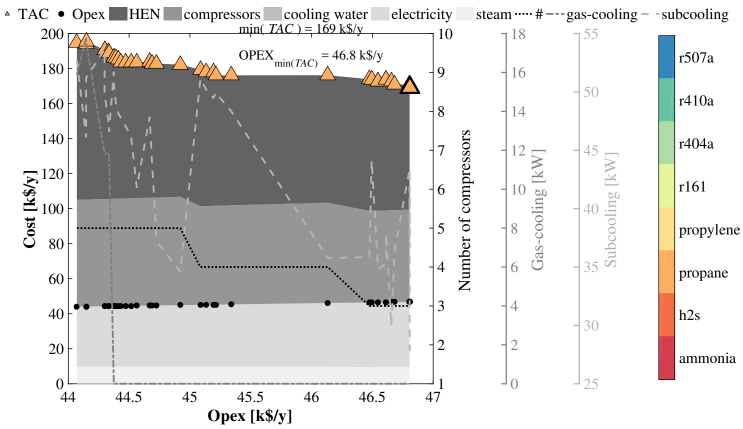
Sets	
P	set of time periods {1,2,3, ...,$\mathsf{n_p}$}
W	set of utility technologies
G	set of heat pumps with one working fluid
COMP	set of compressor types
Variables	
f_p^w	[$\mathsf{f}^{w,\min}$, $\mathsf{f}^{w,\max}$] continuous variable for sizing technology w during period p
y_p^w	{0,1} binary variable related to existence of technology w during p
f^w	[$\mathsf{f}^{w,\min}$, $\mathsf{f}^{w,\max}$] maximum size of technology w
y^w	{0,1} overall existence of technology w
$y^{\,g,i\to j,c}$	{0,1} overall existence of compressor type c between level i and j of heat pump g
Parameters	
$\mathsf{f}^{w,\min}$	minimum size parameter of technology w
$\mathsf{f}^{w,\max}$	maximum size parameter of technology w
$\mathsf{f}^{g,i\to j,c,\min\,/\,\max}$	minimum/maximum size parameter of compressor type c between level i and j of heat pump g
$\mathsf{n}^{c,\max}$	[-] maximum number of staged compressors of type c of heat pump g
$\mathsf{p}^{g,i}$	[bar] pressure at level i of heat pump g
$\mathsf{p}^{c,\min\,/\,\max}$	[bar] minimum/maximum pressure of compressor type c, see Table 26, column: **Pressure**
$\mathsf{PR}^{c,\min\,/\,\max}$	[bar] minimum/maximum pressure ratio of compressor type c, see Table 26, col.: **Press. ratio p. stg.**
$\dot{\mathsf{V}}^{g,i}$	[m^3/h] reference volumetric flowrate at level i of heat pump g
$\dot{\mathsf{V}}^{c,\min\,/\,\max}$	[m^3/h] minimum/maximum volumetric flowrate of compressor type c, see Table 26, col: **Volume flow rate**
$\dot{\mathsf{E}}^{g,i\to j,c}$	[kW] reference power consumption of compressor type c between level i and j of heat pump g
$\dot{\mathsf{E}}^{c,\min\,/\,\max}$	[kW] minimum/maximum power consumption of compressor type c, see Table 26, col: **Power**

B.4.5.4 Post-computational analysis The post-computational analysis serves to re-calculate the objective function and other key performance indicators which had been linearised at the slave level. Here, the nonlinear cost functions are applied and the real cost of the system is derived.

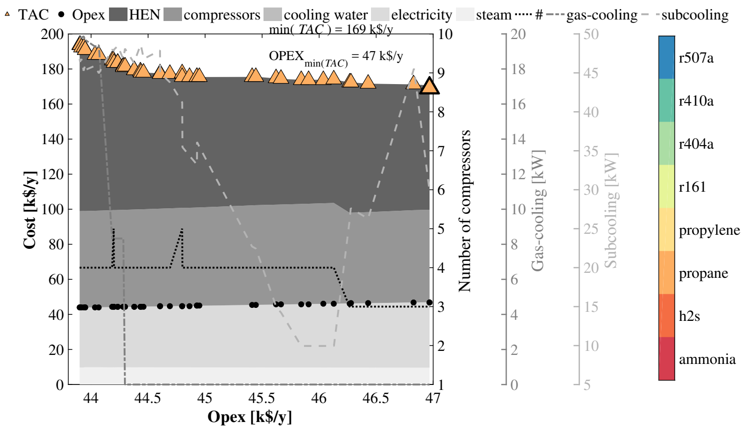
B.5 Compressor selection: benchmarking results



(a) **Original**. No equipment selection, graph adapted from Wallerand et al. [16, 29].



(b) **Master level selection**. Equipment selection during post-compute.



(c) **Slave level selection**. Equipment selection at slave level with integer variables.

Figure 57: Non-dominated frontiers of the different approaches for industrial case *E2* [29].

C Swiss potentials

C.1 Details: food & beverages

C.1.1 Dairies

Table 31: Average consumption values in EU dairies ([106] (for cheese highest consumption inspired by [86]), Table 3.59)

		Milk	Yogurt, others	Cheese	Milk powder	Whey	CH dairy Average[a]
Fuel	GJ/t	0.18	1.5	4.6	3	20	957
Electricity	GJ/t	0.15	2.5	2.9	0.1	3.3	1.241

[a] average based on data SMP [181]: 11% long lasting products (between UHT and powder: 1 GJ/t assumed), 26.6% yogurt or similar, 19.2% milk or similar, rest cheese

C.1.2 Meat production

Table 32: Danish, Swedish and Norwegian meat production data ([106], Table 3.12 & Table 3.15)

		Salami	Var. sausages	Canned meat	Beef, sheep[a]	Poultry[a]	Pork[a]	CH Average[b]
Fuel	GJ/t	3.2-4.5	1.6-3.6	1.7	0.5	0.6	0.9	0.76
Electricity	GJ/t	3.6	2.7-4.7	0.5-1.4	0.3	1	0.5	0.53

[a] UNIDO [182] Table 13, OECD data
[b] average based on data from [a] and PROVIANDE [183]

C.1.3 Bakery products

Energy consumption data for bread baking:

- electricity consumption 60 MJ/t ([184], Table 5)
- thermal energy consumption 4750 MJ/t ([184], Table 5), in agreement with [185], Fig. 8 (only 20% of thermal energy need is for bread heating)

C.2 Overall

C.2.1 Food and beverage (1)

- **Dairy & cheese**
- [10] Ref. [181] states that 3,454,428 t/y of raw milk were processed in 2015: 43.2% cheese from raw milk, 56.8% (fresh) dairy; a total of 191,321 tons of cheese was produced from this.
- [11] Based on Table 30, for dairy CH average, and cheese data from column *Cheese*
- **Sugar**
- [12] 2018: 1,263,462 t/y; 219,000 t/y sugar [186]
- [13] European reference documents for best available techniques (BREF), Tab. 4.110, Electricity 27.72 kWh/t beet, 417 t (beet)/h, Thermal 72.73 MW, conversion beet to sugar see [12] [106]
- **Chocolate**
- [14] 2018: chocolate bars: 104,408, couverture: 36,874 [187]
- [15] Konstantas et al. [188]: Table 2
- [16] Background data from Muller et al. [99]

- **Fresh bread**
- [17] [189] 2018 data
- [18] Eladly et al. [184], Table 5 (french bread)
- [19] From own calculations. No chemical reactions.
- **Beer**
- [1a] From [190] 2018 converted from hectoliters to tonnes assuming a density of 0.1 t/hl.
- [1b] [106], Table 3.76 (with 0.1 t/hl)
- **Tobacco**
- [1c] Ref. [191] from 2016
- [1d] From Ref. [192] 2911 kWh/GCig, from [193]: 50% electricity, 50 % thermal energy
- [1e] From internal industry data
- **Meat**
- [1f] Ref. [183] 2018 data, meat of all kinds (*Fleisch aller Arten*); distribution: 97,363 t beef/y, 284,352 t pork etc./y, 74,060 t chicken/y
- [1g] Ref. [182], Table 13: 0.3, 0.5 GJ (EL,TH)/t beef, 1, 0.6 GJ (EL,TH)/t poultry, 0.5, 0.9 GJ (EL,TH)/t pork
- [1h] From internal industry data

C.2.2 Pulp and paper (3)

- [30] Verband der Schweizerischen Zellstoff-, Papier- und Kartonindustrie [96], page 19. pulp production: 134,856 t/y (*Holzstoff*), assumption from [95] Figure 1.4: 40% chemical, 60% thermo-mechanical pulping
- [31] Average values from BREF [95] Table 4.6: 550-750 kWh (EL)/air dried ton (ADt), 7.5-8.5 GJ (TH)/ADt
- [32] verage values from BREF [95] Table 5.13: 2350 kWh (EL)/t, 150 MJ (TH)/ADt
- [33] Verband der Schweizerischen Zellstoff-, Papier- und Kartonindustrie [96], page 19. total pulp conversion: 1,042,355 t/y (*Verbrauch Faserstoffe*) $\rightarrow$ this number reflects the total pulp converted rather than the total paper produced, it is assumed here that the numbers are more or less equivalent; it is split according to the figure on page 18 into: 52 kg/hab (packaging), 2+20+59+24 kg/hab (white paper)
- [34] Ref. [95] Table 2.9: RCF without de-inking (packaging) paper 300-700 kWh (EL)/t, 1,100-1,800 kWh (TH)/t
- [35] RCF with de-inking (graphic) paper 900-1,400 kWh (EL)/t, 1,000-1,600 kWh (TH)/t

C.2.3 Chemical industry (4)

- [40] Crude oil flow rate. Calculated from advertised refining capacity (10,800 m^3/day [194, 195]) corrected for crude oil density (0.92 t/m3) and assuming non-stop operation (365 d/y).
- [41] Reported in Ocic [196], Table 32, total primary fuel consumption (2,845.4 MJ (fuel)/ ton crude oil, 350 MJ/t (primary fuel for steam)). Ranges provided by BREF [95] 670-7,650 MJ/t.

C.2.4 Cement (5)

- [50] [MJ/t clinker]. Ref. [197] 2018 data: total energy consumption 12,871 TJ, specific energy consumption (SEC) 3.49 GJ/t clinker
- [51] 397 TWh (EL)/y with data from [50], for thermal requirement: difference between SEC from [50] and electricity consumption; double-check: 360 MJ (EL)/t clinker, 3,500 MJ (TH)/t [198]

C.2.5 Steel (7)

- [70] From Ref. [199] (website not available any more) corroborated by [200].
- [71] From BREF [201] Table 8.1: electric arch furnace (EAF) 1,454-2,693 MJ (EL)/t, with hot rolling data from Worrell et al. [202] (Table 2), increased by fraction: (1.52+0.37)/(1.52)

- 72 [202] EAF 790 MJ (TH)/t, hot rolling 1,820 MJ (TH)/t (double-check: EAF BREF [201] 50-1,500 MJ (TH)/t).

C.2.6 Non-ferrous metals (8)

- 80 Ref. [203] from 2018
- 81 Ref. [204] page 9/10 secondary production from new scarp