Evangelia Gioti

Energy Saving Solutions on Cooling and Ventilation Systems at CERN under the aspect of heat recovery

Master's thesis in Sustainable Energy (MSSE) Supervisor: Armin Hafner Co-supervisor: Pierre Andre Calhau Barroca June 2023





Master's thesis

Norwegian University of Science and Technology Faculty of Engineering Department of Energy and Process Engineering

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Institute	Department of Energy and Process Engineering
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Personal Information	
Surname, First Name	Gioti, Evangelia
Date of Birth	
Email	evangelia.gioti@ntnu.no

Supervision and Co-authors	
Supervisor	Armin Hafner
Co-supervisors (if applicable)	Pierre Andre Calhau Barroca
Co-authors (if applicable)	

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Background and objective: CERN in Geneva is committed to improve its environmental footprint and collaborate to the development of sustainable technologies. The laboratory hosts currently about 653 buildings and more than 400 underground structures with largely different cooling and ventilation needs that account up to 100GWh of energy consumption per year. More efficient and environment friendly solutions shall be investigated considering the opportunity cost. Tasks: 1) Map CERN cooling and ventilation systems (technology and energy demand) 2) Review of relevant literature including system design, technology choices and logic of control 3) Simulation of systems in a CERN building by the dynamic software (Modelica/Dymola) 4) Develop methods (comparison of system alternatives) to aid on strategic decision for replacement/improvement of systems considering opportunity cost and sustainability metrics 5) Proposal for further work

Aknowledgements

The work in this Master's Thesis is the final work for a Master's degree in the program of Sustainable Energy, of the Energy and Process Department, at the Norwegian University of Science and Technology in Trondheim. It was carried out in the spring semester of 2023 and it is a continuation of the specialization project written during the autumn semester of 2022. Due to this fact, some of the theory parts existing in the thesis are similar to the ones of the project work. The thesis assignment comprises 30 ECTS credits.

At this point, I would like to thank my supervisor Professor Armin Hafner and my co-supervisor Pierre Andre Calhau Barroce for their support and feedback during these two semesters. I would also like to express my gratitude to my fellow student and friend Magnus Elias Fjereide Enge, with whom we worked together this year to complete our theses which were both parts of the same CERN project.

Abstract

The aim of this report is to map the already existing systems at the CERN campus and propose alternative, more energy efficient solutions. The investigation will be focused specifically on the examination of the existing cooling and ventilation systems in a typical office network. Through this research, upgrade options will be put forth, primarily in the context of changing their working fluid and identifying compatible solutions for waste heat recovery.

In order for this objective to be fulfilled, a literature review is deemed important to give in-depth research into the many components and the variable types of the present heating and cooling systems. In addition, a thorough analysis of five working fluids is provided, along with a comparison of their thermophysical characteristics, operational costs, and sustainability indicators.

The work follows with the description of the main study case of this project and the methodology used to address the task in an optimal way. The system is modelled using Modelica syntax and simulated using Dymola[®] software solvers based on data gathered from the currently installed network. The simulation features two distinct scenarios utilizing the currently used R134a refrigerant and its CO_2 replacement. Each case is looked into with both constant and dynamic loads.

The outcomes of the two models are contrasted and examined, and then recommendations are made for further system improvements.

Sammendrag

Målet med denne rapporten er å kartlegge de eksisterende systemene ved CERN campus og å foreslå alternative, mer energieffektive løsninger. Det vil spesifikt fokuseres på å undersøke eksisterende kjøleog ventilasjonssystemer i et typisk kontornettverk. Gjennom denne studien vil oppgraderingsalternativer foreslås, primært med tanke på å bytte av arbeidsmedium samt identifisering av kompatible løsninger for gjenvinning av spillvarme.

For å oppnå dette målet, anses en litteraturstudie som viktig for å gi en dyptgående innsikt i de mange komponentene i og de ulike typene av dagens varme- og kjølesystemer. I tillegg er en grundig analyse av fem arbeidsmedier presentert. Her sammenlignes termofysiske egenskaper, driftskostnader og bærekraftsindikatorer.

Videre følger en beskrivelse av dette prosjektets hovedstudie og metodikken som er brukt for å løse oppgaven på en optimal måte. Systemet er modellert ved hjelp av Modelica-syntaks og simulert ved hjelp av programvaren Dymola[®] basert på data samlet inn fra det installerte nettverket. Simuleringen inneholder to forskjellige scenarier. I det første scenarioet er arbeidsmediet som brukes i dag, R134a, er benyttet. Mens i det andre scenariet er dagens arbeidsmedium erstattet med CO_2 . Begge scenariene er undersøkt med både konstante og dynamiske laster.

Resultatene av de to modellene undersøkes og sammenlignes. Deretter gis det anbefalinger for ytterligere forbedringer av systemet.

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Table of Acronyms

Abbreviation	Definition
CERN	European Organization for Nuclear Research
HVAC	Heating, ventilation and Air-Conditioning
LHC	Large Hadron Collider
EDF	Électricité de France
CO_2 (R744)	Carbon Dioxide
F-gases	Fluorinated gases
HX	Heat Exchanger
VCC	Vapor Compression Cycle
COP	Coefficient of Performance
HP	Heat Pump
AHU	Air Handling Unit
DH	District Heating
RES	Renewable Energy Source
TES	Thermal Energy Storage
\mathbf{PCM}	Phase Changing Material
TCES	Thermochemical Energy Storage
TCM	Thermochemical Material
GHG	Greenhouse Gas
H_2O	Water
NH_3 (R717)	Ammonia
HC	Hydrocarbon
N_2O	Nitrous Oxide
ODP	Ozone Depletion Potential
GWP	Global Warming Potential
HCFC	Hydrochlorofluorocarbon
CFC	Chlorofluorocarbon
R22	Chlorodifluoromethane
R12	Freon
HFC	Hydrofluorocarbon
HFO	Hydrofluoroolefin
R1234yf	2,3,3,3-Tetrafluoropropene
R1234ze	1,3,3,3-Tetrafluoropropene
TFA	Trifluoroacetic Acid
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
OEL	Occupational Exposure Limit
NBP	Normal Boiling Point
RCL	Refrigerant Concentration Limit
R134a	1,1,1,2-Tetrafluoroethane
PAG	Polyalkylene Glycol
C_4H_{10} (R600a)	Isobutane
R600	Butane
LSHX	Liquid Suction Heat Exchanger
EPDM	Ethylene Propylene Diene Monomer
R1234ze(E)	trans-1,3,3,3-Tetrafluoroprop-1-ene

Abbreviation	Definition
PI	Proportional Integral
SIM	System Information Manager
NEN	Royal Netherlands Standardization Institute

Table of Symbols

Symbol	Definition	Unit
Q	Heat Flow	kW
m	Mass	$_{\rm kg}$
ср	Specific Heat Capacity	$\rm J/(kg^{\circ}C)$
ΔT	Temperature Difference	$^{\circ}\mathrm{C}$
ρ	Density	$ m kg/m^3$
V	Volume	m^3
Tc	Critical Temperature	$^{\circ}\mathrm{C}$
\mathbf{Pc}	Critical Pressure	bar
ho c	Critical Density	$ m kg/m^3$
Ż	Heat Rejection	kW
$\dot{\mathbf{W}}_{\mathrm{C}}$	Compressor Work	kW
$\dot{\mathbf{m}}$	Mass Flow Rate	$\rm kg/s$
h	Specific Enthalpy	J/kg
η	Isentropic Efficiency	-
Δh	Specific Enthalpy Difference	J/kg

1 Introduction

The European organization for nuclear research (CERN) was established in 1954 and today it is supported by 23 nation states that are in charge of all major choices. It is an international organization whose major objective is to create and disseminate information and knowledge resulting from the creation of particle accelerators and detectors used to research the basic physical characteristics of matter. The energy consumption of the systems used in these experiments is significant, but this has never been a major issue in the field of particle physics. As a result of how the community is now approaching sustainability, CERN has established a goal to reduce its rise in energy and water usage to 5% by the end of 2024. To achieve this, some actions must be taken considering the replacement of outdated technology, the addition of more environmentally friendly solutions, and the recycling of waste heat from the current system's installations.[1]

This report, as a continuation of the specialization project [2], will analyze the already installed cooling systems at CERN and recommend better utilization strategies or more effective substitutes. The major study case for this project will be a network with cooling distribution in two typical office rooms. In order to build a more energy efficient complex, that is tailored to CERN's requirements, suggestions for the systems' design, refrigerants, and heat recovery potentials will be examined and compared.

1.1 Background

In this section, a brief update about CERN will take place. Specifically, some information concerning its location and occupied area will be given, along with a detailed reference about the amount of energy and water consumed by its experiments. Further, there will be a part dedicated to the environmental impact of the organization and its future plans to achieve sustainability.

1.1.1 CERN Campus

CERN is built upon 625 hectares of ground along the Swiss-French border, with 79 hectares of fenced property expanding to the Meyrin site and 85 hectares to the Prévessin site [1]. The extent of the campus with the various sites and its relationship to the city of Geneva and the lake is depicted in the following Figure 1.1.

The organization owns 653 buildings, the majority of which date from the 1970s. According to its intended purpose, the land is separated into three categories: academic, scientific, and technical, as shown in Figure 1.2. Almost 17,500 people are employed in these fields. However, the poor thermal insulation and outdated heating, ventilation and air conditioning (HVAC) systems, which lower the energy efficiency of the buildings and raise their energy consumption, due to their old technologies, have a negative impact on the working conditions. Over the years, several reform initiatives have been implemented, although typically, these steps take time due to a lack of funds.[4]



Figure 1.1: Topographic map of CERN's land.[3]



Figure 1.2: Illustrations picturing the land uses in both Meyrin and Prévessin sites.[3]

1.1.2 Energy Consumption

The organization uses 82% of its total energy in the particle accelerators. The remaining portion is split into three parts: 3% for the data center, 3% for the campus infrastructure, and 12% for the experiments.[4] Specifically, 95% of the energy comes from electricity and the remaining 5% originates from fossil fuels [1]. Namely, CERN uses diesel for backup generators, gas for vehicles, and natural gas for heating. When the accelerators are running, 1.3 TWh (4680 TJ) of power is consumed annually.[3] Yet, when the large hadron collider (LHC) is turned off, 64% less electricity is used [5]. This is more clearly demonstrated in Figure 1.3, where the diagram shows that electricity is always present in the maximum amount, followed by steady-state natural gas. When the LHC was shut down between the years 2013-2015 and 2018-2020, there was a huge drop in electricity.



Figure 1.3: CERN's energy consumption during the years 2011-2020.[5]

Concerning the power, CERN is linked to both the French and Swiss grids. Still, it is often supplied by the French electricity company EDF via two 400 kV lines because the grid mix from the Prévessin site is less expensive and contains 87% low carbon.[6][5] The Swiss grid is utilized as a backup in circumstances of electrical repair when the accelerator is not running [6]. The following Figure 1.4 shows how much electricity is used by the various accelerators, the computer center and the buildings in the two campus sites.



Figure 1.4: Electricity usage at CERN.[6]

1.1.3 Water Consumption

The amount of water used at CERN each year is close to 5 million m^3 [3]. It is important to note that the organization obtains 99% of its water needs from Lake

Geneva and the remaining 1% from the water-stressed Pays de Gex region [5]. The LHC accelerator and industrial buildings receive 80% of this amount for cooling, and the other 20% is used for hygienic purposes. This water is then discharged once more into the lake's waterways, and in many cases, into Nant d'Avril.[1]

Figure 1.5, which depicts water consumption over time, clearly demonstrates a decline in water use. Starting with the year 2000, there is a considerable reduction as CERN took action to change the cooling towers' open circuits into closed ones. Following this, the systems began to operate more effectively, leading to a steady decrease. Once more, water use dropped by 47% during the years the LHC was shut down.[5]



Figure 1.5: CERN's water consumption during the years 2000-2020.[5]

1.1.4 Heating Systems

The Meyrin and Prévessin sites each possess a local district heating system with three gas-fired boilers that serve to heat the CERN campus. Each of the 1995-era boilers at the Meyrin facility has a 15 MW capacity. About the Prévessin site, each boiler has a 4.7 MW capacity and was constructed in 1976. The boilers at both locations deliver hot water that is between $110 \,^{\circ}$ C to $140 \,^{\circ}$ C with a return temperature between $90 \,^{\circ}$ C to $105 \,^{\circ}$ C. The heating for the associated buildings in Meyrin's site is distributed by a 25 m pipe. Additionally, water radiators are used to distribute heat throughout the majority of the structures' internal spaces. Only a small number of structures were built early on, with modernized systems that could monitor the temperature. The entire heating system, however, is fairly old and requires regular maintenance in order to prevent any breakdowns that could result in unpleasant leakages.[6]

1.1.5 Cooling Systems

A plethora of cryogenic plants and water cooling towers exist at CERN for cooling all the machinery related to particle accelerators. To function effectively, these superconductive magnets have extremely high cooling requirements. Only for the LHC, 21 cooling plants are located throughout the ring, although only five evaporative cooling towers -two of which are used as a backup- are currently in use.[7] These towers take the return water from the three main cooling circuits, reject the heat through water evaporation, and then restore the cooled water to the circuits [8].

1.1.6 CO₂ Emissions

Based on CERN's Environmental report [5] for the years 2019-2020, the CO_2 emissions released from the organization are separated into two main categories:

- Scope 1: represents direct emissions related to the facilities and the vehicles existing on the campus. These emissions are mostly related to fluorinated gases (F-gases) for particle detection and detector cooling in LHC experiments.[5]
- Scope 2: represents indirect emissions related to the energy utilized for the generation of electricity, steam, heating or cooling.[5]



Figure 1.6: CERN's CO₂ emissions during the years 2017-2020.[5]

From Figure 1.6, it can be observed that in the years 2017-2018 the emissions, both direct and indirect, are much higher than in the years 2019-2020. This is caused due to the operation of the particle accelerator's complex. On the contrary, the direct CO_2 emissions during 2019-2020 reached the numbers of only 78,169 and 98,997 tonnes of CO_2 and the indirect reached 10,672 and 9247 tonnes of CO_2 respectively. Even though the accelerators were not in use, they produced emissions from the detector cooling which was in operation in order to maintain the units. As for Scope 2, until the year 2019, the electricity consumption of CERN's data center facility in Hungary was included in the emissions. From 2020 this centre was no longer in use.[5]

1.1.7 Future Initiatives for Sustainability

The Masterplan 2040 [1] for CERN states that future initiatives must pay close attention to their carbon footprint. Hence, some of the plans aim to improve the working conditions by decentralizing the primary building operations and creating ergonomically built outdoor spaces. The fundamental objective is to make infrastructure systems more energy efficient and, if possible, to achieve some degree of energy independence. To accomplish this, more updated systems must be integrated into the current network. This depicts the Science Gateway project, shown in Figure 1.7, a new structure at CERN with modernized systems that will be fulfilled by the end of 2023.[1]

The heating and cooling systems for both the particle accelerators and the simple working spaces must decrease the energy consumption and overall CO_2 emissions. As a try to do so, CERN developed a plan for gas recuperation, optimization of the current technologies and the replacement of gases with more environmentally friendly ones. This is estimated that will reduce direct emissions by 28% by the end of 2024. Some detectors with F-gas recirculation systems have already been installed in the LHC in order to decrease these gases.[5] Concerning water consumption, the plan is to reduce it by collecting rainwater and circulating it into the buildings.[1]



Figure 1.7: Illustration of Science Gateway project, designed by the architect Renzo Piano.[1]

1.2 Scope of the Project and Introduction to the Next Chapters

This report is an element of an ongoing CERN effort to lower campus energy consumption and CO_2 emissions in the future. A literature review of alternative heating and cooling systems, along with the examination and comparison of various refrigerants will be covered in the following chapters. The reader will gain a better grasp of how each system works along with the optimum fluid for a particular scenario. Further, this work will focus on the description of an existing HVAC network along with its characteristics. From this analysis, a new proposal will arise for the most efficient way to improve this complex and utilize the waste energy being released into the atmosphere. To support the proposal, a simulation of the system with the comparison of two different fluids will take place by the Dymola^(R) software. The main objective of the report will be achieved after a detailed discussion of the findings and a concluding statement. A chapter containing ideas for additional work will also be included.

2 Heating and Cooling Systems

Following the signing of the Paris Agreement [9] in 2019, Europe established the goal of limiting the temperature increase by 1.5-2°C. This suggests that until 2030, Europe will use 32.5% less energy. Since higher energy consumption is associated with European buildings, the rehabilitation of the existing systems and the installation of more energy efficient ones at the new constructions are characterized as required actions. According to studies [10], fossil fuels account for more than 80% of heating and cooling in Europe. As a result, the CO₂ concentration remains high and is still far from the 2050 target of a globe with net-zero CO₂ emissions.[10]

Nowadays, the main priority of European countries is to reduce energy use and decarbonize the environment. To achieve the best output with the least amount of energy waste and operational expenses, engineering experts aim to combine systems. District heating systems combined with heat pumps, thermal energy storage, chillers, and water cooling towers are of particular interest.

2.1 Heating and Cooling Systems fundamentals

The fundamental similarities between the heating and cooling systems are covered in this section. They may operate differently, but they still have some common ground when it comes to the underlying idea. They both rely on whether the heat is added to the conditioned system (a heat source system) or removed from it (a heat sink system), respectively. The thermal energy transmission medium is used in both systems to convey heat. Latent and sensible heat transfer are two additional key concepts in heating and cooling systems, and they are briefly explained here.

2.1.1 Thermal Energy Transport Medium

Several elements can be used as thermal energy transfer mediums in HVAC systems. They typically take the form of a gas, liquid, or solid, and they exchange sensible or latent heat to move thermal energy from or to the system. Latent heat is associated with changes in the medium's phase, whereas sensible heat is associated with changes in temperature. The term "working fluid" or "refrigerant" refers to the described medium. The thermo-physical characteristics of the medium as well as its flow dynamics affect heat transfer [11]. The limits of the system in terms of needed temperatures and capacity, as well as design pressure and safety considerations, determine the optimal working fluid for a given application.

2.1.2 Heat Source

The process heat source is the point in the heating/cooling process where energy is extracted from and transferred to the system's thermal energy transport medium (refrigerant). In other words, this is the point where the system makes thermal contact with the refrigerant, which is operating at a lower temperature. Relatively, if the naming convention is used from the standpoint of the system, this may be thought of as the site of the heat sink.[12]

The prerequisite for transferring heat between two bodies is a temperature difference, which can be accomplished in one of three ways: thermal conduction, thermal convection, or radiation. The most popular method is thermal conduction, which involves utilizing a plate heat exchanger to transfer heat from a conditioned system between the refrigerant and water or air.[12]

2.1.3 Heat Sink

On the other hand, the refrigerant rejects the heat it absorbed at the heat source in the process heat sink. In other words, a heat sink is a point where the system makes thermal contact with the warmer refrigerant.[13]

The same as with the heat source, a temperature difference between the refrigerant and the heat sink is a requirement for heat transfer. At the condenser's input, the heat sink must be colder than the refrigerant.[13]

The heat sink can be categorized into three types: the active, the passive and the hybrid heat sink: [13]

- Active heat sink: in this type, a fan blows cool air over the heat sink's hot surface, allowing the heat to escape into the atmosphere. Although it performs well, it is not appropriate for prolonged operation.[13]
- **Passive heat sink:** here, heat transfer occurs naturally through convection without the aid of any air-supply components. Although its performance is less effective than the active type, it is considered to be more reliable.[13]
- Hybrid heat sink: while not being widely used, this approach incorporates both active and passive properties. It involves control systems, and based on the temperatures in the system, it activates each property.[13]

2.2 HVAC Components

The HVAC systems are in charge of purifying, heating, and cooling the indoor air as well as renewing it. They could consist of a single system or a collection of numerous distinct subsystems. Even if they operate differently or are utilized for other purposes depending on the situation, they all share the same fundamental parts. These components -pumps, compressors, heat exchangers, valves, and fanswill be examined in more detail in the following sections.

2.2.1 Compressors

The mechanical device known as a compressor lowers a gas's volume while increasing its pressure. The saturation temperature increases above the surrounding temperature along with the pressure. An electrical motor is required to supply the necessary work in order to accomplish this. Positive displacement and dynamic functioning compressors are the two primary categories of compressors. Rotary and reciprocating compressors are under the positive displacement category, while centrifugal and axial compressors fall under the dynamic working category.[14]

These devices can also be categorized according to their casing. Compressors can be classified as hermetic, semi-hermetic or open. The compressor and electric motor are enclosed in a closed casing in hermetic and semi-hermetic systems. The semi-hermetic can be opened for specific maintenance tasks in the case that a unit fails, in contrast to the hermetic, which is always closed. The open compressor, on the other hand, lacks a casing, which makes it simpler to maintain and repair when necessary. The piston, screw, and turbo compressors are the most often utilized types of compressors, as indicated in Figure 2.1. Each of them has a separate displacement range of operation.[14]

- **Piston compressor:** it is one of the oldest types of reciprocating compressors. A piston inside a cylinder, which moves upward when compressing gas and downward when recharging the volume to repeat the process, makes up the device. The range of its capability is 100 kW to more than 500 kW. The use of this technology in small systems is fairly common.[14]
- Screw compressor: this kind of compressor belongs to the rotary group. Two intermeshing rotors, one male and one female, operating in parallel, compress the gas by transferring the air from the intake to the outlet inside the casing. The pressure of the gas at the exit is already known because the screw compressor's design yields a set pressure ratio. Large systems with high pressures use this type of compressor.[15]
- **Turbo compressor:** using rotating impellers, this centrifugal compressor compresses the refrigerant. The high pressure refrigerant is forced at the inlet vanes when the impellers begin to rotate, and it is then directed to the diffuser. There, the gas expands and its volume reduces, turning it into a gas with a low speed and high pressure. High suction pressure systems can provide this requirement. Its capacity typically depends on the axis's diameter.[15]



Figure 2.1: Piston, screw and turbo compressors.[14]

2.2.2 Heat Exchangers (HX)

Heat exchangers are passive mechanical devices that are used in order to transfer heat between two fluids that are physically separated by a thin, highly thermally conductive layer and are operating at different temperatures [16]. Condensation and evaporation are the basic processes for heat exchangers, utilized in HVAC systems. A phase shift from high pressure, high temperature vapour to high pressure, high temperature liquid occurs for the refrigerant in the condenser. The condensation process releases heat into the surrounding area. The evaporator operates in the reverse. A low pressure, low temperature vapour is created when a low pressure, low temperature liquid or gas absorbs heat and begins to evaporate.[14]

The construction of the heat exchangers defines the various categories to which each type belongs. The plate, shell and tube, and finned tube heat exchangers are the most widely used types, as shown in Figure 2.2.

- Plate heat exchanger: it is made of multiple parallel metal plates that are spaced apart just enough for the fluid to pass through. The plates are made of materials (usually metals) with high thermal conductivity and a reduced thickness to maximize thermal conductance. The number of plates varies depending on how much surface area is required to exchange the necessary heat. It is thought to be the most effective kind of heat exchanger because of its extremely compact design, suitability for small temperature and pressure changes, and high efficiency.[16]
- Shell and tube heat exchanger: it is made up of many tubes enclosed inside a cylindrical shell. One fluid circulates inside the tubes of the heat exchanger and the other passes through the shell, achieving heat exchange. Low maintenance costs and versatile design characteristics define this type of heat exchanger. It performs well in systems that operate at high temperatures and pressures.[16]
- Finned tube heat exchanger: the parallel fins in this form of the heat exchanger are penetrated by the tubes. One of the fluids moves through the tubes, while the other moves between the fins outside the tubes. Metallic fins help the fluids transfer heat more efficiently. Systems with high temperatures and pressures use it.[16]



Figure 2.2: Plate, shell and tube and finned tube heat exchangers.[14]

2.2.3 Valves

Devices called valves are used to control flow or pressure. These elements are in charge of ensuring that the entire system operates safely and effectively. They are divided into three groups: ball, check, and control valves. There are multiple valves that fall under each category, though they can be distinct into expansion valves, safety relief valves, pressure control valves, differential pressure valves, bypass valves, and float valves based on the application for which they are used.[17]

- Expansion valve: this valve is used to lower the pressure and temperature of the high pressure fluid as it exits the condenser and enters the evaporator. The valve permits the fluid to expand or change phases by lowering pressure.[17]
- Safety relief valve: depending on the system pressure, this valve switches between open and closed. In order to avoid any accidents, it opens when there is an excess of pressure and closes once the pressure has returned to normal levels.[17]
- **Pressure control valve:** this particular type of motorized valve is installed at the condenser's output and regulates the component's pressure to adjust it to the outlet temperature [17].
- Differential pressure valve: while preventing liquid droplets from entering the compressor, it maintains a consistent pressure difference between the condenser and the pressure receiver [17].
- Flash gas bypass valve: the valve is positioned between the evaporator's outlet and the pressure receiver. Its goal is to keep the pressure between these two parts constant.[17]
- Float valve: typically, tanks and flooded evaporators contain this valve. It is implemented for managing and balancing the component's liquid content.[17]

2.2.4 Fans

A fan is a rotor-driven air-displacement device. It consists of a motor that supplies an impeller with kinetic energy so that it can start rotating. The flow is directed by blades that are attached to the impeller. Thanks to electrical motors, electrical energy is transformed into mechanical energy, which is subsequently transformed into pressure difference, creating an air stream. Its work on the gas per unit mass must be less than 25 kJ/kg in order for it to be categorized as a fan and not as a turbo compressor. Metal, aluminium, or plastic are frequently used in their construction. As shown in Figure 2.3, they can be divided into four main groups based on the direction of the flow: propeller, centrifugal, mixed, and tangential fans.[18]

- **Propeller or Axial fan:** this fan has propeller-shaped blades enclosed in a container or a cylinder [19]. Air is driven into the inlet as it flows parallel to the axis before being pushed by the axis to the output. High flow rate to pressure ratios are best served by this type of fan.[18]
- Centrifugal or Radial fan: the most typical fan for commercial ventilation is this one. Air enters axially and begins to radially move the blades. The air is then released at a 90° angle. This fan has a waterwheel-like appearance. Low flow rate to pressure ratios is suitable for it.[18][19]
- Mixed or Compound fan: here, air is introduced axially, but it is expelled at an angle of between 30° and 80°. They are excellent for industrial applications with huge amounts of air at low or moderate pressures, just like centrifugal fans.[18]
- **Tangential or Cross fan:** the blades of this type of fan are parallel to the shaft. The air enters and flows across the impeller's whole length. There, the spinning creates a vortex and the flow is being discharged at the impeller's output. This fan is advised for extremely high flow rates against low resistance.[18]



Figure 2.3: Illustration of multiple types of fans.[18]

2.3 Vapor Compression Cycle

The vapor compression cycle (VCC) is used by both heat pumps and chillers. The primary distinction between a heat pump and a chiller is that the former is made to transfer heat to the heat sink, whereas the latter is made to draw heat from the heat source. In other words, the chiller is made to cool an area, and the heat pump is made to heat it.

Two heat exchangers (an evaporator and a condenser), an electrically powered compressor, and a throttle valve consist the four major components of VCC systems. A working fluid is flowing via the pipes connecting the parts, which are assembled into a closed system. Through the heat exchangers, a secondary (or more) working fluid -typically water, air, or a water/glycol mixture- connects the heat source and heat sink to the system.[20] The VCC is typically identified by the numbers in Figure 2.4, and the cycle runs as follows:

- 1-2: the temperature rises as a result of the high pressure at which the gaseous working fluid is compressed.
- 2-3: the working fluid is condensed and heat is rejected to the heat sink as the superheated gas passes through the condenser. Since this process is isobaric, pressure remains constant.
- **3-4:** the expansion value is where the high pressure, low temperature working fluid goes through an isentropic expansion and emerges as a low temperature, high pressure gas/liquid mixture. Enthalpy stays constant.
- 4-1: the gas/liquid mixture is then transferred to an evaporator, where heat from the heat source is used to evaporate any leftover liquid. The pressure remains the same because this process is isobaric.



Figure 2.4: Schematic diagram of a simple VCC.

The compressor work in a VCC, as previously mentioned, uses the only electricity needed for the cycle. The coefficient of performance (COP), which describes the relationship between electricity used and heat delivered for a heat pump or heat extracted for a chiller, is typically used to describe the efficiency of such systems.[20]

2.3.1 Waste Heat Recovery

The potential for recovering waste heat from industrial processes across a variety of temperatures in Europe is estimated to be 304.13 TWh/year [21]. Based on this potential, it was calculated that industrial heat pumps might use 7% of the waste heat, producing 28.37 TWh of thermal energy per year, which corresponds to 1.5% of Europe's annual heat consumption [22].

Waste heat is the heat that is generated during a process but is not used for any particular function. It can, however, be recovered from heat pumps and added to a different cycle process where it is required. Waste heat that can no longer be used is released into the atmosphere. Heat recovery heat pumps, which include direct and indirect heat recovery systems, function in high temperatures. When the temperature is high enough, it is possible to use the waste heat directly without taking any additional steps. When indirect heat recovery is employed, the temperature can not be elevated to the required levels; therefore, a heat exchanger must be used to boost the temperature to the desired levels. This amount of recovered heat can be used to improve the system's efficiency by reducing energy consumption, or it can be used as a heat source in a different circuit.[23]



Figure 2.5: Schematic diagram of a simple VCC with an indirect circuit for waste heat recovery.

2.4 Heating Systems

A heating system is a complex of various subsystems that are piped into one another. Its function is to transfer heat from an external source into the system. Boilers will be discussed as the primary heating systems in this section.

2.4.1 Boilers

Boilers are vessels filled with water, used for heating purposes. The heating process is known as combustion, and the inner surface of the vessel is known as the furnace. They use gas, oil, coal, or electricity as a heating source. They either heat the water and turn it into steam or keep it warm as a liquid, depending on the distribution system. Boilers are classified as smoke tube boilers or water tube boilers depending on whether they distribute hot water or gas into the pipes. The amount of steam produced determines the size of the boilers. Moreover, a relationship between pressure and steam temperature is noticeable. Thus, the boilers are divided into three categories: low, medium, and high pressure. Oversized boilers have higher capital expenses and are less effective.[24]

In order to continue functioning effectively, they must maintain a steady level of water inside. A feed pump helps to do this by continuously supplying liquid to the boiler. It can either be turned on or off depending on the water level. It should be noted that the water charge varies depending on the pressure boiler. To be more precise, the high pressure boiler holds less water. Further, several safety and charge valves are installed on the system to ensure their safe and effective operation can control the pressure.[24] Figure 2.6 shows the operation process of a boiler.



Figure 2.6: Illustration of a boiler process.

2.5 Cooling Systems

The concept of cooling systems is covered in this section. Similar to heating systems, cooling systems are composed of a variety of different subsystems, but their primary function is to deliver thermal energy in the form of cooling. The investigation is mostly focused on chillers and cooling towers.

2.5.1 Chillers

Chillers are cooling devices that remove heat from an enclosed space and then release it to the environment. This process is carried out by three circuits that every chiller contains: the refrigeration circuit, the chilled water circuit and the condenser circuit.[25] Nonetheless, chillers are split into two categories: compression chillers and absorption chillers. Its main difference is that in the compression chillers, a single device is used to compress the refrigerant, whereas in the absorption chillers the compressor is replaced by an absorption set, a heat exchanger, a pump and a generator. This is because compression chillers utilize electricity to compress the gas, while absorption chillers use heat as their primary energy.[26]

2.5.1.1 Compression Chillers

Compression chillers produce cooling using the VCC, as already mentioned in Section 2.3. Here, the water never comes into contact with the refrigerant while the three circuits are operating. The compressor, evaporator, condenser, and expansion valve are the four basic refrigeration components found in these chillers. However, the cooling medium varies, and on the basis of that, they are divided into air-cooled and water-cooled chillers.[25]

• Water cooled chillers: in this type of chiller the fluid circulates into the refrigeration circuit and exchanges heat with the water. The cooled water, coming from the evaporator, will be pumped into the air handling unit (AHU) to collect all the unwanted heat from the building. While the warm water, coming from the condenser, will be sent to a cooling tower where the heat will be rejected to the ambient air.[25][27]

Due to their size and weight, water chillers are typically installed in the basement. To reduce the noise and vibration from the compressor units and the pumps, the space needs to be well ventilated and insulated. With this particular type of chiller, the condenser and evaporator are both shell and tube heat exchangers with water in the tubes and refrigerant in the shell.[25] Over 200 tons of peak cooling load, water cooled chillers are typically found in medium and large installations. Also, they cost more to be built and maintained than chillers that use air cooling.[27] The following Figure 2.7 provides an illustration of a water-cooled chiller.

• Air cooled chillers: the sole variation between the circuit routes of the air-cooled and watercooled chillers is on the condenser side. The condenser in this instance is a refrigerant to air coil with fans instead of being the same as the evaporator, shell and tube heat exchanger. The fans aid in circulating the air over the coil, causing the fluid to condense and deliver heat to the surroundings. It is important to note that the dry bulb temperature and airflow rate both affect condenser efficiency. As a result, the outside temperature should not exceed 35°C. The air is used by these chillers, as already mentioned, to cool the water as it passes through the structure and absorbs the heat from the AHU.[25] In order to have direct access to outdoor air, air-cooled chillers are installed on the roofs of buildings. They are smaller than water-cooled ones, less expensive and typically installed in smaller plants with capacities under 200 tons. But, because of the fans, they generate a lot of noise and vibration on the roof, which requires careful management. Because of their utilization of external air and lack of water treatment or cooling towers, which could result in significant water waste, they are an affordable solution in terms of operating expenses. However, due to the fact that air has a weak ability to conduct heat, the condenser unit must be larger and operate at greater condensing temperatures, which lowers the compressor's efficiency. Compared to chillers that are water cooled, this results in a higher power input and more CO_2 emissions.[27] The following Figure 2.8 shows an illustration of an air-cooled chiller.



Figure 2.7: Schematic diagram of a water cooled chiller.



Figure 2.8: Schematic diagram of an air cooled chiller.

2.5.1.2 Absorption Chillers

A mixture of water and an absorber, typically lithium bromide, is used in absorption chillers. It is a non-toxic salt drawn to water by nature. In order to separate them again after they have been combined, heat must be applied. The chiller circuit is therefore based on that procedure. From the absorber to the generator tank, the water and refrigerant combination is pumped while passing via a heat exchanger on the low side of the cycle. The mixture fills the generator, forming a reservoir, and heat is applied to start the separation process. Waste heat from hot water or steam flowing through pipes can be used for this purpose. As soon as the separation process begins, hot water turns into vapor and fills the condenser, while lithium bromide returns to its original state and the heavy particles descend to the bottom of the generator, creating a concentrated liquid. This hot liquid moves downward through the heat exchanger before ending up in the absorber, where it will be mixed with water once more to re-start the process.[25]

The refrigerant cycle is the same as the water cooled chillers' with the only difference being that the heat transfer at the evaporator side causes the water to vaporize into the evaporator and be spayed to the absorber to get mixed with the lithium bromide. Heat is produced as these two fluids interact, and this heat must be evacuated once more through the cooling tower. As a result, each process will start over from scratch. [25] Figure 2.9 illustrates a cycle of a simple absorption chiller.

Moreover, absorption chillers must be installed in a specific location since they are bigger and heavier than compression chillers. This is because they include several components and they all have intricate functions. Thus, their expenditures for operation and maintenance are considerably higher. Still, they do not cause a lot of noise or vibration, making them an ideal option for residential buildings. The fact that these chillers use thermal energy and fossil fuels means that they consume less electricity overall, but the absorber units force them to use more water. The usage of fossil fuels increases the CO_2 emissions, as would be predicted.[26]



Figure 2.9: Schematic diagram of an absorption chiller.

2.5.2 Water Cooling Towers

In heat-intensive processes where there is insufficient natural cooling, such as lakes or rivers, evaporative cooling towers are commonly used. Inland nuclear and fossil fuel power facilities are typical applications for large cooling towers, while other process industries and HVAC systems are ideal for smaller cooling towers.[28]

An evaporative cooling tower is a device used to reject heat to the outside air in HVAC systems that utilize water cooling. This type of cooling tower functions as an evaporating heat exchanger, as seen in Figure 2.10. When hot water from a chiller comes into contact with cool, dry air, the dry air absorbs the heat and rejects it to the atmosphere. Through the evaporator, the residual water is cooled to the desired outlet temperature. The heat rejection results in a loss of 1-2% of the water flow.[28] Dry cooling systems, in which heat is transferred without direct contact between a process liquid and ambient air, are also referred to as cooling towers. Due to the latent heat transfer of the phase change described in Section 2.8.2, evaporative cooling is an efficient way to reject heat.[29]



Figure 2.10: Evaporative cooling tower schematic.

Figure 2.10 shows the essential components of an evaporative cooling tower. There is a basin at the bottom where cold water is gathered and released. The dry air inlet is located over the collection container. To increase the amount of time that the hot water and dry air are in touch with each other, a fill material is used. The hot water input is positioned above the fill material, and it is dispersed using spray nozzles to produce tiny droplets that speed up the convection and evaporation processes. An electrically powered fan at the top pushes the hot, humid air outside. Because of the fan's increased air flow, the cooling capacity is boosted.[28]

2.6 Space Heating and Air Conditioning

The thermal energy distribution systems in closed spaces are called space heating and cooling systems. Depending on how they are used, they can produce either warm or cold air. Radiators and air handling units with various types of ventilation are the systems analyzed in this section.

2.6.1 Air Handling Unit (AHU)

Regardless of the type or size, ventilation is vital for today's structures. In order to preserve the best thermal comfort for those within and to stop the spread of contaminants, that could have negative health effects, the air must be renewed. This process is achieved by the air handling unit system. It takes the ambient air and cleans it, through a filter, before it is forwarded to a heating or cooling coil. There, the air gets the desired temperature and afterwards, it is pushed by a fan to a duct network which is responsible for the distribution of the supply air to the designated building areas.[30]

A return duct line pulls the polluted air out of the rooms and by a fan it is forced out to the atmosphere. Some of the air can be directed to the supply line where it will be filtered and forwarded again into the building. This heat recirculation is happening through heat recovery systems which manage to save energy and reduce operating costs. It is worth mentioning that the amount of air in the system is always controlled by the angle of the dampers in the air streams, which varies depending on the people's needs.[30]

There are many types of air handling units, depending on the components they include, but the most simple form, the one that was described above, can be shown in the following Figure 2.11.



Figure 2.11: Schematic layout of a simple air handling unit.

2.6.2 Ventilation Types

Natural ventilation and mechanical ventilation are the most prevalent methods of ventilation. The natural one uses no mechanical systems but instead circulates air through openings by taking advantage of the temperature difference between the inside and outside of the building. Opposite to that, mechanical ventilation regulates the volume and distribution of air in an area using systems with fans and ducts. The usage of mechanical ventilation is required in the majority of non-residential structures. As illustrated in Figure 2.12, this sort of ventilation uses two different types of air distribution: mixing and displacement.[19]

- Mixing ventilation: a diffuser on the ceiling provides the air, which is then distributed evenly throughout the space. The air is getting mixed with the inside air and acquires the same temperature. Pollutants are also getting mixed when the air is mingled. The ventilation regulates the density of indoor pollutants by bringing in enough outdoor air to dilute emissions from inside sources.[19]
- **Displacement ventilation:** here the diffusers are placed close to the floor providing colder temperatures than the air in the surrounding space. When the air is forced higher, thermal plumes will form close to the heat sources. Ducts installed on the ceiling will extract it once it reaches the upper level. By concentrating contaminants in the higher zone and keeping them out of the occupant zone, this sort of ventilation offers the benefit of providing adequate indoor air quality.[19]



Figure 2.12: Layout of mixing and displacement ventilation processes.

2.6.3 Radiators

For indoor settings, radiators serve as heating distribution systems. They can either be standalone or attached to the main system. They are supplied with hot water produced in a heat pump or a boiler and delivered through pipes if they are part of a bigger central system. Based on the elimination of heat loss and the preservation of the proper thermal comfort in the space, the size of a radiator can be determined. To balance the heat losses from the insulation gaps, these systems, known as water radiators, are installed close to openings. Besides that, a wheel head valve or thermostatic radiator valve, which shuts off the hot water flow when the temperature in the room disturbs the occupants' thermal comfort level, can also be used to manually adjust the incoming heat.[31]

On the other hand, radiators that function as independent systems merely need to be plugged into the power grid. They may be dry systems or have a little circulating oil. When the current central heating system is insufficient, electric radiators might serve as an additional heating solution. Nonetheless,
because of their dry nature, they could make the residents feel uncomfortable in terms of temperature by lowering the relative humidity of the enclosed space.[31]

Besides that, radiators are typically made of steel, but they can occasionally be made of copper or aluminium. Although there are many various types of radiators available, panel radiators are the most popular. The following categories apply to the various types: [32]

- segment (column) radiators
- panel radiators
- panel-convector radiators
- **c**onvector radiators
- canal radiators
- $\bullet\,$ smooth- and finned-tube radiators
- surface radiators

2.7 District Heating (DH)

In northern countries, district heating is widely used. It is a centralized system in charge of supplying thermal energy to heating systems in buildings, that are situated far from the heat source. The district heating system consists of a central heat producer that is linked to a series of pipelines that provides hot water to smaller substations. The heat is then transferred from these neighbourhood substations to a heat exchanger and distributed through water radiators inside the buildings.[33] In Europe, the water that is supplied frequently reaches 90°C and is returned at 60°C. Ultimately, the water is making its way back via the pipelines to the central heat producer, where the same cycle will restart.[34]

The majority of residential properties have separate heating and cooling systems, which is one of the main causes of excessive energy usage. These systems run on fossil fuels and the residents have complete control over them. However, district heating might take the place of these systems and link them to a single, massive system that would waste less energy and use a renewable energy source (RES) to minimize CO_2 emissions. This could be a solution for cities that are expected to grow until the year 2050. Furthermore, district heating systems that are currently in place can quickly update their machinery and switch from fossil fuel to renewable sources, enabling them to recycle used energy.[10]

Additionally, various heat sources that cannot be combined on a building level can be used in conjunction with the district heating network. Geothermal energy and solar panels are two suggested methods for meeting electrical needs and fostering some degree of energy independence.[34] Also, the system's ability to be placed close to the heat source results in high energy quality distribution across the network and keeps safety hazards outside of residential areas. Surprisingly, combining heat pumps with the system could lead to heat recovery and the utilization of otherwise wasted energy. Using the extra heat causes the supply temperatures to drop and requires less electricity. As a result, the system's effectiveness is increased and operating expenses are reduced.[10] Figure 2.13 shows an illustration of a district heating system with a heat source, customers, and supply/return water.



Heat Source

Figure 2.13: Schematic view of a district heating system.

2.8 Thermal Energy Storage (TES)

The majority of the world's energy need is for thermal energy [35]. By 2022, most of this demand had already been met by fossil fuels [36]. This is due to their ease of being transported and stored for any time required. They can therefore provide energy whenever and wherever it is needed. Even so, according to the Paris Agreement [9] this demand must soon be covered by carbon-neutral energy sources, including solar and wind power.

Moving forward, a stable energy supply is perceived as somehow being difficult to achieve for renewable energy sources like solar power. Summertime, when the demand for thermal energy is typically at its lowest, defines the period when solar power generation reaches its peak. Hence, by balancing production and consumption, thermal energy storage (TES) is seen as a key technology that assures a reliable energy supply in a system based on renewable energy. TES could increase the overall effectiveness of energy by storing excess heat produced in the summer to be used in the winter. It is important to mention that TES is also possible for more reliable heat sources, as in this case the cooling towers and data center at CERN.



Figure 2.14: TES different classes.

According to the method and material employed, TES is often divided into three categories, as shown in Figure 2.14. They are referred to as thermochemical heat storage, sensible heat storage, and latent heat storage. No matter the storage mechanism, there are three basic stages in the TES process: charging, storing, and discharging. Similar to a battery, the energy is charged when the level is increased, stored when it is kept in the storage, and discharged when it is given back to the user. Figure 2.15 clarifies these stages.[37]



Figure 2.15: TES three main stages.

2.8.1 Sensible TES

Sensible TES involves heating or cooling the temperature of a storage medium to store energy. Here, the initial heating or cooling of a medium is the charging process and the release of this energy is the discharging process. A constant storage temperature is maintained during these processes. The storage medium might theoretically be made of any kind of material but the most commonly used ones are water, dirt, rock beds and sand. The heat capacity and mass of the storage media influence the storage potential for sensible TES. The following Equation 2.1 represents the heat held within a substance.[37]

$$Q = mc_p \Delta T = \rho V mc_p \Delta T \tag{2.1}$$

Where Q is the energy stored, m is the mass of the storage material, V is the volume, ρ is the density, c_p is the specific heat capacity and ΔT is the temperature difference in the material.

Due to the following benefits, sensible TES is the most frequently preferred TES [38]:

- Cheap, predictable, simple technology
- Mature technology
- Quick charging and discharging
- Common storage materials, such as water, are easily available and have a long lifetime
- Possible with large volumes

Although sensible TES provides many benefits, it also has several drawbacks. The following list contains the biggest restrictions [38]:

- Low volumetric storage capacity
- Heat loss can be significant over time

2.8.2 Latent TES

Latent TES involves a phase change in a so-called phase change material (PCM). A PCM is heated or cooled to the melting or evaporation point in order to store energy. The PCM may begin in any phase, including gaseous, liquid or solid. A liquid will solidify when chilled to a temperature below its melting point, while a solid will melt when heated to a temperature above its melting point. The PCM will absorb or release thermal energy during these phase transitions, which correspond to the charging and discharging processes in latent TES. Until the phase change temperature is attained, the PCM will either absorb or release sensible thermal energy, as shown in Figure 2.16. In addition, the PCM will continue to absorb or release latent heat at a steady temperature after the phase change temperature is attained.[37] Figure 2.16 illustrates how, at constant temperatures, latent heat is either emitted or absorbed.



Figure 2.16: Diagram illustrating the phase changes in latent TES.

Some advantages of using latent TES are [38]:

- High volumetric storage capacity compared to sensible, due to the energy required for a phase change
- Easily transported

Some disadvantages of using latent TES are [38]:

- The lifetime of PCM's can be limited due to their corrosivity or phase change cycles
- Low thermal conductivity
- Heat loss can be significant over time

2.8.3 Thermochemical Energy Storage (TCES)

Heat is stored through reversible exothermic/endothermic chemical reactions in thermochemical energy storage (TCES). The Formula [39] below can be used to represent the thermochemical reaction.

$$C + heat \leftrightarrow A + B \tag{2.2}$$

A thermochemical material (TCM), C, as well as two reactants, A and B, are needed for the TCES process. When heat is delivered to C during the charging process in TCES, it chemically dissociates into two components, A and B, in an endothermic reaction. The storage procedure starts when A and B are separated. The components are kept apart and at room temperature, so there should be no heat loss. The degradation of the materials is the primary cause of the energy losses in TCES. When A and B are mixed in the reversed exothermic reaction, the discharging process takes place. Heat is released as C is reformed. Formula 2.3 can be used to describe the discharging process: [39]

$$A + B \leftrightarrow C + heat \tag{2.3}$$

Some advantages of using TCES are:

- Very high volumetric storage capacity compared to sensible and latent TES
- Little to no heat losses due to ambient storage temperatures
- Feasible for long-term storage
- Easily transported

Some disadvantages regarding TCES:

- Relatively high cost
- Possibly short lifetime due to degradation of the materials
- Technically complex
- Still in research and development process

2.8.4 Seasonal and Short-term TES

The amount of energy consumed fluctuates daily, throughout the year, and throughout the day. Thus, both short- and long-term TES can be useful:

- Short-term TES controls supply and demand by delivering stored energy when there is a strong demand. It is employed for load shifting and peak shaving. Peak shaving is the process of using stored energy to ensure a sufficient supply when demand is at its maximum. This allows heat production to be more consistent. Load-shifting refers to the ability to change energy production from a time of heavy load to a time of day when energy can be produced more inexpensively. Stratified hot water tanks are the most typical type of short-term TES. To keep hot water at the top of the tank and cold water at the bottom, they apply the stratification concept.[37]
- To compensate for seasonal variations in energy demand, seasonal or long-term storage is used. This way, energy can be stored during the summer, when heat is typically in surplus, and be used later during the winter. A geothermal heat pump is an example of a seasonal thermal storage system. In the summertime, the heat pump can take advantage of free cooling from the borehole and send heat in return. This thermal energy will then be used again when a heating need will arise.[37]

3 Refrigerants

The history of refrigerants over the years and their classification into generations are covered in this section. Along with that, five distinct working fluids are introduced and compared based on their thermo-physical characteristics and environmental impacts.

The choice of a refrigerant is thought to be crucial for a variety of factors, including public health and environmental concerns as well as the effectiveness of the refrigeration cycle. According to studies [40], 7.8% of greenhouse gas (GHG) emissions come from the refrigeration field. The estimated annual direct emissions from refrigerant leaks are between 10-15%, whereas the estimated annual indirect emissions from electricity produced from fossil fuels globally are between 25-30%.[40] Thus, it appears more crucial than ever to use environmentally friendly refrigerants.

3.1 History of Refrigerants

First off, there are two categories of refrigerants: natural and synthetic. Besides, they can be also grouped according to their chronological time of appearance. First generation refrigerants are those that are naturally occurring. They can be found in the environment and originally appeared in the 1800s without any human influence. These refrigerants are water (H₂O), ammonia (NH₃), carbon dioxide (CO₂), hydrocarbons (HC) and air, more specifically nitrous oxide (N₂O). What is important to be mentioned at this point, is that they almost present no ability to cause ozone depletion potential (ODP) or global warming potential (GWP). However, because of their toxicity and flammability levels, the other generations that include synthetic refrigerants quickly replaced them.[41][40]

Next in line are the second generation refrigerants, which were developed around the 1930s. They are recognized as halogenated refrigerants and are synthesized by combining hydrochlorofluorocarbons (HCFCs) and chlorofluorocarbons (CFCs). The two most well-known of these, which predominated throughout time and were frequently used in air-conditioning systems, were chlorodifluoromethane (R22) and freon (R12). After several years of use, it was discovered that CFCs were contributing to the ODP and that both CFCs and HCFCs were to blame for the GWP. Due to this, the Montreal Protocol [42], an international agreement to safeguard the ozone layer, prohibited the use of second generation refrigerants in 1987. In other words, this agreement called for the suspension of CHC use by 2010 and HCFC use by 2040.[41][40]

Moving to the third generation, ozone-friendly refrigerants were developed. The second generation was replaced by hydrofluorocarbons (HFCs), which were in use up until 2010. However, another issue arose when it was discovered that these refrigerants were raising the GWP. Once again, an international agreement, known as the Kyoto Protocol [43], was signed in 1997 in an effort to lessen the effects. Its main objective was to lower the atmospheric concentration of greenhouse gases, hence reducing the phenomenon of global warming.[41][40]

After 2010, the fourth generation of refrigerants was finally introduced. These are known as hydrofluoroolefins (HFOs), and they are acceptable for direct emissions under the ODP and GWP regulations. R1234yf and R1234ze are two of the most popular ones because they are thought to be excellent choices for low temperature refrigeration systems.[41] Although the fourth generation of synthetic refrigerants exhibits better direct emissions quality than the previous generations, it has been noted that the indirect emissions are higher than anticipated. Even in comparison to the third generation, they emit more indirectly. Their poor thermodynamic performance and large mass flow rates appear to be the cause of this.[40] On top of that, trifluoroacetic acid (TFA), which can be discharged into the atmosphere and end up in groundwater, is present in a significant amount in HFOs. Although it might not be harmful to people, it poses a risk to aquatic organizations.[17]

The refrigeration industry once again turned to natural refrigerants, after so many generations and attempts to develop better fluids. The first generation, which continues to produce direct and indirect emissions with the best impact consequences, is widely distributed across the ecosystem. Its flammability or toxicity can be brought under control with the right implementation of safety precautions, allowing the refrigerants to be used in every situation without any negative effects.

According to the generation they belong to and the time they first arose, the various types of refrigerants can be divided into categories. These details are shown in Table 3.1.

Table 3.1:	$\ Categorization$	$of \ refrigerants$	based on a	the generation	and chronol	ogical order.
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Refrigerants	Generation	Date
Natural	1st generation	1830
CFC	2nd generation	1930
HCFC	2nd generation	1930
HFC	3rd generation	1950
HFO	4th generation	2010

3.1.1 Classification of Refrigerants

The flammability and toxicity levels of refrigerants have been classified by the American society of heating, refrigerating and air-conditioning engineers (ASHRAE) [44]. These categories serve as global safety standards and constitute a uniform code for the refrigeration industry. These are the categories that have been derived from ASHRAE Standard 34:

- Toxicity classification [44]
 - 1. Class A: refrigerants have an *OEL of 400 ppm or greater
 - 2. Class B: refrigerants have an OEL of less than 400 ppm

*Where OEL is the occupational exposure limit

• Flammability classification [44]

The refrigerants will be assigned to classes based on lower flammability limit testing, the heat of combustion and the optional burning velocity measurement.

- 1. Class 1: No flame propagation
- 2. Class 2L: Lower flammability
- 3. Class 2: Flammable
- 4. Class 3: Higher flammability



Figure 3.1: Refrigerant classification based on ASHRAE Standard 34.[44]

Figure 3.1 highlights the four classes with various colours in accordance with their risk assessment while displaying the various levels of flammability and toxicity.

3.2 Ammonia NH₃ (R717)

Ammonia is a natural refrigerant which appears as a colourless gas. It can ascend because of its lower gas density than air at ambient temperature. It is reported to be exceedingly soluble in water and can be liquefied at pressures of 6 bar. The Formula 3.1 for ammonia, which combines atmospheric hydrogen and nitrogen, is as follows: [17]

$$N_2 + 3H_2 = 2NH_3 \tag{3.1}$$

3.2.1 Classification

According to ASHRAE Standards [44], NH_3 is categorized as B2L which means it is toxic despite its low flammability. More specifically, it ignites when the amount of ammonia in the air is between 15-28%.[44] It is a limit hard to reach, since the areas where NH_3 plants are located have to be well ventilated. Given that the auto-ignition temperature is 650°C, the chance of an explosion is rather minimal.[17] Ammonia is a great option for regular usage in refrigeration systems because it presents zero GWP and ODP as a refrigerant [41].

3.2.2 Characteristics

During condensation and evaporation, R717 has a high heat transfer coefficient. Condensation occurs between 20°C and 45°C, while evaporation occurs between -55°C and 10°C. Moreover, it can achieve higher temperatures when it is used as a refrigerant in heat pumps. In order to prevent any damage to the system and oil circulation, the hot gas at the compressor end should not exceed 130°C since the system's critical temperature (Tc) is 133°C. The fluid is marked as the optimal choice for pumps and heat recovery systems due to the elevated compression-end temperature. Additionally, because

its critical pressure (Pc) can reach 113 bar, its volumetric cooling capacity is appropriate for high-temperature heat pumps.[17][45] Its normal boiling point (NBP) is -33.3° C at 1 bar and its critical density (pc) 243.99 kg/m³ [46].

Table 3.2 concentrates all the characteristics of ammonia as a refrigerant and the values for the most important temperatures and pressures.

Categories	Values
Chemical Name	Ammonia
Refrigerant Number	R717
Chemical Formula	$ m NH_3$
Generation	1st (Natural)
Safety Group	B2L
Auto-Ignition Temperature	$650^{\circ}\mathrm{C}$
Occupational Exposure Limit (OEL)	$25~\rm ppm~v/v$
Refrigerant Concentration Limit (RCL)	320 ppm v/v
Molecular Weight	$17.01 \; (g/mol)$
Normal Boiling Point (NBP)	-33.3°C
Critical Pressure (Pc)	113 bar
Critical Temperature (Tc)	133°C
Critical Density (pc)	$243.99~\rm kg/m^3$
Triple Point Pressure	0.0609 bar
Triple Point Temperature	$-77.65^{\circ}\mathrm{C}$
Global Warming Potential (GWP)	0
Ozone Depletion Potential (ODP)	0

 Table 3.2: Ammonia characteristics as a refrigerant.

The following Figure 3.2 illustrates the log P-h diagram of ammonia with its critical point.



Figure 3.2: Log P-h diagram of ammonia.

3.2.3 Utilization

To begin with, 80% of ammonia output goes toward using it as a fertilizer in agricultural processes. Only 2% of the production is converted into a fluid for refrigeration cycles. Its designation as a refrigerant is R717, and it introduces good thermodynamic qualities. Due to its high level of toxicity, it is typically utilized in indirect systems, but it can also be used in direct systems when combined with another liquid coolant, such as glycol or water. Otherwise, as illustrated in Figure 3.3, it is frequently encountered as the higher stage in a cascade system, typically with CO_2 at the lower level. Ammonia is often used in large-scale systems, such as those for food refrigeration.[17]



Figure 3.3: Schematic diagram of a 2-stage cascade system with NH3 at the upper part and CO_2 at the lower part.

3.2.4 System Components

Due to the significant pressure variations between condensation and evaporation, the compressors that would be better suited for R717 are screw and piston compressors. Specifically, piston compressors function between 25°C and 35°C. Consequently, two-stage compression should be used if the system's evaporation temperature is lower than -20°C. Screw compressors, on the other hand, use oil or refrigerant injection to cool down their components, allowing them to run at lower temperatures in a single stage. It should be noted at this time that screw compressors generally cost more than pistons. As the oil from the compressor cannot be completely removed, an oil separator is another essential part of the system.[17]

As for the heat exchangers, plate heat exchangers are considered the optimal choice for ammonia refrigeration systems. They are quite effective, but as a drawback, careful consideration should be given to the material choice. NH_3 plants can only utilise steel and aluminium. This is due to the reaction that occurs when copper or zinc comes into contact with ammonia. Even if the 99.95% purity of NH_3 , used for refrigeration purposes, is very high, only ammonia that is fully dry and 100% pure might safely come into touch with copper. Therefore, this is not feasible as an amount of water must exist to prevent stress corrosion cracking.[17]

3.2.5 Safety Precautions

Ammonia has a pungent smell which makes it easy to identify even at 3 ppm, a concentration which is thought to be non-toxic for humans. Depending on the duration of exposure, it begins to affect human health after 25 ppm, but at 5000 ppm it may be immediately fatal. Since gaseous NH_3 is lighter than air, it might be quickly released to the atmosphere with a suitable ventilation system in case of a leakage. However, because of the high solubility of the refrigerant to water, it will be harder for leakage to be noticed when it comes in contact with it. Hence, heat is emitted and significant amounts of vapour are created when liquid ammonia comes into contact with water. As for the explosion risk, due to the comparatively high auto-ignition temperature, it is highly unlikely to occur indoors while similarly it is considered impossible outdoors.[17]

In order to prevent such accidents, some safety precautions must be taken. According to European Standard EN 378 [47], components like safety or overflow valves are important to avoid the buildup of unnecessary pressure in the system and lower the flammability risk. Further, to safeguard the units, numerous separate safety switches should be installed on the high side of the compressors. It is also considered crucial to install gas detectors to measure the level of ammonia in the room so that, in the event of a leakage, they can alert the employees. Engineers should always wear safety gear whenever they enter a room to fix a leakage.[17][47]

3.2.6 Installation and Operation Costs

Normally, ammonia systems were commonly located outside but recently they have begun to be installed within, in the same space as the other building systems. As long as the ventilation rate stays within the specified range, it is now regarded as a safe alternative. These systems are more expensive than facilities using other refrigerants in terms of capital expenses, but their costs for operation and maintenance are far lower. Thus, they quickly recover their initial investment costs. It is important to note that the system is thought to be very efficient with an increased COP, because of R717's excellent thermodynamic properties. This results in less electricity being used and less CO_2 emissions being released. Nonetheless, R717 is less expensive than synthetic refrigerants due to its low density and easier to be supplied. Finally, ammonia systems have a long lifespan and do not require any challenging maintenance tasks.[17]

3.3 Carbon Dioxide CO₂ (R744)

As a gas, carbon dioxide has no colour or smell. The following Formula 3.2 shows that it is a combination of carbon and oxygen, which makes it a natural refrigerant. The CO_2 gas is quite prevalent in the atmosphere and it is even present in human cells. It has also received a lot of interest recently as a refrigerant.[17]

$$C + O_2 = CO_2 \tag{3.2}$$

3.3.1 Classification

 CO_2 is a part of the 1st generation of refrigerants and is neither toxic nor flammable. It is categorized as A1 and has no auto-ignition temperature.[44] Due to this ability, it can easily be used as a fire agent for extinguishing the fire when it has a concentration of 10% by volume. Moreover, it has a strong odour at very high concentrations and its maximum OEL can reach 0.5% by volume. Despite the fact that CO_2 emissions cause global warming, CO_2 produces a negligible amount of harmful emissions when used as a refrigerant. In particular, its GWP is estimated to be 1 and its ODP is zero.[41] This highlights the safe use of refrigerant.

3.3.2 Characteristics

Carbon dioxide's ability to operate at higher pressures than other refrigerants is a considerable benefit. To achieve this, it can switch between subcritical and transcritical phases depending on the temperatures or pressures under which it is running at the time. At its critical point, where the temperature is 31.1° C and the pressure is 7.38 bar, the phase shifts from subcritical to transcritical. What is more, the gas has a significantly high density and acts more like a liquid in the transcritical area. There, condensation ends and the relationship between temperature and pressure becomes unclear. So the pressure can be controlled by the amount of the refrigerant at the high pressure side.[17]. Its molecular weight is 44.01 (g/mol) and its critical density is 467.6 kg/m³ [46]. Besides that, the refrigerant has the potential to change into a solid form known as dry ice at its triple point, which is at a pressure of 5.17 bar and a temperature of -56.6°C. Good thermal conductivity, low viscosity, and a high specific heat capacity are all characteristics of liquid CO₂.[17]

Table 3.3 concentrates all the characteristics of carbon dioxide as a refrigerant and the values for the most important temperatures and pressures.

Categories	Values
Chemical Name	Carbon Dioxide
Refrigerant Number	R744
Chemical Formula	CO_2
Generation	1st (Natural)
Safety Group	A1
Auto-Ignition Temperature	-
Occupational Exposure Limit (OEL)	$5000~\rm ppm~v/v$
Refrigerant Concentration Limit (RCL)	30,000 ppm v/v
Molecular Weight	$44.01 \; (g/mol)$
Normal Boiling Point (NBP)	-78.4°C
Critical Pressure (Pc)	7.38 bar
Critical Temperature (Tc)	31.1°C
Critical Density (pc)	467.6 kg/m^3
Triple Point Pressure	5.17 bar
Triple Point Temperature	$-56.6^{\circ}\mathrm{C}$
Global Warming Potential (GWP)	1
Ozone Depletion Potential (ODP)	0

Table 3.3: CO_2 characteristics as a refrigerant.

The following Figure 3.4 illustrates the log P-h diagram of CO_2 with its critical point and the different subcritical/transcritical phases.



Figure 3.4: Log P-h diagram of CO₂.

3.3.3 Utilization

 CO_2 is ideal for direct systems in public settings because it is not toxic. The gas can be evacuated directly to the atmosphere even if leakage occurs, without the need for additional safety measures. The ability of CO_2 to attain high temperatures, between 85-90°C, without the necessity of an additional auxiliary system makes it ideal for hot water production systems. Furthermore, because of its capacity to function at temperature glide conditions, it is regarded as a great refrigerant for heat recovery from industrial refrigeration systems. These systems, which go by the name "Booster" systems, exhibit exceptional performance. Figure 3.5 shows a schematic representation of a straightforward booster system.

 CO_2 is also encountered in the lower half of cascade systems, typically working in conjunction with ammonia on the higher part. There, it can effectively take care of the cooling requirements for low and medium temperatures, while ammonia can cover the high pressure side. It is a very effective system, but quite expensive to implement.[17]



Figure 3.5: Schematic diagram of a simple CO_2 booster system.

3.3.4 System Components

As was previously noted, CO_2 operates at high pressures. Screw compressors are the best option for these systems because they can cope well with these circumstances. When the pressures are high, the pressure ratio is getting smaller and as a result the size of the compressor decreases but the efficiency increases. In order to protect the system against high pressures and ensure that the pressure will decrease before hitting the evaporator, numerous types of pressure valves are generally required. Because of its strong thermal conductivity qualities, copper is the most frequently utilized material for CO_2 components. Steel and aluminium are also materials that can be used.[17]

In addition, the condenser is known as a gas cooler when the system is in transcritical mode because it stops condensing. The suction gas heat exchanger for heat recovery is another element employed in this stage. Its function is to use the waste heat after compression and it is often installed before the gas cooler. Pressure receivers and multiple ejectors are utilized in booster systems to increase efficiency by unloading the primary compressor and ensuring better performance by directing CO_2 gas to a parallel compressor. In order to keep the evaporators saturated, they additionally pump liquid to them.[17]

3.3.5 Safety Precautions

The amount of CO_2 that is considered to be ideal in a closed area, is under 800 ppm. Although exposure to high concentrations may cause some breathing problems, the majority of instances can be resolved by getting fresh air. Only when the concentration reaches 50,000 ppm or above, may the effects be considered life-threatening. Electronic devices that alarm for high concentrations should, however, always be implemented for safety reasons. Gas detectors should be positioned low in the room since CO gas is heavier than the air.[17]

When CO_2 is at a standstill, the situation is most severe. If the liquid refrigerant is left in the system, it may be exposed to warm surroundings, which will affect the pressures. Thus, all pipes and components that could trap any liquid must have safety relief valves installed. To prevent these kinds of issues, it is preferable to size the system for a pressure of 90 bar. Moreover, a cold finger system should be used to quickly cool down each component, and special attention should be paid to prevent the formation of dry ice. When a safety valve is opened, such as when doing maintenance, dry ice frequently results in reducing the system's overall effectiveness. If it obstructs the discharge valve and holds the liquid inside, it could be very risky. Even so, technicians should always wear protective gloves since any contact with dry ice might cause frostbite.[17]

3.3.6 Installation and Operation Costs

 CO_2 systems can be installed both inside or outside due to their small size and the lack of significant safety concerns. Consequently, the installation expenses are in logical terms. Concerning the components, the system acquires smaller pipelines because of pressure drop and low fluid viscosity of the fluid. There is less demand for refrigerant in the system and less cycling through the pumps since evaporation heat absorption is higher than that of other refrigerants. As a result, the system as a whole has lower operating expenses and is more cost-effective. As noted before, the compressors have a small swept volume and work more energy efficiently. On the other hand, booster systems with parallel compression typically have higher energy efficiencies, so even though they require more components, their great performance tends to quickly offset the additional expenses. They make a major contribution to the units' lifespan extension.[17]

3.4 1,1,1,2-Tetrafluoroethane (R134a)

R134a belongs to synthetic refrigerants and it was made as the replacement for R12, known as freon, a CFC refrigerant with serious damaging effects on the ozone layer. Its chemical compound is consisted of two carbon atoms, two hydrogen atoms and four fluorine atoms, as it is shown in the following Formula 3.3.[48]

$$C2H2F4 \tag{3.3}$$

3.4.1 Classification

R134a is an HFC refrigerant, meaning it is historically placed in the 3rd generation. It has been classified as A1 class, which makes it non-toxic and non-flammable.[44] Consequently, its auto-ignition temperature is measured to be extremely high, more than 743°C [49]. Since it belongs to the 3rd generation, it presents zero ODP but very high GWP. Specifically, its greenhouse gas emissions are calculated to be around 1430. An amount that causes severe consequences to the environment.[50]

3.4.2 Characteristics

R134a as gas is heavier than air and has the tendency to gather close to the ground level [50]. Its molecular weight is measured to be 102.03 (g/mol), almost 3.5 times heavier than air. It is a high temperature refrigerant which operates with a higher suction pressure than the atmospheric pressure, as most of the HFCs do [17]. As for its specific characteristics, it appears a critical pressure of 40.67 bar and a critical temperature of 101°C [50] [49]. Its NBP can be met at -26.1°C, while its triple point is as low as -103.3°C [17]. Another worth mentioning characteristic is its critical density, which is considered to be quite increased at 508 kg/m³ [50].

Table 3.4 concentrates all the characteristics of 1,1,1,2-Tetrafluoroethane as a refrigerant and the values for the most important temperatures and pressures.

Categories	Values
Chemical Name	1, 1, 1, 2-Tetrafluoroethane
Refrigerant Number	R134a
Chemical Formula	C2H2F4
Generation	3rd (HFC)
Safety Group	A1
Auto-Ignition Temperature	>743°C
Occupational Exposure Limit (OEL)	1000 ppm v/v
Refrigerant Concentration Limit (RCL)	50,000 ppm v/v
Molecular Weight	$102.03 \; (g/mol)$
Normal Boiling Point (NBP)	-26.1°C
Critical Pressure (Pc)	40.67 bar
Critical Temperature (Tc)	101°C
Critical Density (pc)	508 kg/m^3
Triple Point Pressure	0.0039 bar
Triple Point Temperature	-103.3°C
Global Warming Potential (GWP)	1430
Ozone Depletion Potential (ODP)	0

 Table 3.4:
 1,1,1,2-Tetrafluoroethane
 characteristics
 as
 a
 refrigerant.

The following Figure 3.6 illustrates the log P-h diagram of R134a with its critical point.



Figure 3.6: Log P-h diagram of R134a.

3.4.3 Utilization

R134a, as it was mostly created to replace freon, it is commonly used in air conditioning systems in automotive vehicles, refrigerator cases, venting machines and small household refrigerators. It usually operates at medium and high temperatures and can also be met at industrial and commercial chillers. In addition, many manufacturers use it in plastic foam blowing, while pharmaceutical companies use it as a propellant in some aerosol products.[48]

3.4.4 System Components

R134a presents high water solubility which limits its potential to be used in refrigeration systems. If there is even a chance of water being in the system, the lubricating oil will react and corrosion will occur. In order to prevent this from happening, regular cleaning and the installation of highly efficient driers is necessary.[51] Moreover, it can be immiscible with some oils, so polyalkylene glycol (PAG) and polyol ester lubricants are the ones that R134a should be used with [48]. In general, it shows excellent compatibility with most materials, without having any reaction [49]. As for the compressors that are most suitable for this kind of refrigerant, centrifugal, rotary screw, scroll and reciprocating compressors are suggested.

3.4.5 Safety Precautions

Even though R134a is considered to be a non-toxic, non-flammable gas and its OEL is increased at 1000 ppm v/v, extremely high concentrations should be avoided to prevent breathing difficulties [44]. The most appropriate measure to secure safety is to provide proper ventilation with local extraction so the leaked gas can easily be removed from closed spaces without causing asphyxiation problems. Since the gas is heavier than air, with a molecular weight of 102.03 (g/mol), oxygen detectors are recommended to be placed at the ground level to monitor the gathered gas percentage.[49]

Furthermore, its auto-ignition temperature is considered extremely high but when the gas is transported in containers it is under pressure. That means that the area should be well ventilated and great attention should be given to the surrounding temperature. The containers have to be stored in cool places and avoid any heated sources or sunlight, to prevent an explosion.[50] For this reason, regular inspections for any kind of leakages are also highly recommended [49].

3.4.6 Installation and Operation Costs

Since R134a is classified as A1 it can be placed both inside and outside without any restrictions. As mentioned before 3.4.3, it is mostly used for small systems so the installation and charging costs are low. However, the range of operation with high pressures increases the energy use of the components and reduces their lifetime. This results in an increase in the operation and maintenance costs of the system. At this point, it should also be noted that a synthetic refrigerant is more expensive than natural refrigerants and its price will be even higher after some years due to the environmental restrictions from the European regulations (no. 517/2014) [40]. R134a has already been banned from the air conditioning systems as their GWP is higher than 150 [40].

3.5 Isobutane C4H10 (R600a)

Isobutane as a gas is colourless but it has a sweet odour in high concentrations. It is a natural refrigerant with a structural composition of four carbon and ten hydrogen atoms, similar to butane (R600).[52] However, their thermophysical properties differ. R600a does not absorb much water but it is soluble in oil [17]. The chemical consistency of R600a can be observed in the following Formula 3.4.[52] It is also worth mentioning that isobutane took the place of CFCs and HFCs, like R12 and R134a [17].

$$CH(CH_3)3\tag{3.4}$$

3.5.1 Classification

Isobutane belongs to the hydrocarbons category and it is a 1st generation refrigerant. Specifically, it is classified as an A3 class which subsequently ranks it with low toxicity but high flammability.[44] Its auto-ignition temperature is measured to be 460°C. Concerning the environmental footprint, it presents zero ODP and GWP 3 which makes it negligible.[52]

3.5.2 Characteristics

R600a presents the ability to achieve low discharge temperatures and pressures, which makes it suitable for medium, high and very high applications. Its critical temperature is placed high, at 135°C, and its critical pressure drops at 36.45 bar. The refrigerant operates below its critical point for refrigeration purposes and by having pressures above the atmospheric pressure, it prevents oxygen and moisture from entering the system, in case of a leak. What is worth mentioning, is its triple point features, which are significantly low, with the temperature approaching the value of -159.6° C. As for the NBP, it is elevated reaching the temperature of -11.7° C. In general, isobutane shows efficient thermodynamic properties and as a natural gas it can be found in large quantities in the environment.[17][52]

Table 3.5 concentrates all the characteristics of isobutane as a refrigerant and the values for the most important temperatures and pressures.

Categories	Values
Chemical Name	Isobutane
Refrigerant Number	R600a
Chemical Formula	$CH(CH_3)3$
Generation	1st (Natural)
Safety Group	A3
Auto-Ignition Temperature	$460^{\circ}\mathrm{C}$
Occupational Exposure Limit (OEL)	$1000~\rm ppm~v/v$
Refrigerant Concentration Limit (RCL)	$4000~\rm{ppm}~v/v$
Molecular Weight	$58.1 \; (g/mol)$
Normal Boiling Point (NBP)	-11.7°C
Critical Pressure (Pc)	36.45 bar
Critical Temperature (Tc)	$135^{\circ}\mathrm{C}$
Critical Density (pc)	$221 \ \mathrm{kg/m^3}$
Triple Point Pressure	2.29E-07 bar
Triple Point Temperature	$-159.6^{\circ}{ m C}$
Global Warming Potential (GWP)	3
Ozone Depletion Potential (ODP)	0

 Table 3.5:
 Isobutane characteristics as a refrigerant.

The following Figure 3.7 illustrates the log P-h diagram of isobutane with its critical point.



Figure 3.7: Log P-h diagram of isobutane.

3.5.3 Utilization

Isobutane is mostly utilized for small commercial refrigeration systems, fridges, freezers and standalone appliances. Because of its ability to reach very low temperatures, it makes it possible to be selected for both single and multi-stages systems. When it is used for indirect circuits, the systems are larger than the ones for direct use. This is due to the high flammability potential. In order to prevent any accidents, the indoor direct systems have to occupy small spaces and be limited capacity systems with a specific amount of refrigerant circulating in the different stages.[17]

3.5.4 System Components

For hydrocarbons like R600a, reciprocating, rotary and scroll compressors are usually preferred for small and medium systems. They tend to be smaller in size and have lower displacement volumes up to 300 m^3/h . Moreover, isobutane is soluble in oil and by using these kinds of compressors the oil circulating in the system is reduced. When larger systems are required, screw compressors in the semi-hermetic casing can be chosen. However, extra attention must be taken to the quantity of refrigerant inside the component. It has to be a considerable amount in order to prevent any problems with the lubricants. The displacement volume of screw compressors can reach over 1000 m^3/h .[17]

Concerning the heat exchangers, compact or liquid suction heat exchangers (LSHX) are considered appropriate for isobutane systems. Compact heat exchangers appear optimal heat transfer properties and are able to control the flow of the refrigerant passing through the component. Consequently, the amount of oil can also be reduced. As for LSXH, they use counter-flow and can increase the discharge temperatures after the condenser. In addition, they cause the reduction of the refrigerant charges by 5% to 15%. Since the system manages to decrease the refrigerant level, no liquid receivers are required.[17] Another fact is that R600a is compatible with most materials except EPDM rubber, natural rubber and silicone. In most cases though, the one that is usually preferred is copper due to its excellent thermal conductivity abilities.[53]

3.5.5 Safety Precautions

The first priority, as a safety precaution for isobutane, is to minimize the flammability risk. In order to achieve this, electronic devices and tools that could act like a source of ignition should be removed, as much as possible, from the enclosed spaces. Gas detectors are recommended to be placed in the machinery room to alarm for any risk of high concentrations and they should be installed at ground level, as the gas is heavier than air with a molecular weight of 58.1 (g/mol).[52] CO₂ could be an optimal choice to act as a fire extinguishing medium, in this case [17]. The OEL is calculated at 1000 ppm v/v and it should be respected because, in case of a leakage in closed spaces, the gas can display oxygen and cause asphyxiation.[44]

Besides, as already mentioned, the refrigerant charges have to be decreased. This reduction could happen with the addition of multiple circuits in the systems, so the fluid can be divided. Further, flooded systems should be avoided, while dry expansion systems should be preferred. Another measure is to place pressure limitation devices and safety relief valves that could stop the operation of the system if a component fails or the risk of explosion is high. As for the ventilation of the room, it is recommended to be well ventilated and a pipe should be connected to the pressure relief valve to direct the gas immediately outside of the room, into the atmosphere. The pipe has to be sprayed with nitrogen afterwards to cool down.[17]

3.5.6 Installation and Operation Costs

Since isobutane is mostly utilized for small sized systems, fewer installation costs are needed. The components present small swept volumes with lower pressure ratios, which indicates less work, electricity consumption and decreased operation costs. Not only does this increase the system's capacity, but it also creates an overall quieter machine with less noise or vibrations. Hence, fewer chances of system failure and an extended life for the units is succeeded. R600a as a natural refrigerant is cheaper than synthetic refrigerants and easier to get supplied. This leads to less transportation costs and a smooth operation of the different circuits.[17]

3.6 trans-1,3,3,3-Tetrafluoroprop-1-ene (R1234ze(E))

R1234ze(E) falls within the synthetic category as it is an HFO refrigerant. It was developed to replace R134a due to its high GWP. Despite the fact it is a pure molecule, its molecular form is distinct from that of natural refrigerants. It also contains fluorine atoms in addition to carbon and hydrogen atoms, as seen in the following Formula 3.5.[54]

$$CF3CH = CFH \tag{3.5}$$

3.6.1 Classification

R1234ze(E), which is categorized as A2L, belongs to the 4th generation of refrigerants [44]. Although it is thought to have low flammability and toxicity levels, sunlight and hot sources with temperatures above 50°C should be kept out of the area. It is noteworthy to mention that this refrigerant is still non-flammable when blended with air that is 30°C below ambient temperature. Thus, handling and storage are regarded as safe processes.[55] Its auto-ignition temperature is marked at 360°C. Even though it is not a natural refrigerant, it still has a low GWP of approximately 7 and zero ODP.[56] Additionally, due to its low energy usage, it is estimated that it can cut its direct CO_2 emissions by 99.6% while simultaneously reducing its indirect emissions.[54]

3.6.2 Characteristics

The low critical pressure of this refrigerant, 36.4 bar, compared to the high critical temperature, 109.37°C, is its primary characteristic. It is suitable for usage in high temperature systems because of this distinction. The low triple point temperature, which is estimated to be -104.53°C, is another noteworthy aspect. All of these characteristics allow the refrigerant to function across a wide temperature range before going through a phase transition. The values for the critical density and molecular weight are 114.04 (g/mol) and 489.2 kg/m³, respectively. It appears to be a gas that is considerably heavier than air.[56]

Table 3.6 concentrates all the characteristics of R1234ze(E) as a refrigerant and the values for the most important temperatures and pressures.

Categories	Values
Chemical Name	trans-1,3,3,3-Tetrafluoroprop-1-ene
Refrigerant Number	R1234ze(E)
Chemical Formula	CF3CH=CFH
Generation	4th (HFO)
Safety Group	A2L
Auto-Ignition Temperature	$368^{\circ}\mathrm{C}$
Occupational Exposure Limit (OEL)	800 ppm v/v
Refrigerant Concentration Limit (RCL)	16,000 ppm v/v
Molecular Weight	114.04 (g/mol)
Normal Boiling Point (NBP)	-18.97°C
Critical Pressure (Pc)	36.4 bar
Critical Temperature (Tc)	109.37°C
Critical Density (pc)	489.2 kg/m^3
Triple Point Pressure	0.0022 bar
Triple Point Temperature	-104.53°C
Global Warming Potential (GWP)	7
Ozone Depletion Potential (ODP)	0

Table 3.6: R1234ze(E) characteristics as a refrigerant.

The following Figure 3.8 illustrates the log P-h diagram of the R1234ze(E) refrigerant with its critical point.



Figure 3.8: Log P-h diagram of R1234ze(E).

3.6.3 Utilization

R1234ze(E) is frequently utilized as a fluid in chillers and heat pumps that operate at medium or high temperatures. As it is a common medium for these systems, they can be coupled with district heating and cooling systems. Industrial and commercial refrigeration installations, as well as small appliances like vending machines, are additional areas where it can be encountered. Other than that, it is typically seen in conjunction with CO_2 at the upper circuit of cascade systems. It is a refrigerant that may be used for a wide range of applications and this makes it easier for manufacturers to frequently choose it. Furthermore, it has exceptional thermal characteristics and performance that allow it to enable highly efficient operation.[54] [57]

3.6.4 System Components

Reciprocal, scroll, screw, and centrifugal compressors can all be utilized with this synthetic fluid as a refrigerant [54]. A screw compressor with R1234ze(E) can function at evaporation temperatures exceeding 30°C and condensing temperatures up to 80°C [57]. The refrigerant can be utilized in flooded evaporators and LGHXs because it is a pure molecule. Liquid components will boost its thermodynamic properties. The components should utilize particular lubricants and manage the amount of oil that circulates in the system since R1234ze(E) is soluble in oil. Any materials can be in contact with the fluid, with the exception of acrylics, which can be easily damaged.[54]

3.6.5 Safety Precautions

R1234ze(E) has the same issue as isobutane, where large concentrations may result in asphyxiation by lowering the oxygen in the room since its molecular weight is much heavier than air [55]. The OEL for the gas, according to ASHRAE Standards, is 800 ppm, while the RCL is 16,000 ppm [44]. It is advised to install oxygen detectors in the closed spaces to monitor the oxygen levels and sound an alarm if the gas concentrations are abnormally high. Also, a proper ventilation system must ensure that there are extract ducts available in case of an emergency and maintain good air quality.[56]

Despite the fact that the refrigerant is not particularly flammable, the components should not be subjected to heat beyond 50°C [55]. Moreover, all potential spark-causing sources must be eliminated. Even if there is an ignition, the refrigerant's low heat of combustion prevents the spark from spreading into an uncontrollable fire.[54] Another precaution is a thorough inspection of each unit to look for any liquid that may be trapped inside. Since the refrigerant is soluble in oil, the system must be often monitored when it operates under pressure for gas that may become trapped in the oil receiver and cause a leak. With valves monitoring the number of liquid charges, the construction must be tightly sealed.[56]

3.6.6 Installation and Operation Costs

Typically, the entire system is situated outdoors or in machine rooms. The system's low energy usage reduces operating costs while the installation costs are not excessive. In areas with warm weather, the refrigerant would be more energy-efficient due to its high operating temperature range. Besides, the low discharge pressures decrease mechanical stress and increase the components' lifespan. As an outcome, the system performs significantly better and the maintenance expenses are decreased.[54]

The cost of the refrigerant is generally very high as it is estimated to be 10 to 15 times more expensive than R134a, which it replaced [41]. Since R1234ze(E) is a synthetic refrigerant, it will be challenging to be supplied over the following ten years due to the Montreal and Kyoto Protocols [42][43], which forbid the use of these refrigerants in the coming years. Thus, its cost will drastically increase and transportation will be seen as challenging.[54]

3.7 Refrigerants Comparison

A comparison of the aforementioned refrigerants will be carried out in this section. The comparison will be examined in terms of the fluids' generation, environmental effects, and thermo-physical characteristics. To better accomplish this task, the tables and graphics that follow have been designed.

 Table 3.7: Categorisation of refrigerants based on the generation and environmental footprint.

Refrigerants	Class	Generation	ODP	GWP
R717	Natural	1st	0	0
R744	Natural	1 st	0	1
R134a	HFC	3rd	0	1430
R600a	Hydrocarbons	1st	0	3
R1234ze(E)	HFO	4th	0	7

Table 3.7 demonstrates that most of the refrigerants, with the exception of R134a and R1234ze(E), belong to the 1st generation. This indicates that they are natural fluids, while the other two are synthetic refrigerants of the 3rd and 4th generations, respectively. Since they are synthetic, they both have a greater GWP but, like the rest of the natural refrigerants, zero ODP. Nevertheless, R134a with a value of 1430, appears to have the highest GWP of the group. Due to this, R134a is no longer permitted in the majority of applications and has been substituted by R1234ze(E). Ammonia, on the other hand, has no GWP, making it the environmentally friendliest refrigerant on the list.

Categories	R717	R744	R134a	R600a	R1234ze(E)
Safety Group	B2L	A1	A1	A3	A2L
OEL (ppm v/v)	25	5000	1000	1000	800
RCL (ppm v/v)	320	30,000	50,000	4000	16,000
Toxic	Yes	${<}10\%$ No	No	No	No
Flammable	Yes	No	No	Yes	No
Auto-Ignition Temperature (°C)	650	-	>743	460	368

 Table 3.8: Categorisation of refrigerants based on toxicity and flammability.

Moving forward in Table 3.8, the refrigerants are compared based on their safety. From the comparison, the result that only R744 and R134a are classified as A1 fluids arise. Yet, it can be clearly stated that the most optimal choice between them is the R744, since it is also a natural refrigerant. Its value for OEL is the highest among all the other fluids but its RCL is a little bit lower than R134a's. In addition, it is considered non-flammable and non-toxic and as for its auto-ignition temperature, CO_2 does not have one. That is the reason it can be used as a fire extinguishing medium in certain cases.

The only refrigerant in the table that is both flammable and toxic is ammonia, which is categorized as B2L. In contrast to the other fluids, it has an OEL that is significantly low. It is only 25 (ppm v/v), while CO₂ has 5000 (ppm v/v). The RCL value experiences the same thing. However, at this point, it is important to keep in mind that even at 3 ppm, ammonia has a strong odour that makes it very easy to be detected in case of a leakage. Thus, the likelihood of an accident happening is relatively low. In addition, its extremely high auto-ignition temperature makes it more difficult to attain at the point of explosion.

Concerning the other two refrigerants, isobutane is believed to be extremely flammable, making it less safe in comparison to R1234ze(E). For this reason, it is categorized as A3, whereas R1234ze(E) is classified as A2L. In the table, it is in fact the most flammable one. Continuing, their OEL values are practically similar, while R1234ze(E)'s RCL is four times higher than isobutane's. It is interesting to note that isobutane has a higher auto-ignition temperature than R1234ze(E). This is because R1234ze(E), as already explained in Section 3.6.5, is flammable when exposed to temperatures above 50° C for a specific amount of time.

Categories	R717	R744	R134a	R600a	R1234ze(E)
Molecular Weight (g/mol)	17.01	44.01	102.03	58.1	114.04
Normal Boiling Point NBP (°C)	-33.3	-78.4	-26.1	-11.7	-18.97
Critical Pressure Pc (bar)	113	73.8	40.67	36.45	36.4
Critical Temperature Tc (°C)	133	31.1	101	134.5	109.37
Critical Density pc (kg/m^3)	243.99	467.6	508	221	489.2
Triple Point Pressure (bar)	0.0609	5.17	0.0039	2.29E-07	0.0022
Triple Point Temperature (°C)	-77.65	-56.6	-103.3	-159.6	-104.53

Table 3.9: Categorisation of refrigerants based on different pressures and temperatures.

The critical points, triple points, and NBPs of the refrigerants are compared in Table 3.9. Generally, the triple point -the point at which the solid, liquid, and gas phases are in equilibrium- occurs below the NBP. Hence, the conclusion that can be drawn from the results in the table is that CO_2 has a lower NBP than its triple point. The NBP pressure for the majority of refrigerants is 1 bar, however, CO_2 has already reached its triple point at 5.17 bar. This is happening because, at 1 bar this fluid does not have a liquid phase. To clarify the situation, it is solid at 1 bar below -78.4°C and gas at 1 bar above the same temperature. Isobutane has the highest NBP and the lowest triple point. Figure 3.9 shows an example of a typical placement of the triple, boiling and critical points.

The critical points of the refrigerants are illustrated in Figure 3.10 in a more graphic manner. Ammonia and isobutane appear to operate in the same range of temperatures, but ammonia has a higher pressure. In contrast, R1234ze(E) is positioned at a lower temperature but has a pressure that is comparable to that of isobutane. Although it runs at a slightly higher pressure and lower temperature, R134a

is comparable to R134ze(E). CO_2 is the fluid that is outside of the other refrigerants' pressure and temperature ranges. Its critical point is the lowest since it consists of a low temperature refrigerant for subcritical operation. If it has to work at higher temperatures and pressures, it must change to a transcritical phase.



Figure 3.9: Diagram with an example of a typical placement of the triple, boiling and critical point.



Figure 3.10: Diagram with the critical points of the different refrigerants.

4 Study Case

CERN is an organization respected for its working achievements and the possibilities of new discoveries that it offers in the field of physics. However, the time has come to take under consideration the consequences that the experiments cause to the environment and adjust to European legislation accordingly. The aim of this thesis is to map the already existing systems that are used by the organization, acknowledge the problems and suggest new solutions. The investigation will be focused on the cooling and ventilation part of a typical office distribution network at CERN, and more energy efficient proposals will arise.

To begin with, the system is designed for a load of 10 kW. Specifically, the network includes two air-cooled chillers and two AHUs that provide cold air into two office rooms. The chillers operate with the synthetic HFC refrigerant, R134a, which cools the water being directed to the two AHUs in order to cool the air which will be distributed afterwards into the offices. These units are connected to each other by a network of supply and return pipes, utilizing water as a heat transfer fluid. A schematic diagram of this system with the typical examples of the two offices is illustrated in the following Figure 4.1.



Figure 4.1: Schematic diagram of the 10kW system's network, connected to two offices.

In more detail, the system includes:

- 2 chillers with a temperature range of operation 7/12 °C at the cold side and 20/25 °C at the warm side.
- 2 AHUs connected to 2 offices with 18°C supply air and 23°C exhaust air.
- A network of pipes connecting the different units with 7°C supply water and 12°C return water.

In the existing system, the offices are provided with a 10 kW constant load each, which corresponds to the internal heat gains of 29 employees, the technical equipment and lighting. In order to investigate further the way of operation of this complex, it will be designed in the Dymola[®] software. Based on the simulated outcomes the performance of each system will be examined and afterwards, the same complex will be re-designed with a natural fluid as a refrigerant.

The main problem that the existing system faces is the utilization of synthetic refrigerant. As mentioned before, in Section 3.4, R134a has high GWP, which is the reason it is banned in European countries. Consequently, the use of it in CERN must be stopped and replaced by a 1st generation working fluid. In this case, where only cooling is requested, CO_2 is considered to be the best replacement since it presents negligible GWP and high efficiency in low and medium temperatures. Thus, the chillers will be replaced with ones operating with CO_2 and then the two systems will be compared based on their simulation results.

Except for the comparison of the two cases, operating in a constant load, the systems will also be studied as dynamic models with a non-constant load for 24 hours, corresponding to a typical working day. This will aid in observing the system's operation under realistic conditions, focusing on the resulting variations of the chillers' capacity levels and COPs. Moreover, an analysis of the outcomes from the simple form of the heat recovery system existing in the AHUs will arise, along with suggestions for the potential use of the waste heat recovery originating from the CO_2 chiller. In the end, the most sustainable solution will prevail.

5 Methodology

This chapter describes the methodology used to develop the already existing cooling system at CERN, as was described in the Study Case 4. The system is modelled in the dynamic software Dymola in order to be replicated with technical details and examined under realistic conditions. Except for the existing system, a new version of it, which includes the proposed solution for improvement, will also be modelled and described.

5.1 Dymola/Modelica

Modelica is an object-oriented modelling language which, based on mathematical equations, simulates physical systems. Graphical expressiveness requires a modelling environment, in this case, is called Dymola. There are many different libraries in the software that can be used by the user based on the purpose of the simulation. For this project, the standard library and the TLK-Thermo GmbH (TIL 3.12.1, TILMedia 3.12.1) libraries were selected. All the elements required for the dynamic modelling of complex thermal systems are provided by these libraries. More specifically, the Modelica standard library includes components for hierarchical state machines, control systems, and mechanical, electrical, magnetic, thermal and fluid systems. While, components for thermodynamic systems like heat exchangers, compressors, valves and pumps are introduced by TIL 3.12.1. TILMedia 3.12.1 uses external databases like REFPROP to determine the thermo-physical parameters of liquids and gases. Finally, DaVE software -an extension package from Dymola- was used to visualize and plot the results on log P-h and T-s diagrams.[58][59]

5.2 Modelling Approach

In this section, a modelling approach of the simulation in Dymola is elaborated and the main components are explained. Since the system consists of a complex of smaller subsystems and a network of pipes, first each subsystem has to be designed separately. After that, they will all be connected into one big network and a dynamic simulation will be performed.

For this project, the condensing and evaporating temperatures are the only known values. So the rest of the information (pressures, enthalpies) is derived from CoolPack software, which includes a collection of cycles for refrigeration systems. As a modelling approach, several assumptions had to be considered, such as no heat loss in the transport pipes and 100% efficiency in the heat exchangers, which would not be the case for real applications. However, all of the components that are chosen for each subsystem are designed based on the same logic. These shared parameters are displayed below:

• **Compressors:** the compressors used for the simulations are modelled in Dymola using the same component: the premodelled "ReciprocatingCompressor". This compressor component requires an input of the parameters: rotational speed (Hz), displacement (m³) and volumetric, isentropic- and effective isentropic- efficiencies. The compressor efficiencies were all set to a constant of 0.7, which was the preset value for the component. The real efficiencies would vary depending on whether the cycle is running on full load or not, but in the simulations the chillers are constantly in full load. The rotational speed is set to 50 Hz in all the compressors and the displacement has been set after several iterations using different inputs.

• Heat Exchangers: concerning the chillers, a "Plate" heat exchanger was chosen as an evaporator and a "FinAndTube" heat exchanger as a condenser, both with counter-flow. For the AHUs, a "FinAndTube" heat exchanger with cross-flow was selected. The input parameters for the heat exchangers are the heat transfer coefficient (U), the refrigerant and water/air, and the geometry of the heat exchanger. Usually heat transfer coefficient for gases is in the range of 50-100 W/m²K and for liquids in the range of 2000-5000 W/m²K[60].

Regarding the geometry of the heat exchangers, it is decided based on the length, width, pattern angle, wall thickness and the number of plates/tubes. For all the subsystems, their geometry has been decided after several trials and errors. In addition, it should be mentioned that the heat source is water, which exchanges heat directly in the heat exchanger, and the heat sink is air for all the subsystems.

- **Proportional Integral (PI) Controllers:** the "PIControllers" are feedback control loops that receive inputs from other parameters, make the calculations and give the output to the connected component.
- Expansion Valves: the "OrificeValve" is used in all the simulated subsystems. The input parameter for this pre-modelled valve is the effective flow area, which in all cases is regulated by a "PIController". The only difference is that for the chillers the "PIController" regulates the high pressure and the superheat at the outlet of the evaporator, while for the AHUs it regulates the returned air temperature.
- Fans: the "SimpleFan" type of fans, with 0.7 efficiency, is installed in the subsystems to force the air in the correct direction and sometimes to keep the requested temperature.
- **Tubes:** the "Tubes" simulate the pipes and they can be designed with a given length and diameter. They also control the heat transfer and the pressure drop in the pipe network.
- Sensors and Pressure States: different kinds of sensors and pressure states give an overview of the cycle. Sensors are placed before and after every component in order to signal if the cycle is running with the correct values. In some cases, pressure, superheat and temperature sensors are added to give input to the "PIControllers".
- System Information Manager (SIM): it is a necessary element that must be included in the design of every cycle in Dymola in order for the system to be able to run. It defines the substances (liquid, gas, fluid) that are used in every component and includes their properties.

5.3 Study Case Modelled in Dymola

5.3.1 Main System 10kW

A representative image of the main system's model in Dymola is illustrated in Figure 5.1. Here, the two chiller subsystems along with the two AHUs and the offices can be seen as blocks. Except for the offices, the rest of the blocks are connected to each other with a pipeline network which starts from the chillers, supplies the AHUs with 7°C water and then returns at 12°C. From the chilled water, the AHUs cool the intake ambient air and distribute it in the offices at 18°C. Afterwards, the exhaust air returns to the ventilation system at 23°C and is forced out to the environment.

At this point, should be noted that all the blocks with the same name are completely similar to each other concerning the input values and their use. As mentioned in the beginning, each subsystem has first been modelled and simulated separately and then they were linked to the main system. This was achieved by creating partial and modular models. In other words, in the model that was originally created each component was chosen to be placed as "replaceable", which means that can be easily changed anytime with another component that belongs to the same category. Further, the model was made to be partial and by extending it, another identical model was created which is called modular. So, the advantage of this approach is that whenever a value is changed in the partial model it also changes automatically in the modular one. And by linking the modular model to the main system, there is the benefit of studying the partial subsystem individually and then all the changes that have been made are transferred to the main model. By using this modelling method, it becomes easier to detect any errors and an incredible amount of time is saved.



Figure 5.1: Illustration of the main system as it was modelled in Dymola.

The components that can be observed in the main system are the following:

- 1: a "HydraulicCapacitor" which defines the pressure in the liquid circuit.
- 2: a "SimplePump" which pumps the water to the supply pipelines.
- 3: two "OrificeValves" that control the mass flow of the returned water at both chillers' pipelines.
- 4: a "DirectionalControlValve" which directs the supplied water to three different paths and splits equally the mass flow.

The water and air mass flows, used as inputs at the system, were calculated based on the following Equation 5.1 and are better presented in Table 5.1:

$$\dot{Q} = \dot{m}_R c_p \Delta t \tag{5.1}$$

Where, c_p of water is 4.184 (kJ/kg K) and c_p of air is 1 (kJ/kg K).

Table 5.1:	Input	mass	flows	at	the	system.
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Characteristicts	
Mass Flow of Water (kg/s)	0.48
Mass Flow of Air (kg/s)	2

5.3.2 Subsystem 1 (Chiller)

Figure 5.2 illustrates the subsystem which corresponds to the actual model that is inside the chiller block in the main system. The fluid used for the existing chiller is R134a. In Table 5.2, the input parameters of the chiller are presented.



Figure 5.2: Illustration of the R134a chiller (10kW) as it was modelled in Dymola.

The components that are installed in the chiller cycle are the following:

- 1: a "Plate" heat exchanger operating as an evaporator with inlet temperature 12°C and outlet 7°C.
- 2: a "Separator" which splits the lubricating oil from the refrigerant.
- 3: a "ReciprocatingCompressor" with 50 Hz speed.
- 4: a "PIController" connected to the compressor to regulate the displacement based on the suction pressure.
- 5: a "FinAndTube" heat exchanger operating as a condenser with inlet temperature 20°C and outlet 25°C.
- 6: an "OrificeValve" working as an expansion valve.
- 7: a "PIController" connected to the valve to regulate the superheat at 5K.

Characteristicts	
Refrigerant	R134a
Evaporating Temperature (°C)	7
Condensing Temperature (°C)	25
Superheat (K)	5
Suction Pressure (bar)	3.15
Discharge Pressure (bar)	6.65
Mass Flow (kg/s)	0.06
Enthalpy h1 (kJ/kg)	403
Enthalpy h2 (kJ/kg)	425.6
Enthalpy h3 (kJ/kg)	234.3
Enthalpy h4 (kJ/kg)	234.3
Is entropic Efficiency (n_{is})	0.70

Table 5.2: Input parameters for subsystem 1 with R134a.

The CO_2 chiller, which will replace the R134a chiller, has exactly the same design in Dymola as the one in Figure 5.2. The only difference is the different input parameters used, as seen below in Table 5.3.
Characteristicts	
Refrigerant	CO_2
Evaporating Temperature (°C)	7
Condensing Temperature (°C)	25
Superheat (K)	5
Suction Pressure (bar)	37
Discharge Pressure (bar)	64.27
Mass Flow (kg/s)	0.06
Enthalpy h1 (kJ/kg)	438.5
Enthalpy h2 (kJ/kg)	470.5
Enthalpy h3 (kJ/kg)	274.5
Enthalpy h4 (kJ/kg)	274.5
Isentropic Efficiency (n_{is})	0.70

Table 5.3: Inputs parameters for subsystem 1 with CO_2 .

5.3.3 Subsystem 2 (AHU)

In Figure 5.3, the representation of the AHU cycle can be observed, modelled in Dymola, which corresponds to the same named block in the main system. In Table 5.1, the input mass flow rates for air and water are presented.



Figure 5.3: Illustration of the AHU as it was modelled in Dymola.

The components that are installed in the AHU are the following:

- 1: two connected "Tubes" to direct an amount of returned air to the supply pathway achieving heat recovery.
- 2: a "FinAndTube" heat exchanger which uses water to cool the air. The inlet air temperature is 23°C and the outlet 18°C.
- 3: a "SimpleFan", with 0.7 efficiency, which pushes the supply air into the office.
- 4: a "SimpleFan", with 0.7 efficiency, which directs the returned air out of the system.

5.3.4 Subsystem 3 (Office)

Each office corresponds to a 10 kW constant load. Figure 5.4 illustrates the office as a model in Dymola.



Figure 5.4: Illustration of the office, with load 10kW, as it was modelled in Dymola.

The only component used here is the "Volume" (1) representing the office space. It is dimensioned with a volume of 609 m³, as calculated in the following Section 5.5, and it is connected to a "BlockSource" (2) that defines the constant load.

5.4 Main System with Dynamic Load

The system was also modelled with a dynamic load of 24 hours in order to observe how the overall capacity changes throughout the day. The "Volume", representing the office, is now connected to a "FileReader" which takes as inputs the different calculated loads from an Excel file and gives the signal to the system to also start changing temperature and pressure values. The mass flows of the air and water have to remain constant, as was previously explained in Equation 5.1. This time the system was designed with only one subsystem of each kind for time-saving reasons and it is illustrated in the following Figure 5.5.



Figure 5.5: Illustration of the system on a smaller scale with the dynamic load as it was modelled in Dymola.

5.5 Office Volume Calculation based on the Internal Gains

The offices' volume was calculated based on the heat dissipation values from TEK17 [61] and ASHRAE Standard 55 [62]. Thus, according to ASHRAE, one person doing office work emits 1.2 Met, corresponding to 70 W/ m^2 [62]. From the Du-Bois body surface area, arises the fact that the human body has an average surface of 18 m^2 [63]. The heat emission from a person is then calculated in the following Equation 5.2:

$$Heat_{person} = 70(W/m^2) * 1.8(m^2) = 126W/person$$
(5.2)

In addition, the average heat dissipation from a computer is 110 W/person. If the lighting and the other technical equipment's emissions are considered, then an extra 100 W/person can be assumed.[62] So, the final value for the heat coming from equipment installations, corresponding to one person, and the total internal gain value are calculated in Equations 5.3 and 5.4 respectively:

$$Heat_{equipment} = 110(W/person) + 100(W/person) = 210W/person$$
(5.3)

$$Total_{heat} = 210(W/person) + 126(W/person) = 336W/person = 0.336kW/person$$
(5.4)

Since the load of each office is 10 kW and the heat per person is now known, the number of employees can be calculated, as shown in Equation 5.5:

$$Employees = \frac{10(kW)}{0.336(kW/person)} = 29.7, \ so \ 29 \ people$$
 (5.5)

Based on the royal Netherlands standardization institute (NEN) [64], 7 m^2 of space corresponds to each person. From this and the number of employees, the area of the building can arise in Equation 5.6:

$$Area = 29(employees) * 7(m^2) = 203m^2$$
(5.6)

Typically, the height of a floor in a building is 3 m [61] together with the concrete roof slab. In this case, there is only one floor so the volume of each office room can result in the following Equation 5.7:

$$Volume = 203(m^2) * 3(m) = 609m^3$$
(5.7)

5.6 Dynamic Load

The calculation of the dynamic load was made only for 24 hours, based on certain assumptions for a typical working day at CERN, since it is an office space and every day presents almost the same load variation. From Section 5.5 above, the number of employees resulted to be 29 for a 10 kW office. In Table 5.4 the number of people, that are present in the office each hour, is explained along with the assumptions made.

The load for each hour was calculated from the following Equation 5.8.

$$Load = Total_{heat} * Employees_{present} = 0.336kW * Employees_{present}$$
(5.8)

At this point, it should be mentioned that the load can never be zero due to the fact that some of the technical equipment is always turned on. So during the hours that no one or just a few people are present in the office, the load reaches 50% of the heat gains coming from the equipment and lighting.

This means that the minimum load that can be reached is 3.05 kW, calculated from the following Equation 5.9:

$$Load = \frac{Heat_{equipment}(W) * Employees}{2} = \frac{210(W) * 29}{2} = 3045W = 3.05kW$$
(5.9)

As is shown from the dynamic load calculation method followed, only the heat dissipating from the internal gains was taken into account. In realistic conditions, the outdoor temperature, the materials and the thermal bridges of the building are also included but due to the lack of this information, they were considered negligible for this project.

Table 5.4: Calculated load for the employees that are present in the office space every hour during a working day.

Time	Employees	Working Program	Load (kW)
*00:00 - 7:00	0	No one is present	3.05
8:00	15	Working day starts (flexible program)	5.04
9:00	29	All employees are present	10
10:00	29	All employees are present	10
11:00	29	All employees are present	10
12:00	12	Lunch break starts	7.6
13:00	17	Some may go later for lunch break	7.73
14:00	29	All employees are present	10
15:00	29	All employees are present	10
16:00	18	Typical working day ends	6.05
17:00	9	People that started work later may be still in the office	3.05
18:00	2	Some of them may need to work extra hours	3.05
*19:00 -23:00	0	No one is present	3.05

5.7 Equations for Chiller Systems

In this section, useful equations for the calculation of loads, electric power and COP of the system are given. All of them were used in order to figure out the corresponding values.

5.7.1 Compressor Work (\dot{W})

The electrical demand of a heat pump or chiller is represented by the compressor work, as described in Section ??. The following Equation 5.10 is used to compute compressor work.

$$\dot{W} = \frac{\dot{m}(h_{discharge} - h_{suction})}{\eta_{isentropic}}$$
(5.10)

5.7.2 Condenser Heat Rejection $(\dot{Q_C})$

The heat rejection from a condenser is calculated by Equation 5.11. This heat is energy that is being transferred from the system to the heat sink.

$$\dot{Q}_C = \dot{m}_R \Delta h_C \tag{5.11}$$

5.7.3 Evaporator Cooling Effect $(\dot{Q_E})$

The evaporator's cooling effect, commonly known as its heat absorption, is determined by Equation 5.12. The evaporator absorbs heat from the heat source.

$$\dot{Q}_E = \dot{m}_R \Delta h_E \tag{5.12}$$

5.7.4 COP calculations

The COP in a chiller represents its cooling capacity. It is measured by the relationship between the evaporator's cooling output and the compressor's electric input. The COPs for the cold side, hot and cold side are calculated with Equations 5.13-5.14, respectively.

$$COP_{cold\,side} = \frac{\dot{Q}_E}{\dot{W}} \tag{5.13}$$

$$COP_{both\ sides} = \frac{\dot{Q}_C + \dot{Q}_E}{\dot{W}} \tag{5.14}$$

6 Results and Discussion

In this section, the outcomes from the various simulated models in Dymola are presented. The findings are then examined and compared to determine which model performs the greatest, particularly in terms of energy efficiency (COP).

6.1 Main System



Figure 6.1: Illustration of the main system with results from Dymola.

From the results of the main system's simulation, which can be observed in the above Figure 6.1, the conclusion that arises is that the required values for temperatures, pressures and mass flows have been achieved. The differences in some of the results in comparison to the required values are very small. This means that the methodology used, for the system's design in the software, was successful. At this point, it should be mentioned that the figure is a representative image of the main system modelled with R134a as a fluid. However, almost the same results have also been accomplished with the CO_2 as the used refrigerant. For better understanding, the results will be analysed in detail in the following sections.

6.2 Subsystem 1 (Chillers)

In this section, the chillers' results from both refrigerants (R134a, CO_2) will be analysed in more depth and discussed. First, they will be examined as they were originally designed like independent systems and afterwards, they will be studied as subsystems connected to the main system.



Figure 6.2: Illustration of the R134a chiller with results from Dymola.

Figure 6.2, shows the result values of the chiller as an independent system, directly from the simulation in Dymola. Each value comes from the corresponding sensor, representing the pressures, enthalpies, temperatures and mass flows of the cycle. While Table 6.1, gathers all the simulation results from the chiller as an independent and as a connected system along with the required designed values.

Parameters	Independent System	Connected System	Designed Values
Compressor Work (kW)	1.67	1.73	1.34
Heating Capacity (kW)	11.85	12.43	11.34
Cooling Capacity (kW)	10.17	10.7	10
Hot Side Temperatures (^{o}C)	20/25.84	20/26.12	20/25
Discharge Pressure (bar)	7.92	8	6.65
Cold Side Temperatures (o C)	6.95/12	7.63/12.73	7/12
Suction Pressure (bar)	3.15	3.15	3.15
Mass Flow (kg/s)	0.059	0.062	0.059
$COP_{cold \ side}$	6.09	6.18	7.47
$COP_{hot-and cold-side}$	13.2	13.37	15.9

 Table 6.1: Simulation result summary for R134a chiller.

From the above table, it can be seen that the numbers between the independent system and the designed values are not far from each other. Their difference is that the Dymola results for the upper part of the cycle present an almost negligible rise in comparison with the required ones. This is clearly a matter of the cycle's design into the program and the assumptions made about the size of the components (heat exchangers, compressors, valves) since there was no detailed information for the design, given by CERN. Thus, the cooling capacity of the chiller is 10.17 kW when the designed value is set to 10 kW, only 0.17 kW lower. Respectively, the value from the heat rejected from the condenser is 11.85 kW, slightly increased from the 11.34 kW that was requested.

Another worth noting point is that when the chiller operates as a subsystem of the main system its values are increased in comparison with the values of the independent system. This is due to the fact that more components (pump, hydraulic capacitor) are added for the connection of the chiller to the AHU, which makes the overall electrical input of the system rise. Further, for the independent system, the inlet water temperature at the evaporator is constant at 12°C as it is not affected by the cycle but for the connected system, this value is affected by the return temperature from the AHU so it starts changing. However, the temperature that remains constant in all systems is the inlet air temperature at the condenser which is set at 20°C.

As it was expected, the COPs coming from Dymola are also different from the designed ones. Since both cooling and heating loads together with the compressor's work are higher than the designed values, the COPs will be less. Therefore, for the independent system the $COP_{cold\,side}$, which is the most important for a chiller, is calculated to be 6.09 while the requested is 7.47. Further, the $COP_{cold\,side}$ for the connected system is 6.18 which makes it closer to the desired value. In any case, even though it is a little decreased, it is still a COP value that is considered to be very efficient.



Figure 6.3: Illustration of the log P-h and T-s diagrams from R134a chiller cycle.

Figure 6.3 shows the log P-h and T-s diagrams of the simulated independent chiller. One point that could be discussed is the high discharge temperature at the T-s cycle. As can also be seen from the previous Figure 6.2, the specific temperature reaches 47.41°C when the designed temperature is only 39°C. This is probably a problem coming from the size of the compressor since the discharge pressure is also a little bit higher (7.92 bar) than the requested value (6.65 bar), as was presented in Table 6.1. As for the diagrams from the connected system, they would be more-less the same since its values are

not far from the independent system. Once again, the discharge temperature will be higher as it faces the same problem.

6.2.2 CO₂ Chiller

The results for the CO_2 independent chiller can be seen either from Figure 6.4, illustrated exactly as they were at the modelled cycle, or from Table 6.2 along with the results from the connected system and the designed values.



Figure 6.4: Illustration of the CO₂ chiller with results from Dymola.

Parameters	Independent System	Connected System	Designed Values
Compressor Work (kW)	2.09	2.43	1.95
Heating Capacity (kW)	11.94	13.06	11.95
Cooling Capacity (kW)	9.85	10.63	10
Hot Side Temperatures (^{o}C)	20/25.89	20/26.43	20/25
Discharge Pressure (bar)	68.21	68.57	64.27
Cold Side Temperatures (o C)	7.3/12	7.74/12.81	7/12
Suction Pressure (bar)	37	37	37
Mass Flow (kg/s)	0.059	0.069	0.06
$COP_{cold\ side}$	4.72	4.37	5.12
$COP_{hot-andcold-side}$	10.4	9.75	11.26

Table 6.2: Simulation result summary for CO_2 chiller.

From the findings gathered in Table 6.2, it can be observed that the Dymola values for the independent system are almost the same as the designed ones. There is a small rise with the most noticeable one being at the compressor work where the result is 2.09 kW while the requested was 1.95 kW. This is probably due to the fact that the compressor size was not known so the method of trials and errors was used to find an optimal displacement that could reach as close to the design value as possible. Therefore, the discharge pressure resulted to be increased by almost 4 bar from the requested value and consequently, the enthalpy at that point (see Figure 6.4), which is responsible for the compressor work, got raised.

The cooling and heating capacities are close enough to the correct numbers which also make both of the COPs close to the designed ones. However, due to the small exclusion at the capacities and the increased value of the compressor work, they are a little bit lower than the designed COPs. Specifically the $COP_{cold \ side}$ is calculated to be 4.72 while the requested was 5.12. Either way, it is considered a good COP for a chiller.

As happened before, with the R134a chiller, when the CO_2 chiller operates as a connected subsystem its simulation values are augmented in comparison to the same chiller when it functions independently. In this case though, the rise in the numbers is higher than previously. The most worth mentioning difference is between the heating capacity values, where the independent system has 11.94 kW, almost the same as the designed value, and the connected system reaches 13.06 kW. This is due to the compressor's increase which caused the rise in discharge pressure and enthalpy. The enthalpy at the superheated area has a decisive role in the calculation of the condenser's capacity. Moreover, contrary to the R134a case, the COP values here are less than the ones from the independent chiller and the reason behind it is once again the escalation of the electric input.

Moving forward, the log P-h and T-s diagrams of the independent chiller, modelled in Dymola, are illustrated in the following Figure 6.5. From the log P-h diagram, the CO₂ cycle can be seen working subcritical, as it should, while in the log T-s diagram an observation could be mentioned concerning the discharge temperature. It is also shown in Figure 6.2.2, that the value is 59.95°C while the correct one is calculated at 55.3°C. A noticeable increase, which can be again attributed to the compressor's size since the discharge pressure was also raised, as previously discussed. The same stands for the diagrams corresponding to the connected system.



Figure 6.5: Illustration of the log P-h and T-s diagrams from CO₂ chiller cycle.

6.3 Subsystem 2 (AHUs)

The modelled AHU as a separate system is presented in Figure 6.6 with the simulation outcomes. Table 6.3 gathers all the result values for the AHU as an independent (in) and as a connected (co) system with a constant load for the different refrigerants. Along with them, the designed values are given.



Figure 6.6: Illustration of the AHU as an independent system with results from Dymola.

Parameters	AHUin	AHUco (R134a)	AHUco (CO ₂)	Designed Values
Cooling Coil Capacity (kW)	11.18	10.7	10.6	10
Intake Temperature (^{o}C)	23	23	23	23
Supply Temperature (^{o}C)	17.56	18.65	18.71	18
Return Temperatures (o C)	23	23.63	23.69	23
Exhaust Temperature (^{o}C)	23	22.63	22.66	23
Air Mass Flow (kg/s)	2	2	2	2

 Table 6.3: Simulation result summary for the different AHUs.

Based on the findings, the AHU as an independent system has achieved reaching all the designed values except for the supply temperature and the cooling coil's capacity. However, the supply temperature has a negligible difference from the required one. As for the capacity, it seems to be higher than the 10 kW that was asked. This is a matter of design of the heat exchanger in Dymola, probably the size and the number of tubes were not achieved successfully but it still is close enough to operate the system efficiently with the correct temperatures.

Concerning the system when it functions as a subsystem connected to the main network, it appears to surpass the designed values, for both refrigerants. Still, the simulation values are not far from the designed ones and it seems that for both of the fluids, the cooling capacity has dropped. In fact, it has aligned with the cooling capacity of the chillers that the AHUs are connected to, as was presented before in Tables 6.1 6.2. In addition, the supply and return air temperatures have increased since the water temperatures from the chillers were also augmented. This means that when the systems are connected they affect each other's operation, which is an expected outcome. Since the air's mass flow remains constant, the Q and the Δ T have to change as was previously explained in Equation 5.1.

Except for the mass flow, the other value that remains always constant is the intake air temperature because it is set as the ambient air value. This is not true though for the exhaust temperature due to the fact that before the air gets released to the environment, it passes through tubes that connect the exhaust with the incoming path and recover some of the heat which is then directed to the incoming stream. This justifies, for both of the refrigerants, the exhaust temperature values which are below the return temperatures. Yet in this specific case, where the load is at its maximum, the heat recovery is inefficient. This phenomenon will be better explained in the following Section 6.4 with the AHU operating under dynamic load.

6.4 Main System with Dynamic Load

The main system was simulated in Dymola with a dynamic load in order to observe the way it functions under realistic conditions throughout 24 hours. Figure 6.7 shows the results of the simulation caught up in the moment when the load was 10 kW. It is a representative image of the system running with the R134a as a refrigerant, while the same illustration of the system operating with CO_2 can be found in Appendix A.1.

When the system is at 10 kW, it has the same result values for the chiller and the AHU as the ones that were discussed in the previous sections where the load was constant. Nevertheless, the hours that the load varies the numbers for temperatures, pressures and capacities change. The mass flows for water and air remain constant in all cases.



Figure 6.7: Illustration of the Dymola results for the main system operating with R134a and having a dynamic load. The image illustrates the system at a moment when the load is 10 kW.



Figure 6.8: Diagram representing the dynamic load of the systems in relation to 24 hours.

Figure 6.8 shows the dynamic load, that was calculated based on the internal gains in an office room and explained in Section 5.6, in relation to one typical working day schedule. When all of the people are present in the room, the load is set at 10 kW which is the maximum value it can reach. On the other hand, during the hours that some of the employees leave, the load starts decreasing until it drops to 3.05 kW when no one is present in the office. Nonetheless, the load does not go to zero due to the fact that some of the equipment is still on, even during the night. This load is the same input for both systems with R134a and CO_2 refrigerants.

6.4.1 Dynamic Chiller with R134a

The results of the main system running with dynamic load and using R134a as a working fluid are presented in this section. The following diagrams will aid in the understanding of the chillers' operation.

Figure 6.9 below, illustrates the variation in heating and cooling capacities of the chiller throughout the day. These capacities are presented in relation to the compressor's work and as it can be observed when the input load increases, at the hours the employees are in the office, both the Qs and the W are also augmenting. Specifically, the heating capacity from 12.32 kW tops up to 12.43 kW and the cooling capacity from 10.61 kW goes to a maximum of 10.7 kW. They both reach their higher values when the load is 10 kW, the same values as the ones when the system was connected to a constant load. The same stands for the compressor work's number fluctuations.



Figure 6.9: Diagram representing the heating and cooling loads of the R134a chiller in relation to the compressor's work.



Figure 6.10: Diagram representing the $COP_{cold \ side}$ of the R134a chiller in relation to the dynamic load.

The performance of the chiller is shown in Figure 6.10 and it is illustrated in relation to the load variations. From the previous diagram, it was explained that when the input load increases the same happens for the capacities and the compressor work. Nonetheless, with this rise of the values the $COP_{cold\,side}$ decreases, since it is an outcome of their ratio. This happens at the hours that the employees are present in the office and the chiller is expected to function at higher cooling demand, making the system less efficient. The highest $COP_{cold\,side}$ is at 6.22 and the lowest is at 6.18, a difference that is considered quite small.

6.4.2 Dynamic Chiller with CO₂

In this part, the results of the main system running with dynamic load and using CO_2 , as a refrigerant, are presented. The simulation outcomes are illustrated in diagrams.



Figure 6.11: Diagram representing the heating and cooling loads of the CO_2 chiller in relation to the compressor's work.

The above Figure 6.11 shows the fluctuation of the CO_2 chiller's capacities in relation to the compressor's shaft power. As happened before, with the R134a system, both the evaporator and condenser capacities are increased when the internal gains of people and technical equipment are high, during working hours. The cooling load from 10.54 kW elevates to 10.63 kW, while the heating load from 12.94 kW climbs to 13.06 kW. Moreover, the compressor work from 2.40 kW increases to 2.43 kW. All of them, reach the same values as the connected system with a constant 10 kW load. It is worth noting that there is no significant difference in the values even when comparing the lowest and the highest prices.

Ideally, it is better for the compressor's work to vary slightly when a chiller is operating. This is due to the fact that small variations in the compressor's operation aid to maintain a constant temperature and minimise compressor wear and tear. On the other hand, when fluctuations in the compressor's performance are significant they might create temperature swings and make it work under harder conditions, which can increase the energy use and shorten the compressor's lifespan.

Furthermore, the cooling performance of the CO_2 chiller is illustrated in the following Figure 6.12. It can be observed that as the internal gains elevate, the $COP_{cold \, side}$ decreases and the system becomes less efficient. More specifically, it starts at 4.39 when no one is present in the office and it falls down to 4.37 during the hours that all the employees are working and the internal load is 10 kW.



Figure 6.12: Diagram representing the $COP_{cold \ side}$ of the CO_2 chiller in relation to the dynamic load.

6.4.3 Dynamic AHUs

The AHUs for both systems (R134a, $C0_2$) are discussed in the same section as their resulting temperatures are almost the same, making their diagrams look identical. Since the temperatures are the same so is the heat recovery amount the systems achieve.



Figure 6.13: Diagram representing the air temperatures' fluctuations in the AHU in relation to the dynamic load.

Figure 6.13 represents the fluctuations in temperatures corresponding to the variation of the dynamic load. As can be seen, all temperatures during the hours that the employees are not present in the office, remain constant. During that time, the supply air in the room is 16.1°C and the return is 17.6°C. These temperatures give only a 1.5°C difference, which means that the cooling coil does not need to consume much electricity to cover this gap and results in energy savings and less operational costs. The fact that most of the hours of the day are covered by a low load, due to the cause that the building is not residential, aids even more in achieving these savings. However, when the load starts increasing the temperatures follow and this does not apply anymore.

Another important part worth focusing on is the change in the return and the exhaust air lines along the day. During the nighttime and the hours that the load is constant, the return air stream is lower than the exhaust. On the other hand, when the employees start reaching the office, the return air rises until it overpasses the exhaust air, at a load of 10 kW. At this specific time, the return air is also higher than the mixed air, which is the stream resulting from the combination of the incoming and the air from the heat recovery.

In terms of heat recovery, as the load increases the efficiency of the heat recovery system decreases. Higher load results in a higher demand for cooling capacity, which lowers the temperature difference between the exhaust and incoming air streams. Here, which is a case of a cooling system, the heat recovery system extracts the heat from the air and returns it to the heat source. Then the cooler air is directed to the incoming pathway and precools it before it is inserted into the cooling coil. This is achieved when the load is low, the exhaust line is higher than the return and the mixed air is cooled below 23°C. On the contrary, when the return air overpasses all lines the system does not recover the cold air anymore and forces the cooling coil to consume more energy to cool the incoming air. This is the reason the mixed stream reaches 23°C at that time.



Figure 6.14: Diagram representing the heat recovery in the AHU in relation to the dynamic load.

In Figure 6.14 the amount of heat recovery succeeded can be better explained. At the lowest load of 3.05 kW, the system recovers 0.38 kW of heat, which is approximately 12.5% of the total load. It is an amount which can result in energy savings and fewer operation costs but it can not be characterized as significant. Usually heat recovery systems can recover 60-80% of waste heat. In the case of R134a, the return air is 17.6° C, the exhaust 19.2° C and the incoming 23° C. Nonetheless, when the load is 10 kW the heat recovery is 0.04%, almost zero. This is because the return temperature has risen up to 23.63° C while the exhaust is 22.63° C and the incoming is 23° C. The same stands for the CO₂ system just with a negligible variation in the temperatures.

6.5 Systems Comparison

This section is dedicated to comparing the different systems based on their simulation results from Dymola, their opportunity costs and sustainability, and the heat recovery potentials from the chillers.

6.5.1 Simulation Results

The different systems are compared as independent (in), as connected constant (co) systems with 10 kW and as dynamic (dy) with the lowest possible load, 3.05 kW. The comparison will be achieved through tables marked with the aforementioned symbols corresponding to the kind of system referred to along with its refrigerant.

	10 kW		10 kW		3.05 kW	
Parameters	$R134a_{in}$	CO_{2in}	$R134a_{co}$	CO_{2co}	$R134a_{dy}$	CO_{2dy}
COP _{cold side}	6.09	4.72	6.18	4.37	6.22	4.39
Cooling Capacity (kW)	10.17	9.85	10.7	10.63	10.61	10.54
Compressor Work (kW)	1.67	2.09	1.73	2.43	1.71	2.40

 Table 6.4: Summary of all chillers' simulation results.

Starting with the chillers, Table 6.4 provides an overview of all the important results that need to be discussed. The first thing that must be mentioned is that in general, all the independent systems had certain small differences from the designed values from the beginning. For both fluids, the differences were noticed mostly in the upper parts of the chillers with the values being a little bit higher than requested. As was expected, this also affected the COPs that were found to be less than the designed ones. The main reason for that is the method used for the design of the system in Dymola, the kind of components and the sizes that were chosen. However, having small exclusions from the original design is something that can happen in reality when a system is getting built.

Moving to the connected systems, when the load is 10 kW both of the chillers' values increase and surpass the designed ones for both upper and lower parts. This has to do with the rise of the electric energy when chillers and AHUs are connected, which forces the overall heat in the components to elevate. Therefore, the temperatures of the water in the pipes that connect the systems augment and, since the mass flow remains constant, the Qs and all the other values are getting increased too. When the load is dynamic and falls to its lowest value, which is 3.05 kW, the values may decrease but they

still remain higher than the ones of the independent systems. Even though the load drops to less than 50% of the total, the differences in the prices are not significant.

From Table 6.4, it can be observed how COPs are affected by the fluctuations of the load. Specifically for the R134a system, the cooling capacity is higher when the system is connected but the highest $COP_{cold\ side}$ exists when the load is at its lowest. This is natural to occur since the calculation of it, comes from Equation 5.13 which is basically Qe/W. On the other hand, the CO₂ system possesses a higher $COP_{cold\ side}$ when it works as an independent chiller. Apparently, when the system is connected the electric input rises enough to increase the compressor's work in a way that makes the system less efficient. This can also be seen at the time the load has dropped and the $COP_{cold\ side}$ is higher but yet remains lower than the independent one. Consequently, it seems that in terms of operation, based on the design chosen for the modelled systems, the R134a chiller performs more efficiently than the CO₂ chiller.

As for the AHUs, when they operate as independent systems the values are all set according to the requirements with the exception of the cooling coil's capacity which is 11.18 kW. This again is related to the heat exchanger's choice and design method. Nevertheless, when the AHUs are connected as subsystems of the main system the cooling capacities align with the ones from the chillers and start appear fluctuations in the temperatures of the air streams instead. In general, the subsystems have managed to save much energy and operational costs due to the hours the load is low, as the supply and the return temperatures are almost the same, making the systems quite efficient.

In the case the load increases, so do the temperatures resulting in the prevention of achieving efficient heat recovery. This is due to the fact that the demand for cooling capacity elevates and the exhaust air approach dramatically the incoming air temperature. Thus, the only hours that the system can extract some cold air from the return stream and direct it into the supply, in order to precool it and save energy, is when the load is low at 3.05 kW. Even then, the heat recovery succeded is estimated at 12.5% which is not considered enough. The same stands for both AHUs, which gives the conclusion that their chillers, even if they present some small differences between them in relation to the resulted values and design, both affect them in a way which gives the overall systems almost the same results.

Regarding the efficiency of the heat recovery, many aspects can be accounted responsible for it but the main one is the configuration of the system. In this project, the AHUs were designed with a simple form of heat recovery system by using two pipes connecting the exhaust with the incoming stream to transfer some of the extracted cold. This simple form is easily affected by load variations which makes it less efficient in comparison to plate heat exchangers and thermal wheels which are usually preferred. In addition, some AHU systems are built with variable speed drives or other control strategies that allow them to adjust the airflow and temperature setpoints so that their heat recovery efficiency remains consistent regardless of the load changes. These are all parameters that were not taken into account mostly due to the lack of data and the desire to focus more on the chillers.

6.5.2 Opportunity Cost and Sustainability

One of the main differences between the R134a and the CO_2 as refrigerants, is that the first one is a synthetic and the second a natural fluid. Even though both of them have zero ODP the fact that the R134a presents a very high GWP makes it inappropriate for use. As previously mentioned in Section 3, it has already been banned in most refrigeration systems, especially those for air conditioning. On the contrary, CO_2 not only has a negligible footprint but by replacing the current systems at CERN

with it, it will aid in the decarbonization of the whole network. It is worth mentioning that the electric grid in Switzerland is aiming towards a 100% emission-free electricity supply by 2050 [65], which would reduce the carbon footprint of the chillers' operation in the area to practically zero. Thus, CO_2 systems could rightfully be characterized as a sustainable solution.

In terms of safety both the refrigerants are classified as A1 class, which means that the systems using them do not face any specific safety concerns. This automatically reduces the expenses for the installation of expensive safety equipment and maintenance costs. However, the unique ability of the CO_2 to operate with higher evaporation and absorption temperatures than the other fluids allows it to utilize smaller pipes and have less refrigerant circulating into the system. Consequently, the operation costs of the chiller are decreased. In addition, since R134a is synthetic and the European legislation has become stricter [40], its price has been increased and its availability has been limited.

6.5.3 Waste Heat Recovery Potentials

Concerning the potentials of waste heat recovery between the two chiller models, CO_2 is considered the most optimal choice. In general, this natural refrigerant has the ability to reach significantly higher temperatures in the superheated area in contrast to R134a and it is able to recover 40% of that heat when it operates in subcritical mode. While the HFCs refrigerants can only recover 10-15%.[17] Additionally, when it switches to the transcritical phase it can recover even more waste heat. For these reasons, only the CO_2 chiller is further analysed.

To begin with, in the modelled systems the heat is rejected to the environment without taking any advantage of it. With the use of CO_2 though, the waste heat will be a better quality of heat which will be able to be stored in hot water tanks and then used for space heating purposes. The temperature needed for this kind of use is between the range of $30^{\circ}C$ and $55^{\circ}C$ [17]. In general, the use of waste heat can be utilized even when the system operates subcritical. In this specific case though, where the inlet air temperature to the condenser is only $20^{\circ}C$ and the outlet $25^{\circ}C$, the requirements for direct heat recovery are not met. Therefore, the high pressure needs to be increased and by doing so, the operation mode will probably have to switch from subcritical to transcritical. There, the condensation process stops to occur and the relationship between pressure and temperature is not clear.

In the modelled chiller, if the inlet air temperature rises to 45°C, on an extremely hot summer day, the high pressure would reach 111 bar and the outlet air temperature would be almost 52°C, a suitable temperature for the space heating. However, with the rise in the condensing temperature, the electric input also increases making the system less efficient, as can be seen clearly in the diagram calculated in CoolPack and illustrated in Figure 6.15. In order to avoid that, a suction gas heat exchanger should be placed downstream of the compressor to keep the temperature before the gas cooler at a low level, as shown in Figure 6.16. With the implementation of a suction gas heat exchanger, the heat at the superheated area will be recovered and directed into a water loop connected to the water tank. In this way, energy recycling is achieved, the lifespan of the components is extended, which signals the reduction of both operation and maintenance costs, and the environmental footprint is minimized, as much as possible.



Figure 6.15: Diagram illustrating the $COP_{hot-and cold-side}$ of the CO_2 chiller in relation to the inlet air temperature.

Figure 6.15 shows the passing from subcritical operation to transcritical and the way the chiller's performance is affected. At the beginning where the inlet air temperature is 20°C the $COP_{hot-and cold-side}$ value is 10.4, as was previously seen from the simulation model results. Yet, as the temperature increases the $COP_{hot-and cold-side}$ decreases reaching at the end the value of 4.



Figure 6.16: Schematic diagram of the CO_2 chiller with the waste heat recovery circuit.

7 Conclusions

This report aims to raise awareness regarding energy use and the environmental footprint of CERN due to the experiments performed. To achieve this, the currently installed systems at the organization are mapped and new proposals for their replacement with more sustainable solutions are suggested.

To begin with, CERN is a European organization which is dedicated to experiments concerning physics. By using particle accelerators, it consumes a significant amount of energy which is now considered unacceptable. In addition to this, the campus contains building blocks, dating from the 70s, which have been installed with old heating and cooling systems and are supplied by a district heating network with gas-fired boilers. The CO_2 emissions dissipating from them are acknowledged as a considerable source of environmental pollution and the necessity of putting an end to it is now greater than ever.

As for the water usage, needed for the cooling of the systems, it presents a high amount of consumption which needs to be reduced to 5% in the upcoming years. The heat in the systems is rejected from the water evaporation in the cooling towers without being recovered, resulting in huge energy loss. Due to all these reasons, the organization faces forces from the European legislation to minimize its energy utilization and follow the path of sustainability. Thus, a Masterplan has been developed which predicts the construction of energy efficient infrastructures and the optimization or replacement of the systems' technologies in order to reduce the carbon footprint by the year 2040.

Having the environmental aspects in mind, the engineering community has shifted to the preference of using combined systems that are able to achieve waste heat recovery and store thermal energy for later use. By adopting this kind of tactic, the energy and operation costs can be reduced by far and the fossil fuels systems can be eliminated. In this effort for improvement, the limitation in the utilization of synthetic refrigerants has become stricter and the weight has been shifted to the natural fluids.

Through a detailed analysis of natural and synthetic refrigerants, the outcomes that prevailed were that R134a has the highest value for GWP while ammonia has zero impact. Nevertheless, ammonia is a fluid that is both toxic and flammable which classifies it as B2L. The only fluids that were categorized as A1 class are the R134a and the CO_2 , which has no auto-ignition temperature. Since CO_2 belongs to the 1st generation it is automatically considered a better choice. Its critical point is lower than the others' and it is optimal for operation in low and medium temperatures. In case it has to operate in higher temperatures than 31°C the fluid must change from subcritical to transcritical phase. The refrigerant with the highest critical point is ammonia, while R134a, R1234ze(E) and isobutane are placed almost in the same line of working area.

Concerning the study case of this report, a combination of cooling and ventilation systems that exist in a typical office building at CERN was investigated. Specifically, two 10 kW air-cooled chillers operating with R134a provide cold water to two AHUs in order to cool down two office spaces. The aim was to examine the network, address the problems it may faces and propose more advanced solutions. The methodology used for this investigation includes the design of both the existing system and a new similar one with CO_2 as a refrigerant. The design was made in the dynamic software Dymola and a comparison of their simulation results arose. In more detail, the simulations were made with both a constant load of 10 kW and a dynamic load calculated based on the heat dissipating from the internal gains, representing a 24-hour typical working day at the organization. According to the simulation results, all of the systems were validated efficiently with only small exclusions, in some cases, that are considered negligible. A worth noting point is that when the chillers, the AHUs and the offices are connected, operating as a whole network all the values increase a bit due to the rise in the electric input and the thermal energy coming from the different components. Nonetheless, this complex becomes more efficient with the implementation of a dynamic load as the cooling demand is reduced when the employees are not present in the office, making the load drop to 3.05 kW which is less than half of the 10 kW constant one. Thus, the COP rises at that time and the systems' performance becomes more energy efficient with fewer operation costs and energy consumption.

Specifically for the AHUs, when the network operates with a dynamic load the energy savings topup outside the working hours, where the load is at its lowest. During these hours, the supply and the return temperatures in the offices present only a 1.5°C difference which aids the cooling coil to maintain a steady function without high cooling demands. At that time, the heat recovery system which connects the exhaust with the supply air stream succeeds to recover its maximum amount of energy by extracting the cold from the return path and directing it into the supply. This amount is calculated to be 12.5%, a percentage capable of reducing the operating expenses and the overall energy consumption of the system but with the potential of receiving further improvement in order to become more efficient. Still, when the load increases the heat recovery gradually stops working until it reaches 10 kW where it is characterized as inefficient.

What is more, from the comparison of the systems using the two different working fluids the conclusion that CO_2 has more advantages than R134a arose. Its ability to not cause any harmful impact on the environment surpasses every positive aspect of the R134a which presents a high GWP. Except for that, this synthetic refrigerant, like all of the HFCs, is banned from use in refrigeration applications and the European legislation has set strict limits regarding its transportation, making it harder to be supplied and even more expensive. On the contrary, CO_2 as a natural refrigerant is an easy solution regarding its availability and due to the fact that it operates in high evaporation temperatures, its components are smaller and less fluid is needed in the system. All these aspects make it a cost-effective option with reduced installation and operation expenses.

Finally, CO_2 is known for its heat recovery potentials due to its operation in high pressures at the superheated area. The ability to switch from the subcritical to the transcritical phase allows it to work on a wider area than R134a and save more energy. In this case, the chiller has to escalate its discharge pressure by using a suction gas heat exchanger and switching to transcritical mode, in order to store the recovered waste heat in hot water tanks that will be later used for space heating purposes. This solution will aid in minimizing the drop in its performance and it constitutes a sustainable outcome. Consequently, by replacing R134a with CO_2 in the systems it will result in the decarbonization of the CERN network and the reduction of the overall energy consumption.

8 Further Work

The report has fulfilled its obligations to the aforementioned sections, which included a thorough examination of the literature, a description of the primary study case, and simulations of the systems in Dymola. The findings of the investigation and the discussion part did, however, result in some conclusions that might be further examined. Suggestions that could prove valuable for expanding the thesis are covered in this section.

These proposals are listed below:

- Improvement of the design of the heat recovery system in the AHUs in order to achieve a higher percentage of waste energy.
- Simulations in Dymola for the hot water tanks that are connected to the CO₂ chiller to result in the exact amount of waste heat recovered in relation to the dynamic load.
- Implementation of a dynamic load in the systems that takes into account the outside weather temperatures of the building in order to simulate the models in more realistic conditions.
- Simulations with different natural refrigerants and comparison of their performance.
- Scale up the system to a 100 kW network in order to cover the energy needs of a whole office building.
- Replacement of the air-cooled chillers with water-cooled ones that are connected to cooling towers. Calculation of the waste heat recovery that can be achieved from the cooling towers.

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Figure A.1: Illustration of the Dymola results for the main system operating with CO_2 and having a dynamic load. The image illustrates the system at a moment when the load is 10 kW.



