

Simulation and LCA of amine scrubber for CO₂ capture with heat pump and electrode boilers

by

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Abstract

Terms such as "global warming," "net zero," and "CO₂ capture" are frequently encountered in discussions surrounding climate change. Although the mitigation of climate change through CO₂ capture is widely acknowledged, the sustainability of this process depends on the source of energy. This study involves performing simulations and life cycle assessments (LCA) to analyze the environmental impacts of different configurations employing amine-based CO₂ capture. Specifically, certain configurations include an electric boiler, heat pump technology, and mixing the concentrations of CO₂ in the ongoing flue gas by recycling CO₂ from the natural gas combustion, distinguishing them from the conventional method.

For the evaluation of different configurations, Aspen Plus v12.1 was used for simulation and GaBi 8.7 was used for LCA. Pinch analysis, which includes heat integration, was performed to minimize the reboiler duty for specific configurations.

Key results indicate the importance of energy sources in achieving decarbonization. Especially when powered by renewables, configurations employing heat pump technology and electrode boilers exhibit lower emissions and greater net reductions of CO₂ equivalents.

In conclusion, this thesis underscores the importance of the energy source in CO₂ capture sustainability. Heat pump technology and the conventional method employing electrode boilers are both seen as a viable option, especially when operated with renewable electricity, as opposed to the traditional practice of directly burning fossil fuels to generate thermal energy for reboilers. Future investigations could explore the comparison of ammonia based CO₂ capture systems or alternatively, investigate the potential of chilled ammonia-based processes, comparing its environmental impacts with the amine-based approach. This study contributes valuable insights to the development of more sustainable and effective strategies in the global effort to reduce climate change.

Zusammenfassung

Begriffe wie "globale Erwärmung", "Netto-Null", und "CO₂-Abscheidung" sind heute in Diskussionen über den Klimawandel häufig anzutreffen. Obwohl die Abschwächung des Klimawandels durch CO₂-Abscheidung allgemein anerkannt ist, hängt die Nachhaltigkeit dieses Prozesses von der Energiequelle ab. Im Rahmen dieser Abschlussarbeit werden Simulationen und Lebenszyklusanalysen (LCA) durchgeführt, um die Umweltauswirkungen verschiedener Konfigurationen der aminbasierten CO₂ Abscheidung zu analysieren. Bestimmte Konfigurationen umfassen einen Elektrodenkessel, eine Wärmepumpentechnologie, und die Vermischung der CO₂ Konzentrationen im laufenden Rauchgas durch Rückführung von CO₂ aus der Erdgasverbrennung, wodurch sie sich von der herkömmlichen Methode unterscheiden.

Für die Bewertung der verschiedenen Konfigurationen wurde Aspen Plus v12.1 für die Simulation und GaBi 8.7 für die LCA verwendet. Es wurde eine Pinch-Analyse durchgeführt, welche die Integration von Wärme einschließt, um den Reboilerbetrieb für bestimmte Konfigurationen zu minimieren.

Die wichtigsten Ergebnisse zeigen, wie wichtig die Energiequellen für die Dekarbonisierung sind. Insbesondere wenn sie mit erneuerbaren Energien betrieben werden, weisen Konfigurationen mit Wärmepumpentechnologie und Elektrodenkesseln geringere Emissionen und eine größere Nettoreduktion von CO₂ Äquivalenten auf.

Abschließend unterstreicht diese Arbeit die Bedeutung der Energiequelle für die Nachhaltigkeit der CO₂-Abscheidung. Sowohl die Wärmepumpentechnologie als auch die konventionelle Methode mit Elektrodenkesseln werden als umsetzbares Option angesehen, insbesondere wenn sie mit erneuerbarem Strom betrieben werden, im Gegensatz zur herkömmlichen Praxis der direkten Verbrennung fossiler Brennstoffe zur Erzeugung von Wärmeenergie für die Reboiler. Künftige Untersuchungen könnten die vergleich des CO₂, das durch aminbasierte CO₂-Abscheidung gewonnen wird, mit CO₂ aus Ammoniakherstellung und ihre Umweltauswirkungen mit dem aminbasierten Ansatz vergleichen. Diese Studie leistet einen wertvollen Beitrag zur Entwicklung nachhaltigerer und wirksamer Strategien im Rahmen der weltweiten Bemühungen zur Eindämmung des Klimawandels.

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Nomenclature

Abbreviations

- CCS Carbon Capture and Storage
CCU Carbon dioxide Capture and Utilization unit
CCUS Carbon Capture, Usage and Storage
CDR Carbon Dioxide Removal
COP Coefficient Of Performance
COP Conference of Parties
DEA Diethanol Amine
EF Environmental footprint
EU European Union
FU Functional Unit
GHGs Greenhouse gases
GWP Global Warming Potential
ILCD International Reference Life Cycle Data System
IPCC Intergovernmental Panel on Climate Change
ISO International Organization for Standardization
LCA Life Cycle Assessment
LCI Life Cycle Inventory
LCIA Life Cycle Impact Assessment
PCC Post-Combustion Capture
ppm Parts per million
TEA Techno Economical Assessment
UNFCCC United Nations Framework Conventions on Climate Change
- Chemicals**
- CO Carbon monoxide
CO₂ Carbon dioxide

H_2 Hydrogen

MEA Monoethanol Amine

Parameters

ΔH_i Enthalpy of the reaction, (kJ/kmol)

μ_L Viscosity of the absorbent,(mPa s)

ϕ_L Association factor of the absorbent

ϕ_L^* Association factor of the absorbent

$P_{CO_2}^*$ Concentration of $CO_2(g)$ expressed as partial pressure, (bar)

P_{CO_2} Concentration of $CO_2(g)$ expressed as partial pressure, (bar)

$D_{CO_2,L}$ Diffusion coefficient of CO_2 in the gas phase (m^2/s)

K_L^* Liquid- side mass transfer coefficient without reaction (mol/ $m^2/s/kPa$)

K_G Overall mass transfer coefficient (mol/ $m^2/s/kPa$)

M_L Molecular weight of the absorbent L, (g/mol)

p Partial pressure of solute in gas phase, (bar)

p^* Partial pressure of gas in vapor phase over the liquid in equilibrium with the gas, (bar)

V_A Molecular volume of the species A, (m^3/mol)

H Henry's constant

k_i Equilibrium constant

P Total pressure, (bar)

R Universal gas contant

T Temperature, (K)

x Mole fraction of solute in liquid phase.

y Mole fraction of solute in gas phase

y^* Equilibrium mole fraction of solute in gas phase

Chapter 1

Introduction

1.1 Introduction

If you regularly read the newspapers or follow the news, it is difficult to escape without the term global warming in the headlines. From hurricanes to heatwaves, rising sea levels to bid farewell to glaciers, the issue of global warming is consistently mentioned. Comparing today's world with 3 or 4 decades ago, we are seeing extreme weather events and all thanks to human footprint.

Global warming is the term used to describe the gradual increase in the temperature of the earth's surface that has been observed since the preindustrial era (between 1850 and 1900). This phenomenon is mainly caused by human activities, specifically burning fossil fuels, which leads to higher levels of greenhouse gases in the atmosphere of the earth, resulting in the trapping of heat [1].

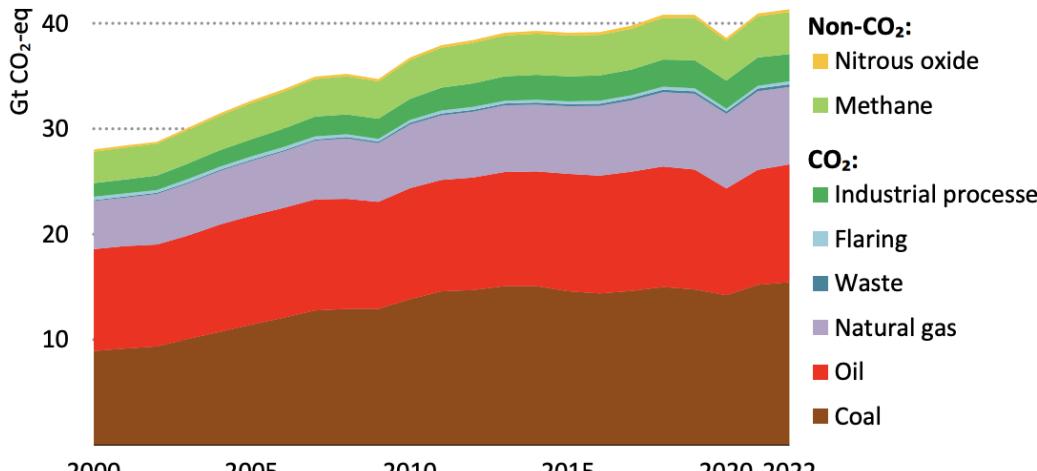
Greenhouse gases (GHGs) are gases present in the atmosphere. These gases have the ability to allow sunlight to enter the atmosphere, but prevent some heat that the earth would normally radiate back into space. Although these gases are necessary to regulate the temperature of the earth, their increased concentration, caused by human activities, increases the greenhouse effect, resulting in global warming.

Source	Global CO ₂ emissions (10 ⁶ t CO ₂ /year)	CO ₂ purity (volume %)
Coal	14,200	12–15
Natural gas	6,320	3–5
Refineries	850	3–13
Cement production	2,000	14–33
Ethylene production	260	12
Iron and steel production	1,000	15
Natural gas production	50	5–70
Ammonia production	150	100

Figure 1.1: Major sources of CO₂ [2]

1.2 History

In 1824, Jean-Baptiste Joseph Fourier made the discovery of the greenhouse effect [4]. However, because of the lack of necessary equipment, he was unable to conduct an experiment to prove his theory. It was not until over 70 years later that Svante Arrhenius



IEA. CC BY 4.0.

Source: Flaring emissions are from IEA analysis based on the [World Bank Global Gas Flaring Reduction Programme](#).

Figure 1.2: Global energy related greenhouse gas emissions, 2000-2022 [3]

provided evidence linking the greenhouse effect to the concentration of carbon dioxide in the atmosphere [5]. Arrhenius also established a correlation between earth's temperature and the concentration of CO₂ in the atmosphere. Subsequently, other scientists, such as Plass and Charles D. Keeling, presented significant evidence supporting the idea that an increase in CO₂ concentration is the primary cause of the increase in average temperature. This led to the World Conference on the Changing Atmosphere, which took place in Toronto, Canada, in 1988. During this conference, it was concluded that CO₂ emissions should be reduced by at least 20% compared to 1988 levels by the year 2005 [6].

Like many situations, humans tend to question everything. In an attempt to discredit these reports, various governments and organizations have claimed uncertainty in the reports. To address this issue, the Intergovernmental Panel on Climate Change (IPCC) was created in 1988 [7]. Its purpose is to provide scientific guidance to policy makers and improve decision-making processes. Together with IPCC, the United Nations Framework Convention on Climate Change (UNFCCC) was founded in Rio de Janeiro, Brazil, in 1992. Its aim is to facilitate intergovernmental negotiations on climate change among nations.

In the following, we will discuss some of the results that have been produced from this framework.

1.Kyoto Protocol, Japan, 1997: It was signed during the Third Conference of Parties (COP-3). It mandated a reduction in greenhouse gas emissions (including carbon dioxide, methane, nitrous oxide, hydrofluorocarbons, perfluorocarbons, and sulfur hexafluoride) "by at least 5% below 1990 levels in the commitment period 2008–2012" for 37 industrialized countries" [8].

2.Paris Protocol, France, 2015: It was signed during COP-21 among 194 states and the European Union. With the purpose of "holding the increase in the global average temperature to well below 2 °C above pre-industrial levels and to pursue efforts to limit the temperature increase to 1.5 °C above pre-industrial levels, recognizing that this would significantly reduce the risks and impacts of climate change" [9].

3.Dubai Protocol, UAE, 2023: It was signed during COP-28 among 197 nations and the European Union. It compelled governments to "speed up the transition away

from fossil fuels to renewables such as wind and solar power in their next round of climate commitments” [10].

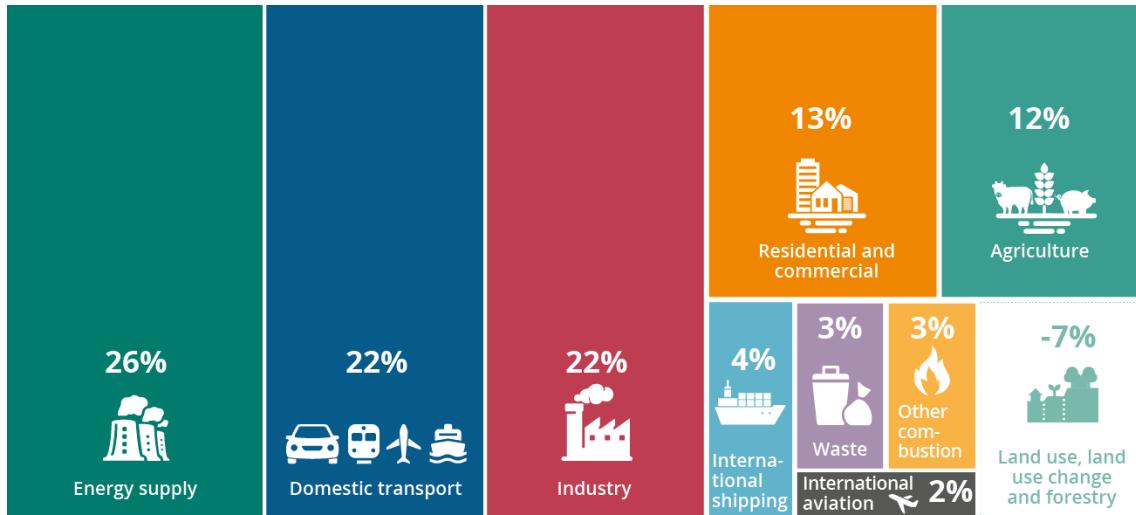


Figure 1.3: Greenhouse gas emissions in the EU [11]

The figure 1.2 and figure 1.6 illustrate global energy-related greenhouse gas emissions and the distribution of GHG emissions by product on a global scale. Also, figure 1.3 shows that energy production continues to be the main contributor to CO₂ emissions. Furthermore, most of global energy consumption is based on fossil fuels, which produce significant amounts of pollutants such as CO₂, CH₄, and NOX.

The global carbon cycle

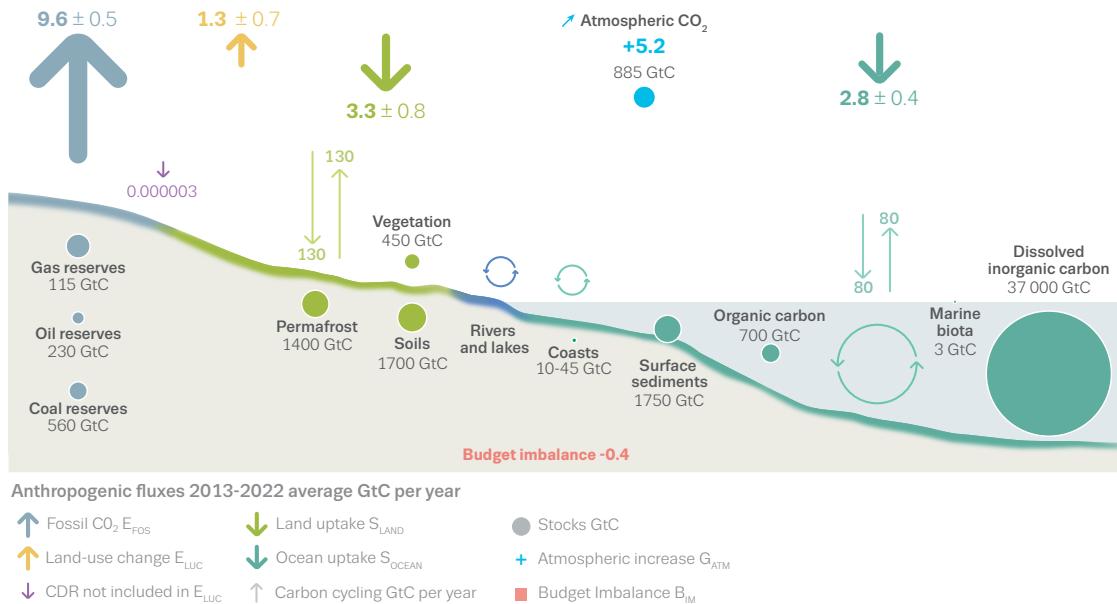


Figure 1.4: The global carbon cycle [12].

Before the industrial revolution, the concentration of CO₂ in the atmosphere of earth was approximately 250 ppm. However, by 2019, this level had reached more than 410 ppm.

The main primary reason for this increase can be attributed to extensive combustion of fossil fuels, namely coal, oil and gas, which are essential to provide the energy needed to support our modern lifestyle [13]. The current global carbon cycle is illustrated in figure 1.4 which shows the imbalance in the carbon cycle caused by anthropogenic activities.

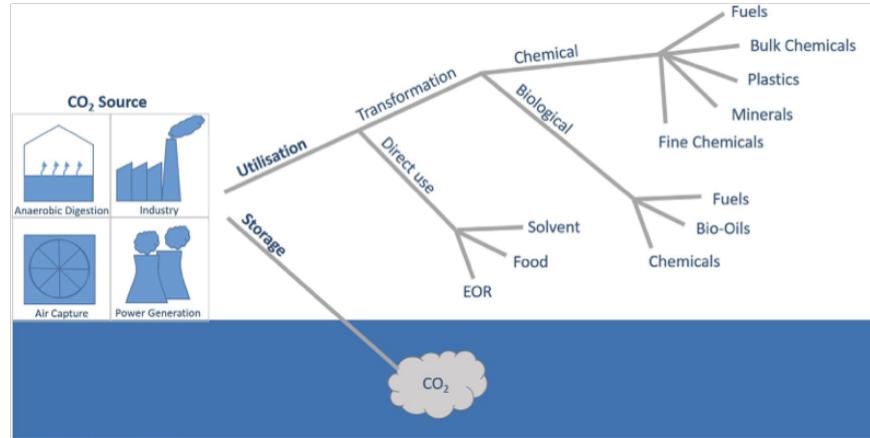
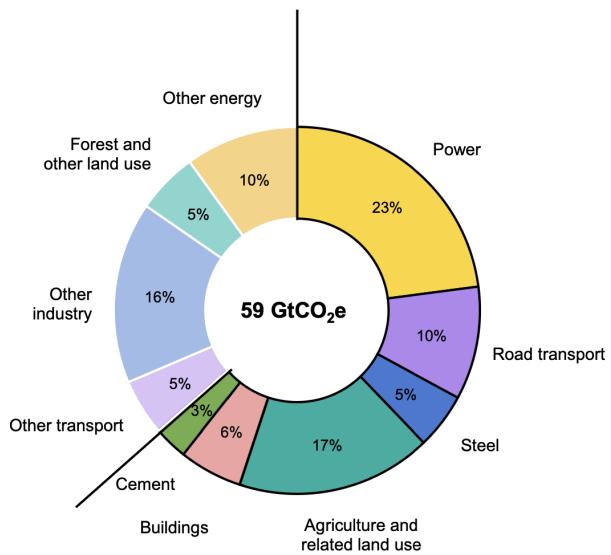


Figure 1.5: CO₂ storage and utilisation options [14]

Based on the above discussion, it can be concluded that CO₂ is the major culprit and that it is crucial to reduce its emissions. To achieve this, it is essential to capture CO₂ and use it directly or transform it into a chemical, biological, or permanently store it in geological formations such as deep saline formations and depleted oil and gas fields, as shown in figure 1.5.



Source: IPCC (2022), [Climate Change 2022: Mitigation of Climate Change](#).

Figure 1.6: Greenhouse gas emissions by sector, 2019 [3]

The commercialization of emerging power generation technologies, such as fuel cells, and the improvement of existing technologies such as solar photovoltaic(PV) and battery storage require more time and innovation to increase electricity production. As a result, we

will continue to rely on fossil fuels for a few more years. However, it is important to mitigate emissions and one way to do this is by capturing CO₂ and using it to produce chemicals, plastics, or in the food industry. By implementing carbon capture and utilization (CCU), the transition from an unsustainable linear economy to a sustainable circular economy is achievable [15].

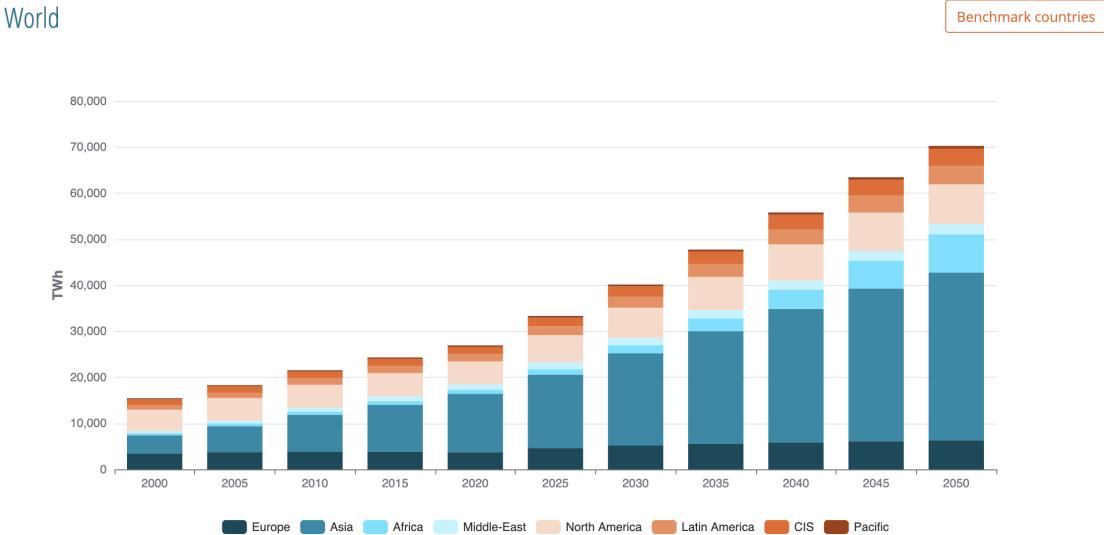


Figure 1.7: Enerdata Forecast of global electricity demand over 2000 - 2050 [16]

According to the Enerdata forecast, worldwide electricity consumption is expected to increase by 3% annually from 2000 to 2050, as illustrated in figure 1.7. The production of electricity from fossil fuels leads to substantial CO₂ emissions. Therefore, the implementation of CCU is essential to reduce these emissions and to achieve the climate change goals. In addition, the use of CCU allows CO₂ to be used as a raw material for the synthesis of fuels or chemicals. This approach is considered the most environmentally sustainable option.

According to the IEA, carbon capture, utilization and storage (CCUS) play a vital role in decreasing CO₂ emissions within the energy industry and reaching a state of net zero emissions. It plays various essential functions, such as tackling emissions from current energy facilities, offering a resolution for industries facing difficulties in reducing emissions, and serving as a foundation for generating clean hydrogen. Moreover, CCUS can help reduce emissions by extracting carbon from the atmosphere, helping to offset inevitable emissions [3]. Additionally, CO₂ utilization, in combination with renewable technologies, contributes directly to nine of the 17 UN Sustainable Development Goals. [17]. Furthermore, as stated by the IPCC, it would be 138% more expensive, on average, to achieve global climate objectives without the implementation of CCS (Carbon Capture and Storage).

This thesis examines post-combustion amine-based carbon capture where energy is supplied by fossil fuels and renewables. In the case of post-combustion carbon capture, more than half of the plant's energy is consumed by the reboiler.

1.3 Goal of the thesis

- The purpose of this thesis is to simulate and evaluate various configurations for carbon dioxide capture, which include seven variations. These configurations either

use fossil fuels, providing thermal energy, or employ heat pumps powered by various sources of electricity.

- The objective is to conduct a comprehensive life cycle assessment using GaBi software, comparing the environmental impacts of each configuration, with the goal of determining the most sustainable approach for amine-based carbon dioxide capture.

1.4 Thesis structure

The thesis comprises a total of seven chapters.

- Chapter 2: Describes CO₂ capture technologies, the science behind absorption, previous investigations related to amine-based carbon capture, and principles of life cycle assessment(LCA).
- Chapter 3: Presents the software tools required for modeling, simulation, and performing life-cycle assessment. The tools used for this thesis are Aspen plus®, GaBi, Coolselector2®, LaTeX, Excel.
- Chapter 4: Discusses phases of life cycle assessment, scope of LCA, connecting GaBi database, and creating a plan, process, and project to calculate environmental impacts.
- Chapter 5: Describes and evaluates the results of seven modeled configurations, drawing comparisons through simulation and LCA.
- Chapter 6: This chapter discusses the key findings and compares them from the results section.
- Chapter 7: Summarizes the research findings and proposes future potential work based on the study.

In this thesis, the following questions are ultimately answered:

1. What is the connection between global energy demand and the escalating global warming phenomenon?
2. What are the reasons for the increasing importance of carbon capture technologies?
3. What provides a competitive advantage to amine-based CO₂ capture, making it the predominant choice over other methods?
4. What is the importance of the Life Cycle Assessment (LCA) tool and simulation in evaluating various configurations to achieve sustainability?
5. What makes heat pumps more advantageous compared to fossil fuels?
6. What are some possible future research paths that could be recommended or conclusions that can be drawn from this study?

Chapter 2

Theoretical background and Literature Review

This chapter gives insight about technologies for CO₂ capture, science behind absorption, a review of relevant literature, and identification of gaps that served as basis for this thesis.

2.1 Carbon dioxide capture usage and storage technologies

2.1.1 Evolution of CO₂ capture, usage and storage (CCUS)

In the previous chapter, it was emphasized that CO₂ constitutes a major contributor to greenhouse gas production. To trace the origins of CO₂ capture technologies, it is essential to revisit the past. In the late 1980s, the scientific community highlighted the increase in atmospheric CO₂ levels, predominantly caused by human activities and leading to climate change. This concern led to the establishment of the Intergovernmental Panel on Climate Change (IPCC) in 1988.

The first IPCC report which was published in 1990 outlined that “the technologies to capture and sequester from fossil fuel combustion deserve investigation, considering the expected continuing dependence on fossil fuels as primary energy sources” [18]. Moreover, the United Nations Framework Conventions on Climate Change (UNFCCC) also stress the importance of this topic, as observed in the previous chapter. As a result, carbon capture technologies were developed to specifically address and mitigate CO₂ emissions from industrial facilities involving combustion processes.

2.1.2 Technologies for carbon capture

Carbon capture and storage (CCS) technologies are classified into three categories as shown in figure 2.1:

- **Pre-combustion capture:** The process involves capturing CO₂ prior to the combustion process through reforming and gasification methods, resulting in the generation of *syngas*—a gaseous mixture of H₂ and CO [7].
- **Oxy-combustion:** The scenario regulates combustion using pure oxygen instead of air. The resulting product is a highly concentrated CO₂, which can be captured and stored [7].
- **Post-combustion:** In this case, CO₂ is captured after combustion. This method is undoubtedly the most appealing method compared to other capture systems [7].

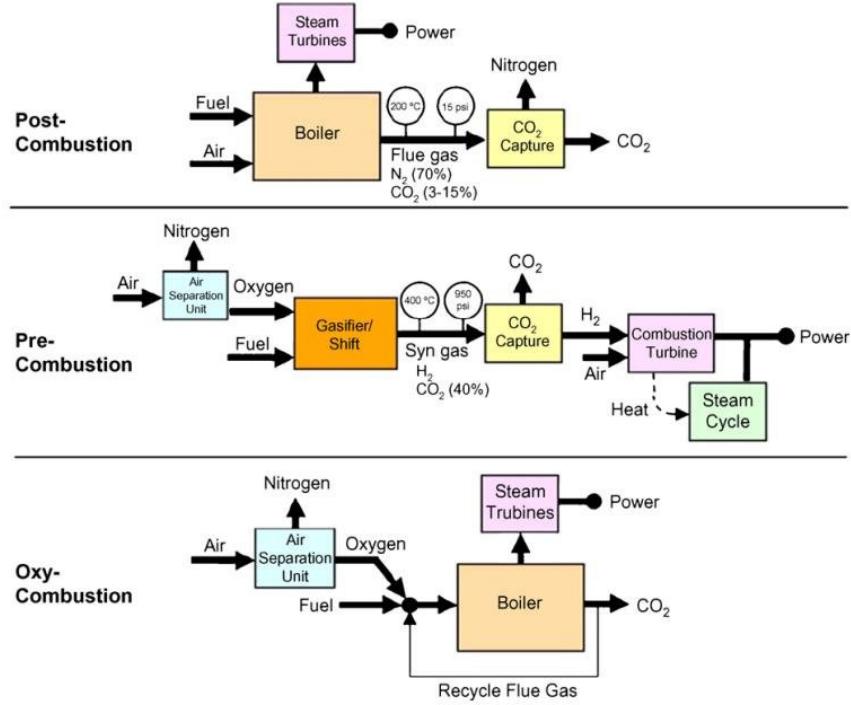


Figure 2.1: Scheme of post-combustion, pre-combustion, and oxy-combustion systems [19]

The figure 2.2 illustrates various CO₂ capture routes, including absorption, membrane, adsorption, and chemical looping, each with its own merits and drawbacks.

On a closer look at the technology categories, it becomes evident that post-combustion capture (PCC) stands out, supported by extensive studies and its ability to retrofit existing power plants, opening the way to a significant reduction in CO₂ emissions in a variety of industrial sectors [21]. Despite its capture efficiency being somewhat lower than that of certain alternatives, the versatility of PCC makes it an integral method in the transition towards sustainability.

2.2 Absorption

Absorption is a gas-liquid mass transfer operation in which a substance is transferred from the gas phase to the liquid phase [22]. The substance absorbed is called the solute, and the other substance in which it absorbs the solute is called the solvent. The absorption rate is governed by the molecular diffusion rate that dominantly controls the interphase mass transfer [22].

Absorption can be categorized into two types:

- **Physical absorption:** Process in which the absorption of a substance, typically a gas, into a liquid occurs without significant chemical reactions. The process is usually reversible, driven by a weak physical force. Examples include the absorption of oxygen in water [23].
- **Chemical absorption:** Process in which the absorption of a substance involves chemical reactions between the gas and the liquid. The process is generally irreversible driven by strong chemical forces. Examples include the absorption of carbon dioxide in an amine solution during carbon capture [23].

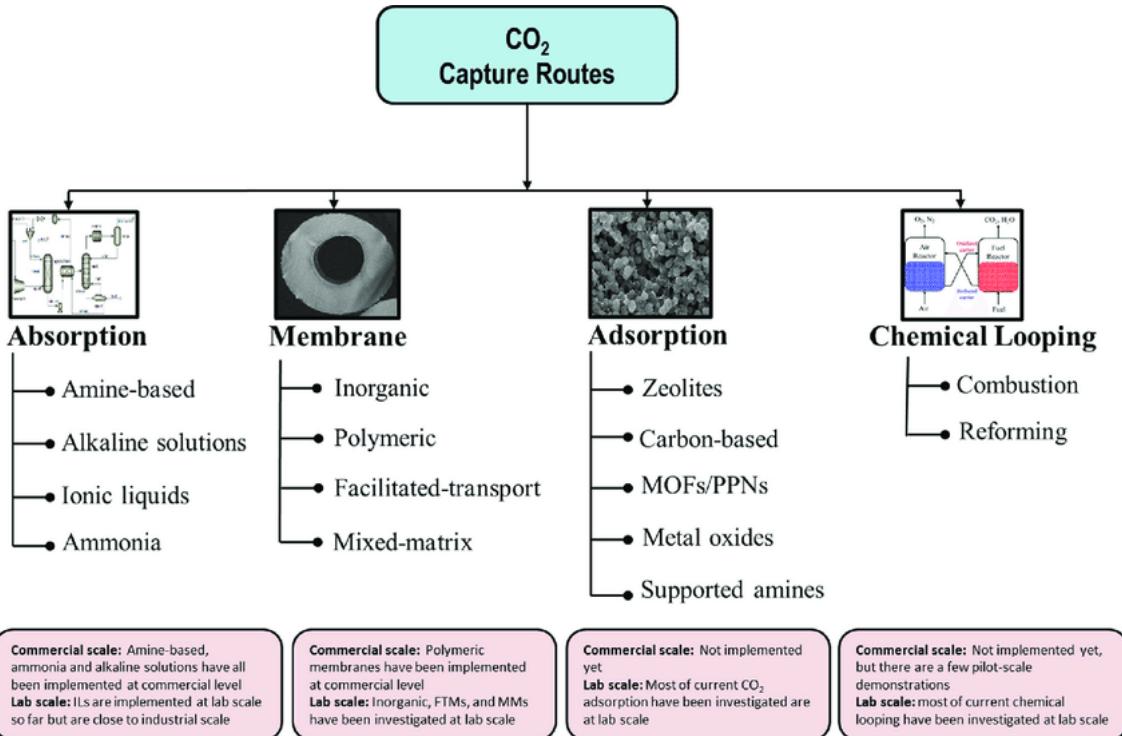


Figure 2.2: CO₂ capture routes [20]

2.2.1 Physical absorption principles

With an understanding of the rate of absorption depending upon the rate of molecular diffusion, let us understand the factors that influence molecular motion, commonly referred to as the driving force.

Temperature and pressure play crucial roles in determining the solubility of gases in liquids, as outlined by Van't Hoff's law of dynamic equilibrium. It explains that, at a constant temperature, an increase in pressure leads to higher solubility, whereas a temperature increase increases heat absorption, leading to a reduction in gas solubility.

Henry's law states that, under constant temperature conditions, the amount of dissolved gas in a liquid is proportional to its partial pressure above the liquid [22].

$$p^* = H \cdot x \quad (2.1)$$

where p^* is the partial pressure of gas in vapor phase over the liquid in equilibrium with the gas;

H is the Henry's law constant;

x represents the mole fraction of solute in liquid phase.

According to Dalton's law, the total pressure of a gas mixture is equal to the sum of the partial pressures of each gas present in the mixture, and this correlation can also be represented using mole fractions and the total pressure [22].

$$p = y \cdot P \quad (2.2)$$

where p is the partial pressure of gas in vapor phase;

P is the total pressure of the system;

y represents the Mole fraction of solute in gas phase.

Combining equations (2.1) and (2.2)

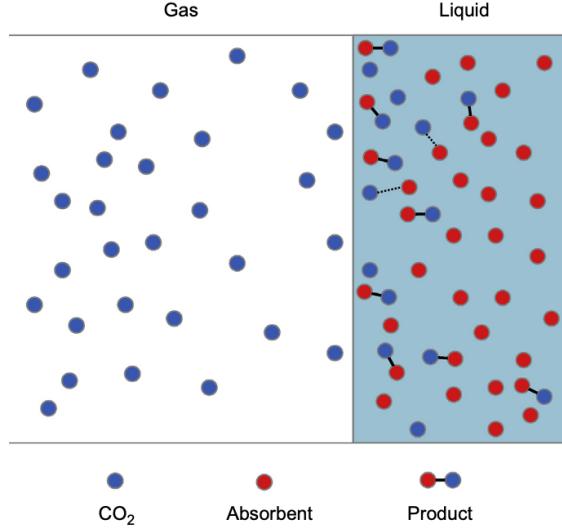


Figure 2.3: Graphical representation of CO_2 gas crossing a gas-liquid interface and undergoing chemical reaction with an absorbent [24]

$$y^* = \frac{H \cdot x}{P} \quad (2.3)$$

where y^* is the equilibrium mole fraction of solute in gas phase.

The equation (2.3) enables us to determine the concentration of the solute in the vapor phase when it reaches a state of equilibrium with the liquid phase.

Employing the same logic to our chemical absorption process between CO_2 and amine based solvent, concentration gradient triggers the absorption of $\text{CO}_2(g)$ into the amine solvent, leading to diffusion, and the process continues until equilibrium is reached [24].

In mathematical terms, the concentration gradient can be expressed as

$$DF = P_{\text{CO}_2} - P_{\text{CO}_2}^* \quad (2.4)$$

where DF is the driving force;

P_{CO_2} is concentration of $\text{CO}_2(g)$ expressed as partial pressure (bar);

$P_{\text{CO}_2}^*$ is concentration of $\text{CO}_2(g)$ at equilibrium expressed as partial pressure (bar);

The rate of achieving equilibrium depends on the driving force and diffusion coefficient. There are many theories to estimate the diffusion coefficient, but the Wilke-Chang correlation is commonly used in absorption applications [24].

$$D_{A,L} = 7.4 \times \frac{10^{-8}(\phi_L \cdot M_L)^{0.5}}{T \cdot \mu_L \cdot V_A^{0.6}} \quad (2.5)$$

where ϕ_L is association factor of the absorbent;

M_L is molecular weight of the absorbent L (g/mol);

T is temperature (K) ;

μ_L is Viscosity of the absorbent ;

V_A is molecular volume of species A (m^3/mol).

As depicted in figure 2.3, the interaction at the interface between the gas and liquid phases is dynamic [24]. The movement of molecules at interface between gas phase to liquid phase and vice versa is caused by diffusion, which is a spontaneous movement of molecules from higher concentration to lower concentration.

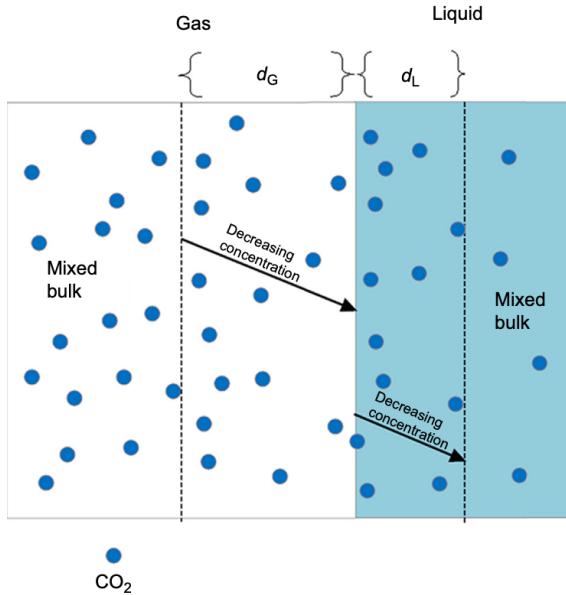


Figure 2.4: Graphical representation of the stagnant film regions of thickness d_G and d_L at the gas-liquid interface [24]

$$N_{CO_2} = K_G(P_{CO_2} - P_{CO_2}^*) \quad (2.6)$$

$$\frac{1}{K_G} = \frac{1}{K_L^*} + \frac{1}{K_G} \quad (2.7)$$

$$k_L^* = \frac{D_{CO_2,L}}{d_L h_{CO_2,L}} \quad (2.8)$$

$$k_G = \frac{D_{CO_2,G}}{d_G RT} \quad (2.9)$$

where N_{CO_2} is the molar flux of CO_2 ; ϕ_L is association factor of the absorbent; K_G is the overall mass transfer coefficient ($mol/m^2/s/kPa$) ; K_L^* is the liquid- side mass transfer coefficient without reaction ($mol/m^2/s/kPa$) ; $D_{CO_2,L}$ is diffusion coefficient of CO_2 in the liquid phase (m^2/s) ; R is the gas constant ($0.008314\ m^3\ kPa/K/mol$) .

From equation (2.6) to equation (2.9), the equations clearly expresses the rate of movement of CO_2 molecules from gas phase to liquid phase at the interface and the same is visualised in figure 2.4 [24].

2.2.2 Chemical absorption principles

Having explored the physical absorption principles like solubility, diffusivity and the factors behind driving force, it is essential to understand chemistry principles behind absorption to gain a holistic understanding. In the upcoming section, our focus will shift towards the reaction between CO_2 and amine solutions chemistry, paving the way for understanding, modeling and simulation in the subsequent chapters.

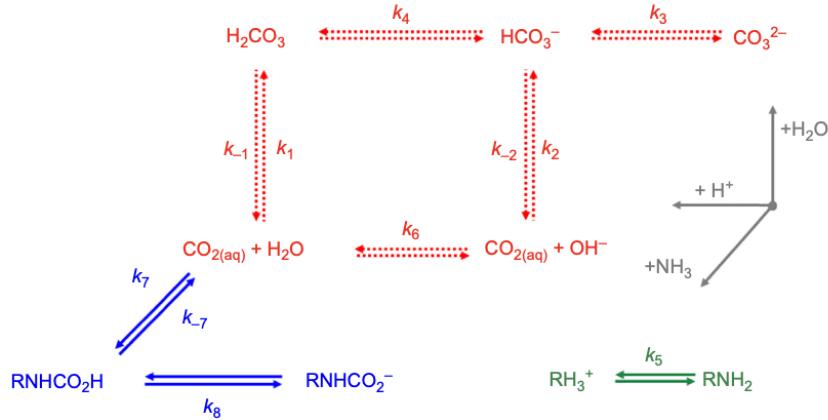
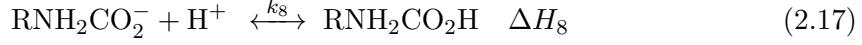
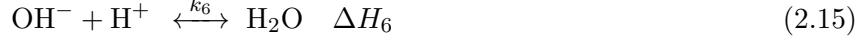
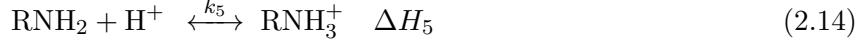
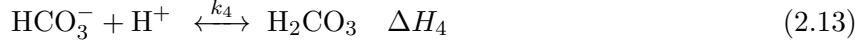
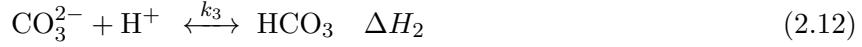


Figure 2.5: Reaction sequences [17]



In equation (2.10), we observe the reaction between CO_2 and water, leading to the formation of carbonic acid, which occurs at a relatively slow rate. Similarly, equation (2.11) shows the formation of bicarbonate through the reaction of CO_2 with hydroxide, also with amine to form carbamic acid shown in equation (2.16) [24].

The slow reactions mentioned above are accompanied by the addition of proton, where carbonates undergoes protonation, equation (2.12) and equation (2.13). Additionally, amine, hydroxide, carbamate also experiences the same depicted in equation (2.14), equation (2.15), and equation (2.16) respectively [24], and the visual representation of reactions is shown in figure 2.5 [24].

The series of reactions outlined in figure 2.5, indicating that the presence of the amine does not affect the interactions between CO_2 and water/hydroxide. Sterically hindered and secondary amines do not take part in carbamate formation, their primary role lies in the protonation equilibrium (k_5). Primary and secondary amines directly interact with CO_2 , leading to the formation of carbamic acid represented in equation (2.16). Under the existing conditions, carbamic acid deprotonates to form carbamate equation (2.17) [24].

Choice of amine The described equations emphasize that the amine's kinetics is a major key factor in governing the CO_2 absorption process. The two important parameters

pH and protonation constant(k_5) [24]. Several studies by different researchers lead to the conclusion that the reactive amine with high protonation constant offers advantages, and the structure of the amine is crucial [24]. The other important parameters are capacity, CO₂ absorption rate, thermal and oxidative degradation, volatility, cost, aerosol emissions and many more.

Amines are classified into three categories according to the number of hydrogen atoms replaced in the NH₃ molecule. They are called primary amines (1°), secondary amines (2°), tertiary amines (3°).

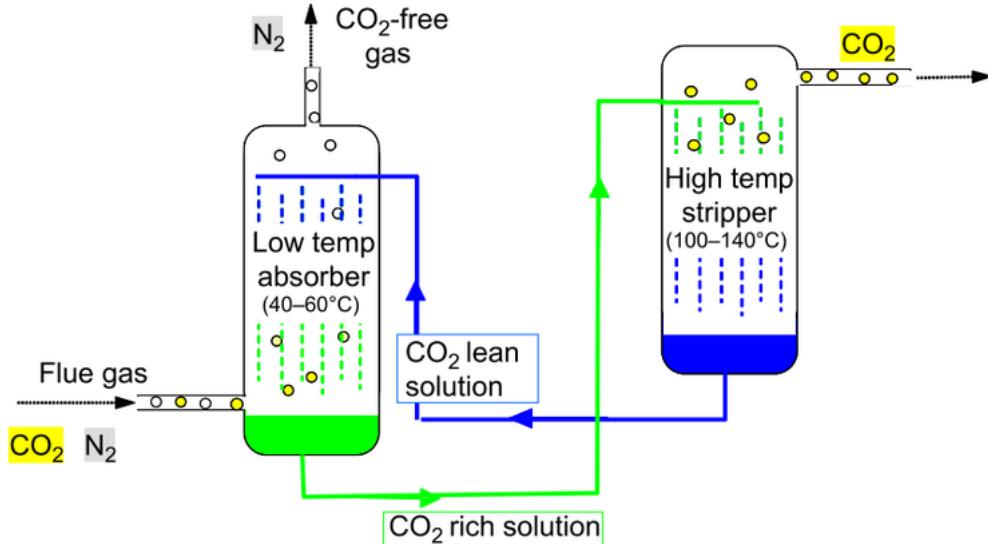


Figure 2.6: Schematic diagram of the amine-based PCC plant [24]

Although secondary and tertiary amines offer advantages over primary amines such as monoethanolamine (MEA) due to the structure advantage to capture CO₂, MEA have certain merits, such as high absorption rate, cost effectiveness, established technology, and availability making it a practical and suitable choice to find the energy requirement, which is the main objective of this research.

2.2.3 Absorber and desorber

The absorption process is carried out in a column called an absorption column or absorption tower. The absorber can be designed as a packed column, a tray column, or a spray column.

The trays can be classified into bubble cap tray, valve tray, and sieve tray, and the packings are of two types: random packing and bubble packing [22].

Desorber, also called a stripper, performs the opposite function of an absorber. It involves a change in temperature or pressure conditions to reverse the absorption process. In the absorber, the solvent (absorbent) is mixed with a gaseous mixture set for removal, and in the desorber (Stripper) it undergoes regeneration, freeing it from dissolved substances. The regenerated solvent is pumped back to the absorption tower to complete the cycle. The figure 2.6, illustrates a comprehensive absorption process, showcasing both an absorber and a desorber.

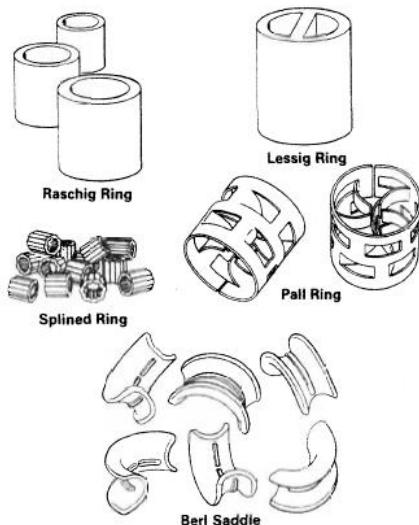


(a) Bubble cap tray

(b) Sieve tray

(c) Valve tray

Figure 2.7: Trays [25]



(a) Random packings [26]



(b) Structured packing [27]

Figure 2.8: Packings

2.3 Combining everything

2.3.1 Absorption

1. Maintaining a low temperature is significant to enhance the attraction for CO₂ absorption.
2. CO₂ moves from the bulk gas volume to the interface between gas and liquid.
3. CO₂ gets absorbed into the absorbing substance.
4. CO₂ interacts with the amine in the solution as described in the equations. This process reduces the CO₂ concentration at the gas-liquid interface, ensuring the continued push for CO₂ to transition from the gas phase to the liquid phase.

2.3.2 Desorption

1. Elevated temperatures are required to ensure the desorption of CO₂.
2. The backward reactions are fast, so the desorption rate is limited only by diffusion.

3. Desorption, being an endothermic process, requires the addition of heat to the absorbent in order to keep the temperature constant.

2.4 Earlier investigations:

The following section summarizes key findings from preliminary examinations addressing the simulation and LCA of the CO₂ absorption process.

Simulation

- In 2016, Stefania Moioli et al. examined the importance of amine scrubbing, particularly using an aqueous MEA solution 30% by weight, as a baseline solvent for post-combustion CO₂ capture. The study highlighted the crucial role of the thermodynamic model in determining the overall heat of absorption and in influencing energy requirements and temperature profiles during solvent regeneration. The simulation results were validated against the experimental data, highlighting the focus on energy saving solutions [28].
- In 2017, Lionel Dubois and Diane Thomas studied ways to make CO₂ capture in cement plants more energy efficient. Using ASPEN HYSYS and different solvents, they found that lean or Rich vapor compression configurations could save about 30% of energy and reduce cooling demands. The research not only focused on operational costs but also considered the overall investment required [29].
- In 2018, Nwaoha Chikezie et al. used ProMax 4.0® simulator to study CO₂ capture from a coal-fired power plant using a mixture of MEA and DEA mixture. The study assessed the impact of various process variables on key parameters. The findings highlighted the significant influence of the reboiler temperature on the dependent variables, with regeneration energy, compressor electrical energy and operational costs playing a crucial role in the process [30].
- In 2022, Tianca Li et al. used the ProMax®5.0 process simulator to design three novel configurations for cement plant flue gases. The study compared the technical and economic advantages of these configurations with a conventional setup. Three cases of flue gas compositions were simulated, including one based on published design parameters and the other two with higher CO₂ content assumptions. The research showed that innovative configurations could reduce regeneration energy by up to 22% and solvent demand by up to 10% [31].

Life cycle assessment(LCA)

- In 2011, Khoo et al. explored mineral carbonation for CO₂ sequestration in Singapore. Life cycle assessment revealed CO₂ avoidance (106.9-175.9 kg/MWh) and varied sequestration effectiveness (32.9%-49.7%). Life cycle costing showed that 105.6 and 127.2 USD/tonne of CO₂ were avoided, but engineering challenges and variable conditions were highlighted [32].
- In 2019, Ben Young et al. explore the environmental impacts of amine solvent-based carbon capture systems in US sectors such as ammonia production, petroleum refining, and power plants. When analyzing complete life cycle inventories, an increase in particulate matter, eutrophication potential, and reduced water consumption per kg of CO₂ eq. are observed. The impacts on acidification potential and particle matter formation are the result of factors such as combustion emissions and the influence of the carbon capture unit [33].

- In 2020, Rosental et al. conducted a life cycle assessment (LCA) on the production from the cradle to the gate of the major organic chemicals using a combination of carbon capture and utilization (CCU) and water electrolysis technologies. The chemicals investigated included methanol, ethylene, propylene, benzene, toluene, and mixed xylenes. The results demonstrated that the use of CCU processes with offshore wind turbine electricity reduced greenhouse gas emissions by 88–97% compared to fossil-based routes, despite an increase in other environmental impacts such as eutrophication and ozone depletion [34].
- In 2021, Yangdong He et al. investigated the environmental benefits of using CO₂ for syngas production, highlighting an energy efficient three step hydrogen production system using iron based chemical loop combustion. With a life cycle emission of 129.98 kg CO₂ eq./MWh, this approach demonstrated a 46.87% reduction in carbon emissions and 18.19% energy savings compared to conventional systems [35].

Key Observations

- In 2002, Anand Rao et al. conducted research on carbon capture and sequestration, emphasizing key factors influencing feasibility and cost. Their findings highlighted the importance of design assumptions, capture system details, and pollution control interactions. In particular, retrofit systems faced higher costs due to less efficient heat integration, while SO₂ emission trading credits provided a slight cost reduction in amine-based capture systems due to the National Acid Rain Control Program [36].
- In 2014, Rosa M. Cuéllar-Franca and Adisa Azapagic conducted a pioneering study that compared carbon capture and storage (CCS) with carbon capture and utilization (CCU) technologies. CCS showed a reduction of 63 to 82% in the potential for global warming, especially in oxy-fuel and integrated gasification plants, but with elevated acidification and human toxicity. On average, CCS exhibited a lower global warming potential compared to CCU options, highlighting environmental considerations [37].
- In 2019, Vega et al. explored the efficacy of post-combustion capture (PCC) using chemical absorption and aqueous amine solvent within CCS. PCC emerges as a promising technology capable of directly capturing up to 90% CO₂ emissions from flue gas after fossil fuel combustion. The article shows the potential to both retrofit and integrate them into new facilities [38].
- In 2021, Tom Terlouw et al. critically reviewed the LCA of carbon dioxide removal (CDR) technologies, cautioning against misinterpreting emissions avoidance as negative emissions. Recommendations include conducting complete LCAs, considering temporal aspects in biomass-related CDR technologies, and ensuring transparency in methodological choices [39].
- In 2022, Rahim Zahedi et al. examined challenges focused on CO₂ capture technologies, focusing on environmental impacts. The study compared the amine and strong hydroxide absorption processes using Aspen HYSYS for simulation of the amine system and Simapro software for the life cycle evaluation. The study found that strong hydroxides had greater negative effects on marine ecotoxicity, while amine absorption utilized 43% more fossil resources. However, amine absorption showed lower environmental impacts of 8% and 3% on human health and ecosystems, respectively, compared to strong hydroxides [40].

- In 2023, Shirmohammadi et al. evaluated the environmental performance of a petrochemical plant that produces urea fertilizer and liquid ammonia. The study focused on the use of excess ammonia to increase urea production through a CO₂ capture and utilization unit (CCU). The CCU plant, which recovered 5500 kg of CO₂ per hour, resulting in a 10% lower carbon footprint compared to the plant without CCU. Despite solar-assisted operation showing slight environmental advantages, the CCU plant increased urea production by approximately 8% [41].

Using Tianci Li et al.[31] as the basis, and adopting the flue gas composition, absorber and stripper design parameters of [30], this thesis conducted an extensive investigation of the energy requirements, especially the reboiler. Although the conventional model relies on fossil fuels to provide energy, my study introduces a heat pump technology to provide energy and heat integration to the model. To understand the merits and demerits of configurations, a detailed life cycle assessment (LCA), examining their environmental impacts over their life cycle. The primary focus is to gain a comprehensive understanding of whether the use of fossil fuels such as natural gas and coal or the adoption of heat pump technology is more effective. This thesis aims to fill this gap by investigating and determining which approach is more sustainable to achieve decarbonization, a study that has not been carried out to the best of my knowledge.

Chapter 3

Modeling and Simulation Methodology

This chapter provides details on the modeling methodology and assumptions used to perform simulations, sensitivity analysis, and a brief overview of heat pumps and refrigerants.

3.1 Modeling in Aspen Plus[®]

AspenTech was founded in 1981 as the Advanced System for Process Engineering (ASPEN)[42]. Aspen Plus v12.1 , a software product of AspenTech, is used in this thesis. The software is used for modeling, simulation, and processing calculations.

Aspen Plus uses three approaches: Sequential modular, Equation oriented and Combinatorial approach. In the sequential modular approach, unit operation blocks are solved in certain sequence, whereas in the equation oriented approach the blocks are solved simultaneously. The third one employs both approaches, since the sequential approach is used to initiate steady state and the equation oriented approach is used for dynamic simulation. This thesis selects the Sequential modular approach for conducting simulations. The table below gives a quick overview of the AspenPlus software procedure.

Title	Description
Set-up	Title, purpose of simulation
Units	Choose units of measurement (SI / English / Metric) for input and output data.
Properties environment	Consists of components and properties(physical and thermodynamic)
Simulation environment	Involves flowsheet (Blocks and Streams)
Run	Simulation and analysis of results

Table 3.1: Steps of AspenPlus software [43]

3.1.1 Process steps

The figure 3.1 depicts the simplified flow diagram of a reactive absorption-stripping for CO₂ capture using post-combustion capture (PCC). It involves a reactive absorption-solvent regeneration process with two main sections: absorption and stripping. In the absorption section, CO₂ is absorbed from the fluegas to the amine solvent (MEA) through a chemical reaction as described in Section 2.2.2 of the previous chapter. In the stripping

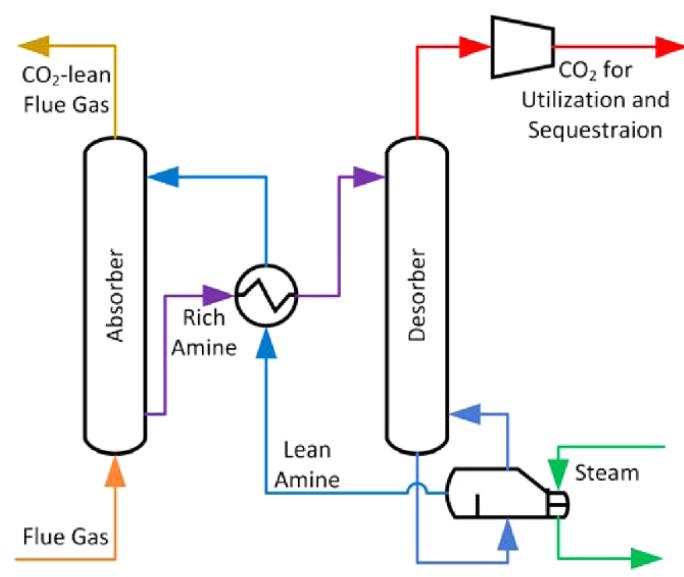


Figure 3.1: Simplified flow diagram of a reactive absorption-stripping plant for CO₂ capture [44].

section, the reverse reaction occurs to release CO₂ back. The two sections are connected by a cross heat exchanger. The rich amine is pumped to the desorber (stripper), and the regenerated solvent completes the cycle through a heat exchanger. The presence of chemical reactions complicates the process, involving various phenomena, as shown schematically in figure 3.2.

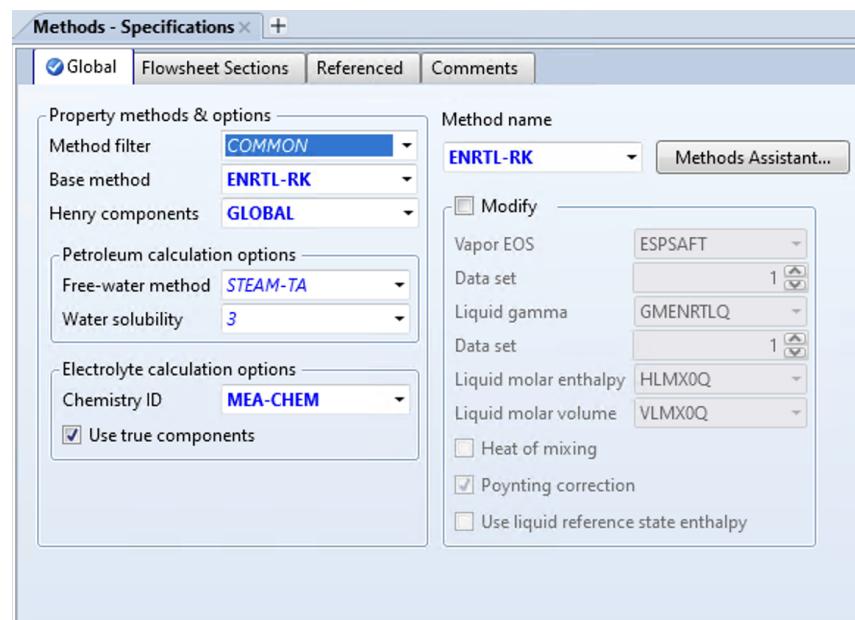


Figure 3.2: Steps involved in the CO₂ capture technique with the reactive absorption-stripping method [7]

3.1.2 Property environment

The property environment consists of components and properties (physical and thermodynamic). The components required for the simulation are shown in figure A1.1. Choosing

the property method is a critical decision, as it serves as the heart of the simulation by calculating the essential thermodynamic and transport properties of the components. As our simulation involves gas and liquid phases, the phase equilibrium calculation is calculated by fugacity, which is done using the γ - γ approach or by the ϕ - γ approach. Given the non-ideal nature of our model attributed to the presence of ions, and based on the findings of the literature survey, the Electrolyte Non-Random Two Liquid - Redlich-Kwong model (ENRTL-RK) emerges as a highly suitable choice and the corresponding equilibrium and kinetic reactions for the process are defined as shown in figure 3.3.



(a) Method specification for the process

Rxn No.	Reaction type	Stoichiometry	Delete
1	EQUIL	MEAH+ + H2O <--> MEA + H3O+	✗
2	EQUIL	2,0 H2O <--> H3O+ + OH-	✗
3	EQUIL	HCO3- + H2O <--> CO3-2 + H3O+	✗
4	KINETIC	OH- + CO2 --> HCO3-	✗
5	KINETIC	HCO3- --> OH- + CO2	✗
6	KINETIC	MEA + CO2 + H2O --> MEACOO- + H3O+	✗
7	KINETIC	MEACOO- + H3O+ --> MEA + CO2 + H2O	✗

(b) Equilibrium and kinetic reactions for the process

Figure 3.3: Simulation environment in Aspen Plus [7]

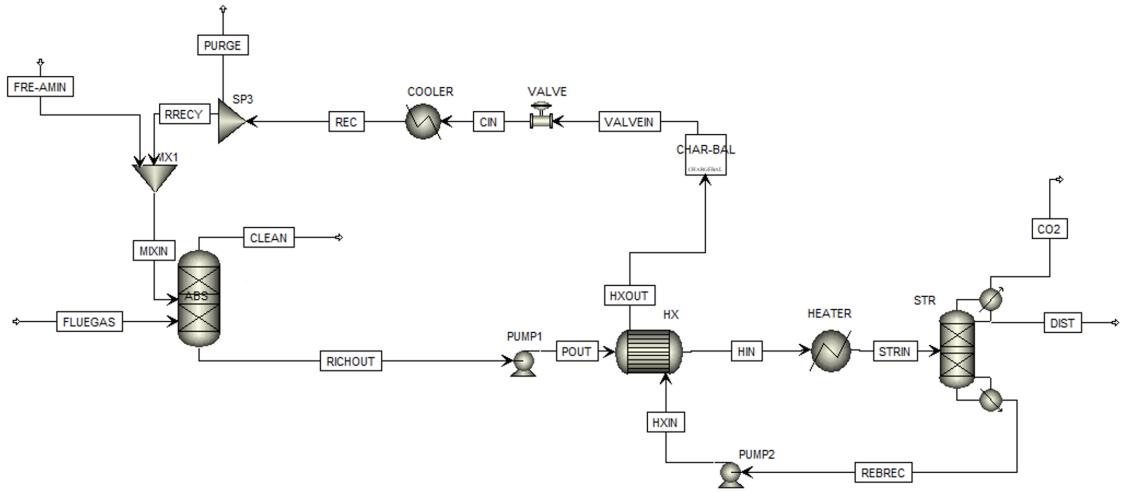


Figure 3.4: Aspen Plus flowsheet

3.2 Heat pump

This study uses heat pump technology to provide energy to the reboiler. The goal is to find the environmental impact by performing an LCA and compare it with the energy supplied by fossil fuels. The following section describes the operation of the heat pump.

Lord Kelvin demonstrated the principles of the heat pump in 1852 [45]. Heat pump is defined as devices that transfer heat from a lower temperature heat source to a higher temperature heat sink [46].

Heat pumps are generally classified into two types.

- 1.) Vapour compression heat pumps
- 2.) Absorption heat pumps

Vapour compression heat pumps operate on a reverse thermodynamic cycle and are powered by an electric motor or an engine-driven compressor. On the other hand, absorption heat pumps do not have a mechanical compressor. Instead, a mixture of two fluids with different vapor pressures. The more volatile fluid evaporates and then recombines with the less volatile fluid. Example water and lithium-bromide [47].

This study focuses on the vapour compression heat pump, and the subsequent section presents the various components and processes involved in its operation shown in figure 3.5 and figure 3.6. The fluid used is called a refrigerant.

3.2.1 Heat pump process

The heat pump process is explained [45] and illustrated in figure 3.6.

- Isobaric evaporation(1-2): The evaporator receives the liquid refrigerant, which then undergoes the boiling process. Heat energy is extracted from either the surroundings or a heat medium.
- Isentropic compression(2-3): The compressor increases the refrigerant pressure from the evaporation pressure to the condensation pressure. When the gas undergoes

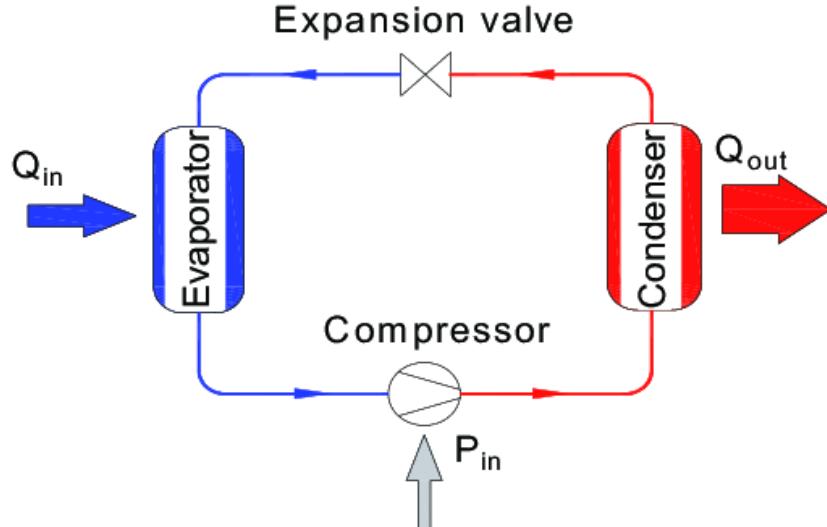


Figure 3.5: Components in heat pump [45]

compression, its internal energy and temperature rise. Achieving isentropic compression in a real process is not possible due to the fact that the fluid's internal friction can never be reduced to zero and heat is inevitably transferred through the cylinder wall.

- Isobaric condensation(3-4): During the process of isobaric condensation, heat energy is released into the surrounding environment through condensation of the refrigerant.
- Isenthalpic regulation(4-1): The evaporator must receive refrigerant in a fully condensed state at low pressure. This is achieved through an isenthalpic change of state, commonly known as throttling.

The coefficient of performance (COP) is used to measure the performance of a heat pump. In heating applications, the performance coefficient is the ratio of work and the output of the condenser. It can be easily determined from the P-H diagram, as illustrated in figure 3.6, by calculating the difference in enthalpy.

In an ideal scenario, the system would not experience any losses. However, in reality, during the isenthalpic compression, there will be some heat exchange with the environment because of factors such as friction or real gas behavior. The same applies to the throttling process, which is not isenthalpic. Additionally, pressure losses are inevitable during the evaporation and condensation processes [49].

The enthalpy of the refrigerant can be calculated by consulting commercially available charts or using software tools like Coolselector®2 developed by Danfoss, or websites such as TLK ENERGY [50].

$$\text{COP} = \frac{Q_{\text{out}}}{W(P_{\text{in}})} = \frac{h_3 - h_4}{h_3 - h_2} \quad (3.1)$$

where Q_{out} - condenser output(kW);

$W(P_{\text{in}})$ - compressor output(kW);

h_2 and h_3 – refrigerant enthalpy before and after the compression (kJ/kg);

h_3 and h_4 – refrigerant enthalpy before and after the condenser (kJ/kg) as shown in figure 3.5.

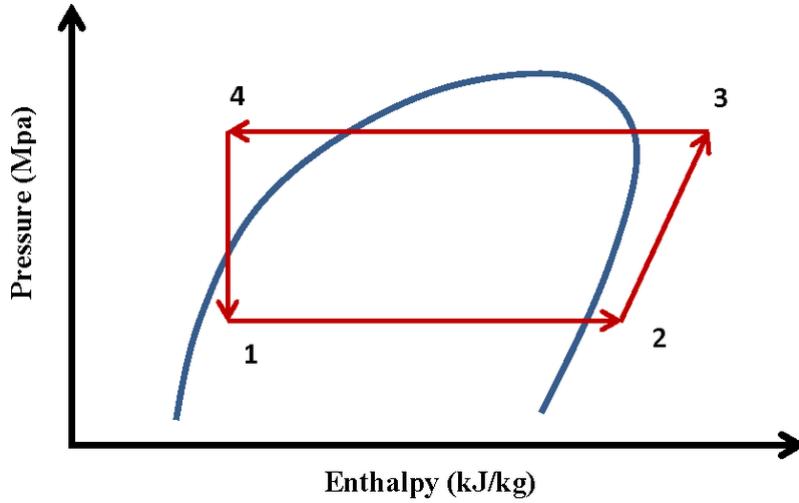


Figure 3.6: Heat pump process in a P-H diagram [48]

3.2.2 Refrigerant

The heat pump system depends on the refrigerant to facilitate the transfer of energy. The selection of refrigerant is mainly determined by its physical, chemical, and physiological characteristics [45]. Researchers have discovered that the emission of certain refrigerants can cause harm to the climate. The classification of refrigerant is illustrated in table 3.2.

In this study, R-1233zd(Solstice[®]), a refrigerant classified as a hydrofluoroolefin (HFO), is used due to its low global warming potential (GWP) , which is typically below 1. This refrigerant also offers additional benefits such as zero ozone depletion potential and non-toxic, non-flammable nature, making it a safer and more environmentally friendly option.

Refrigerant Type	Examples
Chlorofluorocarbons (CFCs)	R-134a, R-410A, R-404A, R-407C
Hydrochlorofluorocarbons (HCFCs)	R-22, R-123
Hydrofluorocarbons (HFCs)	R-134a, R-410A, R-404A, R-407C
Hydrofluoroolefins(HFO)	R-1233zd, R-1234yf,R-1234ze
Natural Refrigerants	Ammonia (R-717), Carbon Dioxide (R-744), Hydrocarbons (Propane - R-290, Isobutane - R-600a)
Blended Refrigerants	R-410A, R-404A, R-407C

Table 3.2: Refrigerant classification [45]

3.3 Simulation data

The simulation parameters used in this thesis were obtained from [30] and are presented in the table shown in table 3.3. This research is also influenced by [31], where the investigation focused on advanced configurations of the PCC process implemented in a cement plant to treat flue gases. The author proposed three novel configurations and compared them with the reference case of [30]. These innovative configurations involve

lean split flow, rich split flow, and vapor recompression. In this study, the vapor recompression configuration is substituted with heat pump technology, addressing a research gap and introducing a heat integration strategy to lower the regeneration duty. Another distinction in this study is the mixing of the combustion flue gas of natural gas with the existing flue gas to increase the CO₂ concentration and analyze its impact on the regeneration duty.

Liquid Composition	
Temperature (°C)	40
Pressure (kPa)	101.5
MEA wt. (%)	30
Columns	
Absorber Packing height (m)	21.95
Packing diameter (m)	10.07
Pressure drop (kPa)	2
Stages	36
Stripper Packing height (m)	15.85
Packing diameter (m)	6.04
Pressure drop (kPa)	10
Stages	26
Reboiler pressure (kPa)	170
Reboiler Temperature (°C)	115

Table 3.3: Liquid composition and column details [30]

3.4 Absorber and desorber temperature

3.4.1 Absorber temperature

Absorption stage in CO₂ capture with amines is significantly affected by fluctuations in temperature, which play a critical role in the effectiveness and success of the process. Decreasing absorption temperatures typically boost the CO₂ solubility in the amine solution, thereby improving the capture efficiency. Nevertheless, extremely low temperatures could result in higher solvent viscosity, which might hinder mass transfer and necessitate extra energy for mixing.

The following information illustrates the differences in absorption based on the temperature of the flue gas.

- Higher flue gas temperature: (Flue gas > lean amine): Reduces the absorption capacity and increases the solvent degradation.
- Equal: Absorption rate is moderate and the energy requirement is balanced.
- Lower flue gas temperature (lean amine > Flue gas): Increases absorption rate which affects the efficiency of the process and reduces the solvent degradation.

3.4.2 Desorber temperature

In the desorption phase of CO₂ capture using amines, temperature is a crucial factor in helping to remove captured CO₂ from the solvent for storage or utilization. Elevated

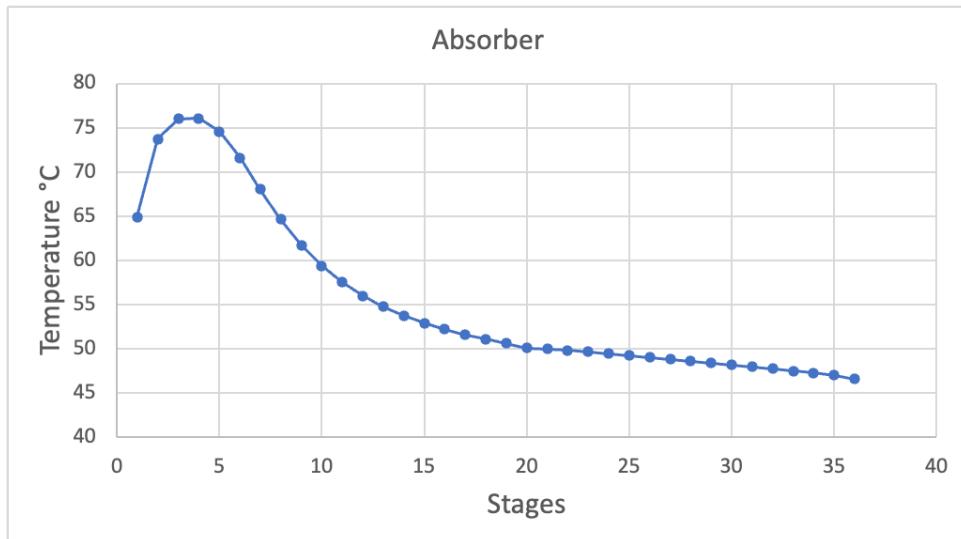


Figure 3.7: Absorber temperature

desorption temperatures typically facilitate the renewal of amine solvents by improving CO₂ release. Nevertheless, excessively high temperatures may result in higher energy consumption and a potential deterioration of the solvent, which can affect its reusability and overall system efficiency.

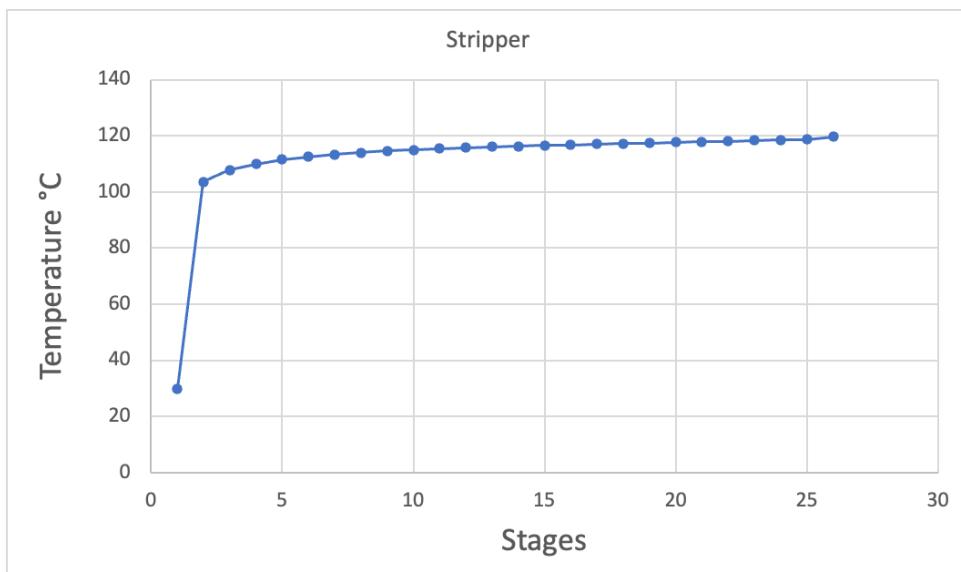


Figure 3.8: Stripper temperature

3.5 Heat integration strategy

Heat integration involves identifying optimal matches between hot and cold process streams to minimize the need for steam, natural gas, or cooling water.

In this thesis, the heat integration strategy is implemented for certain configurations to minimize the energy requirement of the reboiler. The following procedures are adhered to in the heat integration process. Optimization of the process should be ensured before implementing the integration strategy [51]. The composite curves are shown in figure 3.9.

1. Select a lower limit for the operating temperature, for instance, 10 °C.
2. Identify the streams that require heating or cooling.
3. Develop a temperature interval diagram.
4. Create a cascade diagram to identify the pinch point.
5. Decide the optimal configuration for heat exchangers.
6. Determine the most suitable arrangement for heat exchangers.

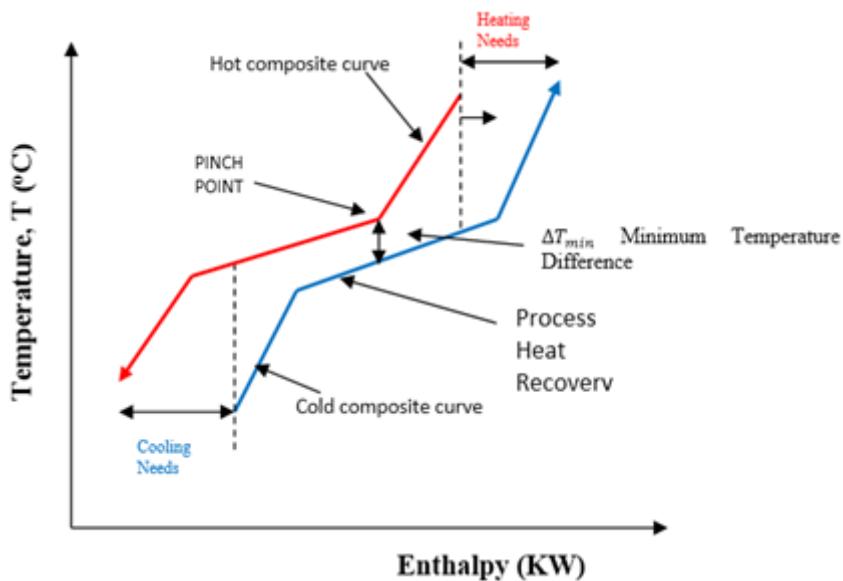


Figure 3.9: Composite curves [52]

Chapter 4

Life Cycle Assessment

4.1 Life cycle assessment

The International Organization for Standardization (ISO) 14000 series standards, focusing on life cycle assessment, provide quantitative methods to evaluate the environmental impacts of a product or service at all stages of its life cycle [53]. ISO 14040 standards are created for managers, which establishes the principles and framework, while ISO 14044 is designed for practitioners, which outlines the requirements and guidelines [54].

LCA defined by ISO 14040: "compilation and evaluation of the inputs, outputs, and the potential environmental impacts of a product system throughout its life cycle" [55].

According to ISO 14044: 2006 standard "Environmental management – Life cycle assessment – Requirements and guidelines" [55], consists of four phases as depicted in figure 4.1.

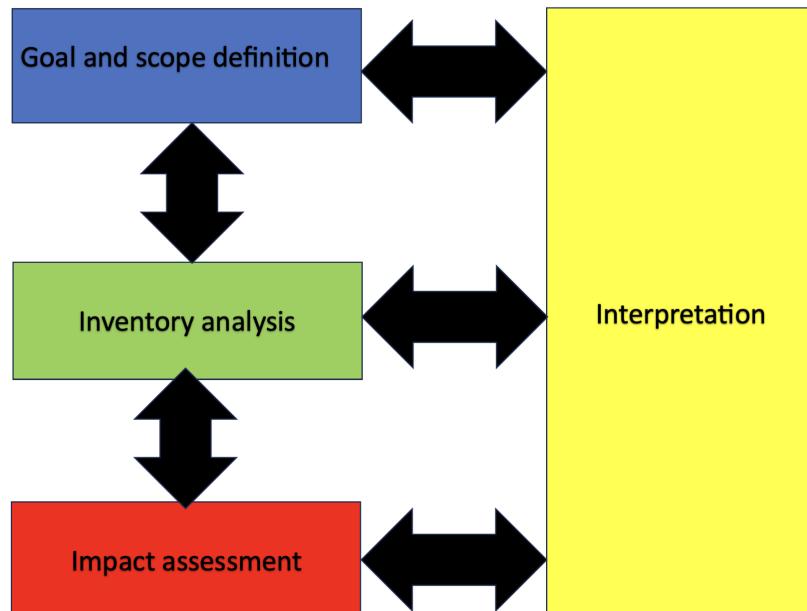


Figure 4.1: Phases of LCA

4.1.1 Phases of life cycle assessment

1. Goal and scope: Includes the boundary of the system and the functional unit that are the backbone of the analysis. The system boundary represents the focus of interest consisting of a single process, multiple processes, or the entire plant. The functional unit is the quantified performance of a product system with a physical unit[56]. Reference flow measures the output of the products generated from processes in the product system to achieve the function specified by the functional unit. The goal and scope also address the purpose behind its execution, the target audience, the product applications, and the comparison aspect of various scenarios or with a benchmark set.

2. Inventory analysis: It includes the collection of data from various sources, such as industry, journals, government published data, and many more, and provides information on the materials flowing into and out of the system. Data are verified before analysis.

3. Impact assessment: The results of the inventory analysis are analyzed for environmental impact, which is done by classifying emissions into impact categories and then characterizing them into common units that are calculated using scientific methodologies for comparison. Examples of impact assessment methods include ReCipe, TRACI, EF, and others.

4. Interpretation: The impact assessment results give information about products or processes that are very useful for decision making. This step also involves finding hotspots, increasing efficiency, among others, as shown in figure 4.2.



Figure 4.2: Business benefits of LCA for Products [56].

4.1.2 Scope of life cycle assessment

The LCA system boundary, which determines the scope of the analysis, can be classified into three different approaches as illustrated in figure 4.3.

1.Cradle to Gate: In this approach, the environmental impact of the product from its extraction or creation ("cradle") through its manufacturing processes, and ending at the factory gate.

2.Cradle to Grave: In this approach, the entire life cycle of a product is considered, from the cradle to the end of life ("grave").

3.Gate-to-Gate: In this analysis, the environmental impacts of a specific stage of the product, typically the manufacturing or production phase, are considered.

After understanding the LCA and its phases, scope, and benefits of performing the LCA, the next step involves calculating the environmental impacts of processes or products using software. There are various options, each having its own merits and drawbacks such as GaBi, OpenLCA, SimaPro, Brightway, one-click LCA, umberto to name a few.

GaBi is known for its user-friendly interface and extensive data base collection. SimaPro offers robust features in modeling and analyzing lifecycles. OpenLCA focuses on flexibility and transparency, and moreover, it is free to conduct the environmental impact analysis.

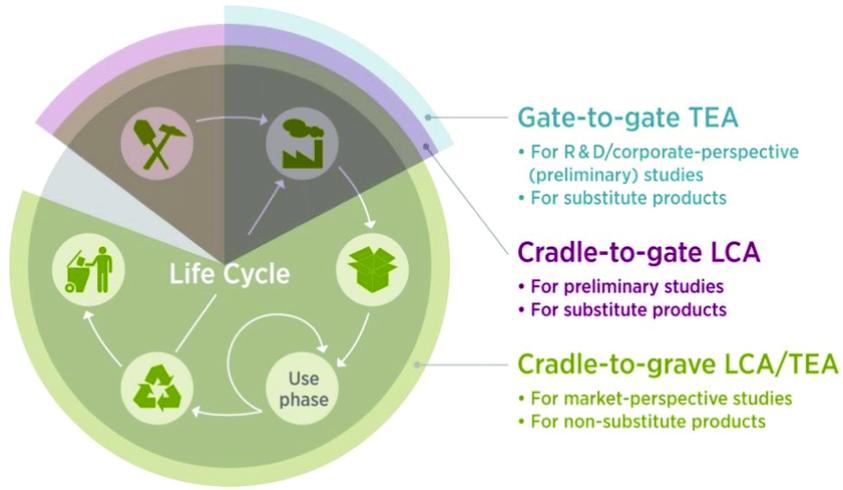


Figure 4.3: Scope of LCA in the product life cycle [57].

The thesis is conducted using GaBi software, and I acknowledge the educational license granted by the company, which facilitates a smooth and efficient analysis. GaBi database information and the GaBi interface are, respectively, shown in figure 4.4 and figure 4.5.

The following outline the steps performed in the GaBi software to calculate environmental impacts.

1. Connect to the database and activate: In this study, the educational database version 8.7 is connected and activated as shown in figure 4.4.

2. Create a new plan: The plan represents the system consisting of processes, flows, and boundaries. In GaBi, there are five types of processes, as illustrated in table 4.1. In this research, we focus on the first two processes. Flows are characterized as elementary and nonelementary flows. Elementary flows are flows that enter a product system coming from a natural environment, whereas non-elementary flows are flows that are valuable substances that are used to connect the process. Non-elementary flows are also called tracked flows, which are used to define environmental impacts of the flow.

3. Adding process and flows: Add processes and flows to the area of the plan object. GaBi has predefined processes and flows that are useful for analysis. Use the "auto-connect" feature to connect flows and processes within the plan. Also, in every plan, one process should be fixed, and a functional unit(FU) is defined in the process, so GaBi calculates all the results in relation to the fixed process.

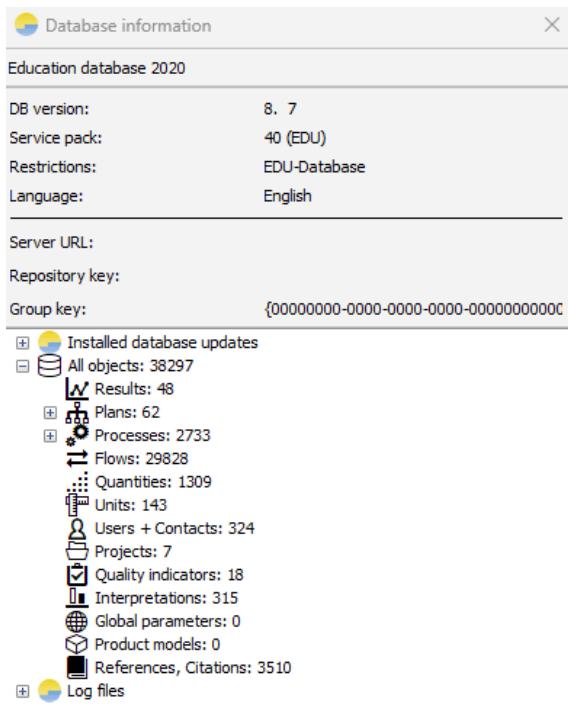


Figure 4.4: GaBi database information

Process	Function
Unit process single operation(u-so)	Referred to as gate-to-gate, which contains data for one specific process step and does not contain LCI data.
Unit process black box(u-bb)	Contains data for multifunctional process or process chain at the plant level.
Aggregated process(agg) or LCI result	Contains data for entire life cycle data, also called cradle-to-gate or grave.
Partly terminated system(p-agg)	Contains all LCI data for the process except for the process or product flow which requires additional modeling.
Avoided product system(aps)	All input and output flows are set to negative values. Used only during allocation modeling.

Table 4.1: Types of process: GaBi - according to the EU ILCD system [58].

4.Creating a new project: Add plan to the newly created project, save the plan within the project and activate the project. It should also be noted that the functional unit of the process and the plan is scaled according to the LCA objective.

5.Interpretation of results: There are many methods available to calculate environmental impacts, such as CML¹, TRACI², environmental footprint (EF) developed by European union(EU), ReCiPe³, IPCC ARS⁴, and the Impact method 2002+, to name a few.

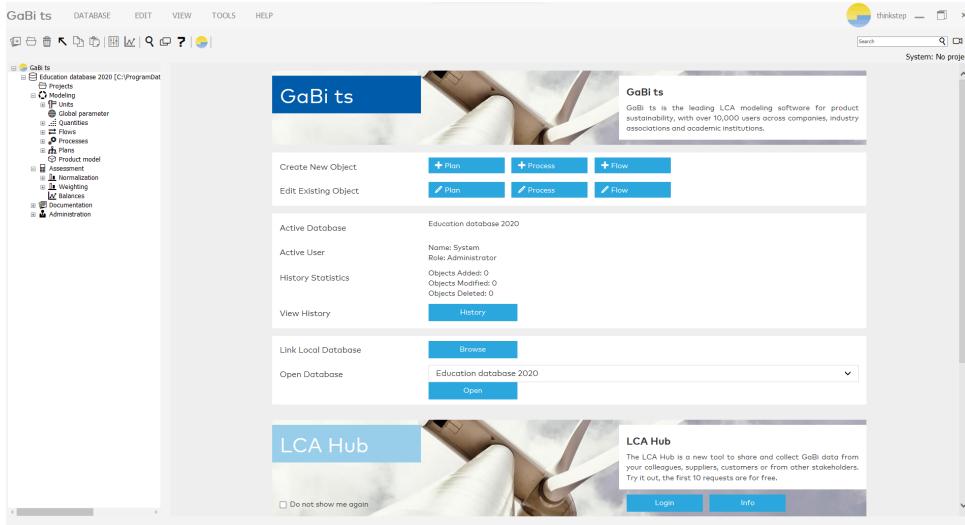


Figure 4.5: GaBi interface [61].

The LCA evaluation for this thesis investigates the following.

- Software: GaBi(8.7), EDU-Database
- Goal: To find out the environmental impact of amine-based CO₂ capture using various configurations.
- Scope: Cradle to gate.
- Functional unit: 1 ton of carbon dioxide (CO₂) captured.
- Impact assessment method: Environmental Footprint (EF 3.0)

¹Centrum voor Milieuwetenschappen Leiden (CML) [59],Leiden University(Netherland)

²Tool for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI), United States Environmental Protection Agency

³Represents the initials of the institutes that were the main contributors of the project and the major collaborators in its design: RIVM, Randboud University, CML and PRé Consultants [60]

⁴Intergovernmental Panel on Climate Change Assessment Reports(IPCC ARS)

4.2 Configuration overview

The figure below illustrates various configurations that were simulated to calculate environmental impacts through Life Cycle Assessment (LCA). The numbers represent the different configurations, while the thermal energy source indicates the type of thermal energy used. The Heat Integration row indicates whether heat integration is implemented or not for each configuration. Each configuration will be discussed in detail in the following chapter.

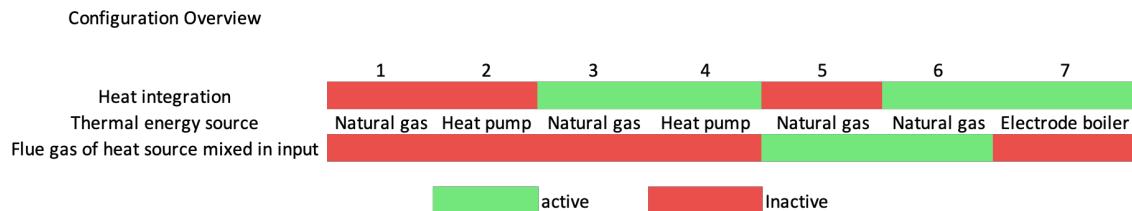


Figure 4.6: Configuration Overview

The following 7 configurations are outlined as follows.

1. Configuration 1: Conventional
2. Configuration 2: Heat pump
3. Configuration 3: Innovative configuration (IC)
4. Configuration 4: Heat pump + Heat integration
5. Configuration 5: Conventional + Flue gas from natural gas combustion (NG)
6. Configuration 6: Innovative configuration(IC) + Flue gas from natural gas combustion(NG)
7. Configuration 7: Innovative configuration(IC) + Electric boiler

Chapter 5

Results

5.1 Sensitivity analysis

Sensitivity analysis is performed on various parameters related to regeneration duty, which is crucial in our study and is performed on Conventional configuration. This analysis aims to examine how changes in one parameter can affect the simulation results. Parameters such as flue gas pressure, heater pressure, heater temperature, molar reflux ratio, molar boil-up ratio, and recycle split fraction are evaluated in relation to regeneration duty. The graphical representation of this analysis can be seen from figure 5.1 to figure 5.6, while the corresponding tabular data are presented from table 5.1 to table 5.6.

Pressure (bar)	Regeneration duty (MJ/kg)
1.035	4.694
1.475	4.690
1.916	4.689
2.356	4.690
2.797	4.693
3.237	4.695
3.678	4.697
4.118	4.6987
4.559	4.700
5	4.701

Table 5.1: Fluegas pressure and Regeneration duty

Heater Pressure (bar)	Regeneration duty (MJ/kg)
2	4.694
2.333	4.715
2.666	4.726
3	4.731
3.333	4.731
3.666	4.732
4	4.732
4.333	4.732
4.666	4.732
5	4.732

Table 5.2: Heater pressure and Regeneration duty

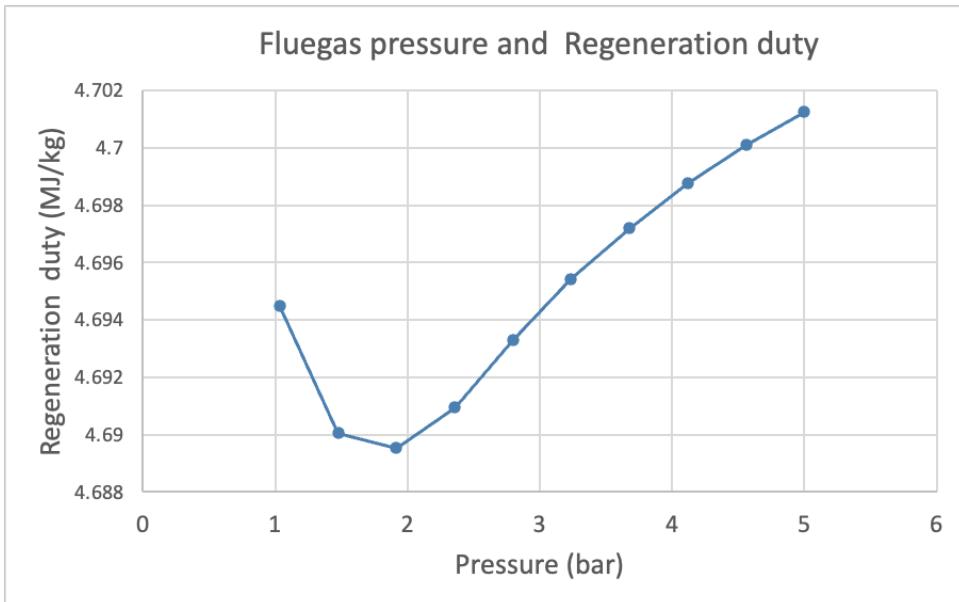


Figure 5.1: Flue gas pressure and Regeneration duty

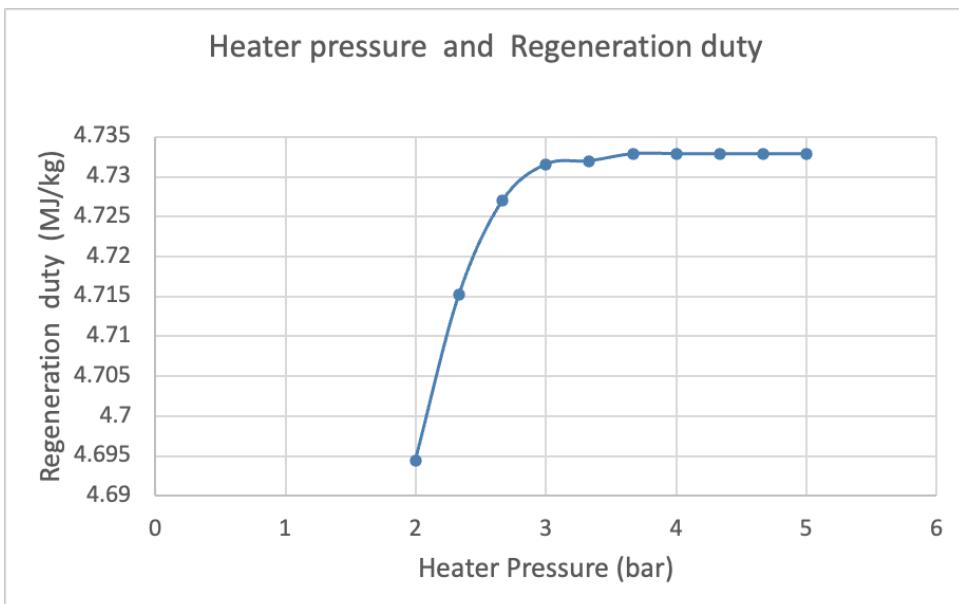


Figure 5.2: Heater pressure and Regeneration duty

From figure 5.1 and figure 5.2, it can be inferred that there is only a slight variation in the regeneration duty value with changes in both flue gas pressure and heater pressure. table 5.1 and table 5.2 shows the tabular data of the pressure of the fluegas and the pressure of the heater against the regeneration duty. This implies that pressure does not significantly influence our simulation results.

Heater temperature (°C)	Regeneration duty (MJ/kg)
95	4.770
97	4.741
99	4.710
100	4.694
101	4.677
103	4.642
105	4.603

Table 5.3: Heater temperature and Regeneration duty

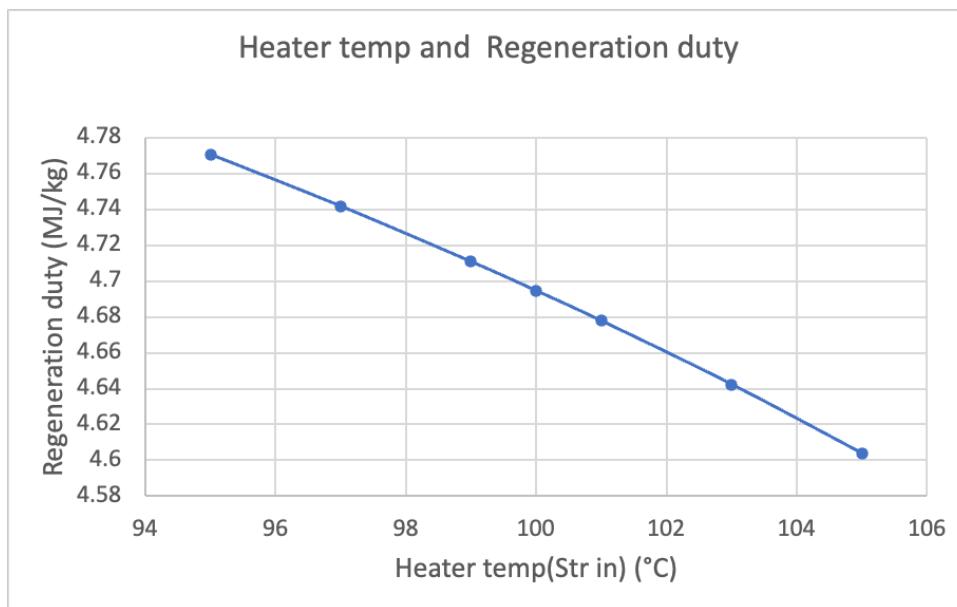


Figure 5.3: Heater temperature and Regeneration duty

Typically, the rich amine solution is preheated before being sent to the stripper. Therefore, from figure 5.3, it can be inferred that a decrease in the heater temperature will result in an increase in the regeneration duty and the tabular data are shown in table 5.3.

Molar reflux ratio	Regeneration duty (MJ/kg)
0.2	4.410
0.4	4.503
0.6	4.578
0.8	4.641
1	4.694

Table 5.4: Molar reflux ratio and Regeneration duty

The molar reflux ratio represents the amount of reflux that flows back into the column to the amount of reflux collected in the distillate. On the other hand, the molar boil-up

ratio is the total vapor flow rate leaving the reboiler divided by the molar flow rate of the more volatile element in the bottom product. By examining the figures shown in figure 5.4 and figure 5.5, it is evident that an increase in the reflux ratio or the boil-up ratio results in a corresponding rise in the regeneration duty and the tabular data is shown in table 5.4 and table 5.5.

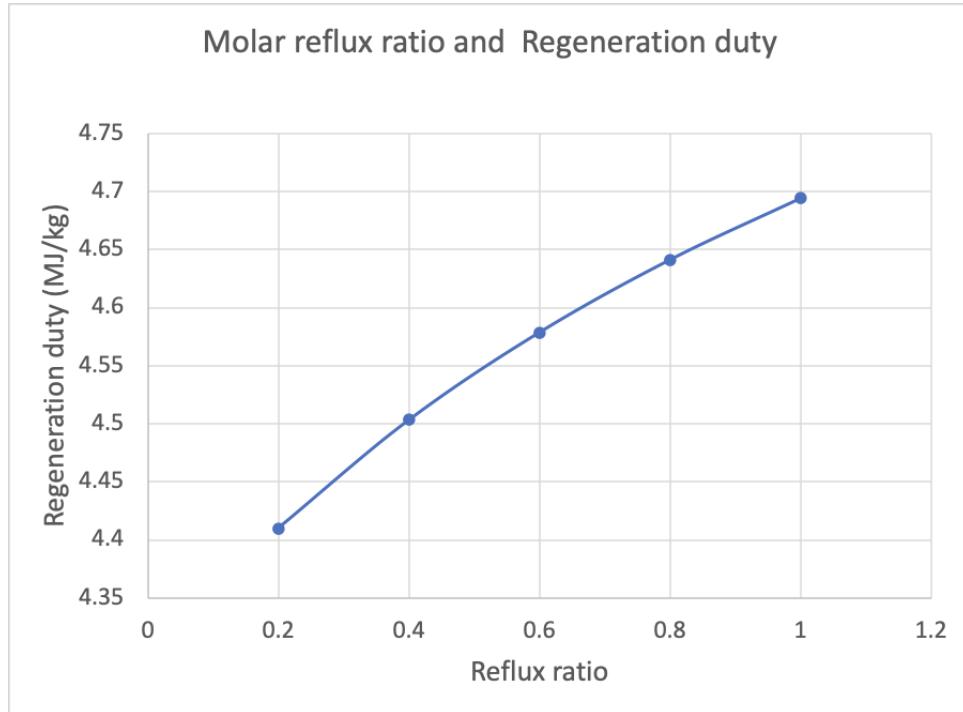


Figure 5.4: Molar reflux ratio and Regeneration duty

Molar boil-up ratio	Regeneration duty (MJ/kg)
0.03	3.754
0.045	3.911
0.06	3.970
0.075	3.987
0.09	3.981
0.2	4.694

Table 5.5: Molar boil-up ratio and Regeneration duty

Finally, the reduction in regeneration duty is observed with an increase in recycle split fraction. However, at a recycle split fraction of 0.8, the regeneration duty unexpectedly reaches a peak. This behavior can be attributed to the higher impurity content, which results in reduced solvent absorption and consequently leads to an increase in duty, as illustrated in figure 5.6 and data in table 5.6.

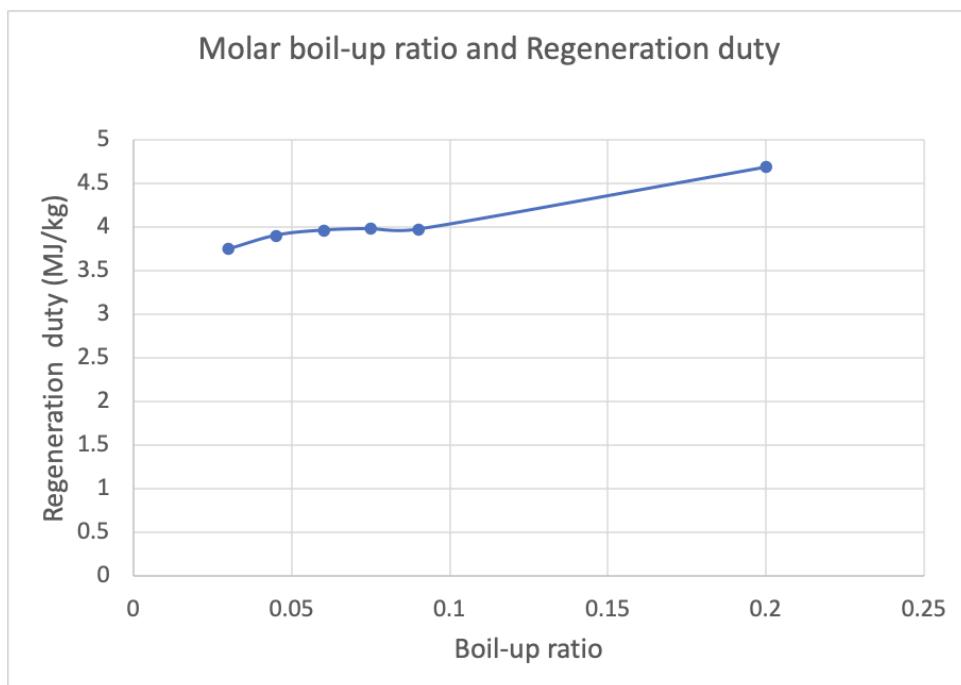


Figure 5.5: Molar boil-up ratio and Regeneration duty

Recycle split	Regeneration duty (MJ/kg)
0.3	4.984
0.425	4.938
0.55	4.858
0.675	4.718
0.7	4.694
0.8	7.374

Table 5.6: Recycle split and Regeneration duty

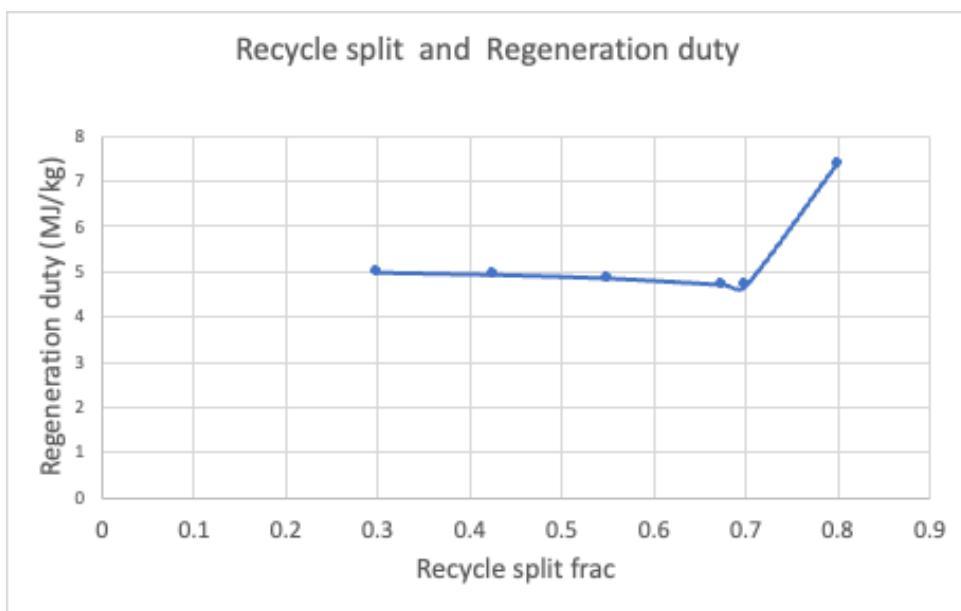


Figure 5.6: Recycle split and Regeneration duty

5.2 Configuration 1: Conventional

The process flow sheet of Configuration 1 [Conventional] is shown in the figure 5.7 and table 5.8 illustrates the table of inputs and outputs in the GaBi plan. Graphical representation of GaBi interface for the Configuration 1 is shown in figure 5.8 and the flue gas input for Configurations 1-4 is also illustrated in table 5.7. It is important to mention that the CO₂ emissions at the output is not a difference between the input CO₂ and the captured CO₂, because some carbon is absorbed into the amine solvent in the form of carbonate species.

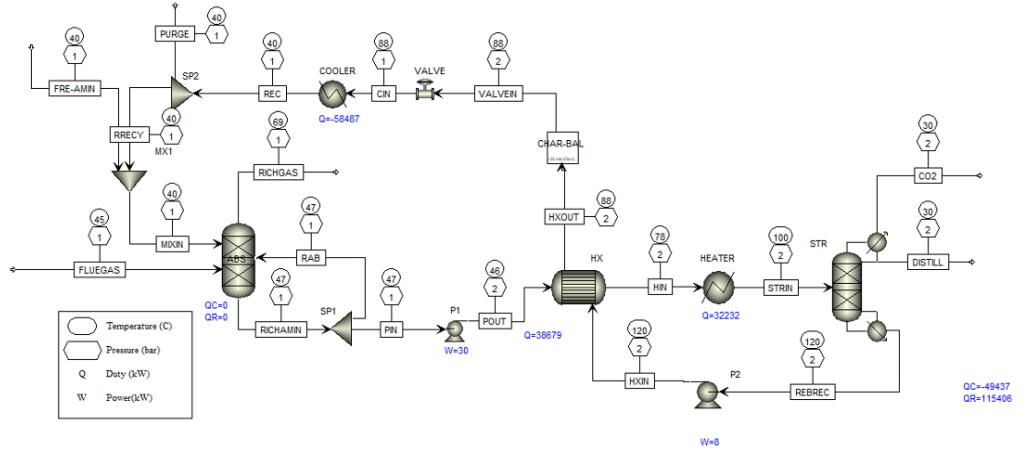


Figure 5.7: Configuration 1: Conventional

	Flows	Amount (kg/sec)
CO ₂	26.9	
N ₂	97.3	
O ₂	17	
H ₂ O (vapour)	37.4	

Table 5.7: Gabi: Input of flue gas for Configurations 1-4

	Flows	Inputs	Outputs	Units
CO ₂	26.9	24.6	kg/sec	
N ₂	97.3	97.3	kg/sec	
O ₂	17	17	kg/sec	
H ₂ O (vapour)	37.4	-	kg/sec	
MEA	311	-	kg/sec	
DE:Electricity, high voltage, at grid	32.3	-	MW	
Thermal energy from natural gas	115	-	MW	
CO ₂ -atmosphere(emissions to air)	-	0.24	kg/sec	

Table 5.8: Configuration 1: GaBi plan - inputs and outputs table

Carbon capture-Conventional -Electricity(Grid mix)
 Process plan: Mass [kg]
 The names of the basic processes are shown.

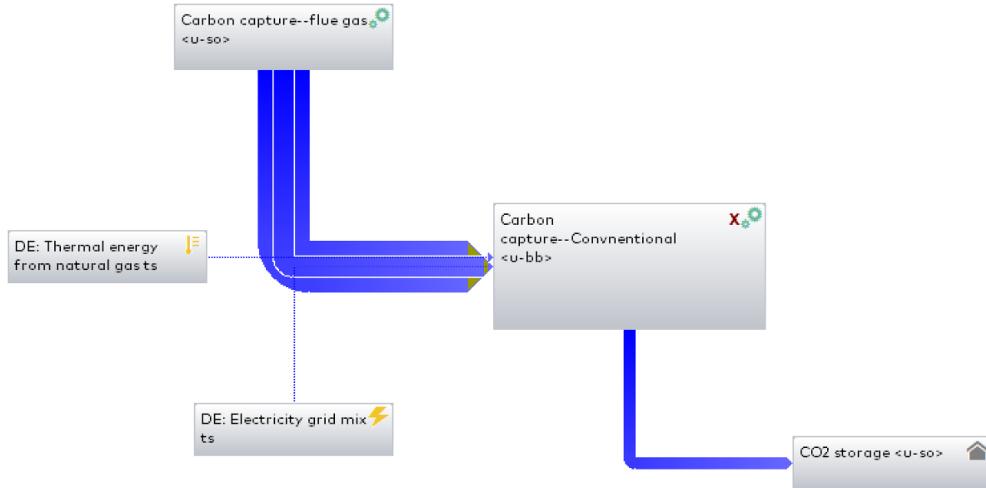


Figure 5.8: Configuration 1: GaBi plan - Electricity - Grid mix

5.3 Configuration 2: Heat pump

The process flow sheet of Configuration 2 [Heat pump] is shown in figure 5.9 and table 5.9 illustrates the table of inputs and outputs in the GaBi plan.

Coefficient of performance (COP): Configuration 2 uses heat pump technology to supply energy to the reboiler, which is shown in figure 5.10. The refrigerant leaves the condenser around 117°C with a pressure of 15 bar and a heat duty (Q) of 115417 KW. On the other hand, the refrigerant leaves the evaporator at 9 °C with a pressure of 1 bar. The power supplied by the compressor (W) is 68248 KW.

The refrigerant used is R-1233zd and the calculated COP (Q / W) for this configuration is 1.79, where Q is the condenser output and W is the supplied work.

Flows	Inputs	Outputs	Units
CO ₂	26.9	24.7	kg/sec
N ₂	97.3	97.3	kg/sec
O ₂	17	17	kg/sec
H ₂ O (vapour)	37.4	-	kg/sec
MEA	313	-	kg/sec
DE: Electricity, high voltage, at grid	101	-	MW
CO ₂ -atmosphere(emissions to air)	-	0.11	kg/sec

Table 5.9: Configuration 2: GaBi plan - inputs and outputs table

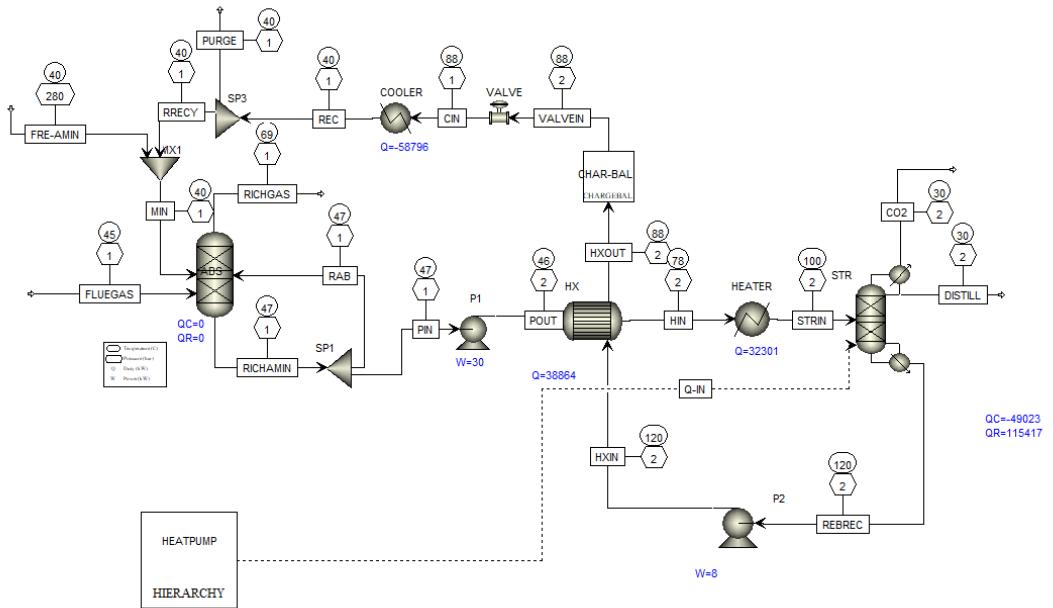


Figure 5.9: Configuration 2: Heat pump

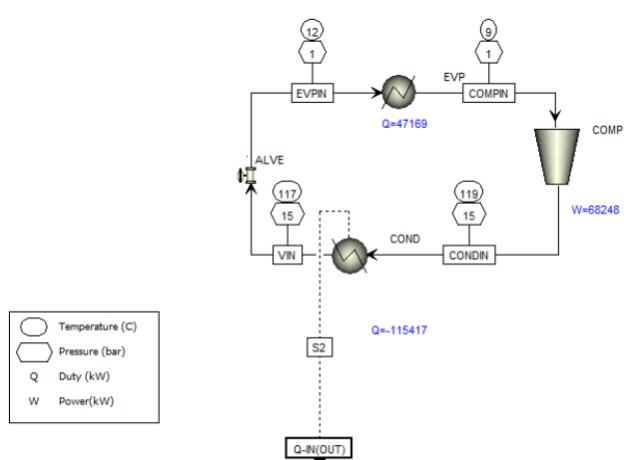


Figure 5.10: Configuration 2: Heat pump simulation

5.4 Configuration 3: Innovative configuration (IC)

The process flow sheet of Configuration 3 [Innovative configuration (IC)] is shown in the figure 5.11 and table 5.10 illustrates the table of inputs and outputs in the GaBi plan. This configuration uses a heat integration strategy to reduce energy requirements of the reboiler.

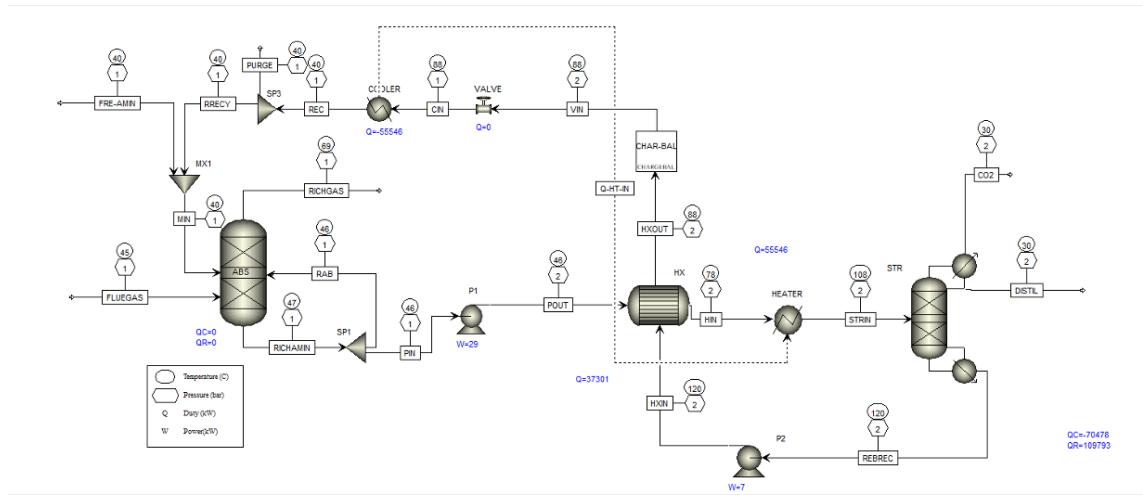


Figure 5.11: Configuration 3: Innovative configuration (IC)

Flows	Inputs	Outputs	Units
CO ₂	26.9	24.2	kg/sec
N ₂	97.3	97.3	kg/sec
O ₂	17	17	kg/sec
H ₂ O (vapour)	37.4	-	kg/sec
MEA	302	-	kg/sec
DE:Electricity, high voltage, at grid	0.035	-	MW
Thermal energy from natural gas	110	-	MW
CO ₂ -atmosphere(emissions to air)	-	0.45	kg/sec

Table 5.10: Configuration 3: GaBi plan - inputs and outputs table

5.5 Configuration 4: Heat pump + Heat integration

The process flow sheet of Configuration 4: Heat pump + Heat integration is shown in the figure 5.13 and table 5.11 illustrates the table of inputs and outputs in the GaBi plan.

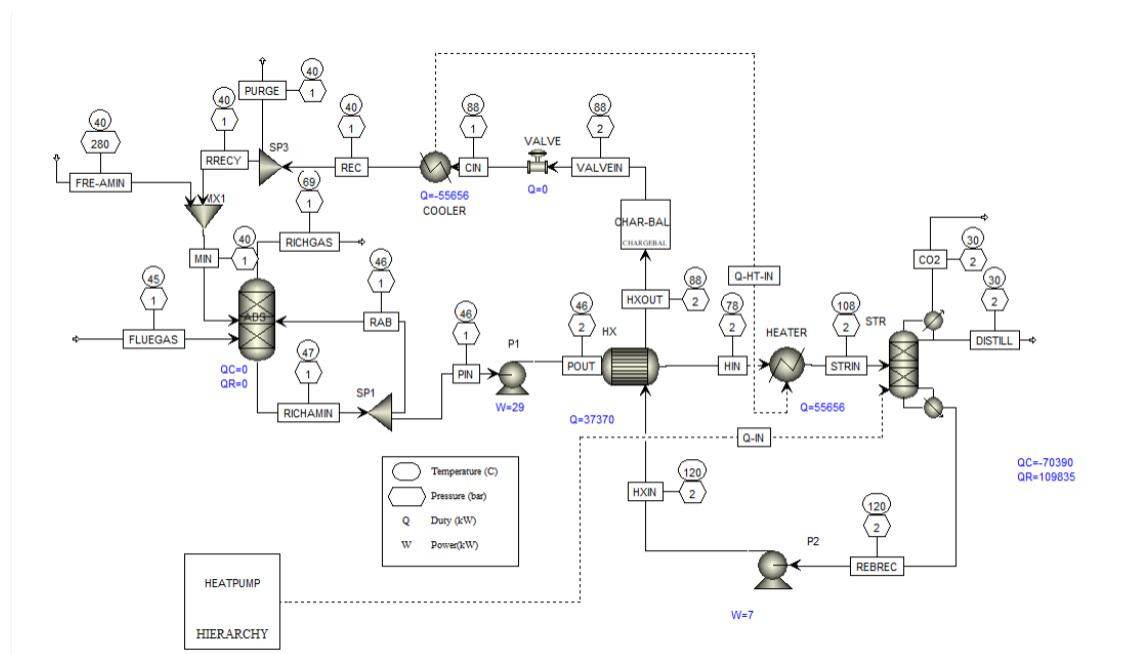


Figure 5.12: Configuration 4: Heat pump + Heat integration

Flows	Inputs	Outputs	Units
CO ₂	26.9	24.6	kg/sec
N ₂	97.3	97.3	kg/sec
O ₂	17	17	kg/sec
H ₂ O (vapour)	37.4	-	kg/sec
MEA	303	-	kg/sec
DE:Electricity, high voltage, at grid	64.9	-	MW
CO ₂ -atmosphere(emissions to air)	-	0.36	kg/sec

Table 5.11: Configuration 4: GaBi plan - inputs and outputs table

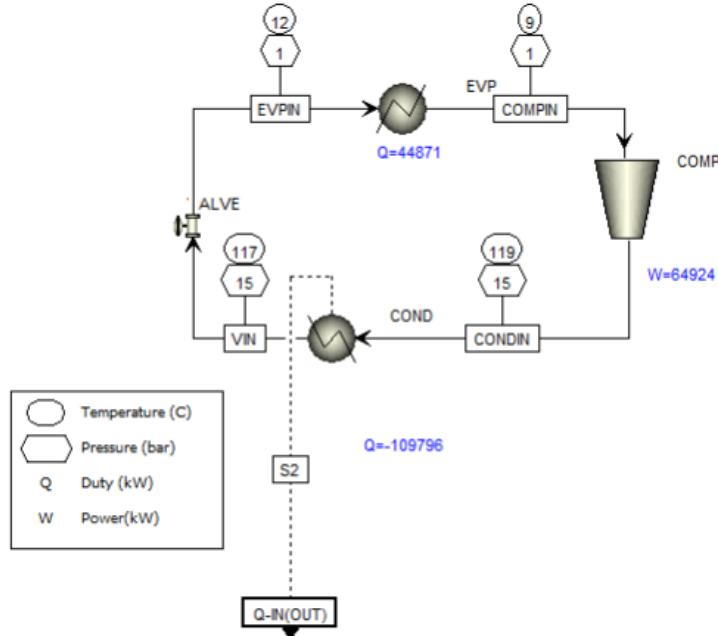


Figure 5.13: Configuration 4: Heat pump (simulation) + Heat integration

Coefficient of performance (COP): Configuration 4, similar to configuration 2, uses heat pump technology to supply energy to the reboiler, which is shown in figure 5.13. The refrigerant used is R-1233zd and the calculated COP for this configuration is 1.69, where Q represents the condenser output and W is the supplied work. Configuration 4 differs from Configuration 2 in that it implements a heat integration strategy.

Calculations:

$$\begin{aligned}
 COP &= \frac{Q}{W} \\
 &= \frac{109796 \text{ [KW]}}{64924 \text{ [KW]}} \\
 &= 1.69
 \end{aligned}$$

5.6 Configuration 5: Conventional + Flue gas from natural gas combustion (NG)

The process flow sheet of Configuration 5 [Conventional + Flue gas from natural gas combustion (NG)] is shown in the figure 5.14 and table 5.13 illustrates the table of inputs and outputs in the GaBi plan. This configuration involves the flue gas generated natural gas combustion, with the combustion supplying energy to the reboiler. The resulting flue gas from the process is then recirculated and combined with the flue gas produced by the cement plant.

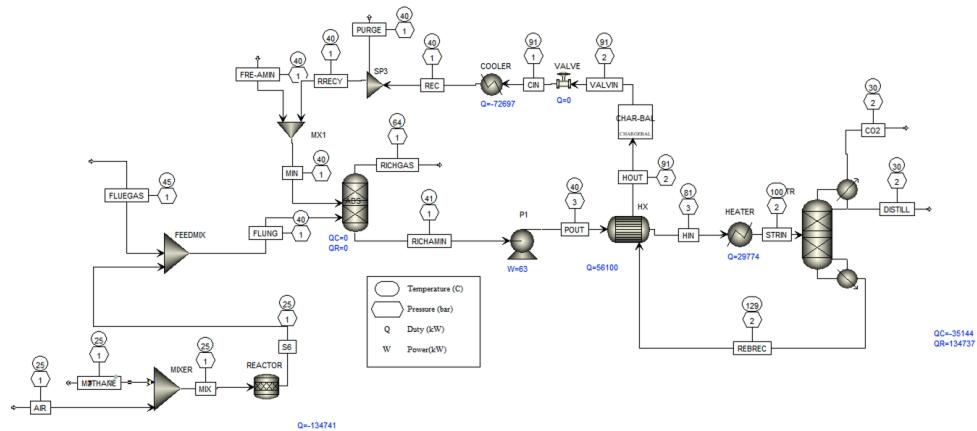


Figure 5.14: Configuration 5: Conventional + NG

Flows	Amount (kg/sec)
CO ₂	33
N ₂	159
O ₂	26.8
H ₂ O (vapour)	42.4

Table 5.12: Gabi: Flue gas input Configuration 5 and Configuration 6

Flows	Inputs	Outputs	Units
CO ₂	33	29.8	kg/sec
N ₂	159	159	kg/sec
O ₂	26.8	26.8	kg/sec
H ₂ O (vapour)	42.4	-	kg/sec
MEA	363	-	kg/sec
DE:Electricity, high voltage, at grid	29.6	-	MW
Thermal energy from natural gas	134	-	MW
CO ₂ -atmosphere(emissions to air)	-	1.73	kg/sec

Table 5.13: Configuration 5: GaBi plan - inputs and outputs table

5.7 Configuration 6: Innovative configuration(IC) + Flue gas from natural gas combustion(NG)

The process flow sheet of Configuration 6 [Innovative configuration(IC) + Flue gas from natural gas combustion(NG)] is shown in the figure 5.15 and table 5.14 illustrates the table of inputs and outputs in the GaBi plan.

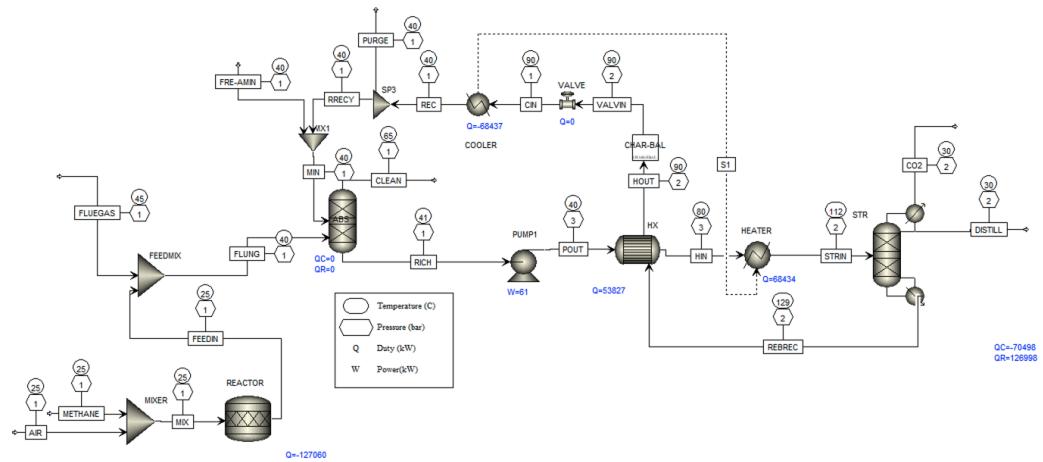


Figure 5.15: Configuration 6: IC + NG

Flows	Inputs	Outputs	Units
CO ₂	33	29.7	kg/sec
N ₂	159	159	kg/sec
O ₂	26.8	26.8	kg/sec
H ₂ O (vapour)	42.4	-	kg/sec
MEA	355	-	kg/sec
DE:Electricity, high voltage, at grid	0.065	-	MW
Thermal energy from natural gas	127	-	MW
CO ₂ -atmosphere(emissions to air)	-	1.34	kg/sec

Table 5.14: Configuration 6: GaBi plan - inputs and outputs table

5.8 Configuration 7: Innovative configuration(IC) + Electric boiler

The process flow sheet of Configuration 7 [Innovative configuration(IC) + Electric boiler] is shown in the figure 5.16 and table 5.15 illustrates the table of inputs and outputs in the GaBi plan. The configuration resembles Configuration 3, with the only distinction being that electricity is used as the energy source instead of thermal energy.

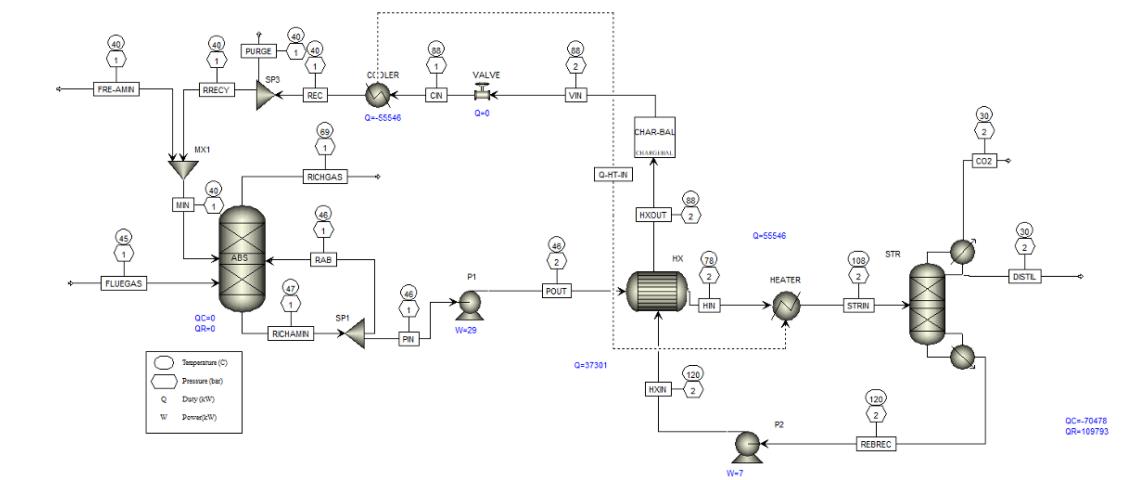


Figure 5.16: Configuration 7: IC + Electric boiler

Flows	Inputs	Outputs	Units
CO ₂	26.9	24.2	kg/sec
N ₂	97.3	97.3	kg/sec
O ₂	17	17	kg/sec
H ₂ O (vapour)	37.4	-	kg/sec
MEA	302	-	kg/sec
DE:Electricity, high voltage, at grid	110	-	MW
CO ₂ -atmosphere(emissions to air)	-	0.45	kg/sec

Table 5.15: Configuration 7: GaBi plan - inputs and outputs table

5.9 Regeneration duty

The image below demonstrates the regeneration duty of seven different configurations, as referenced in figure 5.17. The first two configurations have identical energy requirements, with one relying on fossil fuels, impacting the environment, while the other utilizes a heat pump, which also has environmental implications if the electricity it uses is generated from fossil fuels. Configuration 3 presents a reduction in the reboiler's energy demand through the implementation of a heat integration strategy, a unique feature not explored

in the cited paper [31]. Configurations 3, 4, 5, and 7 have almost the same energy duty, lower than the initial two configurations, due to the implementation of a heat integration strategy that improves the absorption efficiency. Configuration 6 stands out for having a lower energy duty compared to its counterparts.

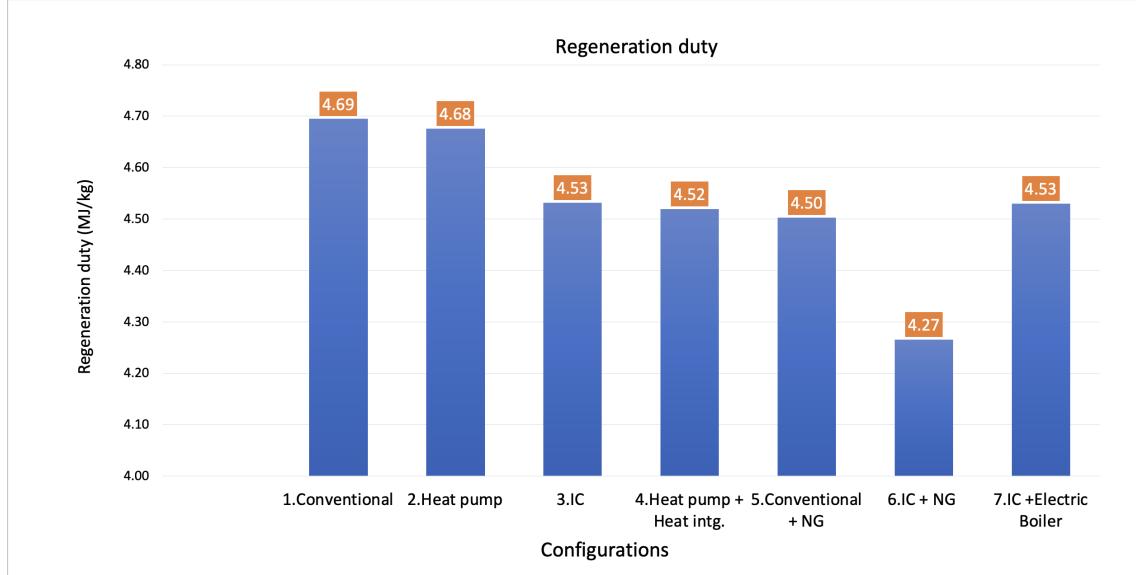


Figure 5.17: Regeneration duty

5.10 Other environmental impacts and simulation metrics

The comparisons of eutrophication terrestrial [Mole of N eq.] and resource use [MJ] for different configurations are illustrated in the images figure 5.18 and figure 5.19. The discussion of these comparisons will be provided in the subsequent chapter. Eutrophication potential refers to the tendency of a substance or activity to increase nutrient levels in water bodies, leading to excessive algae growth and disturbances in the ecosystem. Resource utilization analysis shows the utilization of natural resources, such as energy, water and materials, throughout the life cycle of a product, offering a comprehensive understanding of its environmental impact.

The tables figure 6.3, table 5.17, and table 5.18 illustrate the contribution analysis of climate change and resource utilization, the overall carbon footprint per ton of CO₂ captured, and the simulation metrics for energy.

Contribution analysis of climate change and resource utilization involves evaluating the impacts of different parameters. The total carbon footprint per ton of captured CO₂ measures the total emissions related to the capture, transport, storage, or use of carbon dioxide. This metric is crucial to understanding the environmental consequences of CO₂ capture methods, which helps in decision making to minimize emissions. Simulation data provide various parameters such as heat duty, flow rate, and regeneration duty, which can be used for optimization purposes and identifying hotspots. Detailed simulation outcomes of each configuration are illustrated in Appendix A.

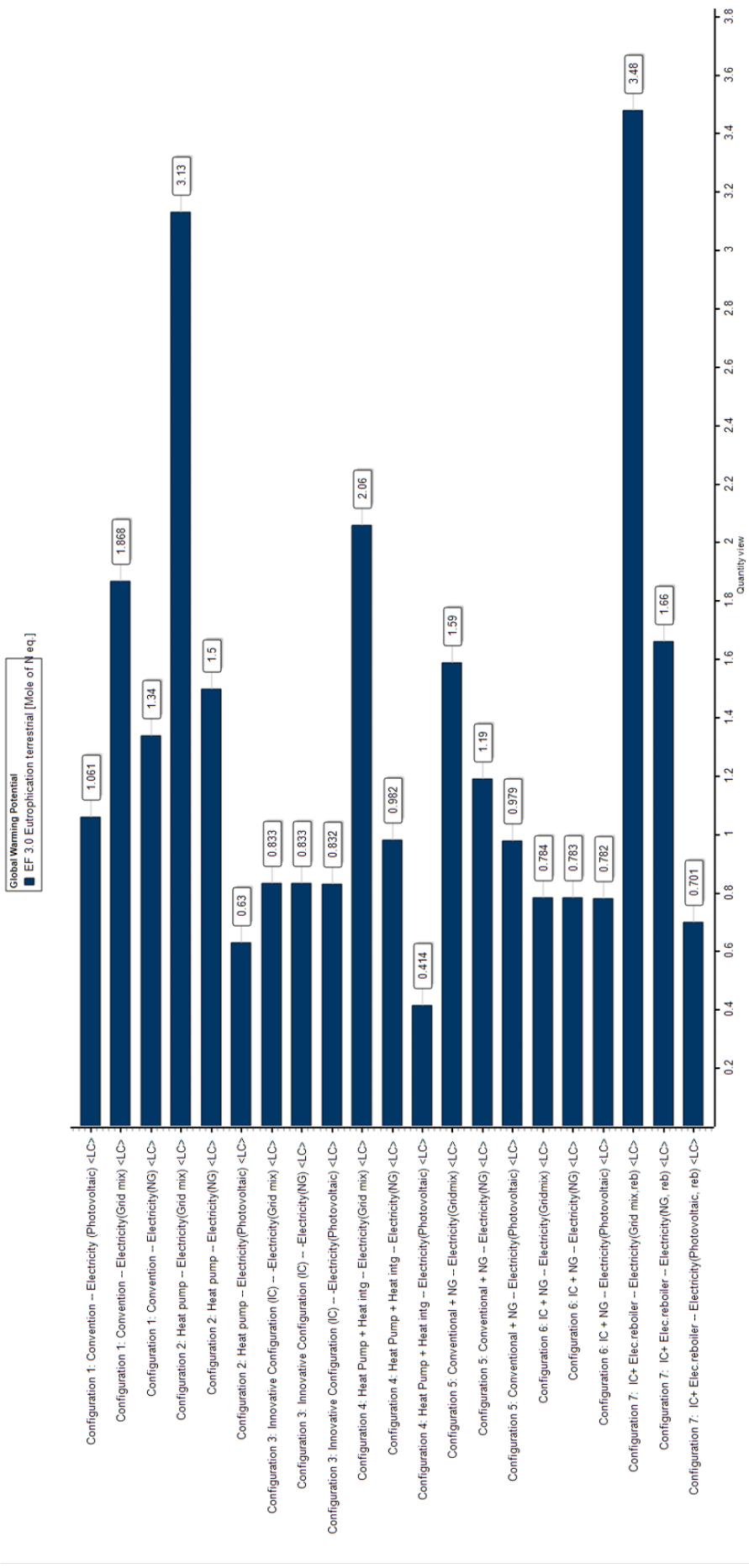


Figure 5.18: Comparison: Eutrophication terrestrial

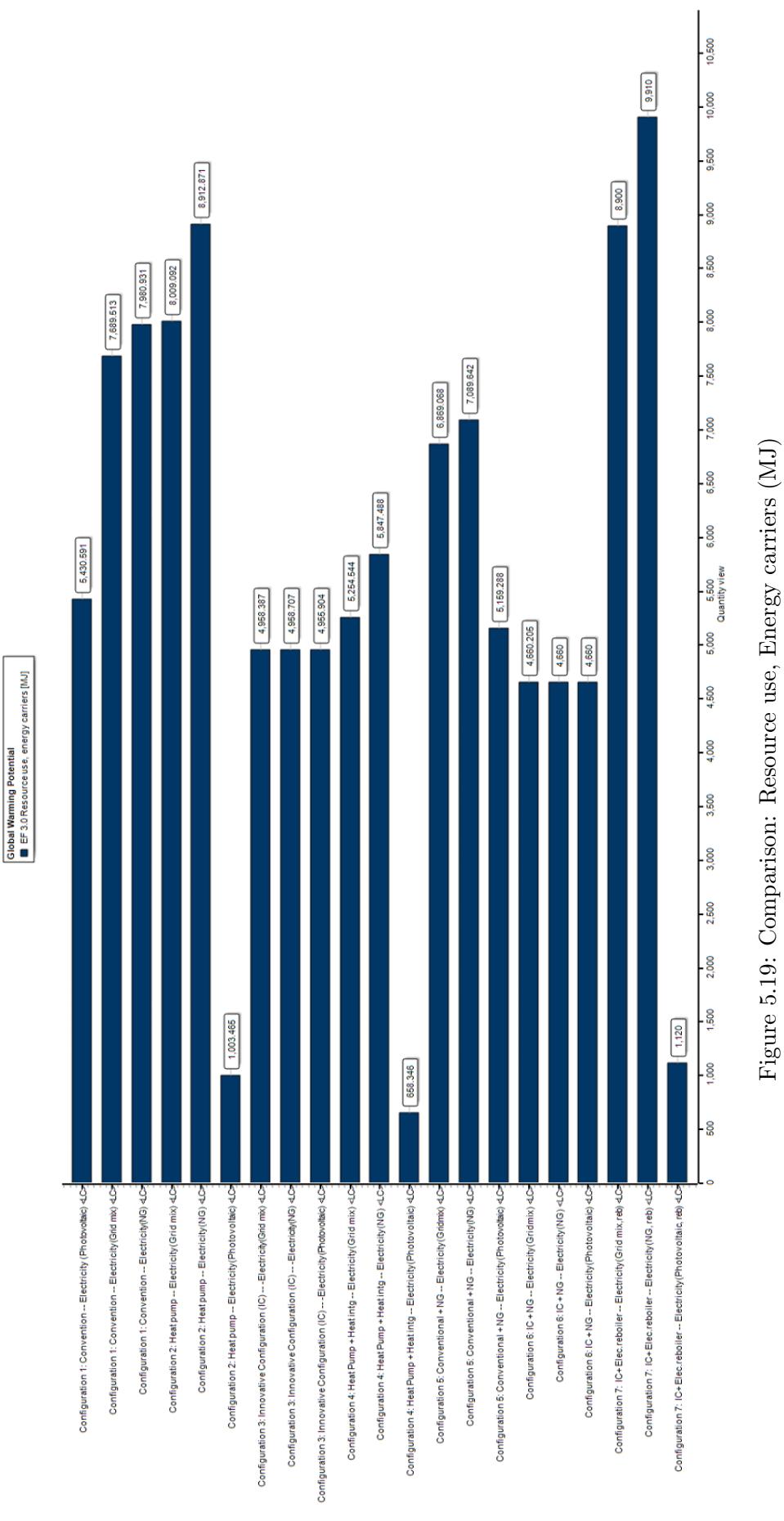


Figure 5.19: Comparison: Resource use, Energy carriers (MJ)

Table 5.16: Contribution analysis: Climate change and Resource use, Energy carriers

Configuration	Climate change (kg CO ₂ eq.)		Resource use, Energy carriers (MJ)	
	Elec. share	Thermal share	Elec. share	Thermal share
Conventional	Gridmix	210	316	2.58×10^3
	NG	177	316	2.87×10^3
	Photovoltaic	25.4	316	3.23×10^3
Heat pump	Gridmix	651	0	8.01×10^3
	NG	550	0	8.91×10^3
	Photovoltaic	78.7	0	1.00×10^3
IC	Gridmix	0.231	305	2.84×10^3
	NG	0.195	305	3.16×10^3
	Photovoltaic	0.027	305	0.356×10^3
Heat Pump + Heat intg.	Gridmix	427	0	5.25×10^3
	NG	361	0	5.85×10^3
	Photovoltaic	51.7	0	658×10^3
Conventional + NG	Gridmix	159	303	1.95×10^3
	NG	134	303	2.18×10^3
	Photovoltaic	19.2	303	245×10^3
IC + NG	Gridmix	0.35	287	4.3×10^3
	NG	0.295	287	4.79×10^3
	Photovoltaic	0.042	287	0.539×10^3
IC + Electric boiler	Gridmix	724	0	8.90×10^3
	NG	612	0	9.91×10^3
	Photovoltaic	87.5	0	1.12×10^3

Table 5.17: Total CO₂ footprint (ton CO₂ eq/ ton of CO₂ captured)

Configuration	Climate change (kg CO ₂ eq.)			CO ₂ Emission to atmosphere (kg) (kg)	Input-CO ₂ (kg)	CF eq.)	(kg) CO ₂	CF eq.)	(ton CO ₂
	Electricity share	Thermal share	Total share CO ₂ eq.)						
Conventional									
	GRIDMIX	21.0	31.6	5.26	9.76	1094.79	-559.03	-0.559	
	NG	17.7	31.6	4.93	9.76	1094.79	-592.03	-0.592	
	PHOTOVOLTAIC	25.4	31.6	341.4	9.76	1094.79	-743.63	-0.743	
Heat pump									
	GRIDMIX	65.1	0	651	4.46	1090.35	-434.89	-0.434	
	NG	55.0	0	550	4.46	1090.35	-535.89	-0.535	
	PHOTOVOLTAIC	78.7	0	78.7	4.46	1090.35	-1007.19	-1.007	
IC									
	GRIDMIX	0.231	305	305.23	18.6	1110.6	-786.76	-0.786	
	NG	0.195	305	305.19	18.6	1110.6	-786.80	-0.786	
	PHOTOVOLTAIC	0.027	305	305.02	18.6	1110.6	-786.97	-0.786	
Heat pump + Heat intg.									
	GRIDMIX	42.7	0	427	14.8	1107.86	-666.06	-0.666	
	NG	36.1	0	361	14.8	1107.86	-732.06	-0.732	
	PHOTOVOLTAIC	51.7	0	51.7	14.8	1107.86	-1041.36	-1.041	
Conventional + NG									
	GRIDMIX	15.9	303	462	58.1	1109.17	-589.07	-0.589	
	NG	13.4	303	437	58.1	1109.17	-614.07	-0.614	
	PHOTOVOLTAIC	19.2	303	322.2	58.1	1109.17	-728.87	-0.728	
IC + NG									
	GRIDMIX	0.35	287	287.35	45.1	1111.78	-779.33	-0.779	
	NG	0.295	287	287.29	45.1	1111.78	-779.38	-0.779	
	PHOTOVOLTAIC	0.042	287	287.04	45.1	1111.78	-779.63	-0.779	
IC + Electric boiler									
	GRIDMIX	72.4	0	724	18.6	1110.6	-368	-0.368	
	NG	61.2	0	612	18.6	1110.6	-480	-0.48	
	PHOTOVOLTAIC	87.5	0	87.5	18.6	1110.6	-1004.5	-1.004	

Table 5.18: Simulation: Energy duty metrics

Configuration	Reboiler (MW)	duty	Stripper heater (MW)	pre- duty	Electricity (MW)	Capture CO_2 (kg/hr)	Capture flow (kg/sec)	CO_2 rate	Regeneration duty (MJ/kg)
Conventional	115.41		32.23		0.03	88495	24.58		4.69
Heat pump	115.42		32.30		68.28	88858	24.68		4.68
IC	109.79	-	-		0.03	87219	24.23		4.53
Heat pump + Heat intg.	109.80	-	-		64.92	87457	24.29		4.52
Conventional + NG	134.03		29.54		0.06	107160	29.77		4.50
IC + NG	126.68	-	-		0.06	106911	29.70		4.27
IC + Electric boiler	109.79	-	-		110	87219	24.23		4.53

Chapter 6

Discussions

6.1 Observations

According to figure 6.1, the following observations can be summarized:

Configuration 1: Conventional

- Configuration 1 shows a significant reduction in carbon dioxide eq. emissions when compared to Configuration 2 by 22. 2% in the grid mix and 9.48% in natural gas. This difference can be explained by the fact that Configuration 1 relies primarily on thermal energy with minimal electricity usage, in contrast to Configuration 2, which relies exclusively on electricity without any thermal energy input. Furthermore, the higher carbon intensity of the grid mix in Configuration 2 is attributed to the various sources of electricity generation, including natural gas, oil and coal, as well as losses during conversion and transmission.
- Configuration 7 can also be justified by the fact that it uses electricity for its operation just as Configuration 2, resulting in a higher intensity of carbon in the operation and achieving a reduction in net emissions in the grid mix and natural gas by 34.17% and 18.92%, respectively.
- Configurations 3 to 6 are expected to achieve greater reductions in CO₂ eq. per ton of captured CO₂ compared to Configuration 1. These reductions range from 4% in Configuration 5, where electricity is sourced from natural gas, to 40.74% in Configuration 3, where energy is obtained from a grid mix. Configuration 2 shows a greater reduction of around 35% when energy is supplied by renewables, such as photovoltaics, which shows the importance of renewables to mitigate climate change.

Configuration 2: Heat pump

- The interesting aspect of Configuration 2 is its use of heat pump technology for CO₂ capture. Despite achieving a COP of 1.69, the energy source that powers the heat pump plays a crucial role in determining the environmental impacts.
- Configuration 2 shows superior reductions of approximately 20-25% compared to other configurations when the energy supplied is from renewables. However, if electricity is sourced from a grid mix and natural gas, the reductions are lower, varying between 10-80% compared to the other configurations.

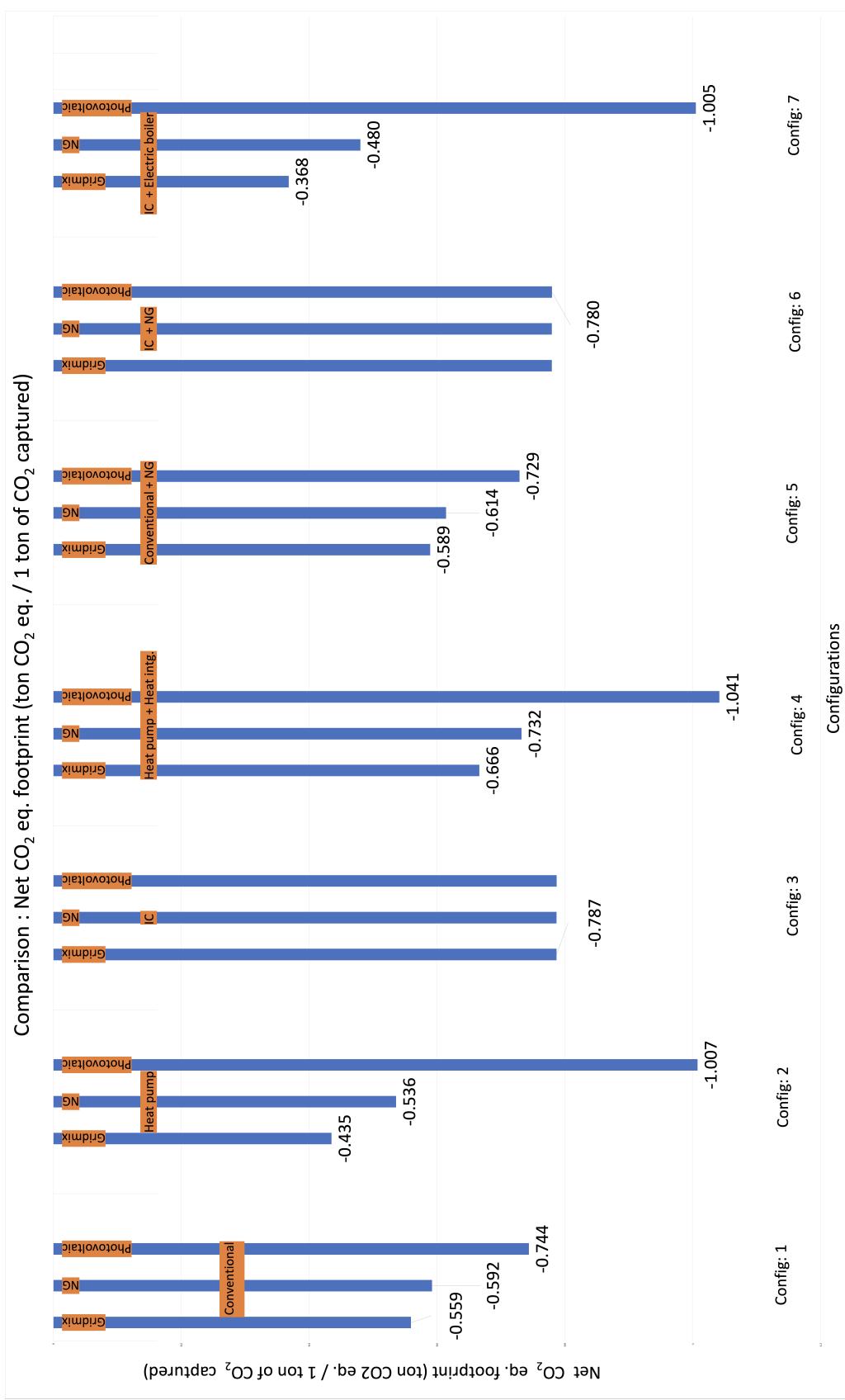


Figure 6.1: Comparison-CO₂ eq. footprint

- Configurations 3 and 6 exhibit a significant reduction of approximately 80% and 45% compared to Configuration 2 when the electricity source is a grid mix and natural gas, respectively, due to its dependence on natural gas as a thermal energy source.

Configuration 3: Innovative configuration (IC)

- Configuration 3 is the one of the Configuration which stands out compared to other cases in this study. It shows a greater reduction of CO₂ eq. in all scenarios except when the energy supply is renewable because the electricity supplied by renewables will have no emissions except during the manufacture, transportation, and installation of the panels.
- If sourced from the grid mix, then Configuration 3 shows a significant net reduction of around 50% and 45% compared to Configurations 7 and 2 and if the source is natural gas, then 40% and 32% for the same.

Configuration 4: Heat pump + Heat integration

- When the energy source is supplied from renewable sources, Configuration 4 emerges as the most sustainable option due to less or no emissions, resulting in overall net reductions of around 29%, 25%, 30%, and 26% compared to Configurations 1, 3, 5, and 6, respectively.
- Similarly to Configuration 3, when the energy source is a grid mix, it also results in a higher net reduction of 45% and 35% in Configurations 7 and 2, respectively, due to the high intensity of carbon in grid mix.

Configuration 5: Conventional + Flue gas from natural gas combustion (NG)

- Configuration 5 replicates Configuration 1, with the difference being the addition of CO₂ input concentration from natural gas combustion, resulting in a reduction of CO₂ concentration in the absorber. This results in small increase in net reduction of 5% and 4% compared to Configuration 1, which can be explained by reduced heat loss, improved mass transfer and absorption efficiency, and reduced dilution of CO₂ in rich amine
- Compared to Configurations 7 and 2, Configuration 5 shows a 38% and 26% greater net reduction when the energy is supplied from the grid mix, which shows the maximum savings potential.

Configuration 6: Innovative configuration(IC) + Flue gas from natural gas combustion(NG)

- Configuration 6 is similar to Configuration 3, except additional CO₂ input from natural gas combustion to the existing flue gas which results in dilution and leads to a decrease in CO₂ concentration in the absorber. It follows in the same way as Configuration 3 where there is a significant net reduction in CO₂ in all cases, except when energy is supplied from renewables.
- Compared to 1,2,5 and 7, it shows a great net reduction impact of 29%, 44%, 25% and 53%, respectively.

Configuration 7: IC + Electric boiler

- Configuration 7 exhibits unusual behavior. In contrast to Configurations 1, 3, 5, and 6 that do not employ heat pump technology, the life cycle assessment for Configurations mentioned above involves supplying thermal energy to the reboiler. However, in Configuration 7, electricity is used as an energy source to generate steam in an electric boiler, which is then used in the reboiler, thereby electrifying the process.
- Configuration 7 demonstrates significant decreases in emissions only when energy is sourced from solar panels. An increase in the net reduction of CO₂ eq. by 26%, 22%, 27%, and 22% is observed compared to configurations 1, 3, 5 and 6, respectively.

6.2 Contribution analysis: Climate change

In the previous section, the net CO₂ eq. footprint was discussed in Configurations where energy is supplied by thermal energy from natural gas or electricity obtained from a variety of sources such as grid mix, natural gas and photovoltaics. Therefore, the following section explains the contribution analysis of electricity and thermal energy shares.

It is important to note that Configurations 2, 4, and 7 do not include a thermal energy share, while Configurations 3 and 6 do not include an electrical share. This can be explained by the fact that former Configurations uses electricity to supply energy from various sources, whereas the latter provide thermal energy from natural gas.

Configuration 1: Conventional

- The contribution analysis from various scenarios or Configurations is illustrated in figure 6.2. Configuration 1 and 5 use both electricity and thermal energy. The proportion of electricity in Configuration 5 is approximately 25% less, and the thermal energy is approximately 4.3% less compared to Configuration 1.
- Due to the combination of thermal energy and electricity from various sources, Configuration 2 has about 68% more electrical share than Configuration 1.
- From figure 6.2, it is clear that in the grid mix for the conventional configuration, the thermal energy contributes the most, followed by electricity, while uncaptured CO₂ plays a smaller role in the overall footprint.

Configuration 2: Heat pump

- As mentioned, Configuration 2 does not have thermal share, so all the configurations have less electrical shares. Configurations 1, 4, and 5 emit less emissions by 67%, 34% and 75% than Configuration 2 when the source is electricity from various sources.
- Configuration 7, similar to Configuration 2, relies on electricity for its operation and produces emissions approximately 11% higher than Configuration 2 when using different electricity sources (gridmix, NG, photovoltaic).
- Configuration 2 only has an electricity contribution, as the whole operation is driven by electricity.

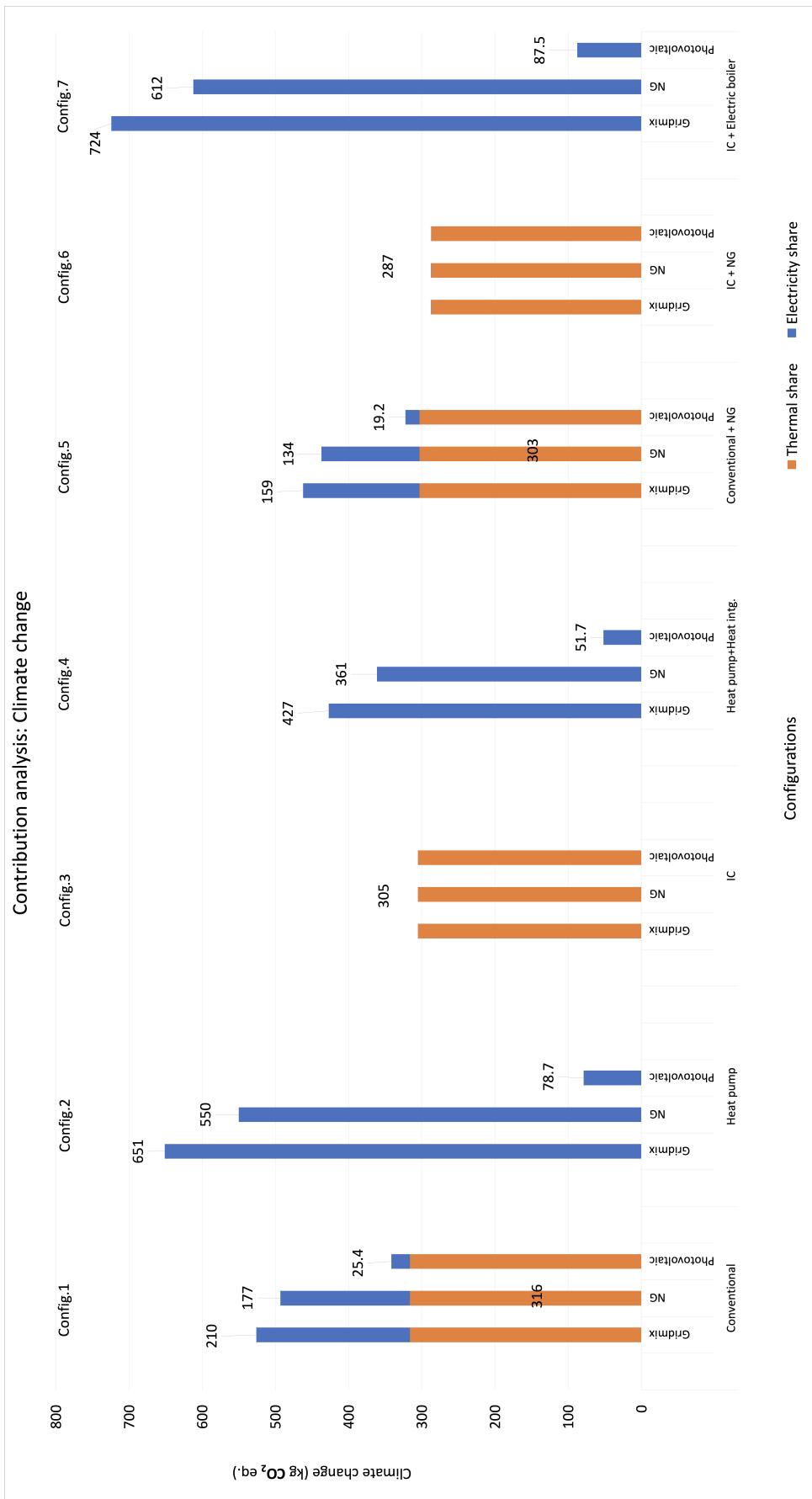


Figure 6.2: Climate change [kg CO₂ eq.]

Configuration 3: Innovative configuration (IC)

- Configurations 3 and 5 show similar thermal share emissions values, with 0.305 and 0.303 t-CO₂-eq. respectively, due to the fact that both use natural gas.
- Configuration 3 shows a slight decrease in the thermal share of 4% than Configuration 3 and 6% increase in the thermal share in Configuration 6.
- It is intriguing to observe that all different sources of electricity have nearly identical values in Configuration 3 and Configuration 6.
- Configurations 3 and 6 show only the thermal contribution and negligible electrical share which shows less carbon footprint when compared to Configuration 1.

Configuration 4: Heat pump + Heat integration

- Configurations 2 and 7 produce higher levels of electrical energy emissions than Configuration 4, by around 52% and 70%, respectively. In contrast, Configuration 5 has 62% lower electrical share compared to Configuration 4.
- Configuration 4 is dominated by the electricity contribution, as the whole operation is driven by electricity. When renewable sources are used, this configuration results in a lower carbon footprint compared to other configurations.

Configuration 5: Conventional + Flue gas from natural gas combustion (NG)

- Compared to Configuration 5, Configurations 1 and 4 have higher electrical share emissions of about 32% and 168% .
- In terms of thermal contribution, Configuration 5 shows a higher thermal contribution of 6% compared to Configuration 6, and the same goes for Configuration 1 with 5%.
- From figure 6.2, it is clear that for Configuration 5, thermal energy contributes the most to the overall footprint, followed by electricity. Uncaptured CO₂ has a negligible impact on the overall footprint.

Configuration 6: Innovative configuration(IC) + Flue gas from natural gas combustion(NG)

- Configurations 1, 3, and 5 depict thermal shares that are roughly 10%, 6%, and 6% higher than that of Configuration 6.

Configuration 7: IC + Electric boiler

- Configurations 2, 4 and 5 show a lower amount of electrical share emissions compared to Configurations 7 by approximately 10%, 41%, and 78%.
- In Configuration 7 of the grid mix, the electricity contribution is the highest compared to other configurations, and no thermal contribution is made as the process is electrified.

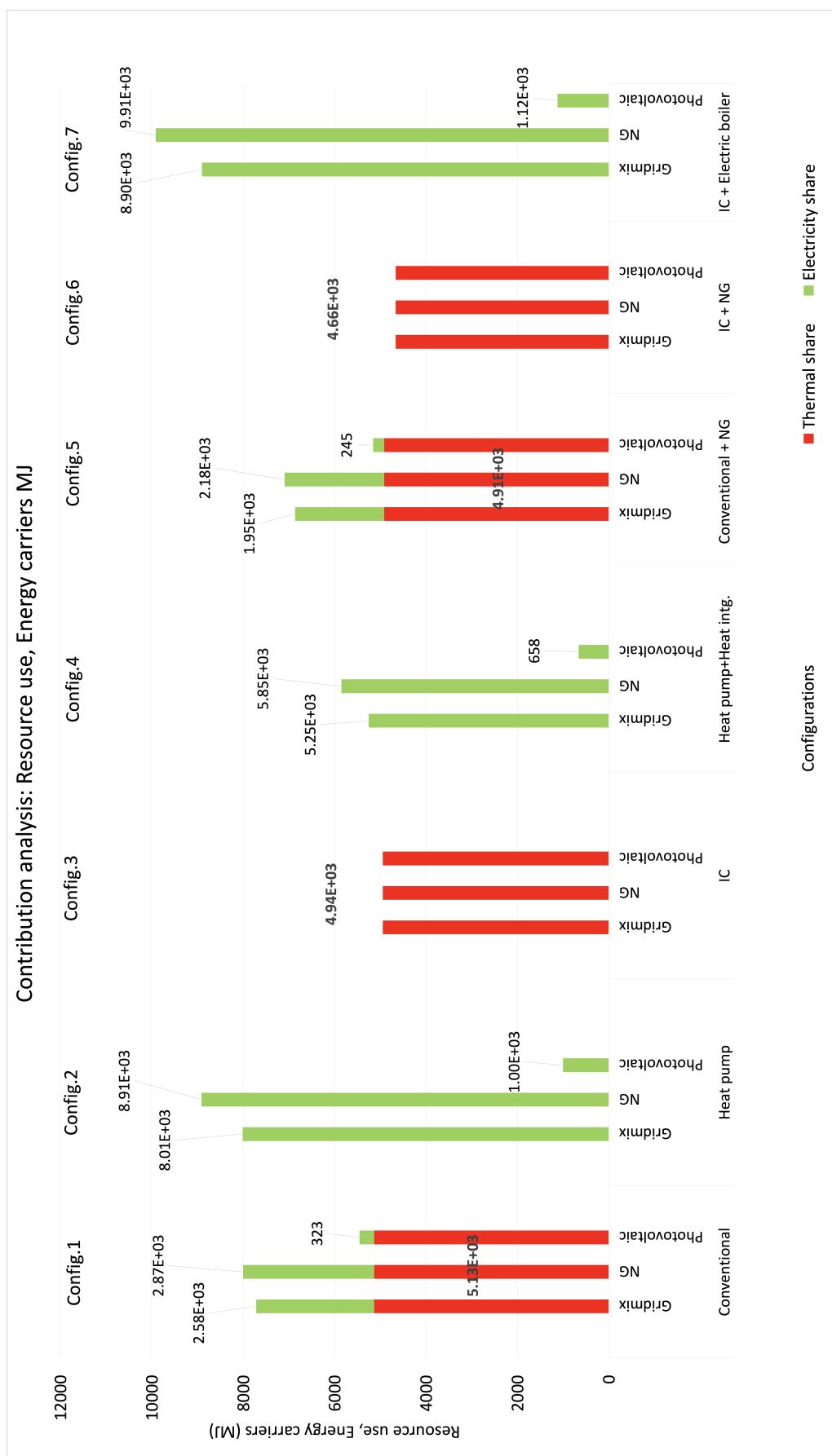


Figure 6.3: Contribution analysis: Resource use, Energy carriers(MJ)

6.3 Contribution analysis: Resource use, energy carriers [MJ]

Resource use, energy carriers [MJ]: It involves using various resources like natural gas, coal, and renewables to generate energy for each configuration in order to meet the specified target of CO₂ capture. It provides information on the efficiency and environmental impact of the configurations.

We have discussed the contribution analysis of climate change, which focuses on both electrical and thermal share and reveals a striking correlation with resource use, expressed in terms of energy carriers measured in megajoules (MJ). The graphical representation of both analyses exhibits a symmetric pattern. As the electrical share increases, there is a clear parallel increase in the utilization of resources to generate electricity, which shows the relationship between the two. The graph clearly shows that the use of energy derived from renewable sources will result in minimal resource consumption, helping to mitigate climate change and improve decision making.

The contribution analysis on resource use is depicted in figure 6.3. The trend of contributions to resource use is similar to contribution analysis to climate change, with Configurations 2, 4, and 7 lacking a thermal energy element, and Configurations 3 and 6 not including the electricity component.

The values displayed in table 5.16 represent the share of electrical energy and thermal energy from climate change and resource use, energy carriers [MJ].

6.4 Other impacts

Acidification terrestrial and freshwater [Mole of H+ eq.] and Land Use [Pt]

The importance of choosing the electrical source is highlighted in the acidification of terrestrial and fresh water [Mole of H + Eq.] and land use [Pt]. Photovoltaic electricity demonstrates a reduced potential for acidification. Similarly, in the Land Use category, the electricity from the grid mix shows the greatest impact on land use.

The eutrophication potential of different configurations is demonstrated in figure 5.18. The eutrophication potential reveals intriguing patterns such as Configuration 2, when powered by electricity from natural gas, exhibits the lowest eutrophication potential compared to grid mix for the same, highlighting the importance of considering natural gas as an energy source to mitigate certain environmental impacts. Detailed LCA results of each configuration are shown in Appendix B.

Chapter 7

Conclusion and Future works

Configuration 2 (heat pump) and Configuration 7 (IC + Electric boiler), produces high emissions compared to all other configurations due to carbon intensity in grid mix and natural gas. Configurations 3 to 6 have lower emissions compared to Configuration 1 due to the heat integration strategy(Configuration 3,4) or burning natural gas(Configuration 5,6) directly to produce thermal energy. Configuration 2 exhibits fewer emissions compared to all other configurations when the source of energy supply is renewable, such as photovoltaic. The contribution analysis of climate change and fossil resource use is correlated because resource consumption is necessary for energy production.

Configuration 2 and Configuration 7 are viable choices when the energy source comes from renewables. Configuration 4, which includes a heat pump and heat integration, presents a feasible alternative showing lower emissions compared to other configurations. Configuration 3 is also a wise choice when applying the heat integration strategy shown in figure 6.1.

The simulation in this study uses parameters from Chikezie Nwaoha et al. [30]. In all scenarios, these parameters remain unchanged. However, adjustments to parameters could be studied in future work, including variations in the composition of the flue gas, operating conditions, and the use of different solvents or combinations of solvents. Furthermore, the life cycle assessment (LCA) in this study only accounts for a limited number of energy sources, namely grid mix, natural gas, photovoltaics, and thermal energy from natural gas, while the future study could also investigate the use of alternative energy sources such as hydropower, wind, ocean energy, and more.

In addition, this research focuses on the capture of CO₂ from cement production and uses amine solvent for absorption, but the capture of CO₂ from ammonia production or the absorption of CO₂ with chilled ammonia process could be explored to compare the distinctions between the two solvents and their life cycle assessments(LCA).

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Appendix A: Simulation results

Components - Specifications					
	Component ID	Type	Component name	Alias	CAS number
Select components					
▶	MEA	Conventional	MONOETHANOLAMINE	C2H7NO	141-43-5
▶	H2O	Conventional	WATER	H2O	7732-18-5
▶	CO2	Conventional	CARBON-DIOXIDE	CO2	124-38-9
▶	H2S	Conventional	HYDROGEN-SULFIDE	H2S	7783-06-4
▶	H3O+	Conventional	H3O+	H3O+	
▶	OH-	Conventional	OH-	OH-	
▶	HCO3-	Conventional	HCO3-	HCO3-	
▶	CO3-2	Conventional	CO3--	CO3-2	
▶	HS-	Conventional	HS-	HS-	
▶	S-2	Conventional	S--	S-2	
▶	MEA+H	Conventional	MEA+	C2H8NO+	
▶	MEACOO-	Conventional	MEACOO-	C3H6NO3-	
▶	N2	Conventional	NITROGEN	N2	7727-37-9
▶	O2	Conventional	OXYGEN	O2	7782-44-7
▶	CO	Conventional	CARBON-MONOXIDE	CO	630-08-0
▶	H2	Conventional	HYDROGEN	H2	1333-74-0
▶	CH4	Conventional	METHANE	CH4	74-82-8
▶	ETHYL-01	Conventional	ETHYL-MERCAPTAN	C2H6S-1	75-08-1
▶	N-HEX-01	Conventional	N-HEXANE	C6H14-1	110-54-3
*					
<input type="button" value="Find"/> <input type="button" value="Elec Wizard"/> <input type="button" value="SFE Assistant"/> <input type="button" value="User Defined"/> <input type="button" value="Reorder"/> <input type="button" value="Review"/>					

Figure A1.1: Overview of the components-specifications tab.

Column Internals Summary		
Summary		
► Number of Trayed/Packed stages	36	Value Units
► Total height	21,95	meter
► Total head loss (Hot liquid height)	0,435267	meter
► Total pressure drop	0,0435602	bar
► Number of sections	1	
► Number of diameters	1	
► Pressure drop across sump		bar
► Total residence time	0	sec

Sections							
	Start Stage	End Stage	Diameter	Section Height	Internals Type	Tray Type or Packing Type	Section Pressure Drop
► CS-1	1	36	10,07 meter	21,95 meter	PACKING	MELLAPAK	0,0435602 bar

(a) Column internal summary-Absorber

Column Internals Summary		
Summary		
► Number of Trayed/Packed stages	24	Value Units
► Total height	15,85	meter
► Total head loss (Hot liquid height)	0,144302	meter
► Total pressure drop	0,0144687	bar
► Number of sections	1	
► Number of diameters	1	
► Pressure drop across sump		bar
► Total residence time	0	sec

Sections							
	Start Stage	End Stage	Diameter	Section Height	Internals Type	Tray Type or Packing type	Section Pressure Drop
► CS-1	2	25	6,04 meter	15,85 meter	PACKING	MELLAPAK	0,0144687 bar

(b) Column internal summary-Stripper

Figure A1.2: Column internals

Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status						
		Units	FLUEGAS	CO2	RICHGAS	MIXIN	DISTILL	PURGE				
Mass Solid Fraction			0	0	0	0	0	0	0	0	0	
Molar Enthalpy	MBtu/lbmol	-51,8969	-167,274	-26,7096	-123,717	-122,971	-124,374					
Mass Enthalpy	kJ/kg	-4523,1	-8978,59	-2404,95	-12600,7	-15777,8	-12669,9					
Molar Entropy	kJ/kmol-K	-33,2767	-1,08153	-0,462577	-194,242	-162,328	-193,761					
Mass Entropy	kJ/kg-K	-1,24688	-0,0249579	-0,0179066	-8,50544	-8,95422	-8,48591					
Molar Density	kmol/cum	0,0514913	0,0680207	0,0358388	44,6138	55,0184	44,8589					
Mass Density	kg/cum	1,3742	2,94762	0,925813	1018,86	997,412	1024,27					
Enthalpy Flow	kW	-808025	-223238	-336892	-3,931608e+06	-66374,4	-1,21734e+06					
Average MW		26,6879	43,3341	25,8327	22,8374	18,1287	22,8332					
+ Mole Flows	kmol/hr	24097,7	2065,53	19521,6	48990,7	835,39	15148,7					
+ Mole Fractions												
- Mass Flows	kg/hr	643118	89508	504297	1,11882e+06	15144,5	345893					
MEA	kg/hr	0	1,3542e-05	511,129	262289	0,0513161	72350,8					
H2O	kg/hr	134739	941,238	91500	790851	15005,3	245410					
CO2	kg/hr	96865,6	88495	845,114	0,0118877	31,9421	0,00748361					
H2S	kg/hr	0	0	0	0	0	0					
H3O+	kg/hr	0,069231	0	0	7,6543e-07	0,000163024	3,88838e-07					
OH-	kg/hr	1,95315e-06	0	0	7,90728	9,95164e-06	1,90196					

Figure A1.3: Configuration 1: Conventional

Material	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids				
				Units	CCU.FLUEGA	CCU.CO2	CCU.RICHGA	CCU.MIN	CCU.DISTILL	CCU.PURGE		
Mass Solid Fraction					0	0	0	0	0	0	0	
Molar Enthalpy	MBtu/lbmol	-51,8968	-167,274	-26,8545	-123,717	-122,97	-124,4					
Mass Enthalpy	kJ/kg	-4523,09	-8978,6	-2420,99	-12593,2	-15778,2	-12662,1					
Molar Entropy	kJ/kmol-K	-33,2759	-1,08161	-0,574619	-194,205	-162,325	-193,883					
Mass Entropy	kJ/kg-K	-1,24685	-0,0249597	-0,0222713	-8,49877	-8,95434	-8,48429					
Molar Density	kmol/cum	0,0514909	0,0680207	0,035851	44,5845	55,0191	44,8328					
Mass Density	kg/cum	1,37419	2,94762	0,924057	1018,8	997,392	1024,52					
Enthalpy Flow	kW	-808023	-224154	-339539	-3,93953e+06	-64738,7	-1,22376e+06					
Average MW		26,6879	43,3342	25,8008	22,851	18,1281	22,8521					
+ Mole Flows	kmol/hr	24097,7	2074,01	19568,9	49284,2	814,812	15225,4					
+ Mole Fractions												
- Mass Flows	kg/hr	643119	89875,4	504893	1,12619e+06	14771	347932					
MEA	kg/hr	0	1,3438e-05	554,023	264022	0,0494677	72756,6					
H2O	kg/hr	134740	945,114	92535,5	795387	14635,9	246570					
CO2	kg/hr	96865,7	88858,4	361,952	0,0126277	31,1581	0,00762829					
H2S	kg/hr	0	0	0	0	0	0					
H3O+	kg/hr	0,0692279	0	0	8,01513e-07	0,000159853	3,9475e-07					
OH-	kg/hr	1,95307e-06	0	0	7,9386	9,6436e-06	1,90095					

Figure A1.4: Configuration 2: Heat pump

Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status						
		Units	FLUEGAS	CO2	RICHGAS	MIN	DISTIL	PURGE				
Mass Solid Fraction			0	0	0	0	0	0	0	0	0	
Molar Enthalpy	MBtu/lbmol	-51,8968	-167,271	-26,8177	-123,87	-123,036	-124,627					
Mass Enthalpy	kJ/kg	-4523,09	-8978,4	-2413,21	-12497,4	-15760,8	-12528					
Molar Entropy	kJ/kmol-K	-33,2759	-1,0797	-0,396944	-195,757	-162,483	-195,868					
Mass Entropy	kJ/kg-K	-1,24685	-0,0249156	-0,0153565	-8,49109	-8,94837	-8,46498					
Molar Density	kmol/cum	0,0514909	0,0680207	0,0358342	44,2668	54,9831	44,3804					
Mass Density	kg/cum	1,37419	2,94762	0,926262	1020,55	998,376	1026,9					
Enthalpy Flow	kW	-808023	-220017	-338492	-3,77785e+06	-132210	-1,15704e+06					
Average MW		26,6879	43,3341	25,8485	23,0544	18,1579	23,1387					
+ Mole Flows	kmol/hr	24097,7	2035,78	19535,2	47215,7	1663,12	14369,1					
+ Mole Fractions												
- Mass Flows	kg/hr	643119	88218,7	504957	1,08853e+06	30198,8	332482					
MEA	kg/hr	0	2,19659e-05	491,156	260173	0,167602	71313,2					
H2O	kg/hr	134740	927,119	91453,7	758618	29853,2	231295					
CO2	kg/hr	96865,7	87219,3	1571,56	0,0122739	63,3075	0,00751995					
H2S	kg/hr	0	0	0	0	0	0					
H3O+	kg/hr	0,0692279	0	0	7,69583e-07	0,000259858	3,84777e-07					
OH-	kg/hr	1,95307e-06	0	0	7,35429	2,6101e-05	1,74935					

Figure A1.5: Configuration 3: Innovative configuration(IC)

Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status		
	Units	FLUEGAS	CO2	RICHGAS	MIN	DISTILL	PURGE	
Mass Liquid Fraction		0,16146	0	0	1	1	1	
Mass Solid Fraction		0	0	0	0	0	0	
Molar Enthalpy	MBtu/lbmol	-51,8968	-167,27	-26,9787	-123,865	-123,036	-124,648	
Mass Enthalpy	kJ/kg	-4523,09	-8978,38	-2430,35	-12489,5	-15760,8	-12519,5	
Molar Entropy	kJ/kmol-K	-33,2759	-1,0795	-0,487867	-195,72	-162,483	-196,001	
Mass Entropy	kJ/kg-K	-1,24685	-0,0249112	-0,0188947	-8,48439	-8,94837	-8,4635	
Molar Density	kmol/cum	0,0514909	0,0680207	0,0358126	44,2358	54,9831	44,3516	
Mass Density	kg/cum	1,37419	2,94761	0,924695	1020,44	998,377	1027,11	
Enthalpy Flow	kW	-808023	-220617	-341364	-3,78843e+06	-131640	-1,159e+06	
Average MW		26,6879	43,3341	25,8203	23,0682	18,1579	23,1584	
+ Mole Flows	kmol/hr	24097,7	2041,34	19583,4	47337,2	1655,95	14391	
+ Mole Fractions								
- Mass Flows	kg/hr	643119	88459,4	505651	1,09199e+06	30068,6	333272	
MEA	kg/hr	0	2,20281e-05	515,586	261169	0,166896	71532,2	
H2O	kg/hr	134740	929,649	92447,7	760357	29724,4	231557	
CO2	kg/hr	96865,7	87457,1	1247,28	0,0129349	63,0343	0,00758848	
H2S	kg/hr	0	0	0	0	0	0	
H3O+	kg/hr	0,0692279	0	0	8,00865e-07	0,000258726	3,87534e-07	

Figure A1.6: Configuration 4: Heat pump + Heat integration

Material	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	
	Units	FLUNG	CO2	RICHGAS	MIN	DISTILL	PURGE		
Mass Solid Fraction		0	0	0	0	0	0		
Molar Enthalpy	MBtu/lbmol	-41,9733	-167,708	-22,7124	-123,367	-122,97	-123,885		
Mass Enthalpy	kJ/kg	-3594,73	-8966,84	-2007,9	-12615,1	-15777,6	-12689,8		
Molar Entropy	kJ/kmol-K	-25,1074	-3,53928	0,935471	-193,823	-162,263	-193,169		
Mass Entropy	kJ/kg-K	-0,924457	-0,0813559	0,0355549	-8,52092	-8,95057	-8,50674		
Molar Density	kmol/cum	0,0489195	0,0922997	0,0362573	44,6573	54,9781	44,9177		
Mass Density	kg/cum	1,32861	4,01537	0,953952	1015,8	996,685	1019,98		
Enthalpy Flow	kW	-938270	-269221	-441050	-4,58061e+06	-2652,66	-1,42481e+06		
Average MW		27,1591	43,5036	26,3106	22,7467	18,1287	22,7077		
+ Mole Flows	kmol/hr	34597,7	2484,55	30055,1	57467	33,3867	17800,5		
+ Mole Fractions									
- Mass Flows	kg/hr	939644	108087	790767	1,30718e+06	605,259	404209		
MEA	kg/hr	0	7,6576e-06	507,913	318340	0,00128593	89647,1		
H2O	kg/hr	152755	840,236	117509	928097	599,618	288546		
CO2	kg/hr	118871	107160	4818,19	0,00908001	1,73439	0,00561029		
H2S	kg/hr	0	0	0	0	0	0		
H3O+	kg/hr	0,0725254	0	0	6,74257e-07	9,50147e-06	3,3381e-07		

Figure A1.7: Configuration 5: Conventional + Flue gas from natural gas combustion (NG)

Material	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids	Status				
		Units	FLUNG	CO2	CLEAN	MIN	DISTILL	PURGE		
Mass Solid Fraction			0	0	0	0	0	0	0	0
Molar Enthalpy	MBtu/lbmol		-41,9733	-167,703	-22,744	-123,554	-123,113	-124,195		
Mass Enthalpy	kJ/kg		-3594,73	-8966,55	-2012,3	-12463,8	-15740,2	-12481,2		
Molar Entropy	kJ/kmol-K		-25,1074	-3,53665	0,880867	-196,013	-162,609	-196,218		
Mass Entropy	kJ/kg-K		-0,924457	-0,0812953	0,0335063	-8,50101	-8,93803	-8,47778		
Molar Density	kmol/cum		0,0489195	0,0922996	0,0362277	44,1498	54,9011	44,2157		
Mass Density	kg/cum		1,32861	4,01537	0,952411	1017,99	998,812	1023,37		
Enthalpy Flow	kW		-938270	-268591	-442059	-4,41931e+06	-111212	-1,34378e+06		
Average MW			27,1591	43,5037	26,2896	23,0577	18,1929	23,145		
+ Mole Flows	kmol/hr		34597,7	2478,8	30082	55359,3	1398,1	16746,3		
+ Mole Fractions										
- Mass Flows	kg/hr		939644	107837	790843	1,27646e+06	25435,6	387593		
MEA	kg/hr		0	2,12919e-05	558,932	320578	0,149031	89570,1		
H2O	kg/hr		152755	837,179	118288	887896	25072,6	268904		
CO2	kg/hr		118871	106911	4067,01	0,00981726	71,9168	0,00582284		
H2S	kg/hr		0	0	0	0	0	0		
H3O+	kg/hr		0,0725252	0	0	6,93515e-07	0,000252104	3,34379e-07		
OH-	kg/hr		1,70626e-06	0	0	9,86955	1,98198e-05	2,34427		

Figure A1.8: Configuration 6: Innovative configuration(IC) + flue gas from natural gas combustion(NG)

<input checked="" type="checkbox"/> Mixed	Cl Solid	NC Solid	Flash Options	EO Options	Costing	Comments																																														
<div style="border: 1px solid #ccc; padding: 5px;"> ▲ Specifications <div style="display: flex; justify-content: space-between;"> <div style="flex: 1;"> Flash Type Temperature Pressure <div style="border: 1px solid #ccc; padding: 5px; margin-top: 10px;"> State variables <table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td>Temperature</td> <td style="text-align: center;">25</td> <td>C</td> </tr> <tr> <td>Pressure</td> <td style="text-align: center;">1</td> <td>bar</td> </tr> <tr> <td>Vapor fraction</td> <td colspan="2"></td> </tr> <tr> <td>Total flow basis</td> <td colspan="2">Mole</td> </tr> <tr> <td>Total flow rate</td> <td style="text-align: center;">500</td> <td>kmol/hr</td> </tr> <tr> <td>Solvent</td> <td colspan="2"></td> </tr> </table> </div> <div style="flex: 1;"> Composition Mass-Frac <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th>Component</th> <th>Value</th> </tr> </thead> <tbody> <tr><td>HCO3-</td><td></td></tr> <tr><td>CO3-2</td><td></td></tr> <tr><td>HS-</td><td></td></tr> <tr><td>S-2</td><td></td></tr> <tr><td>MEAH+</td><td></td></tr> <tr><td>MEACOO-</td><td></td></tr> <tr><td>N2</td><td></td></tr> <tr><td>O2</td><td></td></tr> <tr><td>CO</td><td></td></tr> <tr><td>H2</td><td></td></tr> <tr><td>CH4</td><td></td></tr> <tr><td>ETHYL-01</td><td></td></tr> <tr><td>N-HEX-01</td><td style="text-align: right;">1</td></tr> </tbody> </table> </div> </div> </div> </div>							Temperature	25	C	Pressure	1	bar	Vapor fraction			Total flow basis	Mole		Total flow rate	500	kmol/hr	Solvent			Component	Value	HCO3-		CO3-2		HS-		S-2		MEAH+		MEACOO-		N2		O2		CO		H2		CH4		ETHYL-01		N-HEX-01	1
Temperature	25	C																																																		
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<div style="border: 1px solid #ccc; padding: 5px; margin-top: 10px;"> Reference Temperature <div style="display: flex; justify-content: space-between;"> <div style="flex: 1;"> Volume flow reference temperature <input style="width: 100px; height: 25px; border: 1px solid #ccc; border-radius: 5px; padding: 2px; margin-bottom: 5px;"/> C </div> <div style="flex: 1;"> Component concentration reference temperature <input style="width: 100px; height: 25px; border: 1px solid #ccc; border-radius: 5px; padding: 2px; margin-bottom: 5px;"/> C </div> </div> </div>																																																				

Figure A1.9: Methane input

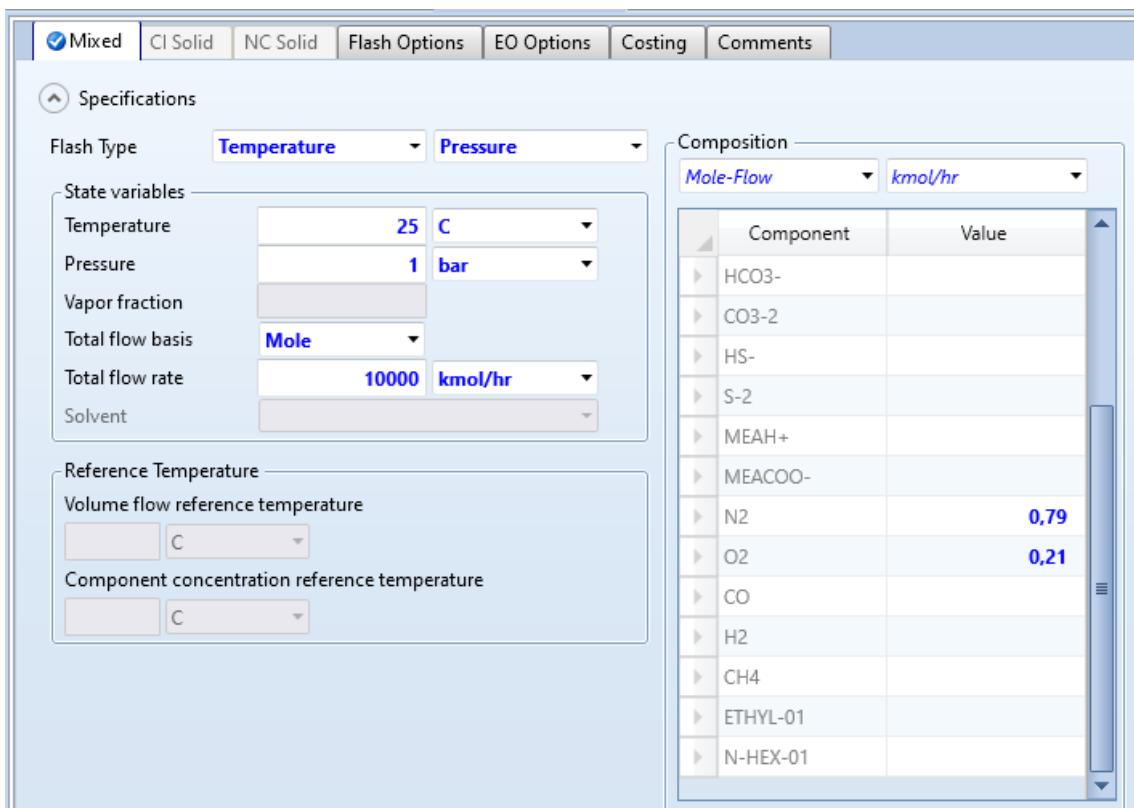


Figure A1.10: Air input

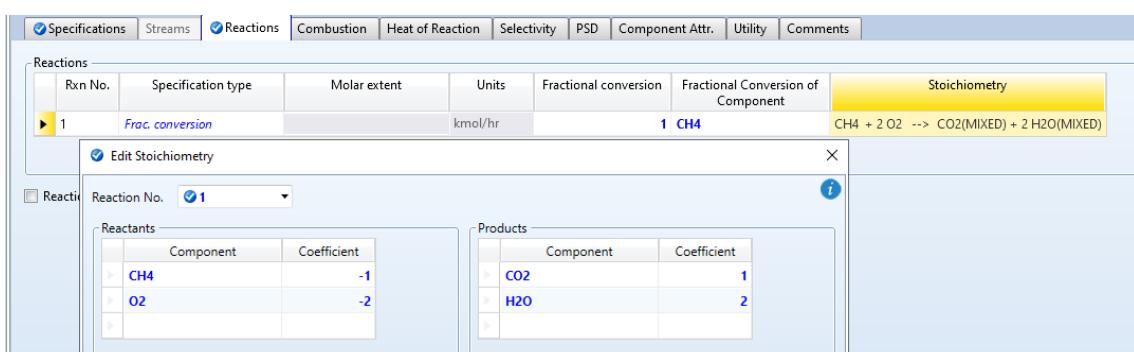


Figure A1.11: Natural gas combustion - reaction

Appendix B: LCA results

Table B1.1: Configuration 1: Conventional

Quantities	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.529	0.333	0.32
Cancer human health effects [CTUh]	7.01×10^{-08}	5.34×10^{-08}	4.40×10^{-08}
Cancer human health effects (Inorganic) [CTUh]	8.13×10^{-18}	4.14×10^{-20}	2.64×10^{-18}
Cancer human health effects (Metal) [CTUh]	2.26×10^{-08}	2.02×10^{-08}	1.62×10^{-08}
Cancer human health effects (Organic) [CTUh]	4.75×10^{-08}	3.31×10^{-08}	2.78×10^{-08}
Climate Change [kg CO ₂ eq.]	526	494	342
Climate Change (biogenic) [kg CO ₂ eq.]	2.94	0.752	0.65
Climate Change (fossil) [kg CO ₂ eq.]	523	493	341
Climate Change (land use change) [kg CO ₂ eq.]	0.534	0.014	0.031
Ecotoxicity freshwater [CTUe]	1.06E+03	88	197
Ecotoxicity freshwater (Inorganic) [CTUe]	708	78.6	141
Ecotoxicity freshwater (Metals) [CTUe]	342	7.84	53.6
Ecotoxicity freshwater (Organic) [CTUe]	4.94	1.54	2.09
Eutrophication freshwater [kg P eq.]	8.75×10^{-04}	2.74×10^{-05}	5.92×10^{-05}
Eutrophication marine [kg N eq.]	0.174	0.121	0.096
Eutrophication terrestrial [Mole of N eq.]	1.87	1.34	1.06
Ionising radiation - human health [kBq U235 eq.]	19.5	0.128	2.57
Land Use [Pt]	1.32×10^{03}	13	158
Non-cancer human health effects [CTUh]	2.96×10^{-06}	2.47×10^{-06}	2.22×10^{-06}
Non-cancer human health effects (Inorganic) [CTUh]	5.31×10^{-07}	1.88×10^{-07}	1.79×10^{-07}
Non-cancer human health effects (Metals) [CTUh]	2.42×10^{-06}	2.28×10^{-06}	2.03×10^{-06}
Non-cancer human health effects (Organic) [CTUh]	4.90×10^{-08}	5.31×10^{-08}	3.83×10^{-08}
Ozone depletion [kg CFC-11 eq.]	6.37×10^{-12}	2.02×10^{-14}	9.76×10^{-11}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.477	0.366	0.305
Resource use, energy carriers [MJ]	7.71×10^{03}	8.00×10^{03}	5.45×10^{03}
Resource use, mineral and metals [kg Sb eq.]	9.62×10^{-05}	2.83×10^{-05}	8.47×10^{-04}
Respiratory inorganics [Disease incidences]	3.87×10^{-06}	2.00×10^{-06}	2.58×10^{-06}
Water scarcity [m ³ world equiv.]	4.81	0.602	5.91

Table B1.2: Configuration 2: Heat pump

	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Quantities			
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.978	0.371	0.33
Cancer human health effects [CTUh]	1.12×10^{-7}	5.94×10^{-8}	3.04×10^{-8}
Cancer human health effects (Inorganic) [CTUh]	2.52×10^{-17}	4.51×10^{-20}	8.10×10^{-18}
Cancer human health effects (Metal) [CTUh]	2.99×10^{-8}	2.25×10^{-8}	9.91×10^{-9}
Cancer human health effects (Organic) [CTUh]	8.17×10^{-8}	3.69×10^{-8}	2.05×10^{-8}
Climate Change [kg CO ₂ eq.]	651	550	78.7
Climate Change (biogenic) [kg CO ₂ eq.]	7.63	0.838	0.523
Climate Change (fossil) [kg CO ₂ eq.]	642	549	78.1
Climate Change (land use change) [kg CO ₂ eq.]	1.63	0.015	0.07
Ecotoxicity freshwater [CTUe]	3.10×10^{03}	97.8	437
Ecotoxicity freshwater (Inorganic) [CTUe]	2.04×10^{03}	87.4	283
Ecotoxicity freshwater (Metals) [CTUe]	1.05×10^{03}	8.69	151
Ecotoxicity freshwater (Organic) [CTUe]	12.3	1.72	3.42
Eutrophication freshwater [kg P eq.]	2.66×10^{-3}	3.04×10^{-5}	1.29×10^{-4}
Eutrophication marine [kg N eq.]	0.3	0.135	0.057
Eutrophication terrestrial [Mole of N eq.]	3.13	1.5	0.63
Ionising radiation - human health [kBq U235 eq.]	60.3	0.14	7.73
Land Use [Pt]	4.08×10^{03}	14.2	464
Non-cancer human health effects [CTUh]	4.26×10^{-6}	2.75×10^{-6}	1.96×10^{-6}
Non-cancer human health effects (Inorganic) [CTUh]	1.27×10^{-6}	2.09×10^{-7}	1.81×10^{-7}
Non-cancer human health effects (Metals) [CTUh]	2.97×10^{-6}	2.54×10^{-6}	1.77×10^{-6}
Non-cancer human health effects (Organic) [CTUh]	4.65×10^{-8}	5.92×10^{-8}	1.34×10^{-8}
Ozone depletion [kg CFC-11 eq.]	1.97×10^{-11}	2.16×10^{-14}	3.03×10^{-10}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.752	0.408	0.219
Resource use, energy carriers [MJ]	8.01×10^{03}	8.91×10^{03}	1.00×10^{03}
Resource use, mineral and metals [kg Sb eq.]	2.42×10^{-4}	3.15×10^{-5}	2.57×10^{-3}
Respiratory inorganics [Disease incidences]	8.05×10^{-6}	2.22×10^{-6}	4.02×10^{-6}
Water scarcity [m ³ world equiv.]	14.2	1.14	17.6

Table B1.3: Configuration 3: Innovative configuration(IC)

	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Quantities			
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.206	0.206	0.206
Cancer human health effects [CTUh]	3.30×10^{-08}	3.30×10^{-08}	3.30×10^{-08}
Cancer human health effects (Inorganic [CTUh])	3.49×10^{-20}	2.60×10^{-20}	2.88×10^{-20}
Cancer human health effects (Metal [CTUh])	1.25×10^{-08}	1.25×10^{-08}	1.25×10^{-08}
Cancer human health effects (Organic [CTUh])	2.05×10^{-08}	2.05×10^{-08}	2.05×10^{-08}
Climate Change [kg CO ₂ eq.]	305	305	305
Climate Change (biogenic) [kg CO ₂ eq.]	0.468	0.465	0.465
Climate Change (fossil) [kg CO ₂ eq.]	305	305	305
Climate Change (land use change) [kg CO ₂ eq.]	0.009	0.008	0.008
Ecotoxicity freshwater [CTUe]	55.6	54.5	54.6
Ecotoxicity freshwater (Inorganic) [CTUe]	49.4	48.7	48.7
Ecotoxicity freshwater (Metals) [CTUe]	5.24	4.87	4.92
Ecotoxicity freshwater (Organic) [CTUe]	0.958	0.954	0.955
Eutrophication freshwater [kg P eq.]	1.80×10^{-05}	1.70×10^{-05}	1.71×10^{-05}
Eutrophication marine [kg N eq.]	0.075	0.075	0.075
Eutrophication terrestrial [Mole of N eq.]	0.831	0.831	0.83
Ionising radiation - human health [kBq U235 eq.]	0.101	0.080	0.082
Land Use [Pt]	9.52	8.08	8.24
Non-cancer human health effects [CTUh]	1.53×10^{-06}	1.53×10^{-06}	1.53×10^{-06}
Non-cancer human health effects (Inorganic) [CTUh]	1.17×10^{-07}	1.17×10^{-07}	1.17×10^{-07}
Non-cancer human health effects (Metals [CTUh])	1.41×10^{-06}	1.41×10^{-06}	1.41×10^{-06}
Non-cancer human health effects (Organic) [CTUh]	3.28×10^{-08}	3.28×10^{-08}	3.28×10^{-08}
Ozone depletion [kg CFC-11 eq.]	1.98×10^{-14}	1.28×10^{-14}	1.20×10^{-13}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.226	0.226	0.226
Resource use, energy carriers [MJ]	4.95×10^{03}	4.95×10^{03}	4.94×10^{03}
Resource use, mineral and metals [kg Sb eq.]	1.76×10^{-05}	1.75×10^{-05}	1.84×10^{-05}
Respiratory inorganics [Disease incidences]	1.24×10^{-06}	1.24×10^{-06}	1.24×10^{-06}
Water scarcity [m ³ world equiv.]	0.232	0.227	0.233

Table B1.4: Configuration 4: Heat pump + Heat integration

	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Quantities			
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.642	0.244	0.216
Cancer human health effects [CTUh]	7.32×10^{-8}	3.90×10^{-8}	1.99×10^{-8}
Cancer human health effects (Inorganic) [CTUh]	1.65×10^{-17}	2.96×10^{-20}	5.31×10^{-18}
Cancer human health effects (Metal) [CTUh]	1.96×10^{-8}	1.48×10^{-8}	6.50×10^{-9}
Cancer human health effects (Organic) [CTUh]	5.36×10^{-8}	2.42×10^{-8}	1.34×10^{-8}
Climate Change [kg CO ₂ eq.]	427	361	51.7
Climate Change (biogenic) [kg CO ₂ eq.]	5	0.55	0.343
Climate Change (fossil) [kg CO ₂ eq.]	421	360	51.3
Climate Change (land use change) [kg CO ₂ eq.]	1.07	0.010	0.045
Ecotoxicity freshwater [CTUe]	2.03×10^{03}	64.2	287
Ecotoxicity freshwater (Inorganic) [CTUe]	1.34×10^{03}	57.3	185
Ecotoxicity freshwater (Metals) [CTUe]	686	5.7	98.8
Ecotoxicity freshwater (Organic) [CTUe]	8.04	1.13	2.25
Eutrophication freshwater [kg P eq.]	0.001	2.00×10^{-5}	8.47×10^{-5}
Eutrophication marine [kg N eq.]	0.197	0.0886	0.037
Eutrophication terrestrial [Mole of N eq.]	2.06	0.982	0.414
Ionising radiation - human health [kBq U235 eq.]	39.6	0.091	5.07
Land Use [Pt]	2.67×10^{03}	9.32	305
Non-cancer human health effects [CTUh]	2.79×10^{-6}	1.81×10^{-6}	1.28×10^{-6}
Non-cancer human health effects (Inorganic) [CTUh]	8.35×10^{-7}	1.37×10^{-7}	1.19×10^{-7}
Non-cancer human health effects (Metals) [CTUh]	1.95×10^{-6}	1.67×10^{-6}	1.16×10^{-6}
Non-cancer human health effects (Organic) [CTUh]	3.05×10^{-8}	3.88×10^{-8}	8.80×10^{-9}
Ozone depletion [kg CFC-11 eq.]	1.29×10^{-11}	1.41×10^{-14}	1.99×10^{-10}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.493	0.267	0.144
Resource use, energy carriers [MJ]	5.25×10^{03}	5.85×10^{03}	658
Resource use, mineral and metals [kg Sb eq.]	0.0001	2.07×10^{-5}	0.001
Respiratory inorganics [Disease incidences]	5.28×10^{-6}	1.46×10^{-6}	2.64×10^{-6}
Water scarcity [m ³ world equiv.]	9.32	0.74	11.5

Table B1.5: Configuration 5: Conventional + Flue gas from natural gas combustion (NG)

Quantities	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.444	0.296	0.285
Cancer human health effects [CTUh]	6.00×10^{-08}	4.73×10^{-08}	4.02×10^{-08}
Cancer human health effects (Inorganic) [CTUh]	6.17×10^{-18}	3.68×10^{-20}	2.00×10^{-18}
Cancer human health effects (Metal) [CTUh]	1.97×10^{-08}	1.79×10^{-08}	1.49×10^{-08}
Cancer human health effects (Organic) [CTUh]	4.03×10^{-08}	2.94×10^{-08}	2.54×10^{-08}
Climate Change [kg CO ₂ eq.]	462	438	323
Climate Change (biogenic) [kg CO ₂ eq.]	2.32	0.66	0.59
Climate Change (fossil) [kg CO ₂ eq.]	460	437	322
Climate Change (land use change) [kg CO ₂ eq.]	0.406	0.012	0.025
Ecotoxicity freshwater [CTUe]	811	78	161
Ecotoxicity freshwater (Inorganic) [CTUe]	547	69.7	117
Ecotoxicity freshwater (Metals) [CTUe]	260	6.96	41.6
Ecotoxicity freshwater (Organic) [CTUe]	3.94	1.37	1.78
Eutrophication freshwater [kg P eq.]	6.6×10^{-04}	2.43×10^{-05}	4.84×10^{-05}
Eutrophication marine [kg N eq.]	0.148	0.107	0.088
Eutrophication terrestrial [Mole of N eq.]	1.59	1.19	0.979
Ionising radiation - human health [kBq U235 eq.]	14.8	0.114	1.97
Land Use [Pt]	1.00×10^{03}	11.5	121
Non-cancer human health effects [CTUh]	2.56×10^{-06}	2.19×10^{-06}	2.00×10^{-06}
Non-cancer human health effects (Inorganic) [CTUh]	4.26×10^{-07}	1.67×10^{-07}	1.60×10^{-07}
Non-cancer human health effects (Metals) [CTUh]	2.13×10^{-06}	2.02×10^{-06}	1.83×10^{-06}
Non-cancer human health effects (Organic) [CTUh]	4.40×10^{-08}	4.71×10^{-08}	3.59×10^{-08}
Ozone depletion [kg CFC-11 eq.]	4.83×10^{-12}	1.80×10^{-14}	7.39×10^{-11}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.408	0.324	0.278
Resource use, energy carriers [MJ]	6.87×10^{03}	7.09×10^{03}	5.16×10^{03}
Resource use, mineral and metals [kg Sb eq.]	7.65E-05	2.51×10^{-05}	6.4×10^{-05}
Respiratory inorganics [Disease incidences]	3.19×10^{-06}	1.77×10^{-06}	2.21×10^{-06}
Water scarcity [m ³ world equiv.]	3.69	0.503	4.52

Table B1.6: Configuration 6: Innovative configuration(IC) + Flue gas from natural gas combustion(NG)

	Electricity (Gridmix)	Electricity (NG)	Electricity (Photovoltaic)
Quantities			
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	0.195	0.194	0.194
Cancer human health effects [CTUh]	3.11×10^{-08}	3.11×10^{-08}	3.11×10^{-08}
Cancer human health effects (Inorganic [CTUh])	3.80×10^{-20}	2.45×10^{-20}	2.88×10^{-20}
Cancer human health effects (Metal [CTUh])	1.18×10^{-08}	1.18×10^{-08}	1.18×10^{-08}
Cancer human health effects (Organic [CTUh])	1.93×10^{-08}	1.93×10^{-08}	1.93×10^{-08}
Climate Change [kg CO ₂ eq.]	288	288	287
Climate Change (biogenic) [kg CO ₂ eq.]	0.442	0.438	0.438
Climate Change (fossil) [kg CO ₂ eq.]	287	287	287
Climate Change (land use change) [kg CO ₂ eq.]	9.2×10^{-03}	8.3×10^{-03}	8.3×10^{-03}
Ecotoxicity freshwater [CTUe]	53	51.3	51.5
Ecotoxicity freshwater (Inorganic) [CTUe]	46.9	45.9	46
Ecotoxicity freshwater (Metals) [CTUe]	5.15	4.59	4.66
Ecotoxicity freshwater (Organic) [CTUe]	0.905	0.899	0.9
Eutrophication freshwater [kg P eq.]	1.75×10^{-05}	1.60×10^{-05}	1.61×10^{-05}
Eutrophication marine [kg N eq.]	0.070	0.070	0.070
Eutrophication terrestrial [Mole of N eq.]	0.784	0.783	0.782
Ionising radiation - human health [kBq U235 eq.]	0.108	0.075	0.079
Land Use [Pt]	9.8	7.62	7.86
Non-cancer human health effects [CTUh]	1.44×10^{-06}	1.44×10^{-06}	1.44×10^{-06}
Non-cancer human health effects (Inorganic) [CTUh]	1.10×10^{-07}	1.10×10^{-07}	1.10×10^{-07}
Non-cancer human health effects (Metals) [CTUh]	1.33×10^{-06}	1.33×10^{-06}	1.33×10^{-06}
Non-cancer human health effects (Organic) [CTUh]	3.09×10^{-08}	3.09×10^{-08}	3.09×10^{-08}
Ozone depletion [kg CFC-11 eq.]	2.26×10^{-14}	1.20×10^{-14}	1.75×10^{-13}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.213	0.213	0.213
Resource use, energy carriers [MJ]	4.66×10^{03}	4.66×10^{03}	4.66×10^{03}
Resource use, mineral and metals [kg Sb eq.]	1.66×10^{-05}	1.65×10^{-05}	1.79×10^{-05}
Respiratory inorganics [Disease incidences]	1.17×10^{-06}	1.16×10^{-06}	1.17×10^{-06}
Water scarcity [m ³ world equiv.]	0.221	0.214	0.223

Table B1.7: Configuration 7: IC + Electric boiler

	Electricity (Grid mix, reb)	Electricity (NG, reb)	Electricity (Photovoltaic, reb)
Quantities			
Acidification terrestrial and freshwater [Mole of H ⁺ eq.]	1.09	0.413	0.366
Cancer human health effects [CTUh]	1.24×10^{-07}	6.61×10^{-08}	3.38×10^{-08}
Cancer human health effects (Inorganic) [CTUh]	2.8×10^{-17}	5.01×10^{-20}	9.01×10^{-18}
Cancer human health effects (Metal) [CTUh]	3.32×10^{-08}	2.51×10^{-08}	1.1×10^{-08}
Cancer human health effects (Organic) [CTUh]	9.08×10^{-08}	4.1×10^{-08}	2.28×10^{-08}
Climate Change [kg CO ₂ eq.]	724	612	87.5
Climate Change (biogenic) [kg CO ₂ eq.]	8.48	0.931	0.581
Climate Change (fossil) [kg CO ₂ eq.]	714	611	86.9
Climate Change (land use change) [kg CO ₂ eq.]	1.81	0.017	0.077
Ecotoxicity freshwater [CTUe]	3.45×10^{03}	109	485
Ecotoxicity freshwater (Inorganic) [CTUe]	2.27×10^{03}	97.2	314
Ecotoxicity freshwater (Metals) [CTUe]	1.16×10^{03}	9.65	167
Ecotoxicity freshwater (Organic) [CTUe]	13.6	1.91	3.8
Eutrophication freshwater [kg P eq.]	2.96×10^{-03}	3.38×10^{-005}	1.43×10^{-04}
Eutrophication marine [kg N eq.]	0.333	0.15	0.064
Eutrophication terrestrial [Mole of N eq.]	3.48	1.66	0.70
Ionising radiation - human health [kBq U235 eq.]	67	0.155	8.59
Land Use [Pt]	4.53×10^{03}	15.8	516
Non-cancer human health effects [CTUh]	4.73×10^{-06}	3.06×10^{-06}	2.17×10^{-06}
Non-cancer human health effects (Inorganic) [CTUh]	1.41×10^{-06}	2.32×10^{-007}	2.01×10^{-007}
Non-cancer human health effects (Metals) [CTUh]	3.3×10^{-06}	2.82×10^{-06}	1.97×10^{-06}
Non-cancer human health effects (Organic) [CTUh]	5.17×10^{-08}	6.58×10^{-08}	1.49×10^{-08}
Ozone depletion [kg CFC-11 eq.]	2.19×10^{-011}	2.4×10^{-014}	3.37×10^{-010}
Photochemical ozone formation - human health [kg NMVOC eq.]	0.836	0.453	0.244
Resource use, energy carriers [MJ]	8.9×10^{03}	9.91×10^{03}	1.12×10^{003}
Resource use, mineral and metals [kg Sb eq.]	2.6×10^{-005}	3.5×10^{-005}	2.8×10^{-005}
Respiratory inorganics [Disease incidences]	8.95×10^{-006}	2.47×10^{-006}	4.47×10^{-006}
Water scarcity [m ³ world equiv.]	15.8	1.27	19.6