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Master's Thesis

Thesis for obtaining the diploma **MASTER**

**In :** Mechanical Engineering

**Option : Energy**

**Presented by :**

Akki Abdellah Mohammed Elamine and BENLARBI Nadir

**Thesis**

# "ASPEN Plus Simulation of $CO_2$ Capture Technologies for Sustainable Hydrogen Production."

Defended in front of the jury composed of :

| | | | | |
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graduating class **2023 - 2024**

# Dedication AKKI Abdellah Mohammed Elamine

This thesis is dedicated to:
This humble work is dedicated to the martyrs, the steadfast, and the honourable souls who stand unwavering in **Gaza**. Their courage, resilience, and sacrifice inspire us all. May this dedication serve as a tribute to their unwavering spirit and a call for peace, justice, and solidarity.

To my parents, **Brahim** and **Benchatti Halima**, whose unwavering support and encouragement have been my greatest source of strength throughout this journey, I express my heartfelt gratitude. And to my dear grandparents, whose unwavering belief in me has fueled my determination, this work stands as a tribute to your love and support.

To my mentor, **Dr. Bensenouci**, and my co-supervisor, whose guidance and wisdom have been invaluable, thank you for shaping my academic path.

To my friends and colleagues, your constant encouragement has made this experience memorable and fulfilling.

Lastly, to my partner, **BenLarbi Nadir**, for your endless patience, love, and understanding during the many late nights and early mornings—thank you. May this work honor the memory of those who came before us and pave the way for those who will follow.

# Dedication BenLarbi Nadir

This thesis is dedicated to:

**The sake of Allah, my Creator.**

**And my Master,My great teacher and messenger, Mohammed (May Allah bless and grant him), who taught us the purpose of life.**

It is with genuine gratitude and warm regard that

I dedicate my dissertation work to my family and many friends. A special feeling of gratitude to my loving **parents** , whose words of encouragement and push for tenacity ring in my ears. My **grandparents**, who helped me in all things great and small and have never left my side. they are very special.

I also dedicate this work to my Colleague **AKKI Abdellah Mohammed Elamine**, who helped me a lot in this work. and give special thanks to all my friends specially **Abdessalam Lakhdari and Abimouloud Mohamed Laid**.

My supervisors: **Pr BENSENOUCI Ahmed** and **Dr MERDJANI AbdelHakim**. May Allah grant you health and happiness and long life.

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First and foremost, we must acknowledge our limitless thanks to Allah, their-Magnificent; the Ever-Thankful, for His help and bless. We are totally sure that this work would have never become truth, without his bless.

# Abstract

This thesis presents a comprehensive evaluation of various carbon capture technologies for post-combustion $CO_2$ capture from power plant flue gas. The study compares the performance and cost-effectiveness of several commercially available technologies, including chemical solvents, membrane separation, and adsorption processes. The simulation results demonstrate that solvent-based technology such as MEA is effective for capturing $CO_2$ from flue gas, but is limited by their high operating costs and energy requirements. The membrane-based technology, on the other hand, showed promising results, with high $CO_2$ capture rates and lower energy requirements compared to the solvent-based technologies. The study highlights the importance of understanding the underlying thermodynamics and kinetics of the capture process, as well as the need for optimized design and operation of the capture unit. Overall, this thesis provides a comprehensive analysis of carbon capture technologies for post-combustion $CO_2$ capture from power plant flue gas and highlights the potential for innovative solutions to address the challenges of climate change mitigation.

# Keywords

Carbon capture , Post-combustion $CO_2$ capture ,Carbon capture and storage (CCS) , Simulation modeling , Numerical modeling , Experimental testing.

# Résumé

Cette thèse présente une évaluation complète de diverses technologies de capture du carbone pour la capture du $CO_2$ post-combustion à partir des gaz de combustion des centrales électriques. L'étude compare la performance et le rapport coût-efficacité de plusieurs technologies disponibles sur le marché, y compris les solvants chimiques, la séparation par membrane et les procédés d'adsorption.

Les résultats de la simulation démontrent que la technologie à base de solvants comme le MEA est efficace pour capturer le $CO_2$ des gaz de combustion, mais est limitée par ses coûts d'exploitation élevés et ses besoins énergétiques importants. La technologie à base de membranes, en revanche, a montré des résultats prometteurs, avec des taux de capture de $CO_2$ élevés et des besoins énergétiques inférieurs par rapport aux technologies à base de solvants.

L'étude souligne l'importance de comprendre la thermodynamique et la cinétique sous-jacentes du processus de capture, ainsi que la nécessité d'une conception et d'une exploitation optimisées de l'unité de capture.

Dans l'ensemble, cette thèse fournit une analyse complète des technologies de capture du carbone pour la capture du $CO_2$ post-combustion à partir des gaz de combustion des centrales électriques et met en lumière le potentiel de solutions innovantes pour relever les défis de l'atténuation du changement climatique.

# Mote Clé

Capture du carbone, Capture du $CO_2$ post-combustion, Capture et stockage du carbone (CSC), Modélisation par simulation , Modélisation numérique, Tests expérimentaux.

# الملخص:

تقدم هذه الأطروحة تقييمًا شاملاً لمختلف تقنيات احتجاز الكربون لاحتجاز ثاني أكسيد الكربون بعد الاحتراق من غاز المداخن لمحطات توليد الطاقة. تقارن الدراسة أداء وتكلفة العديد من التقنيات التجارية المتاحة، بما في ذلك المذيبات الكيميائية، وفصل الأغشية، وعمليات الامتزاز.

تُظهر نتائج المحاكاة أن تقنية المذيبات مثل پيا فعالة في احتجاز ثاني أكسيد الكربون من غاز المداخن، لكنها محدودة بسبب تكاليف التشغيل العالية والمتطلبات الطاقية المرتفعة. من ناحية أخرى، أظهرت تقنية الأغشية نتائج واعدة، مع معدلات احتجاز عالية لثاني أكسيد الكربون ومتطلبات طاقية أقل مقارنة بتقنيات المذيبات.

تسلط الدراسة الضوء على أهمية فهم الديناميكا الحرارية والحركية الأساسية لعملية الاحتجاز، بالإضافة إلى الحاجة إلى تصميم وتشغيل محسنين لوحدة الاحتجاز.

بشكل عام، تقدم هذه الأطروحة تحليلًا شاملاً لتقنيات احتجاز الكربون لاحتجاز ثاني أكسيد الكربون بعد الاحتراق من غاز المداخن لمحطات توليد الطاقة، وتسلط الضوء على الإمكانيات لحلول مبتكرة لمواجهة تحديات التخفيف من تغير المناخ.



**الكلمات الدلالية:** احتجاز الكربون ، احتجاز ثاني أكسيد الكربون بعد الاحتراق ، احتجاز وتخزين الكربون نمذجة المحاكاة ، النمذجة العددية ، الاختبار التجريبي

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# Acronyms

| | |
|---|---|
| **ATR** | auto thermal reforming |
| **AMP** | 2-amino-2-methyl1-propanol |
| **BECCS** | Bioenergy with carbon capture and storage |
| **CCS** | carbon capture and storage |
| **CLC** | Chemical looping combustion |
| **CLP** | calcium looping process |
| **CO2** | carbon dioxide |
| **CFB** | circulating fluidized beds |
| **CO** | carbon monoxide |
| **CAMD** | computer-aided molecular design |
| **DESs** | deep eutectic solvents |
| **EOR** | enhanced oil recovery |
| **EOS** | Equation of State |
| **GT** | gas turbine |
| **ILs** | ionic liquids |
| **IRCC** | integrated reforming combined cycle |
| **IGCC** | Integrated Gasification Combined Cycle |
| **LVC** | Lean Vapor Compressor |
| **LNG** | liquefied natural gas |
| **LVC** | Lean Vapor Compressor |
| **LVC** | Lean Vapor Compressor |

| | |
|---|---|
| **LCOE** | levelized cost of electricity |
| **MOFs** | metal-organic frameworks |
| **MEA** | Monoethanolamide |
| **MDEA** | methyl diethanol amine |
| **NGCC** | natural gas combined cycle |
| **PTSA** | pressure-temperature swing adsorption |
| **PZ** | piperazine |
| **PCC** | post-combustion carbon capture |
| **PSA** | pressure swing adsorption |
| **PR** | Peng-Robinson |
| **RK** | Redlich-Kwong |
| **SSF** | Stripper Split Feed |
| **SRK** | Soave-Redlich-Kwong |
| **SSF** | Stripper Split Feed |
| **TSA** | temperature swing adsorption |
| **VLE** | Vapour-Liquid Equilibrium |
| **VSA** | vacuum swing adsorption |
| **WGS** | water-gas-shift |

# General Introduction

In the pursuit of sustainable energy solutions, the production of hydrogen via methane reforming has garnered significant attention. Previous research, notably the work by **Belkacem Benregga** and **Mohammed Boudali Tedjani**, supervisors by: **Pr BENSENOUCI Ahmed** and Dr **MERDJANI AbdelHakim**. explored hydrogen production through gasification of methane using the **Aspen Hysys** software. Their findings underscored a critical concern: both biogas and natural gas-based hydrogen production processes release substantial amounts of carbon dioxide into the ambient air.

Given the urgent need to mitigate greenhouse gas emissions, our work builds upon this foundation. We focus on capturing $CO_2$ a potent greenhouse gas to contribute to air purification and environmental preservation. By employing innovative technologies, we aim to address the environmental impact associated with hydrogen production methods.

This thesis delves into three distinct $CO_2$ capture technologies, namely $CO_2$ capture from natural gas power plants using (Monoethanolamide (MEA)), $CO_2$ capture from coal power plants using MEA, and $CO_2$ capture from syngas for Integrated (Integrated Gasification Combined Cycle (IGCC)) applications using MEA. Through these efforts, we strive to enhance the sustainability of energy production while minimizing the release of harmful pollutants.

Our thesis consists of

* **Introduction:** A general overview of the topic, including the significance and relevance of hydrogen production by vapour reforming of methane, the research question and objectives, and the scope of the study.

* **Chapter 1:** Entrance to Brief history of hydrogen and Technologies for hydrogen production, and the relevant process conditions and parameters of Technology for $CO_2$ Capture, we discussed how carbon dioxide is produced and its role, and Methodology. Advantages and Limitations of Each Technology.

* **Chapter 2:** we explain The Thermodynamic Properties of $CO_2$ Mixtures, Experimental Data of $CO_2$ and $CO_2$ Mixtures, Evaluations for the Thermodynamic Properties Calculations of $CO_2$ Mixtures, and Evaluation of Cubic EOS for Predicting VLE and Volume of $CO_2$ Mixtures.

* **Chapter 3:** We Simulation of Carbon Dioxide Capture By defining the software we are using (Aspen Plus), we simulate the three mentioned techniques, with the simulation steps.

* **Chapter 4:** Results and Discussion - Presentation of the simulation results, including the production rates of carbon dioxide, and discussion of the implications of the results for the design and optimization of the $CO_2$ capture process.

* **Conclusion:** A summary of the main findings and implications of the study, as well as recommendations for future research or applications.

# 1

# Technology of $CO_2$ Capture

## 1.1 Brief history of hydrogen

Hydrogen, the first element on the periodic table with an atomic number of 1, is truly in a class by itself. It does not belong to any family of elements. Although hydrogen is a nonmetal, it is placed on the left side of the periodic table along with the first group of alkali metals, but obviously, hydrogen does not belong to the alkali metals family.

Hydrogen is the most abundant element in the universe; it is found as interstellar gas and as the chief constituent of main-sequence stars. Helium is the other element similar to hydrogen in its simplicity and abundance and is placed on the same row at the right side of the periodic table. Although helium is a noble gas, and hence it is chemically inert, hydrogen reacts with all sorts of other elements and makes variety of useful compounds. For instance, the bonding of hydrogen with carbon forms the backbone for a vast collection of organic molecules, known as hydrocarbons. Similarly, by bonding with oxygen, hydrogen makes water, the single most important compound on the Earth.

Although hydrogen is the most abundant element, it makes up only about $0.14\%$ of the Earth's crust by weight. It occurs, however, in vast quantities as part of the water in oceans, ice packs, rivers, lakes, and the atmosphere. As part of innumerable carbon compounds, hydrogen is present in all animal and vegetable tissue and petroleum. Even though it is often said that there are more known compounds of carbon than of any other element, the fact is that, because hydrogen is contained in almost all carbon compounds and also forms a multitude of compounds with all other elements (except some of the noble gases), hydrogen compounds may be more numerous. Elementary hydrogen finds its principal industrial application in the manufacture of ammonia; a compound of hydrogen and nitrogen, and in the hydrogenation of carbon monoxide and organic compounds to make a variety of chemicals and fuels.

Hydrogen has also been considered as a potential source of power and transportation and, perhaps in the future, as a source of abundant clean energy.

The purpose of this chapter is to provide an overview of hydrogen, its physical and chemical properties, and an overview of industrial production and uses in chemical and energy industries.

**1766:** Henry Cavendish, a British scientist, first identified hydrogen as a distinct element after observing a gas evolved by the reaction of zinc metal with hydrochloric acid. In a demon-

stration to the Royal Society of London, Cavendish applied a spark to hydrogen gas that yielded water ($H_2O$). This discovery led to his later finding that $H_2O$ is made of hydrogen and oxygen.

**1783:** Jacquest Alexander Cesar Charles, a French physicist, launched the first hydrogen balloon flight known as Charliere. This unmanned balloon flew to an altitude of 3 km. Three months later, Charles himself flew in his first manned hydrogen balloon.

**1788:** Based on the discoveries of Cavendish, the French chemist Antoine Lavoisier gave hydrogen its name, which was derived from the Greek words: **"hydro"** and **"genes,"** meaning **"water"** and **"born of."**

**1800:** English scientists William Nicholson and Sir Anthony Carlisle discovered the process of **"electrolysis."**

**1838:** Swiss chemist Christian Friedrich Schoenbein discovered the fuel cell effect that produced electric current and pure water by combining hydrogen and oxygen gases.

**1845:** Sir William Grove, an English scientist and judge, demonstrated Schoenlein's discovery on a practical scale by creating a **"gas battery."** He earned the title **"father of the fuel cell"** for his achievement.

**1874:** Jules Verne, a French author, prophetically examined the potential use of hydrogen as a fuel in his popular work of fiction entitled The Mysterious Island.

In **1889:** Ludwig Mond and Charles Langer attempted to build the first fuel cell device using air and industrial coal gas.

**1920:** German engineer Rudolf Erren converted the internal combustion engines of trucks, buses, and submarines to use hydrogen or hydrogen mixtures. During this period, British scientist and Marxist writer, J.B.S. Haldane, introduced the concept of renewable hydrogen.

**1952:** The United States of America conducted its first nuclear test of a fusion device, or **"hydrogen bomb"** at Eniwetok in the Marshall Islands.

**1958:** The United States formed the National Aeronautics and Space Administration (NASA). NASA's space program currently uses the most liquid hydrogen worldwide, primarily for rocket propulsion and as a fuel for fuel cells.

**1959:** Francis T. Bacon of Cambridge University in England built the first practical hydrogen-air fuel cell. The 5-kW system powered a welding machine. He named his fuel cell design the

**"Bacon cell."** Later that year, Harry Karl Ihrig, an engineer for the Allis Chalmers Manufacturing Company, demonstrated the first fuel cell vehicle: a 20-horsepower tractor. Hydrogen fuel cells, based upon Francis T. Bacon's design, have been used to generate onboard electricity, heat, and water for astronauts aboard the Apollo spacecraft and all subsequent space shuttle missions.

**1970:** Electrochemist John O'M. Bockris coined the term **"hydrogen economy"** during a discussion at the General Motors (GM) Technical Centre in Warren, Michigan. He later published Energy: The Solar-Hydrogen Alternative, describing his envisioned hydrogen economy in which he explains how could cities in the United States be supplied with energy derived from the sun.

**1973:** The OPEC oil embargo and the resulting supply shock suggested that the era of cheap petroleum had ended and that the world needed alternative fuels. Consequently, the development of hydrogen fuel cells for conventional commercial applications began.

**1974:** The International Association for Hydrogen Energy (IAHE) was formed at the Hydrogen Economy Miami Energy Conference (THEME), the first international conference that Prof. T. Nejat Veziro glu of the University of Miami, Florida, organized to discuss hydrogen energy.

**1976:** The International Journal of Hydrogen Energy (IJHE) was established by T. Nejat Veziro glu as its editor-in-chief, and published by Pergamon Press, to provide a platform for hydrogen energy-related scientific papers.

**1977:** The International Energy Agency (IEA) was established in response to global oil market disruptions. IEA activities included the research and development of hydrogen energy technologies. The U.S. Department of Energy (DOE) was also created during this time.

**1989:** The National Hydrogen Association (NHA) was formed in the United States with 10 members. Today, the NHA has nearly 100 members.

**1990:** The United Nations International Standards Organization (ISO), at the initiative of Gustar Grob of Switzerland, established the ISO/TC-197 Committee to prepare the international standards for hydrogen energy technologies.

**1992:** The world's first solar-powered hydrogen production plant at Solar Wasserst off-

Bayern, a research and testing facility in Southern Germany, became operational.

**1994:** Daimler Benz demonstrated its first NECAR I (new electric car) fuel cell vehicle at a press conference in Ulm, Germany.

**1998:** Iceland unveiled a plan to create the first hydrogen economy by 2030 with Daimler Benz and Ballard Power Systems.

**1999:** The Royal Dutch/Shell Company committed to a hydrogen future by forming a hydrogen division. Europe's first hydrogen fuelling stations were opened in the German cities of Hamburg and Munich.

**2000:** Ballard Power Systems presented the world's first production-ready PEM fuel cell for automotive applications at the Detroit auto show.

**2004:** The world's first fuel cell-powered submarine undergoes deep-water trials (German Navy).

**2013:** Honda unveiled its new FCEV concept hydrogen fuel-cell vehicle at the Los Angeles auto show, promising to market the car initially in Japan and the United States in 2015 followed by a European introduction. Chiyoda Corp. plans to build what it describes as the world's first large-scale power plant fuelled mainly by hydrogen ($70\%$) and natural gas ($30\%$).

## 1.2 Technologies for hydrogen production

Research on hydrogen production [1] is geared toward power generation [2] and is a substitute for fossil fuels. This section presents [3] hydrogen production and contention it identified the production mechanisms, chemical reactions, process efficiency, and by-products. [4]

### 1.2.1 Electrolysis

Electrolysis is a process by which a breakdown of the water molecule is generated ($H_2O$) by the action of electric current flow, generated [5] from sources such as solar or nuclear, [6] in environmental conditions ( $25\,^{\circ}\mathrm{C}$. y 1 atm), a chemical reaction occurs

$$2\mathrm{H}_2O \rightarrow 2H_2 + O_2\ . \tag{1.1}$$

If the electrolysis is carried out at low [7] temperatures, there is an increase in the consumption of electrical energy and generates greater inefficiency in the process for high temperatures, the energy consumption [8] increases, but the efficiency is considered acceptable.

### 1.2.2 Natural gas steam reforming

Kalamaras et al. indicate that $50\%$of global hydrogen demand occurs through steam-reforming natural gas. In the United States, $95\%$ of production is done by this method. This [9] technology is the cheapest and uses natural gas, mainly methane, it is an endothermic process because it exposes natural gas to steam with high temperatures. [10] The reactor

Rx01:

$$\mathrm{CH}_4 + H_2O \rightarrow CO + 3H_2\ . \tag{1.2}$$

Rx02:

$$\text{CO}+\text{H}_2O \rightarrow CO_2 + H_2. \tag{1.3}$$

Rx03:

$$\text{CH}_4 + 2H_2O \rightarrow CO_2 + 3H_2\ . \tag{1.4}$$

The reforming process has two reactions, one of reforming and the other of oxidation, finally, the hydrogen ($H_2$) is separated. Catalysts such as nickel–boron–alumina xerogel improve the efficiency of the reaction. in figure1.1 the monolithic catalyst FeCr Alloy coated with ruthenium (Ru), among other things. [11]

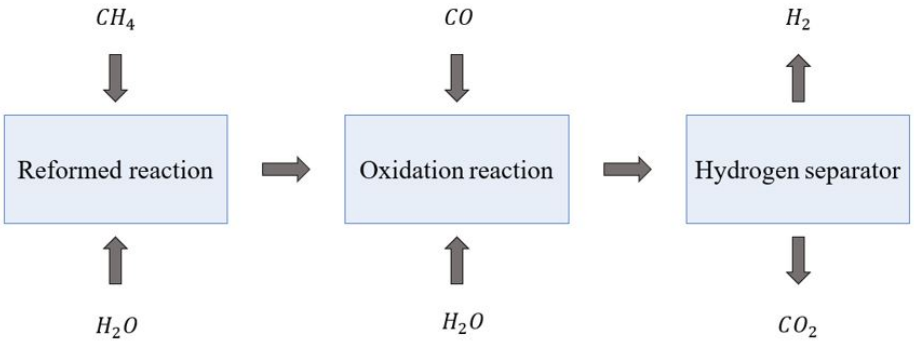


**Figure 1.1:** Natural gas steam reforming process.

Methane is one of the most critical raw materials for hydrogen production under this method. [12] However, biomass is investigated as a surrogate due to its environmental effects and cost reduction. Recently, reforming technology has improved the production of hydrogen to purified hydrogen. Iulian Elli and Basile propose that hydrogen perm-selective membrane be incorporated into a reactor, improving the chemical reaction and obtaining purified $H_2$ in a single

reactor. This membrane must be permeable and thermally [13] stable using palladium, palladium alloys, and an inorganic membrane such as niobium and tantalum.

### 1.2.3 Pyrolysis

Pyrolysis consists of the decomposition of solid organic material in the absence of oxygen and high temperatures, [14] through the application of heat temperature of 500 °C is reached for biomass and 1200 °C for coal. **Figure**1.2 presents the chemical [15] reaction; the results depend on raw material, temperature, pressure, and process time gaseous products such as hydrogen ($H_2$), carbon monoxide ($CO$) and carbon dioxide ($CO_2$), liquids such as hydrocarbons and solids such as carbonaceous residues and coke are obtained. [16]

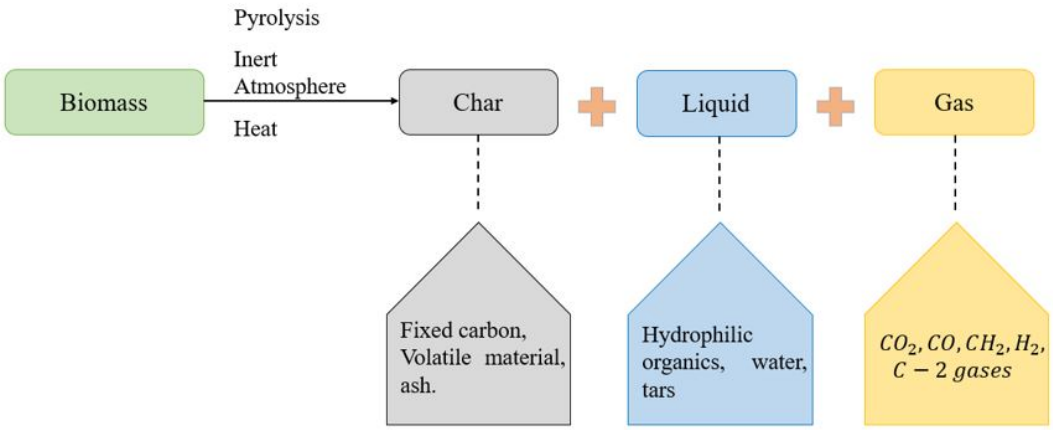


**Figure 1.2:** Pyrolysis process in biomass.

Rx03:

$$CnHn \rightarrow CO + CO + CmHm + Tar + Carbon \tag{1.5}$$

## 1.3 Carbon ($CO_2$) capture technologies

Carbon capture technologies play a crucial role in mitigating the effects of greenhouse gas emissions on the environment. These technologies are designed to capture carbon dioxide from industrial processes and prevent it from entering the atmosphere. By implementing carbon capture technologies, industries can significantly reduce their carbon footprint and contribute to global efforts to combat climate change. In this overview, we will explore the various types of carbon capture technologies and their applications in different industries. We will also examine the benefits and challenges associated with the implementation of these technologies, providing a comprehensive understanding of their role in creating a sustainable future.

## 1.4 What is carbon capture?

Carbon capture technologies refer to a set of methods and systems designed to capture carbon dioxide emissions produced by various sources such as power plants and industrial facilities. These technologies aim to prevent the release of carbon dioxide into the atmosphere, thus helping to mitigate climate change. Carbon capture can involve various techniques, including post-combustion capture, pre-combustion capture, and oxyfuel combustion. The captured carbon dioxide can then be stored underground or utilized in other industrial processes. Overall, carbon capture technologies play a crucial role in reducing greenhouse gas emissions and combating global warming.

## 1.5 How is carbon capture works?

Carbon capture technologies work by capturing carbon dioxide emissions from sources like power plants or industrial facilities, preventing them from entering the atmosphere. These technologies use various methods such as absorption, adsorption, or membrane separation to capture the carbon dioxide, which can then be stored underground or utilized in other processes, e.g.: One example of a carbon capture technology is carbon capture and storage CCS, which involves capturing carbon dioxide emissions from sources like power plants and storing them

underground to prevent their release into the atmosphere. Another example is direct air capture, a technology that removes carbon dioxide directly from the air using chemical processes. Additionally, Bioenergy with carbon capture and storage (BECCS) is a method that combines bioenergy production with carbon capture and storage to achieve negative emissions. These technologies play a crucial role in reducing greenhouse gas emissions and combating climate change by capturing and storing carbon dioxide before it enters the atmosphere.

There are several methods and technologies available for decarbonizing fuel gas production. These include carbon capture and storage [17], biomass gasification, electrolysis of water to produce hydrogen, and the use of renewable energy sources such as wind and solar to power fuel gas production. Each route has its advantages and challenges, and the choice of decarbonization route will depend on factors such as cost, availability of resources, and the specific requirements of the end-use applications. [18] In the following sections, we will delve into each carbon capture method in more detail to provide a comprehensive understanding of the options available for decarbonizing fuel gas production.

## 1.6 Pre-combustion

Pre-combustion carbon capture appears before the combustion process, in this process, fuel is oxidized using a gasification process, which produces syngas (a gas mixture of predominantly $CO_2$ and $H_2$) [19], and the produced $CO$ is converted into $CO_2$ then it's captured before combustion as shown in figure 1.3

Pre-combustion carbon capture uses chemical and physical methods to catch $CO_2$ from syngas. Chemical absorbent, such as carbonates and physical solvents like polypropylene glycol and methanol, are used in large scale to capture $CO_2$ [20], Carbon capture technologies have been gaining significant attention as the world seeks to mitigate the effects of greenhouse gas emissions on the environment. In recent years, there has been a growing interest in pre-combustion carbon capture technologies due to their potential to capture carbon dioxide before it is released into the atmosphere.

One of the primary considerations in evaluating pre-combustion carbon capture technologies

is their efficiency and cost. Understanding the expenditure and energy consumption associated with these technologies is crucial for assessing their viability and practicality on a larger scale.

Efficiency analysis involves examining the capability of the technology to capture carbon dioxide from the source, whether it's natural gas, coal, or biomass while minimizing energy input and maintaining high capture rates. This can be measured by looking at the overall process efficiency [18], including the energy penalty associated with implementing the carbon capture technology.

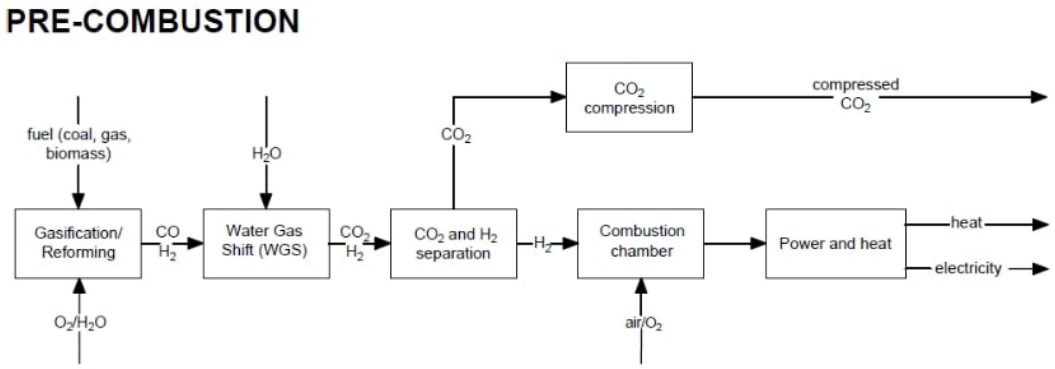


**Figure 1.3:** pre-combustion Diagram

Cost analysis, on the other hand, encompasses evaluating the capital and operating costs of the pre-combustion carbon capture processes. This includes the costs of equipment, infrastructure, maintenance, and the overall cost of electricity generation with the integrated carbon capture system [21].

To conduct a comprehensive assessment of pre-combustion carbon capture technologies, it is essential to delve deeper into the specific methods and processes involved, considering the varying characteristics of different feedstocks and the associated challenges. Understanding the unique technical and economic features of these technologies is critical in order to make informed decisions regarding their implementation and scalability.

| Highlights | | |
|---|---|---|
| Software | Methodology | Efficiency |
| Aspen Plus | The objective of this study was to explore pre-combustion $CO_2$ capture techniques specifically applied to natural gas power plants. The authors aimed to assess the feasibility, efficiency, and potential environmental impact of implementing pre-combustion capture using auto thermal reforming auto thermal reforming (ATR) and methyl diethanol amine (MDEA) processes. ATR The study investigates the production of hydrogen ($H_2$) fuel from natural gas within the liquefaction facility using ATR. MDEA Absorption: The syngas generated during $H_2$ production is treated to remove $CO_2$ using MDEA. $H_2$ as Fuel: The purified $H_2$ is then utilized as the primary fuel in the plant's gas turbines. [22] | 50% |
| Aspen Plus | this study was to evaluate the performance of a biomass-integrated combined power plant with post-combustion $CO_2$ capture. The study involved several steps: Designing the combined power plant layout, including biomass gasification, power generation, and $CO_2$ capture. And developing detailed process models for each component (gasifier, gas turbine, steam cycle, and $CO_2$ capture unit). The study provided insights into the trade-offs between power generation efficiency and $CO_2$ capture efficiency. It highlighted the importance of selecting appropriate $CO_2$ capture methods to minimize energy penalties. The researchers discussed the feasibility of integrating biomass-based power plants with $CO_2$ capture for sustainable energy production. [23] | 90% |
| Aspen Plus | identify the most important solvent characteristics in the $CO_2$ capture process. Additionally, the authors aimed to determine how these characteristics contribute to the total cost of $CO_2$ separation and analyze the economic feasibility of current deep eutectic solvents deep eutectic solvents (DESs) reported in the literature. [24] The study contributes valuable insights into the economic viability of using deep eutectic solvents for pre-combustion $CO_2$ capture. It highlights the importance of optimizing solvent properties and understanding their impact on overall process costs. | 85% |

| | | |
|---|---|---|
| Aspen HYSYS GT PRO and GT MASTER | analyse the performance of a pre-combustion $CO_2$ capture process integrated into a natural gas combined cycle (NGCC) power plant. The researchers aimed to evaluate both the design (steady-state) and off-design (transient) behaviour of the system. [25] The study focused on an integrated reforming combined cycle (IRCC) process. In this process: Natural gas is reformed into syngas (a mixture of hydrogen and carbon monoxide). The CO in the syngas is converted to $CO_2$ in shift reactors. The $CO_2$ is then captured from the syngas.The resulting hydrogen-rich fuel is used in a gas turbine (GT) within a combined cycle setup. The IRCC process achieved very low $CO_2$ emissions (typically below $100$ g $CO_2$/net kWh electricity) compared to a state-of-the-art NGCC (around $365$ g $CO_2$/net kWh electricity).Detailed HRSG design for IRCC cycles. Insights into subsystem efficiency losses. Quantification of efficiency potential.Addressing model uncertainties. | $93\%$ and $95\%$ |
| Aspen HYSYS | Optimize the design of a pre-combustion $CO_2$ capture plant. The researchers aimed to incorporate experimental knowledge into the optimization process. The study involved detailed process modeling and Solvent Selection: Choosing an appropriate solvent for $CO_2$ capture. Optimizing operating conditions (e.g., temperature, pressure) for maximum efficiency. The study provided insights into: [26] Optimal solvent selection. Energy-efficient process configurations. Trade-offs between cost and performance. Contributions included: Improved understanding of $CO_2$ capture plant design. Practical guidelines for implementing optimized designs. | between $85\%$ and $90\%$ |
| Aspen Plus | the pre-combustion decarbonization route for electricity production with $CO_2$ capture. The researchers focused on pre-combustion technologies applied to two different fuels: natural gas and coal, as they constitute a significant portion of global electricity production from fossil fuels. briefly touched on pre-combustion $CO_2$ capture in industrial settings, particularly projects involving $CO_2$ storage or enhanced oil recovery (EOR). [17] Research activity in pre-combustion decarbonization for power production was more focused on coal. Natural gas-based plants faced challenges due to complexity and costs, making them less competitive. | range from $80\%$ to over $90\%$ |

| | | |
|---|---|---|
| Aspen Plus<br>ChemCAD<br>COMSOL<br>Multiphysi cs | explore various $CO_2$ capture approaches in thermal power plants.Specifically, the researchers investigated pre-combustion, post-combustion, and oxy-combustion technologies. For gasification applications, the researchers focused on partial oxidation processes. [27] Fuel inside the gasifier was partially burned to produce synthesis gas (syngas) containing hydrogen ($H_2$),carbon monoxide (CO), and minor constituents. The syngas was then processed in a water-gas-shift (WGS) reactor to increase $CO_2$ concentration. | 92% |
| Aspen Plus<br>Aspen HYSYS | The objective of this study was to develop cost-efficient pre-combustion $CO_2$ capture and oxy-fuel technologies for power generation based on fossil fuels. The project aimed to substantially reduce the cost of $CO_2$ capture. ENCAP (ENhanced CAPture of $CO_2$) was a major technology development project funded by the 6th Framework Programme of the European Commission. It involved leading European power and energy industries, equipment suppliers, research institutes, and universities. [28] The research provided insights into the feasibility of pre-combustion and oxy-fuel technologies. It contributed to understanding the trade-offs between technical performance and cost reduction. | range from 41% to over 44% |
| Aspen-Plus<br>ChemCAD<br>COMSOL<br>Multiphysi cs | highly efficient and stable pre-combustion $CO_2$ capture process based on calcium looping. The focus was on producing high-purity hydrogen ($H_2$) while capturing $CO_2$. [21] The research demonstrated that calcium looping could achieve high $CO_2$ capture efficiency while producing high-purity hydrogen.Stability improvements were crucial for practical implementation. The study contributed to advancing pre-combustion $CO_2$ capture technologies. | 51% |
| Aspen Plus | this study was to evaluate and compare three different carbon capture processes applied to coal power plant Pre-combustion. [29] The study compared the costs and levelized cost of electricity (LCOE) for each capture technology. Findings revealed that pre-combustion was the most costly, with an investment approximately 1.6 times higher than the oxy-fuel process. The research emphasized the importance of considering both technical and economic aspects when evaluating carbon capture technologies. | range from 85% to over 90% |

| | | |
|---|---|---|
| Aspen Plus<br>Aspen HYSYS - ChemCAD<br>MATLAB<br>COSMO-RS<br>VASP | was to review and analyze various aspects related to pre-combustion carbon capture and the incorporation of ionic liquids (ILs) in this process. reviews several aspects related to pre-combustion capture and ILs. [20] It covers Carbon dioxide separation technologies.<br>Research progress in pre-combustion capture. Pilot plant and commercial facilities. Modeling approaches, with a focus on computer-aided molecular design (CAMD). | ranging from 80% and 90% |
| Aspen Plus | The study aimed to optimize the design of an IGCC power plant with pre-combustion $CO_2$ capture using different solvents. The focus was on evaluating the performance of various physical and chemical solvents for $CO_2$ capture. Among the evaluated solvents, dimethyl ethers of polyethylene glycol were found to be more energy-efficient for $CO_2$ capture. [30] Economic analysis revealed that implementing pre-combustion $CO_2$ capture using dimethyl ethers of polyethylene glycol led to an increase in capital cost (ranging from 19.55% to 22.55%) depending on the desired $CO_2$ capture rate. | ranging from 70% to over 90% |
| Aspen HYSYS | This study was to assess the feasibility and effectiveness of the HBGS process for capturing $CO_2$ from gas streams before combustion. [31] The study aimed to evaluate the potential of clathrate hydrates as a separation medium. | range from 70% to 90% |
| Aspen Plus<br>Aspen HYSYS<br>MATLAB | The objective was to evaluate membrane-based strategies for capturing $CO_2$ from gas streams before combustion. [32] The study aimed to assess the feasibility, efficiency, and potential of membrane separation processes. | 92% |
| Aspen Plus<br>Aspen HYSYS<br>gPROMS<br>MATLAB<br>SuperPro | Aimed to assess the feasibility and competitiveness of different $CO_2$ capture options. It focused on integrated energy conversion systems, considering thermodynamic, economic, and environmental aspects. The methodology was applied to fossil fuel-fed power plants. [33] By systematically comparing options, the study aimed to guide decision-making for $CO_2$ capture implementation. | 49.6% |

| | | |
|---|---|---|
| ELCOGAS 14 MWth | demonstrate the feasibility of capturing $CO_2$ and producing $H_2$ in an IGCC plant using solid fossil fuels and wastes as the main feedstock. Additionally, the aim was to obtain economic data to scale the technology to the full Puertollano IGCC capacity in synthetic gas production. [34] fully integrated into the existing IGCC Plant, with all outlets recycled back to the plant. The operation focused on capturing $CO_2$ and producing $H_2$ as additional steps of the existing syngas purification systems of the IGCC process. pre-combustion carbon capture technology, which involves de-carbonisation of fuel (synthetic gas) before combustion in a combined cycle to produce electricity. This technology is commonly used in chemical plants for various products but was applied for electricity production in this project. | 90% |

**Table 1.1:** of pre-combustion.

## 1.7 Post-combustion

carbon dioxide (CO2) capture methods involve the extraction of CO2 from the flue gas emitted during industrial processes, typically following combustion in facilities like power plants. These capture units are strategically positioned downstream of purification systems, such as desulfurization (which removes sulfur compounds), denitrogenating (eliminating nitrogen compounds), and dedusting (filtering out particulate matter) installations. This setup ensures that the flue gas undergoes preliminary treatment to remove impurities before entering the CO2 capture unit [35] This sequential arrangement helps optimize the efficiency and efficacy of the CO2 capture process. Various technologies, including chemical absorption, adsorption, and membrane separation, are utilized for post-combustion CO2 capture. These methods are crucial in mitigating greenhouse gas emissions and addressing climate change concerns by capturing CO2 emissions from industrial activities. In conventional power units, post-combustion technologies are often prioritized. However, a significant barrier exists to their widespread adoption. This barrier stems from the relatively low partial pressure of CO2 in the flue gas. Typically, the flue gas operates under atmospheric pressure, and the concentration of $CO_2$ falls within the range of 13–15% Consequently, the driving force for CO2 capture is also low in these conditions [36]

### 1.7.1 Absorption solvent-based methods:

Post-combustion technologies can be categorized based on the specific processes employed for capturing carbon dioxide. These methods include various approaches such as chemical absorption, adsorption, and membrane separation. Each method offers distinct advantages and challenges, influencing their suitability for different applications and operating conditions. Despite the challenges posed by the low partial pressure of CO2, ongoing research and development efforts continue to improve the efficiency and effectiveness of post-combustion CO2 capture technologies, aiming to address environmental concerns associated with CO2 emissions from power generation and industrial processes.

Commercially available post-combustion technologies are capable of capturing a significant portion of CO2 from flue gas streams. The amine method, for instance, is estimated to capture approximately 85–95% of the CO2 present in flue gas [14], achieving a purity level exceeding 99.95%. In addition to traditional solvents like amine-based-MEA [37], DEA, ammonia, and piperazine, there are now alternative solvents developed for CO2 capture processes. Solvent blends offer enhanced absorption properties by combining different types effectively. Primary and secondary amines exhibit high absorption rates, while tertiary amines possess greater capacity. For instance, blending MEA with a small amount of piperazine (PZ) can significantly improve absorption rates, as PZ demonstrates a 50-fold greater speed compared to MEA. Another approach involves using a solution of 2-amino-2-methyl1-propanol (AMP) with PZ promotion. Studies have indicated that a mixture containing $25wt\%$ AMP and $5wt\%$ PZ can serve as a viable substitute for MEA [38].

ILs represent a novel alternative to conventional amines. These low melting point salts consist of a large organic cation and various anions, offering a wide range of compound properties. ILs can either physically or chemically absorb CO2, depending on pressure conditions. Extensive research and articles have provided significant insights into this technology.

To reduce energy consumption, new-generation solvents such as water-free solvents and biphasic solvents have been proposed. The presence of water in solvents increases the energy demand for regeneration processes. Novel water-free solvents, including non-aqueous organic amine, blends like methanol and ethylene glycol, amino silicones, or amines with a superbase,

have been observed. Researchers have demonstrated that solvent mixtures based on ethylene glycol, employed in the chemisorption process, can achieve CO2 capture efficiencies of up to 95% [39].

DESs, such as choline chloride and ethylene glycol at a 1:2 mole ratio, are gaining attention. These fluids consist of organic halide salts and metal salts or a hydrogen bond donor. DESs share similarities with ILs but are more cost-effective and environmentally friendly. Utilizing DESs can lower the vapor pressure of solvents, reduce corrosion effects, and require less energy in regeneration processes.

The physical absorption method involves using chemically inert solvents to physically absorb $CO_2$. Absorption typically occurs in water or organic absorbers such as methanol or N-methyl-2-pyrrolidone. This method yields optimal results for low-pressure applications. At elevated temperatures and high pressures of the separated gas, this method is particularly effective for capturing $CO_2$ from the coal gasification process. Within this approach, distinct processes are delineated, each employing specific solvents such as SelexolTM, RectisolTM, IfpexolTM, FluorTM, PurisolTM, SulfinolTM, and MorphysorbTM [40] [41].

### 1.7.2 Adsorption-physical separation:

Adsorption is a process that utilizes a solid surface to extract carbon dioxide from a mixture, employing methods such as adsorption, absorption, and cryogenic separation [41] Physical adsorption involves the use of various porous materials like activated carbon, alumina, metallic oxides, or zeolites to absorb carbon dioxide [42]. Activated carbons, containing amorphous carbon, offer a cost-effective solution with a large surface area that can be modified for enhanced pore structure. However, their weak binding energy with carbon dioxide necessitates a high level of microporosity for effective carbon capture.

Zeolites, crystalline aluminosilicates, possess excellent adsorption properties for $CO_2$ capture, albeit they are hydrophilic. The presence of water diminishes their efficacy by weakening the interactions between bonded compounds. A promising alternative is the use of metal-organic frameworks (MOFs) in adsorption processes. MOFs, comprising metal ions or clusters linked by organic ligands, offer advantages such as design flexibility, ease of synthesis, high

porosity, and customizable pore properties [43].

Silica, another adsorption material, is non-carbonaceous and boasts a large surface area and pore size, ensuring high mechanical stability. Mesoporous silica materials incorporate amine-based substances for $CO_2$ capture. Various methods of adsorption include pressure swing adsorption (PSA), temperature swing adsorption (TSA),vacuum swing adsorption (VSA), and pressure-temperature swing adsorption (PTSA).

### 1.7.3 Membrane separation

The membrane separation process begins by directing the flue gas to an absorber to lower its temperature to the operating temperature required for the membrane. Then, the flue gas is conveyed to the membrane. This technique employs various modules [44], including spiral wound, flat sheet, and hollow fibre configurations.

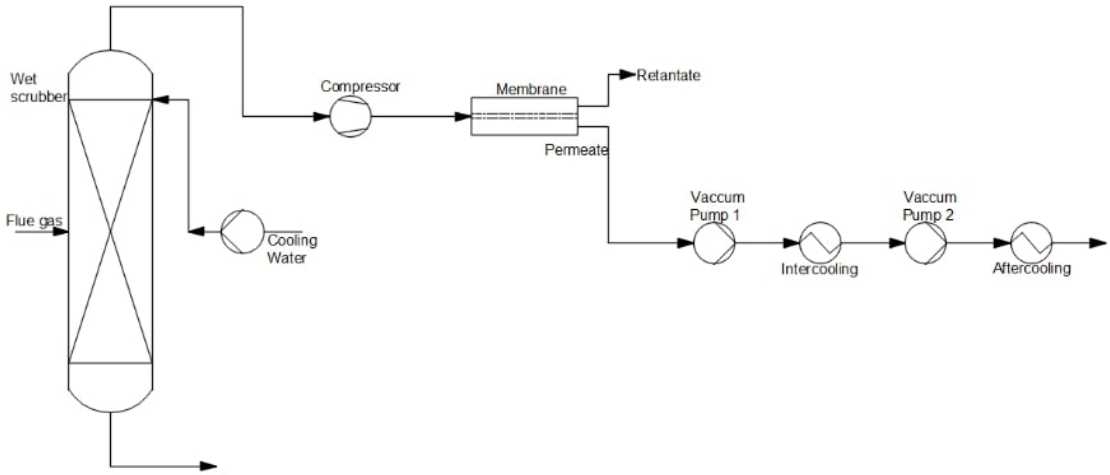


**Figure 1.4:** scheme of the post-combustion $CO_2$ capture method using a membrane separation process.

Two categories of membrane capture technology exist gas separation membranes and gas absorption membranes. In gas separation membranes, the gas containing $CO_2$ is introduced at the high-pressure side, and carbon dioxide is collected at the low-pressure side. Conversely, in the gas absorption system, a solid micro-porous membrane facilitates gas flow and absorption. This system achieves a high $CO_2$ removal rate by minimizing issues such as flooding, foaming, channelling, and entertainment. The underlying principles of both membrane systems are

as follows, Membranes must possess specific properties for effective gas separation, including proper permeability and selectivity [45]. There are three main types of membrane materials: polymeric (organic), ceramic (inorganic), and hybrid membranes. Polymeric membranes are cost-effective to produce, exhibit relatively high gas flux, and maintain mechanical stability. However, they generally have lower selectivity for $CO_2/N_2$, typically below 100 when it's expected to be around 200. Ceramic membranes, particularly those based on zeolites and their derivatives, offer high selectivity but are more challenging to manufacture [45]. Hybrid membranes, which are modifications of inorganic membranes at the surface, combine the advantages of both polymeric and ceramic membranes, offering flexibility, low production costs, and high selectivity.

For post-combustion capture, commercially available polymeric membranes such as PRISM, Polaris, PolyActive, PermSelect, and Medal are commonly utilized. An emerging approach involves the experimental use of metal-organic frameworks (MOFs) in membrane applications. MOFs present advantageous properties for membrane use, including large surface areas, adjustable pore sizes, and controllable pore-surface properties [43].

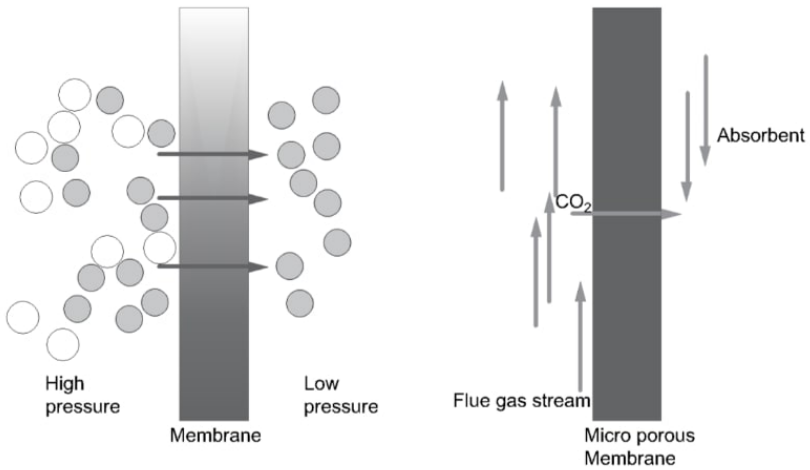


**Figure 1.5:** Principle of Left a gas separation membrane, right a gas absorption membrane

### 1.7.4 Chemical looping combustion CLC and calcium looping process CLP

Chemical looping technology employs two reactors: an air reactor and a fuel reactor, both containing fluidized beds coupled for carrier transport. In the air reactor, metal particles like iron, manganese, or copper undergo oxidation with oxygen from the air, forming metal oxides. These oxides are then transported to the fuel reactor, where they react with the fuel, undergoing reduction during combustion and producing energy along with a flue gas stream rich in $CO_2$ and $H_2O$. This flue gas can be condensed to obtain pure $CO_2$ [46] [47]. A variant of chemical looping is the calcium looping process, which involves a reversible reaction between calcium oxide and carbon dioxide. The initial reaction, carbonation, occurs in the first reactor, forming calcium carbonate. This carbonate is then transferred to the calciner, where the reversible reaction yields a high-purity $CO_2$ stream $(> 95)\%$. Heat for this reaction is generated by burning fuel in an oxygen atmosphere, sometimes categorizing the CLC capture method as a form of oxy-combustion. The reactors, typically circulating fluidized beds (CFB), facilitate solid transport, with cyclones separating solid and gaseous mass streams.

Calcium looping technology offers several advantages, utilizing inexpensive sorbents like lime and partially desulfurizing flue gas. Additionally, the process benefits from mature high-temperature fluidized bed technology [42] [1], which can be employed for power generation.

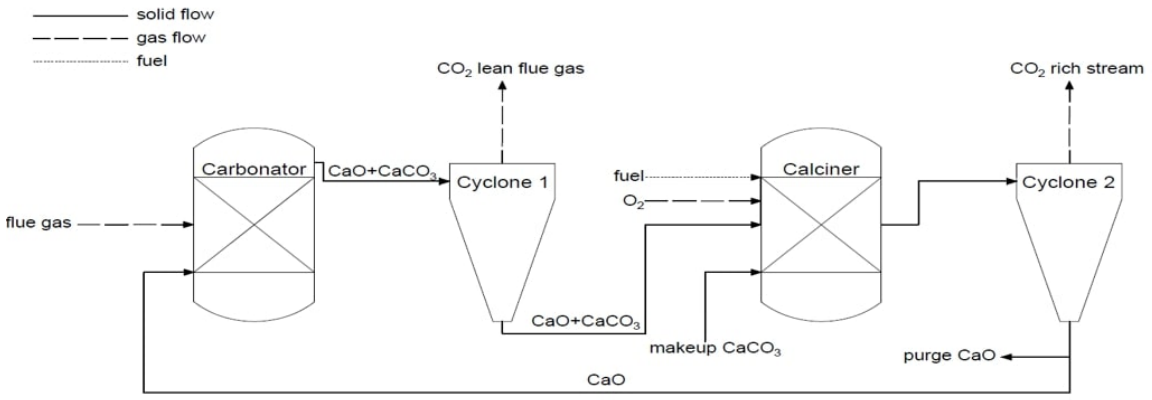


**Figure 1.6:** Scheme of the calcium looping process (brought from [1]).

### 1.7.5 Cryogenic method:

The cryogenic carbon capture technology utilizes liquefied natural gas (LNG) to supply cold energy for $CO_2$ capture. This approach is employed in both oxyfuel combustion and post-combustion carbon capture systems to extract $CO_2$ from flue gas. Cryogenic $CO_2$ capture allows for the production of high-purity $CO_2$, reaching up to $99.17\%$. The process involves compression, expansion, separation, and cooling stages. However, its adoption is limited due to its relatively high operational costs [48]. In post-combustion carbon capture [48] [49], the cryogenic method is implemented through various approaches.

### 1.7.6 Application of absorption-based post-combustion capture method

The absorption-based post-combustion capture method is widely preferred due to its efficiency and relatively lower energy consumption. MEA, and MDEA, and PZ are among the most commonly utilized amine solvents in large-scale industries [50]. Various classified technologies are employed in adsorption, absorption, and membrane separation processes.

conducted an analysis of the challenges and commercial applications of post-combustion carbon capture (PCC) technology, focusing on solvents for absorption, bed configurations for adsorption, and membrane processes. Among adsorption processes, TSA stands out as highly effective compared to PSA and VSA. However, TSA consumes significant energy during regeneration. In chemical absorption, MEA emerges as the preferred solvent for $CO_2$ capture due to its excellent absorption and desorption rates, especially when mixed with other solvents. Nonetheless, solvent absorption processes entail high energy consumption for regeneration, and losses may occur through evaporation and chemical degradation, leading to reduced absorption capacity [29].

Lungkadee et al. conducted simulation analyses of retrofitting a post-combustion capture unit with a 300 MW power plant. Using MEA amine for carbon capture, the absorber and desorbed were designed to achieve $90\%$ $CO_2$ capture capacity with $30wt.\%$ MEA. Another simulation analysis of NGCC power plants utilizing PZ solvent showed improved performance compared to MEA solvent, particularly with $40wt.\%$ PZ solvent, resulting in significant enhancements in capture efficiency [51], energy consumption, and capture cost.

conducted a comparative study of 30 different amine solutions ($30wt.\%$) used for post-combustion carbon capture. Using a solvent screening setup, hexamethylenediamine exhibited the highest $CO_2$ loading of 1.35 [52], while triethanolamine showed the lowest $CO_2$ loading of 0.39 compared to other amines.

| Highlights | | |
|---|---|---|
| Software | Methodology | Efficiency |
| Aspen Plus | The primary objective of the study was to develop efficient methods for capturing $CO_2$ from post-combustion flue gases. The authors proposed novel approaches that integrate $CO_2$ capture with hydrogen production within the same process. [53] By combining these two processes, the overall energy efficiency can be improved. | Efficiency aimed is around $90\%$ |
| Aspen Plus EBSILON® Professional | This comprehensive review focuses on post-combustion $CO_2$ capture technologies specifically applicable to coal-fired power plants. The paper reviews process designs for both chemical absorption and membrane-based separation. Optimization methods include adjusting operational parameters, process modifications, and membrane module types. [36] | $80\%$ and $90\%$ |
| Aspen HYSYS | In this study, the authors simulated the post-combustion $CO_2$ capture process using Aspen Hysys TM software. The focus was on different configurations of the absorption-regeneration process specifically applied to cement flue gases.the authors focused on three alternative configurations: [54] Stripper Split Feed (SSF) Lean Lean Vapor Compressor (LVC) A combination of SSF and LVC. These configurations aim to optimize the absorption-regeneration process | Around $85\%$ |

| | | |
|---|---|---|
| Aspen Plus | Comparison of Absorption, Adsorption, and Membrane Technologies: The absorption process has the best performance in terms of $CO_2$ purity and recovery rate but is the most energy-demanding. [55] The membrane process is the most energy-efficient but has a lower recovery rate and $CO_2$ purity compared to absorption. The adsorption process shows similar performance to the membrane process but requires more energy. Energy Consumption: The membrane process has the lowest energy consumption at 2.88 GJ t $CO_2$ The adsorption process has an energy consumption of 3.25 GJ t $CO_2$ Absorption process has an energy consumption of 3.85 GJ t $CO_2$ | Absorption Process $75\%$ $77\%$ $75.2\%$ |
| Aspen Plus | The methodology in Kazuya Goto, Katsunori Yogo, Takayuki Higashii involves using numerical approaches and simulation tools to evaluate various CCS systems at power plants, considering different types of power generation units, and analyzing the efficiency penalty of coal-fired power plants with CCS. The study also includes the performance evaluation of solid-based and membrane-based $CO_2$ capture systems, aiming to reduce the regeneration energy of scrubbing solvents and develop advanced technologies like solid sorbents and membranes. [56] | Efficiency around $85\%$ |
| Aspen Plus<br>Aspen HYSYS<br>MATLAB | The paper introduces the concept of sequential combustion in steam methane reformers for hydrogen and power production, leading to cost reduction, increased efficiency, and a reduction in the size of the capture plant. [57] The paper discusses the importance of electricity and hydrogen in a zero-carbon economy, the cost-effectiveness of natural gas reforming with carbon capture and storage for low-carbon hydrogen production, a novel technique for reducing costs through integration of carbon capture systems, a commercial-scale demonstration of sequential combustion in an SMR, and the development of an integrated model for power and hydrogen plants with $CO_2$ capture. | $92\%$ |

| | | |
|---|---|---|
| ProTreat® | The main findings mentioned in the paper include: Selection of a $40\%$ wt formulation of PZ (piperazine)/AMP (amino-methyl-propanol) in a 1:2 M ratio as the most representative of the current state of the art for $CO_2$ capture technology. [58] Significant improvement in generation efficiency for power plants using PZ AMP compared to MEA-based processes, resulting in a $27\%$ wt improvement in energy consumption for capture and compression in ultra-supercritical coal-fired power plants and a $16\%$ wt improvement in natural gas combined-cycle plants. Techno-economic analysis results showing the impact of PZ/AMP on the levelized cost of electricity (LCOE) and $CO_2$ avoidance costs for power plants integrated with carbon capture and storage (CCS). | Around $90\%$ |
| Aspen Plus<br>Aspen Plus Dynamics | The methodology involves developing steady-state and dynamic models for an MEA-based $CO_2$ capture process using Aspen software, followed by control studies to evaluate different control approaches. [59] NMPC-based approaches are preferred due to handling nonlinear optimization problems, MPC-based approaches outperform PID-based ones, and balancing fast tracking with robustness is crucial in control system design. | $90\%$ |
| Aspen Plus | focusing on dual-stage membrane systems with a $90\%$ capture ratio. The study evaluated permeate purity, specific energy requirements, specific $CO_2$ emissions. Additionally, economic aspects such as the cost of $CO_2$ captured and avoided, including potential revenues from $CO_2$ valorization through EOR, were assessed. Sensitivity analysis was performed to understand the impact of economic parameter changes on specific costs of $CO_2$ capture and emission avoidance. [60]indicate that dual-stage membrane systems are comparable to chemical absorption methods in terms of efficiency penalties and specific $CO_2$ emission reductions. The membrane configurations were found to be cost-competitive or more cost-effective than conventional amine-based systems. The economic performances of the dual-stage membrane systems were consistent with existing literature, with specific costs of $CO_2$ capture being lower or comparable to previous studies using the same type of polymeric membrane. The study utilized MEMSIC simulation software to evaluate $CO_2$ capture from the exhaust flue gas of a coal-fired power plant, providing valuable insights into the technical and economic feasibility of membrane systems for post-combustion capture. | Nearly $90\%$ |

| | | |
|---|---|---|
| Aspen Plus<br>MATLAB | several key findings: Comparison of pre-and post-combustion $CO_2$ capture processes using chemical absorption technology. Integration of chemical absorption in pre-combustion processes to enhance the quality of syngas in Integrated Gasification Combined Cycle (IGCC) technologies. Analysis of how air/fuel ratios impact syngas composition and low heating value (LHV) in pre-combustion $CO_2$ capture. Evaluation of the energy balance, considering the heat needed for solvent regeneration and energy gain from syngas treatment. Emphasis on the significance of $CO_2$ capture efficiency, L/G ratio, and $CO_2$ flow in both pre and post-combustion scenarios. Discussion on the potential economic implications of employing chemical absorption for $CO_2$ mitigation in power plants. These findings contribute to understanding the efficiency and feasibility of utilizing chemical absorption for $CO_2$ capture in different combustion processes, highlighting its potential benefits for enhancing energy production and reducing carbon emissions. [61] | $90\%$ |

**Table 1.2:** of post-combustion.

## 1.8 Oxy-combustion $CO_2$ capture

In oxy-combustion, exhaust gases from combustion in an oxygen-enriched atmosphere primarily consist of carbon dioxide and water vapor, with minimal nitrogen content. Condensation of water vapor enables $CO_2$ separation, typically at temperatures higher than ambient conditions, except during the condensation process at very low partial pressures. Oxygen for combustion is generated via the air separation process, providing oxygen purity of around $95\%$ Oxy-combustion technology finds application primarily in solid fuel-fired boilers like pulverized coal boilers (PCs) or circulating fluidized bed boilers (CFBs), with increasing consideration for integration into energy systems with gas turbines. Two types of oxy-combustion boilers are distinguished: low temperature and high-temperature boilers. Low-temperature boilers involve combustion in oxygen mixed with recirculated exhaust gases, resulting in flame temperatures similar to those in air-powered units. In contrast, high-temperature boilers can reach temperatures exceeding $2400\,^{\circ}\mathrm{C}$.

The advantages of oxy-combustion include reduction in nitrogen oxide (NOx) emissions, smaller boiler dimensions, simplified $CO_2$ capture compared to other methods, applicability in existing technologies, and lower mass flow rate of exhaust gases (approximately $75\%$ less compared to air combustion). However, oxy-combustion has its drawbacks, including high material requirements due to elevated temperatures, reduced efficiency (as the oxygen production process consumes energy), and high capital costs [37].

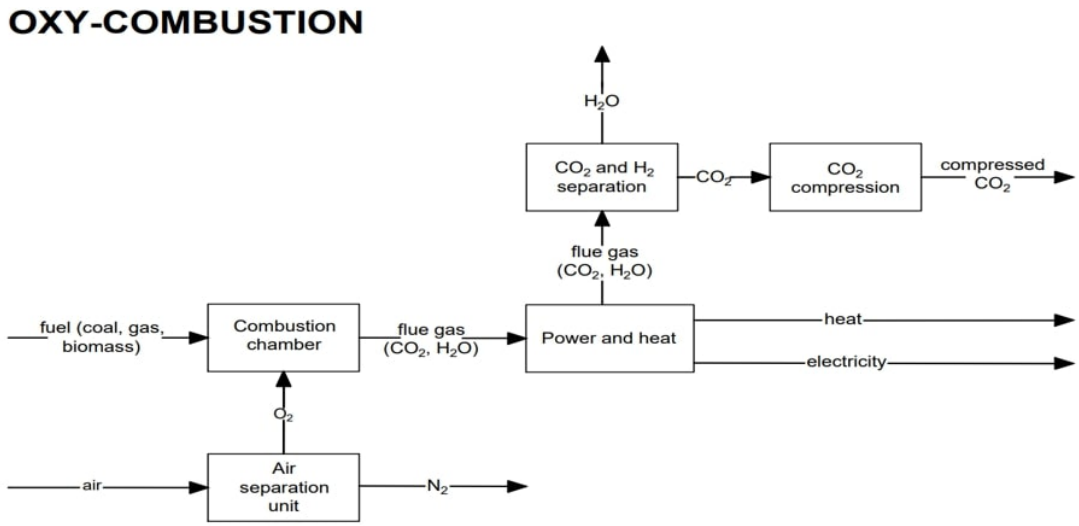


**Figure 1.7:** Diagram of electricity generation heat production with oxy-combustion $CO_2$ capture.

Oxy-combustion methods are primarily implemented at laboratory and pilot scales, with notable installations including the Callide Power Station and Compostilla Thermal Power. At the Callide Power Station, a 30 MWe experimental unit commenced operation in 2012, supplied with a nominal flow of $98\%$ pure oxygen at 19,200 $\mathrm{m}^3/\mathrm{h}$ to the boiler. Various fuel types, such as Callide coal and Minerva coal, were investigated, resulting in a daily $CO_2$ production of 75 tons via cryogenic capture technology. The unit concluded its operations after a successful demonstration in 2016 [62]. Similarly, the OXYCFB 300 project at Compostilla Thermal Power involved the development of a pilot power plant unit with $CO_2$ capture based on oxy-combustion technology. Equipped with a circulating fluidized bed boiler and a pulverized coal-fired boiler, the installation had a thermal power capacity of 30 MWth and 20 MWth respectively, handling a flue gas stream of 800 $\mathrm{m}^3/\mathrm{h}$ The cryogenic method facilitated a daily $CO_2$ separation capacity of 3–5 tons [63].

Oxy-combustion technology extends beyond solid-fueled units to systems equipped with gas turbines, as demonstrated in the Negative $CO_2$ Emission Gas Power Plant project. This concept combines oxy-combustion with $CO_2$ capture from flue gas, potentially achieving negative emission levels by utilizing $CO_2$-neutral fuel like sewage sludge. The use of a prototype spray-ejector condenser (SEC) aids in the $CO_2$ capture process by condensing water vapour from exhaust gases.

Unlike other $CO_2$ capture technologies, oxy-combustion carbon capture requires minimal process modifications. By using oxygen for combustion instead of air, the nitrogen content in flue gas is eliminated, leaving behind primarily carbon dioxide and water vapour. This reduces energy consumption for $CO_2$ separation. The air separation unit (ASU), responsible for oxygen extraction from air, constitutes the most energy-intensive part of the oxyfuel combustion process.

To enhance efficiency and $CO_2$ capture, oxyfuel combustion carbon capture is integrated with moderate and intense low-oxygen dilution (MILD). This approach, known as MILD oxy-combustion carbon capture (MOFC), offers multiple benefits, including improved plant efficiency, enhanced $CO_2$ purity, and reduced energy consumption. Notably, oxy-fuel combustion CCS technology utilized in the Allam cycle achieves higher efficiencies compared to combined cycle power plants with carbon capture units. The Allam cycle incorporates heat generated from the ASU to heat $CO_2$, which is then recycled to the combustion chamber, enhancing cycle efficiency [64].

| Highlights | | |
|---|---|---|
| Software | Methodology | Efficiency |
| COMSOL Multiphysics<br>Aspen Plus<br>Aspen HYSYS | Oxy-fuel combustion involves burning fuel using an oxidizer mixture of pure oxygen and recycled exhaust gases (mainly $CO_2$). The absence of nitrogen in the oxidizer reduces the volume of flue gas, simplifying $CO_2$ capture. Oxy-fuel combustion technology can be applied with slight modifications to existing power plants or new power plants. [65] It is particularly relevant for carbon capture due to its compatibility with existing infrastructure. | around 90% |
| Aspen Plus<br>COMSOL Multiphysics<br>ANSYS Fluent<br>MATLAB | Oxygen Carrier Selection: Identify suitable solid materials (e.g., metal oxides) that can release oxygen during combustion. Fuel Reactor Design: Develop a reactor system where fuel reacts with the oxygen carrier.Oxygen Carrier Regeneration: Separate the oxygen carrier from the flue gas and regenerate it by supplying air or pure oxygen. [66] Integration with Power Plants: Evaluate how CLC can be integrated into existing or new power plants. | ranging from 80% to over 90% |
| ANSYS Fluent<br>CONVERGE CFD<br>OpenFOAM<br>AVL FIRE | In oxy-combustion, pure oxygen or oxygen-enriched air replaces regular air for combustion. The resulting flue gas primarily consists of $CO_2$ and water vapor due to the absence of nitrogen. [67] The captured $CO_2$ may require purification and compression for transportation and storage. It can be stored in geological formations (carbon capture and storage, CCS) or utilized in industrial processes like enhanced oil recovery or chemical production. | 90% |
| Aspen Plus Aspen HYSYS<br>gPROMS | CCUS methods aim to capture $CO_2$ from large industrial sources. This research area is crucial due to socio-economic challenges and the rising fees related to $CO_2$ emissions in the European Union. Improve the efficiency of energy conversion processes. Reduce energy demand. [37] Utilize renewable energy sources (hydropower, wind, biomass, solar cells, nuclear power). Increase green hydrogen usage produced from water electrolysis using renewable energy. | 90% |

| | | |
|---|---|---|
| Aspen plus<br>Aspen HYSYS<br>ChemCAD<br>SimSci PRO/II<br>gPROMS PR EOS in gPROMS | The heart of oxy-fuel $CO_2$ capture systems is the compression and purification unit. The authors delve into the design, operation, and challenges associated with this critical component. [68] They explore various technologies for compressing and purifying $CO_2$ -rich flue gases. The methodology considers the integration of oxy-fuel $CO_2$ capture with existing energy systems. It explores how these technologies can be seamlessly incorporated into power plants and industrial processes. These analyses help evaluate the feasibility and performance of compression and purification units. | ranging from $90\%$ to $95\%$ |
| Aspen Plus<br>Aspen HYSYS<br>gPROMS | The methodology likely involves CFD modelling to simulate oxy-coal combustion processes. CFD allows for detailed analysis of flow patterns, temperature distribution, and species transport. [69] The methodology may include modelling radiative heat transfer within the combustion chamber. Understanding radiation effects is crucial for accurate predictions. The methodology may involve the validation of models using experimental data. | ranging from $80\%$ $83\%$ |
| CFD | Oxy-fuel combustion involves using a combination of oxygen (with purity $> 95\%$) and recycled flue gas (RFG) as the oxidant for coal combustion. [70] The resulting gas mainly consists of $CO_2$ and water vapor. After purification and compression, the $CO_2$ is ready for storage. | Nearly $90\%$ |
| FACTSage 6.0. | Oxygen combustion leads to higher temperatures compared to conventional air combustion. [71] Fuel properties and heat exchanger limitations necessitate temperature moderation. Recycled flue gas helps achieve this moderation. | above $90\%$ |
| Aspen plus | Based on hot gas clean-up, membrane-enhanced $CO_2$ conversion, and direct $CO_2$ condensation. [72] Utilizes hot gas clean-up, oxygen membranes, and calcination-carbonation loops. Technically challenging but energetically favourable. All selected IGCC concepts can realize $CO_2$ capture rates up to $99\%$. | $96\%$ |
| Aspen HYSYS | assess the feasibility and efficiency of various carbon capture approaches in the context of Integrated Gasification Combined Cycle (IGCC) plants. It focuses on oxy-fuel combustion, pre-combustion, and post-combustion capture technologies. Technically challenging but energetically favourable. [73] | ranging from $65\%$ $95\%$ |

**Table 1.3:** of oxy-combustion.

## 1.9 Advantages and Limitations of Each Technology

### 1.9.1 Advantages and Limitations of Pre-Combustion Technology

| | |
|---|---|
| • Efficiency Enhancement: Pre-combustion capture improves the overall efficiency of natural gas power plants by capturing $CO_2$ before combustion.<br>• Hydrogen Production: The process involves producing hydrogen $(H_2)$ from natural gas, which can be used as a clean fuel.<br>• Integration with Existing Plants: Pre-combustion capture can be integrated into existing natural gas power plants, minimizing the need for major modifications. [22] | • Costs: Implementing pre-combustion capture may incur additional capital costs due to equipment and process modifications.<br>• Gas Turbine Redesign: Using $H_2$ as the primary fuel in gas turbines requires redesigning components, which can be challenging for commercial deployment.<br>• State-of-the-Art Technology: To achieve significant advantages over benchmark technologies like MEA absorption, better membrane permeability and lower costs are needed. [22] |
| • Comprehensive Analysis: The study conducts a thorough techno-economic analysis of a biomass-based combined power plant integrated with post-combustion $CO_2$ capture. It considers both technical feasibility and economic viability.<br>• Carbon Reduction: The captured $CO_2$ surpasses emissions from the entire energy system, contributing to overall carbon reduction.<br>• Efficiency Considerations: The study calculates the artificial thermal efficiency of the system and explores how efficiency changes with carbon capture efficiency, aiding informed decision-making. [23] | • Specific Biomass-Based Plant: The study focuses on a particular biomass-based combined power plant.<br>• Generalization Challenges: Generalizing the findings to other plant configurations or feedstocks may require additional investigations. Economic Considerations: The techno-economic analysis is valuable, but actual economic feasibility depends on factors like membrane costs, installation, and maintenance. Balancing performance with cost-effectiveness is crucial. Additionally, the degree of $CO_2$ capture should align with overall plant performance, and beyond a certain value, $CO_2$ capture efficiency becomes flexible for a net- $CO_2$ negative emission plant. [23] |

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| • Deep Eutectic Solvents (DESs): The study focuses on DESs as potential candidates for $CO_2$ capture. DESs offer advantages like low volatility, tunability, and environmental friendliness.<br>• Promising Mixtures: The study screens out mixtures of allyl triphenylphosphonium bromide (ATPPB) and diethylene glycol (DEG) due to their high $CO_2$ solubility, showing promise for efficient $CO_2$ capture.<br>• Comprehensive Analysis: By adopting a rate-based modeling approach, the research identifies crucial solvent characteristics in the $CO_2$ capture process. It analyzes how these characteristics impact the total cost of $CO_2$ separation, considering both technical and economic aspects. [24] | • Mass Transfer Correlations: The choice of mass transfer correlations impacts estimated process costs. The Selexol process remains more economical when using the Hanley and Chen correlations, where liquid viscosity strongly affects mass transfer.<br>• Specific Findings: The study's findings pertain to the studied DESs and the Selexol process. Generalizing these results to other systems or feedstocks requires further investigation.<br>• Economic Considerations and Membrane Stability: While the study analyzes the economic feasibility of DESs, actual costs depend on factors like membrane materials, fabrication, and installation. Balancing performance with cost-effectiveness and ensuring long-term membrane stability are crucial aspects. [24] |
| • Deep Eutectic Solvents (DESs): The research investigates DESs as potential solvents for $CO_2$ capture. DESs offer advantages like low volatility, tunability, and environmental friendliness.<br>• NGCC Integration: The study focuses on integrating the $CO_2$ capture process into a natural gas combined cycle (NGCC) power plant. NGCC plants are widely used for efficient power generation.<br>• Techno-Economic Analysis: The research provides a detailed techno-economic analysis of pre-combustion $CO_2$ capture integrated into NGCC power plants. By considering technical feasibility and economic viability, it offers valuable insights for practical implementation. [25] | • Off-Design Challenges: Achieving optimal performance during off-design conditions (such as load variations) can be challenging. Dynamic behavior and transient effects need further consideration.<br>• Specific to NGCC Plants: The findings are specific to natural gas combined cycle (NGCC) power plants.<br>• Cost Considerations: While the study analyzes the economic feasibility of deep eutectic solvents (DESs), actual costs depend on factors like membrane materials, fabrication, and installation. Balancing performance with cost-effectiveness is essential. [25] |

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| • Efficiency Enhancement: Optimization techniques are applied to improve overall efficiency and cost-effectiveness. Real-world behavior and performance are considered during this optimization process.<br>• Application Context: The research focuses on practical implementation of DESs in $CO_2$ capture processes. [26] | • Off-Design Challenges: Achieving optimal performance during off-design conditions (such as load variations) can be challenging. Dynamic behavior and transient effects need further consideration.<br>• Specific to Pre-Combustion $CO_2$ Capture: The findings are specific to the pre-combustion $CO_2$ capture process.<br>• Generalization Considerations: Extrapolating the results to other types of capture processes or different feedstocks may necessitate additional investigations. [26] |
| • Plant Layouts and Assessments: The study examines plant layouts proposed in literature for both natural gas and coal power plants. It includes heat and mass balances, as well as economic assessments for these layouts.<br>• Pre-Combustion $CO_2$ Capture: The research discusses different sections within a power plant with pre-combustion $CO_2$ capture. It presents available technologies and their advantages, focusing on the decarbonization route for electricity production.<br>• Application to Natural Gas and Coal: The study covers pre-combustion technologies applied to natural gas and coal, recognizing their significance as global sources of electricity. [17] | • Research Focus: Research on pre-combustion decarbonization has primarily centered around coal rather than natural gas.<br>• Challenges for Natural Gas: Natural gas-based plants encounter complexity and cost challenges, making them less competitive compared to post-combustion $CO_2$ capture.<br>• Industry Applications: The study briefly discusses pre-combustion $CO_2$ capture in industry, particularly projects involving $CO_2$ storage or enhanced oil recovery (EOR). [17] |
| • Fuel Sources: The paper considers both natural gas and coal as fuel sources for thermal power plants.<br>• Capture Method Applicability: It highlights the applicability of different capture methods to these fuels.<br>• Technical and Economic Aspects: The paper discusses the technical and economic aspects of each capture method, providing valuable information for decision-making in power plant design and operation. Additionally, it provides an overview of pre-combustion technologies for $CO_2$ capture in thermal power plants, covering various methods to help readers understand different approaches. [27] | • Plant-Specific Variability: Limitations can vary based on specific plant configurations and operational conditions.<br>• Engineering Assessments and Economic Factors: Real-world applications necessitate detailed engineering assessments. The actual costs depend on factors like materials, installation, and operation, emphasizing the importance of balancing performance with cost-effectiveness. [27]<br>• Scope and Generalization: The findings are specific to thermal power plants using natural gas or coal. Extrapolating these results to other types of power plants may require additional investigations. |

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| • The Enhanced Capture of $CO_2$ (ENCAP) project, funded by the European Commission, aims to develop technologies for capturing at least $90\%$ of $CO_2$ emissions and reducing capture costs by $50\%$. The project involves collaboration among leading European power industries, equipment suppliers, research institutes, and universities.<br>• The study focuses on technical and economic aspects related to pre-combustion $CO_2$ capture and oxy-fuel technologies for power generation. It provides valuable information for decision-making in designing and operating power plants. [28] | • Pre-combustion $CO_2$ capture and oxy-fuel processes are the focus of the findings.<br>• Extrapolating these results to other carbon capture methods or different fuel sources may necessitate further investigations.<br>• The study highlights the need for additional research to understand the applicability of these findings beyond the specific processes mentioned. [28] |
| • High Efficiency: The calcium looping process demonstrates high efficiency in capturing $CO_2$ from fuel gas mixtures before combustion.<br>• Stability: The method is stable, ensuring consistent performance over time.<br>• High-Purity $H_2$ Production: Calcium looping enables the production of high-purity hydrogen ($H_2$), which is valuable for various applications. [21] | • Capital Costs: Implementing calcium looping may involve higher capital costs due to the need for specialized equipment and materials.<br>• Complexity: The process requires careful design and operation, considering multiple interacting components.<br>• Energy Consumption: While efficient, calcium looping still consumes energy during the capture and regeneration cycles. [21] |
| • Important Carbon Capture Technology: Pre-combustion capture is crucial for mitigating global warming. It aims to capture $CO_2$ before combustion occurs.<br>• Review of Physical Solvents: The study explores physical solvents for pre-combustion capture using physical absorption, enhancing efficiency.<br>• Solubility Models: The research examines various solubility models for predicting $CO_2$ solubility, aiding in process design. [29] | • Energy and Environment Challenges: While post-combustion capture is established, it has energy and environment-related issues. Pre-combustion capture aims to address these drawbacks.<br>• Ionic Liquids (ILs): Incorporating ILs in pre-combustion capture has gained attention. However, challenges remain in terms of research gaps and modeling approaches. [29] |

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| • Important Carbon Capture Technology: Pre-combustion capture is a crucial technology for mitigating global warming. It aims to capture $CO_2$ before combustion occurs.<br>• Physical Solvents: The review explores physical solvents for pre-combustion capture using physical absorption, which can enhance efficiency.<br>• Solubility Models: The study examines various solubility models for predicting $CO_2$ solubility, aiding in process design. [20] | • Energy and Environment Challenges: While post-combustion capture is established, it has energy and environment-related issues. Pre-combustion capture aims to address these drawbacks.<br>• Ionic Liquids (ILs): Incorporating ILs in pre-combustion capture has gained attention. However, challenges remain in terms of research gaps and modeling approaches. [20] |
| • High Efficiency: Pre-combustion capture is generally more efficient compared to post-combustion methods.<br>• High $CO_2$ Concentration: The shifted synthesis gas stream in pre-combustion capture is rich in $CO_2$, making it easier to remove before hydrogen combustion.<br>• Proven Technology: ELCOGAS's pilot plant uses commercially available technology, ensuring feasibility and reliability. [30] | • Higher Capital Costs: The base gasification process for pre-combustion capture can be more expensive than traditional pulverized coal power plants.<br>• Safety Concerns: Storing captured $CO_2$ may pose risks due to potential leakages and environmental contamination.<br>• Unproven Deep Ocean Storage: Deep Ocean storage remains untested, and its effectiveness is uncertain. • Microbial Breakdown: In basal formation storage, microbes in volcanic rocks might break down carbonates to methane. [30] |
| • High $CO_2$ Capacity: The HBGS process exhibits a high capacity for capturing $CO_2$ from fuel gas mixtures, making it an effective option for pre-combustion capture.<br>• Water as a Solvent: The use of water as a solvent in the HBGS process is advantageous. Water is abundant, cost-effective, and environmentally friendly, contributing to the overall feasibility of $CO_2$ capture. [31] | • Thermodynamic and Kinetic Factors: A thorough assessment of the thermodynamic and kinetic factors is essential for the successful implementation of the HBGS process. These factors impact the efficiency and effectiveness of $CO_2$ capture.<br>• Economic Considerations: While the HBGS process has advantages, economic feasibility remains a challenge. Balancing the costs associated with implementation, operation, and maintenance is crucial. [31] |

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| • Membrane gas separation is a potential solution for capturing $CO_2$ from coal gasification processes. By selectively separating $CO_2$, it contributes to reducing greenhouse gas emissions.<br>• The study focuses on integrating membrane gas separation into an integrated gasification combined cycle (IGCC) process, allowing for efficient $CO_2$ capture within the overall power generation system. Additionally, $H_2$ -selective membranes could enhance the efficiency of hydrogen production in pre-combustion. [32] | • Membrane gas separation in real-world gasification processes involves intricate components and interactions. Factors such as membrane performance (permeability and selectivity), stability, and durability under operating conditions are critical. Additionally, economic feasibility is impacted by membrane materials, fabrication, and installation costs.<br>• Achieving high $CO_2$ selectivity may come at the expense of permeability, making it challenging to strike the right balance between selectivity and overall process efficiency. Furthermore, scaling up membrane systems from lab-scale to industrial applications poses significant engineering challenges, emphasizing the importance of ensuring consistent performance and reliability at larger scales. [32] |
| • The methodology considers thermodynamic, economic, and environmental aspects simultaneously, providing a comprehensive view of $CO_2$ capture options.<br>• Decision-makers can make informed choices by assessing trade-offs between efficiency, costs, and environmental impacts. Additionally, the study guides the optimal design of $CO_2$ capture processes within integrated energy conversion systems. [33] | • Modeling approaches inherently involve simplifications and assumptions, impacting the accuracy of results. The validity of these assumptions plays a crucial role.<br>• The availability and reliability of data significantly influence the accuracy of analysis. However, due to the intricate nature of real-world energy systems, the method might not fully capture all complexities, particularly in large-scale industrial applications. [33] |
| • High Efficiency: Pre-combustion capture is generally more efficient compared to post-combustion methods.<br>• High $CO_2$ Concentration: The shifted synthesis gas stream in pre-combustion capture is rich in $CO_2$, making it easier to remove before hydrogen combustion2.<br>• Proven Technology: ELCOGAS's pilot plant uses commercially available technology, ensuring feasibility and reliability. [34] | • Higher Capital Costs: The base gasification process for pre-combustion capture can be more expensive than traditional pulverized coal power plants.<br>• Safety Concerns: Storing captured $CO_2$ may pose risks due to potential leakages and environmental contamination.<br>• Unproven Deep Ocean Storage: Deep Ocean storage remains untested, and its effectiveness is uncertain.<br>• Microbial Breakdown: In basal formation storage, volcanic rock microbes might break carbonates into methane. [34] |

**Table 1.4:** Advantages and Limitations of Pre-Combustion

### 1.9.2 Advantages and Limitations of Post-Combustion Technology

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| • Feasibility of the Hypogen strategies.<br>• Comparable overall cost of the concepts with conventional post-combustion capture process.<br>• Reduction in overall capture cost by using high-pressure $CO_2$ partial pressure with advanced solvents like 2-amino-2-methyl-1-propanol (AMP).<br>• Cost competitiveness of using polymeric membrane for hydrogen production.<br>• Reduction in regeneration energy and overall cost of $CO_2$ avoided with flue gas circulation when using AMP as a solvent.<br>• Potential for further improvement by applying more developed solvents, processes, and membranes. [53] | • Slow reaction kinetics of sterically hindered amines leading to larger absorber size.<br>• High capital investment due to the slow kinetics of AMP solvent.<br>• Need for additional hydrogen purification step when using polymeric membrane for hydrogen production.<br>• Uncertainty in membrane cost estimation.<br>• Slow kinetics of AMP solvent compared to primary amine solvents. [53] |
| • Membrane-based separation technology is a promising competitor to chemical absorption technology due to its lower energy consumption and environmental impact.<br>• Chemical absorption technology is mature, but its energy-intensive nature is driving research towards finding alternatives.<br>• Various optimization methods have been developed for chemical absorption processes to minimize energy consumption and costs.<br>• Membrane materials, such as polymeric membranes, are easier to manufacture, possess better thermal stability, and have lower energy consumption compared to ceramic membranes.<br>• Hybrid systems demonstrate lower efficiency loss compared to MEA-based absorption and cascade membrane systems for $CO_2$ separation degrees below $90\%$. [36] | • Chemical absorption technology, specifically MEA-based process, is energy-intensive and costly, which hinders its implementation in conventional coal-fired power plants.<br>• Membrane-based separation technology is constrained by the properties of current membrane materials, limiting its $CO_2$ capture ability, especially at higher separation degrees.<br>• Practical problems, such as limited compressor or vacuum pump capabilities, hinder the application of membrane-based separation technology in dealing with typical flue gas.<br>• The energetic and economic evaluations of both technologies vary based on different conditions and assumptions, making it challenging to draw universal conclusions. [36] |

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| • Significant regeneration energy savings (around $24\%$) achievable with alternative configurations of the absorption-regeneration process.<br>• Reduction of the condenser cooling energy by $55\%$ with the SSF configuration, $25\%$ with the LVC configuration, and $40\%$ with the combined SSF-LVC configuration.<br>• Energy consumption reduction by the $CO_2$ capture process applied to cement flue gases.<br>• The LVC configuration is highlighted as a good option for efficiently reducing the energy consumption of the $CO_2$ capture process applied to cement flue gases. [54] | • The study does not provide results or analysis on the Stripper Overhead Compression (SOC) configuration or other solvents, indicating a limitation in the scope of the study.<br>• The paper mentions the need for further comparison with the new Acid Gas Package developed by Aspen Hysys, suggesting a potential limitation in the completeness of the current findings.<br>• The study acknowledges the focus on MEA $30\%$ as the solvent and suggests exploring other solvents, indicating a limitation in the generalizability of the results to different solvent types. [54] |
| • The membrane process is the least energy-consuming. • The absorption process exhibits the best performances in terms of $CO_2$ purity and recovery rate.<br>• The adsorption process requires more energy but fulfils the three imposed criteria.<br>• The absorption process is very demanding in terms of energy but exhibits an excellent grade of purity of $CO_2$ and a relatively high efficiency. [55] | • The simulations were limited to a maximum concentration of $30wt\%$ in MEA due to potential corrosion issues beyond that concentration.<br>• The membrane process reaches a lower recovery rate than the other two processes and a significantly smaller $CO_2$ purity than the absorption process.<br>• The absorption process is the most demanding in terms of energy.<br>• The adsorption process requires more energy compared to the membrane process.<br>• The energy consumption of the adsorption process could be reduced if combined TSA and VSA were used. [55] |
| • The advantages mentioned in this paper include:<br>• An approximate $2\%$ efficiency improvement in coal-fired power plants with CCS.<br>• Development of novel solvents for chemical absorption processes.<br>• Improved power plant efficiency through flow sheet modifications.<br>• Reduction of health, safety, and environmental risks associated with CCS. [56] | • The $10\%$ efficiency penalty for coal-fired power plants with CCS.<br>• The need to reduce the regeneration energy of $CO_2$ scrubbing solvents.<br>• Challenges in developing new solvents suitable for high-pressure regeneration.<br>• The potential for advancements in solid sorbents and membrane technologies to reduce the efficiency penalty in $CO_2$ capture. [56] |

| | |
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| • Decarbonization: The technologies contribute to decarbonization efforts by producing low-carbon hydrogen and electricity, which are essential for transitioning to a zero-carbon economy.<br>• Cost-Effectiveness: Natural gas reforming with carbon capture and storage (CCS) is considered a cost-effective option for industrial-scale production of low-carbon hydrogen, laying the foundation for increased use of hydrogen across various sectors.<br>• Increased Efficiency: The integration of gas turbine engines with hydrogen production technologies leads to a significant increase in net power output and efficiency, reducing operating costs.<br>• Flexibility: The design considerations for flexible operation allow for the generation of low-carbon hydrogen independently of low-carbon electricity, providing operational flexibility and potential cost reductions.<br>• Technological Innovation: The study presents new insights into the design and operation of reformers integrated with gas turbines and $CO_2$ capture systems, showcasing technological advancements in the field. [57] | • Significant improvements in efficiency and cost reduction in hydrogen and power production.<br>• Increased power generation with higher efficiency.<br>• Reduction in investment and operation costs associated with the carbon capture system.<br>• Enhanced mass transfer and solvent capacity in the carbon capture process.<br>• Flexibility in operation for low-carbon hydrogen generation independently of low-carbon electricity. [57] |
| • Improved generation efficiency for power plants using PZ/AMP technology compared to MEA solutions.<br>• Energy consumption reduction for capture and compression.<br>• Cost reduction in terms of levelized cost of electricity and $CO_2$ -avoided cost.<br>• Minimal impact on total capital requirement due to improved energy performance.<br>• Enhanced heat integration and lower specific reboiler duty. [58] | • Physical and chemical properties of amines in solution affecting process performance.<br>• Amine costs impacting overall feasibility.<br>• Ecotoxicity and biodegradability requiring assessment for environmental impact.<br>• Waste streams generated from amine degradation in flue gas service.<br>• Additional capital and operational costs of PCC plant implementation. [58] |

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| • Development of advanced model-based controllers like MPC and $H_2$ robust controllers for efficient operation of the $CO_2$ capture process.<br>• Consideration of economic objectives in control system design to optimize operating costs.<br>• Superior performance of MPC-based approaches compared to PID-based ones in maintaining $CO_2$ capture rate and temperature control. [59] | • Computational expense of NMPC compared to LMPC.<br>• Uncertainties in the process due to factors like changing flue gas composition, solvent degradation, and measurement noise.<br>• Energy penalty for $CO_2$ removal impacting power plant efficiency in MEA-based CO2 capture processes.<br>• Assumptions made in modeling, such as equilibrium assumptions and uncertainties in $CO_2$ absorber performance. [59] |
| • Membrane technology being competitive and attractive for reducing $CO_2$ capture costs and footprint.<br>• Development of low-cost, durable membranes with improved permeability and selectivity.<br>• Potential for membrane systems to be economically competitive compared to amine absorption processes for $CO_2$ capture, especially for geological storage. [60] | • The paper highlights uncertainties in membrane thickness at an industrial scale, the ageing effects of membrane modules, the impact of minor components on the membrane separation performance, and economic assumptions affecting cost estimations. It also discusses the energy analysis of membrane systems, the effects of membrane integration within power plants, and the economic implications of $CO_2$ capture at different purity levels.<br>• The study compares single- and dual-stage membrane system concepts, evaluating their energy and economic performances for $CO_2$ capture from flue gases of a coal-fired power plant. [60] |
| • The advantages of using chemical absorption with amines for post-combustion $CO_2$ capture, as discussed in the document, include high efficiency, mature technology, and low cost compared to other methods. The use of amine-based solvents in the chemical absorption process allows for fast $CO_2$ absorption/desorption rates, high $CO_2$ capacity, low degradation rate, low viscosity, and low amine volatility.<br>• the energy consumption in the process is mainly dependent on the desorption process, making it essential to reduce the energy penalty of $CO_2$ desorption. [61] | • The limitations mentioned in the document regarding the use of chemical absorption with amines for post-combustion $CO_2$ capture include:<br>• Low carbon dioxide capture capacity per unit absorbent.<br>• Amine degradation is caused by components in flue gas like $SO_2$, NOX, and oxygen, leading to a high absorbent makeup rate.<br>• High equipment corrosion rate.<br>• High energy consumption for solvent regeneration. [61] |

**Table 1.5:** Advantages and Limitations of Post-Combustion

### 1.9.3 Advantages and Limitations of Oxy Combustion technology

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| • Oxy-fuel combustion inherently produces a flue gas rich in $CO_2$, making it suitable for carbon capture. • The concentrated $CO_2$ stream simplifies subsequent capture processes.<br>• The absence of nitrogen reduces energy losses associated with nitrogen separation.<br>• Oxy-fuel combustion can enhance overall thermal efficiency in power plants.<br>• Oxy-fuel combustion can be applied with slight modifications to existing power plants or new ones.<br>• It is particularly relevant for retrofitting existing infrastructure. [65] | • Providing pure oxygen can be energy-intensive and costly. • Ensuring a reliable and efficient oxygen supply is essential.<br>• High oxygen concentrations may cause corrosion in equipment.<br>• Proper material selection and design are critical.<br>• Ensuring stable combustion under varying conditions is challenging.<br>• Flame stability and control mechanisms need careful attention. [65] |
| • CLC inherently produces a flue gas rich in $CO_2$, making it suitable for carbon capture. • The concentrated $CO_2$ stream simplifies subsequent capture processes.<br>• The absence of nitrogen reduces energy losses associated with nitrogen separation.<br>• CLC can enhance overall thermal efficiency in power plants. • CLC can be applied with slight modifications to existing power plants or new ones.<br>• It is particularly relevant for retrofitting existing infrastructure. [66] | • Providing pure oxygen can be energy-intensive and costly.<br>• Ensuring a reliable and efficient oxygen supply is essential.<br>• High oxygen concentrations may cause corrosion in equipment.<br>• Proper material selection and design are critical.<br>• Ensuring stable combustion under varying conditions is challenging.<br>• Flame stability and control mechanisms need careful attention. [66] |
| • Oxy-fuel combustion inherently produces a flue gas rich in $CO_2$, making it suitable for carbon capture.<br>• The concentrated $CO_2$ stream simplifies subsequent capture processes.<br>• The absence of nitrogen reduces energy losses associated with nitrogen separation.<br>• Oxy-fuel combustion can enhance overall thermal efficiency in internal combustion (IC) engines.<br>• Oxy-fuel combustion can be applied with slight modifications to existing IC engines or new ones.<br>• It is particularly relevant for retrofitting existing infrastructure. [67] | • Ensuring a reliable and efficient oxygen supply is essential.<br>• High oxygen concentrations may cause corrosion in engine components.<br>• Proper material selection and design are critical.<br>• Ensuring stable combustion under varying conditions is challenging.<br>• Flame stability and control mechanisms need careful attention. [67] |

| | |
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| • Oxy-fuel combustion results in flue gas streams with a higher $CO_2$ concentration compared to conventional air combustion.<br>• Oxy-fuel $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs.<br>• The paper likely discusses how compression and purification units can be optimized to minimize energy penalties during $CO_2$ capture.<br>• Efficient design can lead to lower energy consumption for $CO_2$ compression. [37] | • Implementing oxy-fuel combustion and $CO_2$ capture involves significant capital and operational costs.<br>• The authors may discuss the economic challenges associated with large-scale deployment.<br>• Suitable long-term storage sites for captured $CO_2$ are essential.<br>• Identifying and securing these sites can be a limitation.<br>• Compliance with applicable environmental legislation is crucial.<br>• Stricter regulations may impact the feasibility of oxy-fuel $CO_2$ capture. [37] |
| • Oxy-fuel combustion results in flue gas streams with a higher $CO_2$ concentration compared to conventional air combustion.<br>• This facilitates more efficient $CO_2$ capture.<br>• Efficient design can lead to lower energy consumption for $CO_2$ compression.<br>• Oxy-fuel $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs. [68] | • Implementing oxy-fuel combustion and $CO_2$ capture involves significant capital and operational costs.<br>• The authors may discuss the economic challenges associated with large-scale deployment.<br>• Identifying and securing these sites can be a limitation.<br>• Stricter regulations may impact the feasibility of oxy-fuel $CO_2$ capture. [68] |
| • Oxy-coal combustion results in flue gas streams with a higher $CO_2$ concentration compared to conventional air combustion.<br>• This facilitates more efficient $CO_2$ capture.<br>• Oxy-coal $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs. [69] | • Suitable long-term storage sites for captured $CO_2$ are essential.<br>• Identifying and securing these sites can be a limitation.<br>• Implementing oxy-coal combustion and $CO_2$ capture involves significant capital and operational costs.<br>• The authors may discuss the economic challenges associated with large-scale deployment. [69] |

| | |
|---|---|
| • Oxy-fuel $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs.<br>• discusses how compression and purification units can be optimized to minimize energy penalties during $CO_2$ capture.<br>• Efficient design can lead to lower energy consumption for $CO_2$ compression. [70] | • Compliance with applicable environmental legislation is crucial.<br>• Stricter regulations may impact the feasibility of oxy-fuel $CO_2$ capture.<br>• Implementing oxy-fuel combustion and $CO_2$ capture involves significant capital and operational costs.<br>• The authors may discuss the economic challenges associated with large-scale deployment.<br>• Suitable long-term storage sites for captured $CO_2$ are essential. [70] |
| • Higher $CO_2$ concentration due to oxy-fuel combustion. • Integration with existing infrastructure.<br>• Reduced energy penalties with optimized compression units. [71] | • High costs associated with cryogenic air separation.<br>• Availability of suitable $CO_2$ storage sites.<br>• Environmental regulations and corrosion risks. [71] |
| • Oxy-fuel $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs.<br>• Oxy-fuel combustion results in flue gas streams with a higher $CO_2$ concentration compared to conventional air combustion.<br>• This facilitates more efficient $CO_2$ capture. [72] | • Compliance with applicable environmental legislation is crucial.<br>• Stricter regulations may impact the feasibility of oxy-fuel $CO_2$ capture.<br>• Implementing oxy-fuel combustion and $CO_2$ capture involves significant capital and operational costs.<br>• The authors may discuss the economic challenges associated with large-scale deployment. [72] |
| • Oxy-fuel combustion results in flue gas streams with a higher $CO_2$ concentration compared to conventional air combustion.<br>• This facilitates more efficient $CO_2$ capture.<br>• Oxy-fuel $CO_2$ capture can be integrated into existing power plants and industrial processes without major modifications.<br>• Utilizing the same infrastructure reduces implementation costs. [73] | • Compliance with applicable environmental legislation is crucial.<br>• Stricter regulations may impact the feasibility of oxy-fuel $CO_2$ capture.<br>• Suitable long-term storage sites for captured $CO_2$ are essential.<br>• Identifying and securing these sites can be a limitation. [73] |

**Table 1.6:** Advantages and Limitations of Oxy-Combustion

# 2

# The Thermodynamic Properties Of CO2 Mixtures

# 2.1 Introduction

Understanding the thermodynamic properties of $CO_2$ mixtures is essential for optimizing CCS systems, which aim to reduce $CO_2$ emissions from industrial sources such as coal-fired power plants. Accurate predictions of properties like VLE are key to designing effective $CO_2$ purification processes and ensuring efficient and safe $CO_2$ transport. [74] Here's a detailed look at how these properties and various factors CCS systems:

## 2.1.1 Importance of Thermodynamic Properties

### A) Vapour-Liquid Equilibrium VLE

Design of Purification Processes: VLE data is crucial for understanding the separation of $CO_2$ and other gases during capture. Accurate VLE information aids in designing efficient purification processes, ensuring the captured $CO_2$ meets the required purity standards for transportation and storage. [74]

Operational Efficiency: Knowledge of VLE allows better control of operating conditions in $CO_2$ capture units, enhancing separation efficiency and reducing energy consumption.

### B) High-Density $CO_2$ Transportation

Avoiding Two-Phase Flow: To ensure cost-effective and safe transportation, $CO_2$ should be transported in a high-density, single-phase state. Accurate thermodynamic data helps set the appropriate transportation conditions (pressure and temperature) to prevent two-phase flow, which can cause operational issues and increase energy costs. Pipeline Design: Reliable data on $CO_2$ mixtures' properties is essential for designing pipelines and other transportation infrastructure to handle high-density $CO_2$, minimizing risks and ensuring safety. [75]

## 2.2 Experimental Data and Theoretical Models

### 2.2.1 Challenges with Experimental Data

**Range of Conditions:** CCS processes operate across a wide range of pressures and temperatures, including supercritical conditions, making it challenging to collect comprehensive experimental data.

**Multi-Component Mixtures:** $CO_2$ mixtures from flue gases contain various impurities (e.g., $CH_4$, $H_2$S), complicating the experimental determination of their thermodynamic properties.

### 2.2.2 Theoretical Models

**Equation of State Equation of State (EOS):** Models such as Peng-Robinson Peng-Robinson (PR) and Redlich-Kwong-Soave Soave-Redlich-Kwong (SRK) EOS are used to predict the properties of $CO_2$ mixtures. These models offer a mathematical framework for estimating VLE and other properties under various conditions. [76] **Model Limitations:** The accuracy of different models varies depending on the specific properties, components, and conditions. For instance, PR and SRK models have been tested for binary $CO_2$ mixtures with components like $CH_4$ and $H_2S$, but comprehensive evaluations for broader applications are limited.

## 2.3 Implications for CCS System Design and Operation

### 2.3.1 Defining $CO_2$ Purity Guidelines

**Technical and Safety Requirements:** Understanding the thermodynamic properties of CO2 mixtures helps establish precise guidelines for $CO_2$ purity, considering technical feasibility, safety, and environmental impacts.

**Economic Optimization:** Accurate thermodynamic data enables the optimization of capture and transportation processes, reducing costs and improving efficiency.

### 2.3.2 Development of New Technologies

**Innovation in Capture Systems:** Advances in understanding $CO_2$ mixtures can drive the development of new capture technologies, enhancing the overall performance of CCS systems.

**Handling Impurities:** Better knowledge of how impurities affect $CO_2$ mixtures can lead to improved purification methods and more robust transportation systems.

## 2.4 Necessary Thermodynamic Properties and Potential Operation

### 2.4.1 Conditions of CCS:

The necessary thermodynamic properties and potential operation conditions of CCS systems play a crucial role in the design, optimization, and operation of processes related to capturing, transporting, and storing $CO_2$ emissions. [77]

| | Phase equilibrium | Volume | Enthalpy | Entropy |
|---|---|---|---|---|
| *Capture* | | | | |
| Compression | √ | √ | √ | √ |
| Purification | √ | √ | √ | √ |
| Refrigeration | √ | | √ | √ |
| *Transportation* | | | | |
| Pipline | √ | √ | √ | √ |
| Small tanks | √ | √ | √ | √ |
| Large tanks | √ | | √ | √ |
| *Storage* | | | | |
| Injection | √ | √ | √ | √ |
| Storage | √ | √ | | |

**Table 2.1:** Thermodynamic Properties

## 2.5 Operating Windows of the CCS Processes

The operating windows of CCS processes define the optimal temperature and pressure ranges for conducting various stages of carbon capture, transportation, and storage. By adhering to these operating windows, engineers can design and operate CCS systems effectively, ensuring the successful mitigation of greenhouse gas emissions and contributing to climate change mitigation efforts. [74]

| CCS process | P(MPa) | T(K) |
|---|---|---|
| $CO2CompressionPurification$ | 0 to 11 | 219.15 to 423.15 |
| Initial Compression | 0 to 3 | 293.15 to 423.15 |
| Dehydration | 2 to 3 | 283.15 to 303.15 |
| Purification | 2 to 5 | 219.15 to 248.15 |
| Further Compression/pumping | 5 to 11 | 283.15 to 303.15 |
| $CO2Transport$ | 0.5 to 20 | 218.15 to 303.15 |
| Pipline | 7.5 to 20 | 273.15 to 303.15 |
| Small tanks | 1.5 to 2.5 | 238.15 to 248.15 |
| Large tanks | 0.5 to 0.9 | 218.15 to 228.15 |
| $CO2Storage$ | | |

**Table 2.2:** Estimated operation conditions (**P** and **T**) of the CCS processes

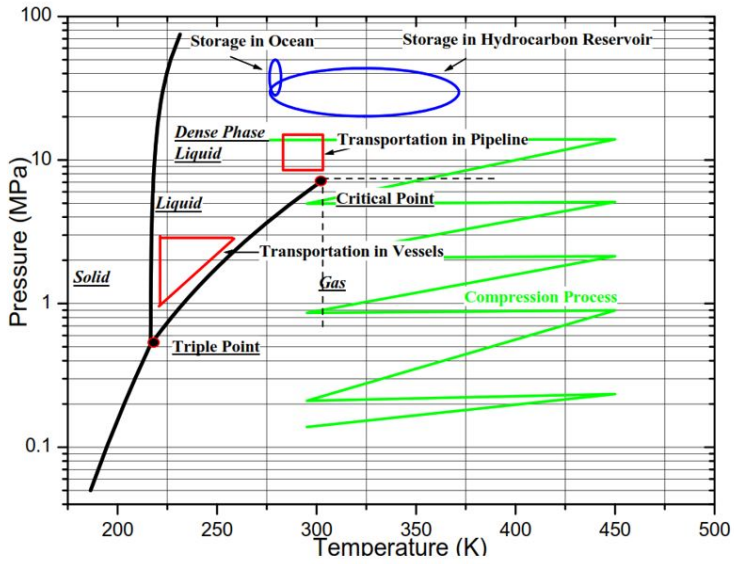



**Figure 2.1:** Potential pressure and temperature windows of the CCS systems

## 2.6 $CO_2$ Mixtures Impurities

While technically feasible, achieving high purity $CO_2$ from the flue gas of fossil fuel-fired power plants can lead to increased costs and energy requirements, thereby reducing power plant efficiency. Finding an optimal balance between the demands of purification, transport, storage, and legal and environmental considerations is crucial.

The characteristics of $CO_2$ streams captured from power generation vary depending on the $CO_2$ capture technology used. For instance, $CO_2$ captured from post-combustion using an amine solution is relatively clean, with H2O as the primary impurity. In contrast, $CO_2$ streams from oxy-fuel combustion can contain higher levels of impurities and $CO_2$ from IGCC processes typically has a more complex composition, including various hydrocarbons like $CH_4$.

Based on fuel conversion processes and the types of major impurities, captured CO2 streams can be categorized into two types: [76]

### 2.6.1 Oxidizing $CO_2$ Streams

These contain residual $O_2$ and sulfur contaminants mainly in the form of $SO_2$ (e.g., $CO_2$ captured from oxy-fuel and post-combustion processes).

### 2.6.2 Reducing $CO_2$ Streams

These have almost no residual $O_2$ and sulfur contaminants primarily as $H_2$S (e.g., $CO_2$ captured from coal gasification processes such as IGCC).

The main differences between these types of $CO_2$ streams are the concentrations of non-condensable impurities such as $N_2$, Ar, and $O_2$, and the types of sulfur impurities due to the different redox conditions—SO2 in oxidizing $CO_2$ streams and $H_2$S in reducing $CO_2$ streams.

Therefore, this research considers impurities such as $N_2$, $O_2$, AR, $H_2$O, $CH_4$, $SO_2$, and $H_2S$ when studying the thermodynamic properties of $CO_2$ mixtures, covering the most significant non-$CO_2$ components found in captured $CO_2$ streams.

## 2.7 Experimental Data of $CO_2$ and C$O_2$ Mixtures

Accurate experimental data for both pure $CO_2$ and $CO_2$ mixtures are essential to verify and calibrate calculation models. Since the 1980s, many high-accuracy experiments have been conducted on pure $CO_2$ properties. Research on the thermodynamic properties of $CO_2$ mixtures has focused on impurities like water, hydrocarbons, nitrogen, and hydrogen sulfide due to their significance in natural gas processing and enhanced oil recovery (EOR). Consequently, extensive data is available for CO2 mixtures with $H_2$O, $N_2$, $CH_4$, and $H_2$S, covering a wide range of temperatures and pressures. However, data on $CO_2$ mixtures containing $O_2$, Ar, and $SO_2$ remain limited, despite the importance of these impurities for CCS processes, particularly in oxy-fuel combustion technology.

Available experimental data of pure CO2 are summarized in table 2.3 Different kinds of Properties including volume, $C_p$, VLE, and excess enthalpy are included.

| Source | Year | Type | P(MPa) | T(K) | Uncertainty |
|---|---|---|---|---|---|
| Holste [78] | 1987 | Volume | 215 - 448 | 0.1 - 50.0 | P:$\pm$0.01% T:$\pm$0.01$K$ |
| Emst et al [79] | 1989 | Cp | 303.15 - 393.15 | 0.1 - 90 | - |
| Duschek [80] | 1990 | VLE | 217 - 340 | 0.3 - 0.9 | P:$\pm$0.02% T:$\pm$0.003$Ka$ |
| Gilgen et al [81] | 1992 | Volume | 220 - 360 | 0.3 - 13.0 | V:$\pm$0.0015 - 0.04% |
| Brachthuser [82] | 1993 | Volume | 233 - 523 | 0.8 - 30.1 | V:$\pm$0.02 - 0.04% |
| Moller et al [83] | 1993 | Excess Enthalpy | 230 - 350 | 15 - 18 | - |
| Fenghour [84] | 1995 | Volume | 329.82 - 697.81 | 3.032 - 34.203 | P:$\pm$0.02% T:$\pm$0.01$K$ |
| Klimeck et al [85] | 2001 | Volume | 240 -470 | 0.5 - 30 | P:$\pm$0.016% T:$\pm$0.004$K$ |

**Table 2.3:** Summary of the available experimental data for pure CO2

The available experimental data on $CO_2$ mixtures containing impurities ($N_2$, $O_2$, Ar, $SO_2$, $CH_4$, $H_2O$, and $H_2S$) are summarized in Table 2.4.

These data primarily focus on VLE properties and volume and are predominantly for binary CO2 mixtures.

| Source | Year | Type | Mixture | T(K) | P(MPa) | Uncertainty |
|---|---|---|---|---|---|---|
| Caubet [86] | 1901 | TPVX | CO2/SO2 | 311 - 511 | 1.4 - 69 | |
| Reamel [87] | 1944 | TPxy | CO2/CH4 | 303.15 - 393.15 | 0.1 - 90 | |
| Steckel [88] | 1945 | PTxy | CO2/H2S | 221 - 288,15 | 0.1 - 3.6 | |
| Bierlein et al [89] | 1953 | PTVX | CO2/H2S | 273 - 370 | 1.5 - 8.5 | P:±0.02 % T:±0.04$K$ |
| Donnelly [90] | 1954 | TPxy | CO2/CH4 | 167 - 301 | 2.0 - 7.4 | |
| Muirbrook [91], [92] | 1965 | TPxy | CO2/O2 CO2/N2 CO2/N2/O2 | 273,15 | 5.5 - 12 | P:±0.1 % |
| Kestin [93] | 1966 | TPVX | CO2/Ar | 293.15 - 303,15 | 0.101 - 2.58 | P:±0.5 % T:±1$K$ |
| Greenwood [94] | 1969 | TPxy | CO2 /H2O | 723 - 1073 | Up to 50 | |
| Fredenslund [95] | 1970 | TPxy | CO2 /O2 | 223.15 - 283,15 | 1 - 13 | P:±0.5 % T:±0.02$K$ |
| Arai [96] | 1971 | PVTx | CO2/N2 CO2/CH4 | 253 - 288 | 5 - 15 | P:±0.01$atm$ T:±0.01$k$ |
| Sarashine [97] | 1971 | PVTx | CO2 /Ar | 288,15 | 5.69 - 9.77 | P:±0.01$atm$ T:±0.01$k$ |
| Davalos [98] | 1976 | PTxy | CO2/CH4 | 303.15 | 0.9 - 8.5 | |
| Altunin [99] | 1977 | Comp | CO2/Ar | 303.15 | 0.29 - 10.75 | |
| Mraw [100] | 1978 | TPxy | CO2/CH4 | 89 - 208 | 0.5 - 6.3 | |
| Somait [101] | 1978 | TPxy | CO2/H2O | 270 | 3 - 12 | P:±0.015$atm$ T:±0.02$k$ |
| Zawisza [102] | 1981 | TPVX | CO2/N2 | 323 - 473 | Up to 3.3 | P:±0.03 % T:±0.05$k$ |
| Dorau [103] | 1983 | TPVX | CO2/N2 | 223.15 - 273,15 | 3 - 20 | |
| Patel [104] | 1988 | TPVX | CO2/H2O | 323 - 498 | Up to 10.34 | P:±0.01 % T:±0.01$k$ |
| Esper [105] | 1989 | TPVX | CO2/N2 | 205 - 320 | 0.1 - 48 | P:±0.015 % T:±0.01$k$ |
| Stemer [106] | 1991 | TPVX | CO2/H2O | 673 - 2973 | 200 - 600 | P:±1 % T:±1 % |
| Fenghour [107] | 1994 | TPVX | CO2/H2O | 415 - 700 | 6 - 35 | P:±0.02 % T:±0.01$K$ |
| Seitz [108] | 1999 | TPVX | CO2/H2O | 600 | 10 - 100 | P:±0.01$MPa$ T:±0.01$K$ |

**Table 2.4:** Summary of the available experimental data for binary $CO_2$ mixtures

## 2.8 Method Evaluations for the Thermodynamic Property Calculations of $CO_2$ Mixtures

The correlation and prediction of mixture behaviors are central topics in applied thermodynamics. For phase equilibrium calculations, there are two main types of thermodynamic methods: liquid activity coefficient-based models and equation-of-state EOS based models. Activity coefficient models are ideal for representing highly non-ideal liquid mixtures at low pressures and can handle mixtures of any complexity. In contrast, EOS methods are applicable over wide temperature and pressure ranges, including sub-critical and super-critical regions. For ideal or slightly non-ideal systems, thermodynamic properties for both the vapor and liquid phases can be computed with minimal component data. However, EOS methods tend to have relatively poor accuracy for liquid phase calculations.

Given the wide range of operating conditions in CCS processes and the need for various thermodynamic properties, EOS methods are generally more applicable than activity coefficient methods. This is because activity coefficient methods are limited to low-pressure scenarios (typically below 10 atm) and involve more complex procedures to calculate other properties, such as volume, enthalpy, and entropy.

A semi-empirical EOS relates volume, pressure, temperature, and composition of substances in mathematical forms. Any thermodynamic property can be derived from it using appropriate thermodynamic relations. However, developing such semi-empirical equations requires extensive experimental data over a wide range of conditions, making progress slow and limited to a few pure fluids.

EOS can be divided into two categories: specialized EOS, such as Span's EOS for $CO_2$, and general EOS, such as the van der Waals EOS. Specialized equations offer better accuracy but are limited to specific substances. For example, Span's EOS is specific to $CO_2$. General EOS can further be divided into those with simple structures, like the Redlich-Kwong (RK) EOS, and those with complex structures, like the Benedict-Webb-Rubin (BWR) EOS. While complex general equations may yield better results due to more parameters, their calculation procedures are more complicated, especially for derived properties like enthalpy and entropy.

Additionally, their complexity makes integration into commercial software like Aspen Plus and IPSpro more difficult if they are not originally included.

From an engineering perspective, a general EOS with a simple structure and reasonable accuracy is preferable. Cubic equations of state have very simple structures. Since van der Waals proposed his EOS in 1873, many modified versions of cubic EOS with two or more parameters have been developed to improve predictions of volumetric and phase equilibrium properties of fluids. It is well established that a cubic EOS can satisfactorily model phase equilibrium. In this work, the RK EOS was modified for gaseous $CO_2$ and $CO_2$/$H_2O$ mixtures, and the reliability of cubic EOS was evaluated for predicting the thermodynamic properties of $CO_2$ mixtures.

## 2.9 Evaluation of Cubic EOS for Predicting VLE and Volume of $CO_2$ Mixtures

The Peng-Robinson (PR) EOS, developed from the Redlich-Kwong (RK) EOS, is designed to predict both liquid volume and vapor pressure, thereby enhancing VLE predictions. It is recommended for hydrocarbon processing applications, including gas processing, refining, and petrochemical processes. [77]

PR equation Mathematical formula:

$$\mathrm{P} = \frac{\mathrm{RT}}{\mathrm{(V\text{-}b)}} - \frac{\mathrm{a}\,\alpha}{\mathrm{V(V+b)+b(V\text{-}B)}} \tag{2.1}$$

Where:

- **P** is the pressure.
- **T** is the temperature.
- **V** is the molar volume.
- **R** is the universal gas constant.
- **a** and **b** are parameters specific to the components in the mixture,.
- $\alpha$ is a temperature-dependent parameter.

### 2.9.1 a Parameter:

The parameter **a** accounts for the attractive forces between molecules. It is calculated using the critical temperature $T_c$ and critical pressure $P_c$ of the substance:

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \tag{2.2}$$

### 2.9.2 b Parameter:

The parameter b accounts for the volume occupied by the molecules themselves (repulsive forces). It is calculated using the critical pressure $P_c$ and critical temperature $T_c$:

$$b = 0.07780 \frac{RT_c}{P_c} \tag{2.3}$$

The Redlich-Kwong EOS is the earliest modification of the van der Waals EOS, enhancing the modeling of intermolecular attraction. It is more suitable for systems at low pressures.

RK equation Mathematical formula:

$$P = \frac{RT}{V-b} - \frac{\frac{a}{T^{0.5}}}{V(V+b)} \tag{2.4}$$

Where:

• **P** is the pressure.

• **R** is the universal gas constant.

• **T** is the temperature.

• **V** is the molar volume.

• **a** and **b** are parameters specific to the components in the mixture.

### 2.9.3 a Parameter:

The parameter **a** accounts for the attractive forces between molecules and is calculated using the critical temperature $T_c$ and critical pressure $P_c$ of the substance:

$$a = 0.42748 \frac{R^2 T_c^{2.5}}{P_c} \tag{2.5}$$

### 2.9.4 b Parameter:

The parameter b accounts for the volume occupied by the molecules themselves (repulsive forces) and is calculated using the critical temperature $T_c$ and critical pressure $P_c$:

$$b = 0.08664 \frac{RT_c}{P_c} \tag{2.6}$$

the Soave-Redlich-Kwong equation of state, which is an improvement over the original Redlich-Kwong Redlich-Kwong (RK) equation of state. The SRK equation incorporates a correction factor introduced by Soave to enhance the accuracy of phase behavior predictions, especially for mixtures [109].

SRK equation Mathematical formula:

$$P = \frac{RT}{V + c - b} - \frac{a}{(V + c)(V + b + c)} \tag{2.7}$$

Where:

• **P** is the pressure.

• **R** is the universal gas constant.

• **T** is the temperature.

• **V** is the molar volume.

• **a** and **b** are parameters specific to the components in the mixture.

• $\alpha$ is the Soave correction factor.

## 2.10 Impact of Impurity on Thermodynamic Properties of $CO_2$

### 2.10.1 Mixtures and Different Processes Involved in the CCS Systems

Impurities significantly affect system design, operation, and optimization by altering the thermodynamic properties of $CO_2$ mixtures. the relationships between thermodynamic properties and some system parameters of $CO_2$ purification and transportation are summarized in Table 2.5.

| | Operation conditions | | Energy consumption | | Configuration design | | Performance | |
|---|---|---|---|---|---|---|---|---|
| | PUR | TRA | PUR | TRA | PUR | TRA | PUR | TRA |
| DP | √ | | √ | | | | √ | |
| BP | | √ | √ | | | √ | √ | |
| DBDP | | | √ | | √ | | | |
| Heat Capacity | | | √ | √ | | | | |
| Enthalpy | | | √ | √ | | | | |
| Entropy | | | √ | √ | | | | |
| Volume | | | | | | √ | | √ |

**Table 2.5:** Relationship between Thermodynamic Properties and system parameters

The variation in impurity content affects the VLE properties of $CO_2$ mixtures, particularly their boiling and condensing behaviors. Physical separation should occur in the two-phase region, meaning that at a constant temperature, the operating pressure must be above the condensing pressure and below the boiling pressure of the mixtures. Unlike separation, transportation must be conducted above the boiling pressure for safety reasons. Consequently, changes in VLE properties necessitate adjustments to the operating conditions of $CO_2$ compression and purification systems, such as discharge pressure and condensation temperature, as well as transport systems. The $CO_2$ purity of the separation product corresponds to the $CO_2$ mole fraction at the bubble point, so any changes in boiling behavior will affect separation performance. Additionally, the design of the separation unit depends on the difference between boiling and dew points. A larger difference allows for a simpler system, like a multi-stage flash, whereas closer boiling and dew points require a distillation column.

Impurity content also impacts the enthalpy, entropy, and heat capacity of $CO_2$ mixtures. Since energy consumption in compression and refrigeration processes depends on **enthalpy and entropy** changes, impurities can significantly influence overall energy consumption.

Moreover, the variation of impurity content will vary the effective $CO_2$ volumes (ECV) of $CO_2$ streams, which is defined as:

$$ECV = \frac{V_{co2}}{V_{co2} - mixture} \tag{2.8}$$

ECV can directly impact the efficiency and economic aspects of CO2 transport and storage, making it crucial for the design of these systems.

Compared to other $CO_2$ capture methods, such as pre-combustion and post-combustion capture, oxy-fuel combustion is expected to produce $CO_2$ streams with relatively high levels of impurities. This introduces greater challenges for $CO_2$ processing, including dehydration, purification, and compression [110]. The focus here is on impurities in the oxidizing $CO_2$ streams captured from oxy-coal combustion. This chapter first analyzes the impact of impurities on the thermodynamic properties of $CO_2$ mixtures, then further discusses how these impurities affect the various processes involved in CCS systems.

## 2.11 Impact of Impurity on Thermodynamic Properties of $CO_2$ Mixtures

According to Table 2.5, the impacts of impurities on VLE, heat capacity, enthalpy, and volume were investigated individually, given their significance to system design and operation.

### 2.11.1 Impact on VLE:

Figure 2.2 illustrates phase diagrams for $CO_2$/Ar, $CO_2/N_2$, and $CO_2/O_2$ at 223.15 K. In area A, the CO2 mixtures are in the liquid phase; in area C, they are in the gas phase; and in area **B**, between **A** and **C**, two phases coexist. To better understand the VLE behaviors of CO2 mixtures in CCS applications, the concentration ranges of impurities were adjusted to reflect probable concentrations in CCS processes. Based on the composition windows presented, the mole fractions of Ar, $N_2$, and $O_2$ were set between $0-5\%$, $0-15\%$, and $0-7\%$, respectively, as shown in the right-side diagrams in Figure 2.2.

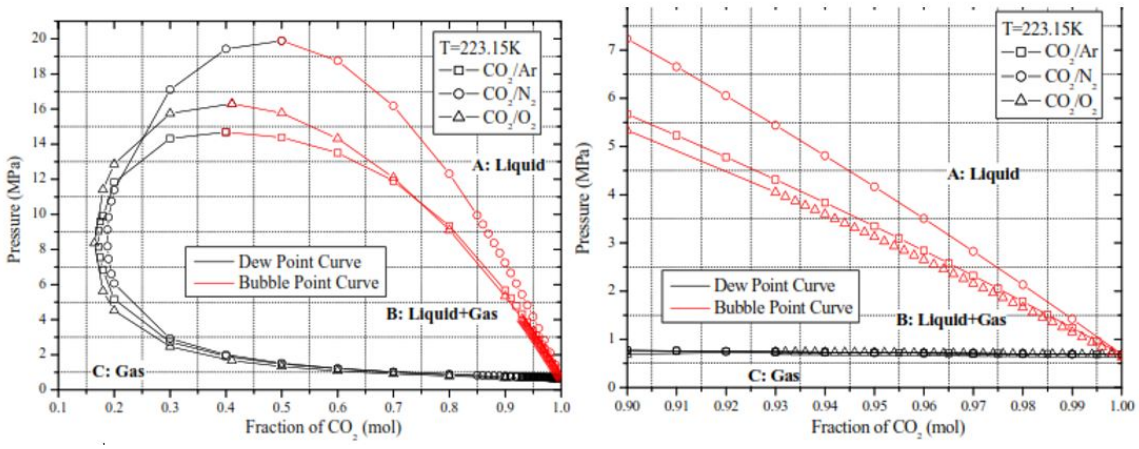



**Figure 2.2:** Comparison of VLE characteristics among the binary $CO_2$ mixtures containing non-condensable impurities: Ar, $O_2$ and $N_2$

In contrast to the saturated state of pure $CO_2$, the presence of non-condensable gases increases both the boiling and condensing pressures of $CO_2$ mixtures. In cases of relatively high $CO_2$ purity, such as $CO2 > 70mol\%$, impurities notably affect the bubble point more than the dew point. Among the impurities, variations in N2 content have the most significant impacts on both the dew and bubble points of $CO_2$ mixtures. Additionally, $CO_2/N_2$ mixtures exhibit the largest disparity between bubble and dew points.

In contrast to the effects of non-condensable gases, $SO_2$ has an opposite influence on the VLE properties of $CO_2$ mixtures. Figure 2.3 illustrates the VLE behavior of $CO_2/SO_2$ mixtures. Because $SO_2$ possesses a higher critical point compared to $CO_2$, its presence in $CO_2$ mixtures leads to an elevation in the condensing temperature at a given pressure or, conversely, a reduction in the condensing pressure at a certain temperature.

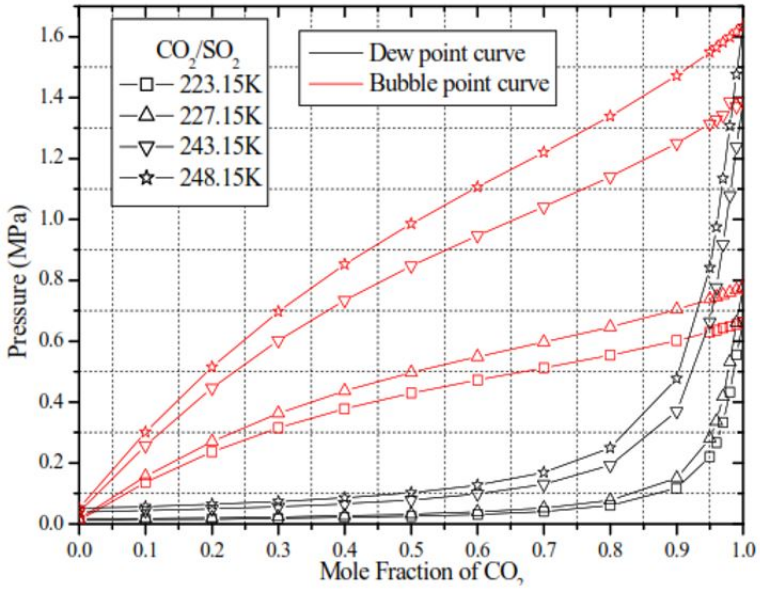



**Figure 2.3:** The VLE characteristics of the $CO_2$ mixtures containing condensable impurity $SO_2$

### 2.11.2 Impact on Heat Capacity:

Heat capacity, enthalpy, and entropy are crucial thermodynamic parameters for $CO_2$ mixtures as they influence heat transfer and energy consumption in $CO_2$ compression/purification processes.

The temperature-dependent heat capacities of pure substances ($CO_2, SO_2, N_2, O_2$, and Ar) have been computed using an empirical equation [111].

$$C = C_1 + C_2 \left[\frac{C_3}{T} \sinh\left(\frac{C_3}{T}\right)\right]^2 + C_4 \left[\frac{C_5}{T} \cosh\left(\frac{C_5}{T}\right)\right]^2 \tag{2.9}$$

This is depicted in Figure 2.4. The heat capacities of the pure substances follow a decreasing order of $CSO_2 > CCO_2 > CO_2 > CN_2 > C_Ar$. Additionally, it's evident that $O_2, N_2$, and Ar exhibit less temperature dependence in their heat capacities.

The heat capacity of a $CO_2$ mixture could be calculated by the following equation:

$$C_{\text{mixture}} = \sum_{i=1}^{n} [C_i * X_i] \tag{2.10}$$

where $CC_i$ represents the heat capacity of the pure component. At an identical operating temperature, the inclusion of $SO_2$ will elevate the heat capacities of $CO_2$ mixtures, whereas the presence of Ar, $O_2$, and $N_2$ will diminish them. This suggests that $CO_2/SO_2$ mixtures could potentially absorb or release more. heat for the same changes in temperature at compared with that of $CO_2/N_2$, $CO_2/O_2$ and $CO_2$/Ar mixtures.

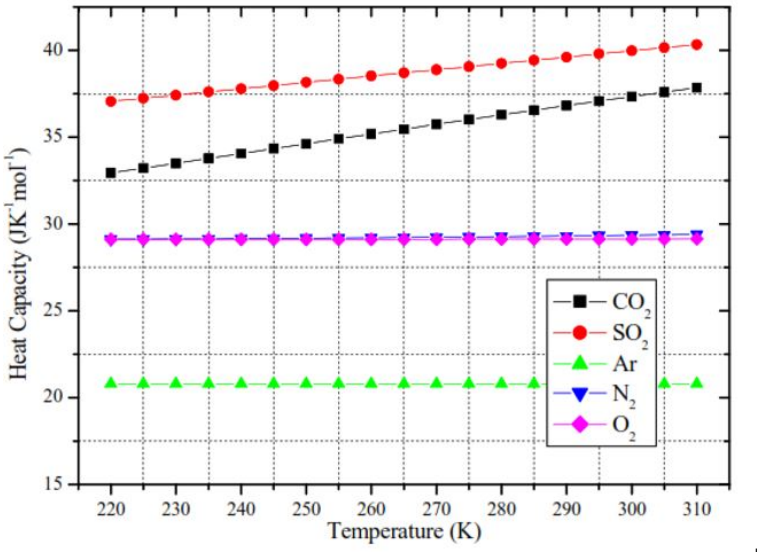



**Figure 2.4:** Heat capacity of different components at different temperatures

### 2.11.3 Impact on Enthalpy:

The enthalpy of a real gas can be determined using the following equation:

$$h(t,p) = \int_{T_0}^{T} \sum y_i C_{p,i}\, dT + \int_{p \longmapsto (0)}^{p} \left[ v - T(\frac{\partial v}{\partial T})_p \right] dP \tag{2.11}$$

Figure 2.5 illustrates the enthalpies of various $CO_2$ mixtures at 303.15K and 3MPa. It's evident that only the inclusion of $SO_2$ raises the enthalpy of $CO_2$ mixtures, primarily attributed to its higher heat capacity compared to $CO_2$.

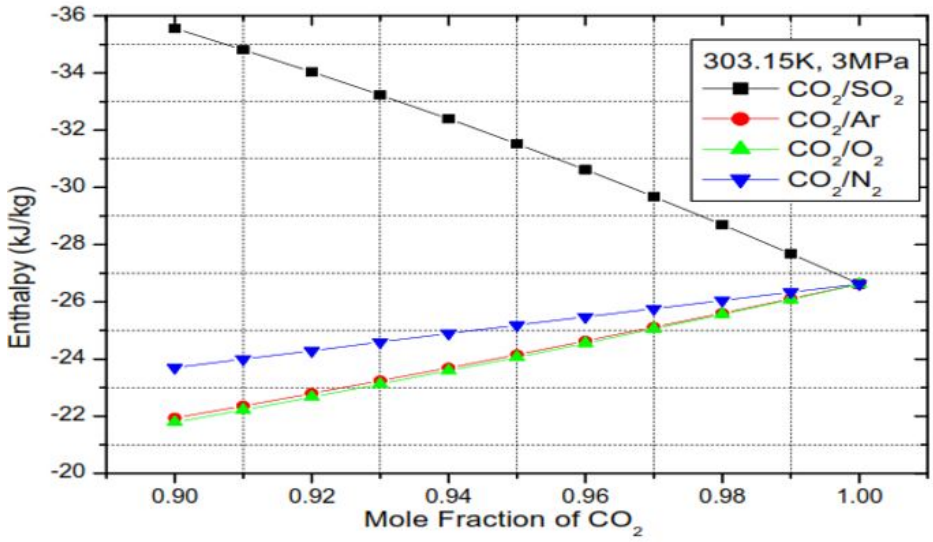



**Figure 2.5:** Enthalpy of different gaseous $CO_2$ mixtures

### 2.11.4 Impact on volume:

The impact of impurities on the volumes of $CO_2$ mixtures depends on their molecular weights. Since $SO_2$ has a higher molecular weight than $CO_2$, while Ar, $O_2$, and $N_2$ have lower molecular weights, only $SO_2$ increases the molecular weight of $CO_2$ mixtures. Consequently, $SO_2$ causes the volumes of $CO_2$ mixtures to increase, whereas the other impurities cause them to decrease. The following Figure shows the volumes and densities of binary $CO_2$ mixtures at different $CO_2$ compositions.

The impact of impurities on the volumes of $CO_2$ mixtures depends on their molecular weights. Since SO2 has a higher molecular weight than $CO_2$, while Ar, $O_2$, and $N_2$ have lower molecular weights, only $SO_2$ increases the molecular weight of $CO_2$ mixtures. Consequently, $SO_2$ causes the volumes of $CO_2$ mixtures to increase, whereas the other impurities cause them to decrease. The following Figure shows the volumes and densities of binary $CO_2$ mixtures at different $CO_2$ compositions.

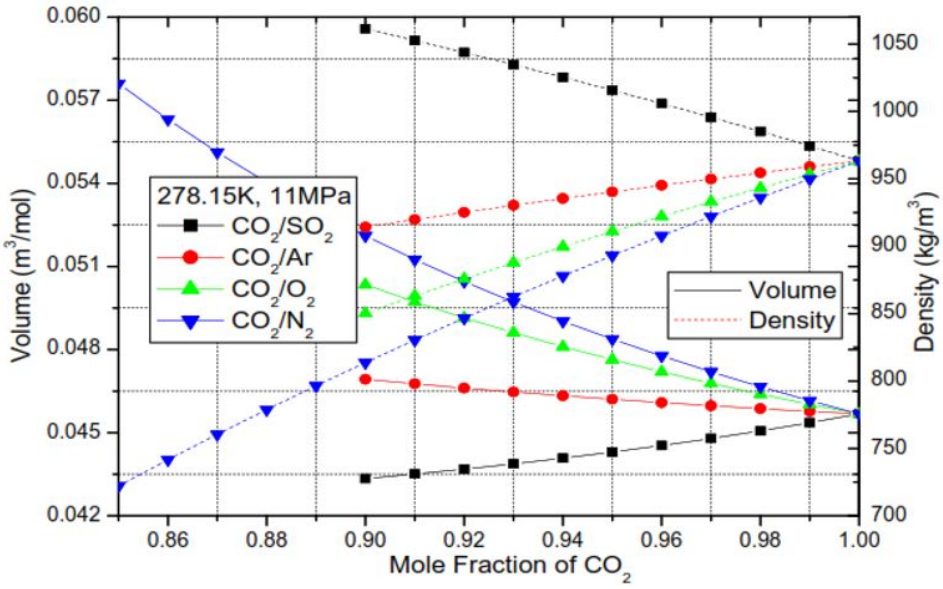



**Figure 2.6:** Volumes and densities of $CO_2$ mixtures at different $CO_2$ compositions.

# 3

# Simulation of Carbon Dioxide Capture

## 3.1 Definition of a Program Aspen

**ASPEN** is an acronym for Advanced System for Process Engineering. It is based on a flowsheet simulation. A flowsheet simulation is a computer software used to quantitatively model a chemical processing plant, which, in addition to the core reactor unit, also includes pre- and post-treatment steps. Thus, the simulation of an entire chemical process, starting from the raw material to the final finished product, is symbolically represented by different icons where each icon stands for a unit operation, chemical process, input/output material stream, input/output energy stream, or input/output electric/pneumatic signal.

### 3.1.1 Aspen Plus

is located between the group of simulators using the sequential strategy, in the same way as other simulators such as **PRO II and CHEMCAD** Thus, it is composed of a group of simulation or program units (subroutines or models) represented through blocks and icons, to which the pertinent information must be provided to solve the mass and energy balances. However, it is important to mention that in the last versions of this simulator, the possibility to work with the simultaneous or equation-oriented strategy has been included, allowing the modelling of systems and processes much more complex, highly integrated and with a high number of recycles.

### 3.1.2 Aspen Hysys

is a process simulator widely used at an industrial level, especially in a project's conceptual design and detailed engineering, control, optimization and process monitoring stages. The most important applications of **Aspen Hysys** correspond to the industries of oil and gas processing, and some industries of air separation. All these practices take advantage of this simulator architecture that permits the integration of the steady-state and dynamic models in only one unit. In this way, it is possible to bring together the stages of process design with the rigorous analysis of the dynamic behaviour and the control of the same, to evaluate instantly the effects that the decisions in the detailed design step have over the dynamic and controllability of the process.

## 3.2 Global schematic of the hydrogen production station simulated by Aspen

In the Last Year, the goal was to model and simulate the production of hydrogen by the vapor-forming technique of natural gas using the **Aspen Hysys** software. Once the process design is fully completed in the software, a comparative study between two types of natural gas is conducted. And output the emitted carbon dioxide ratio. To reduce the emission and spread of carbon dioxide, we decided to complete the process of capturing $CO_2$ using the **Aspen PLUS** software and using several important techniques.

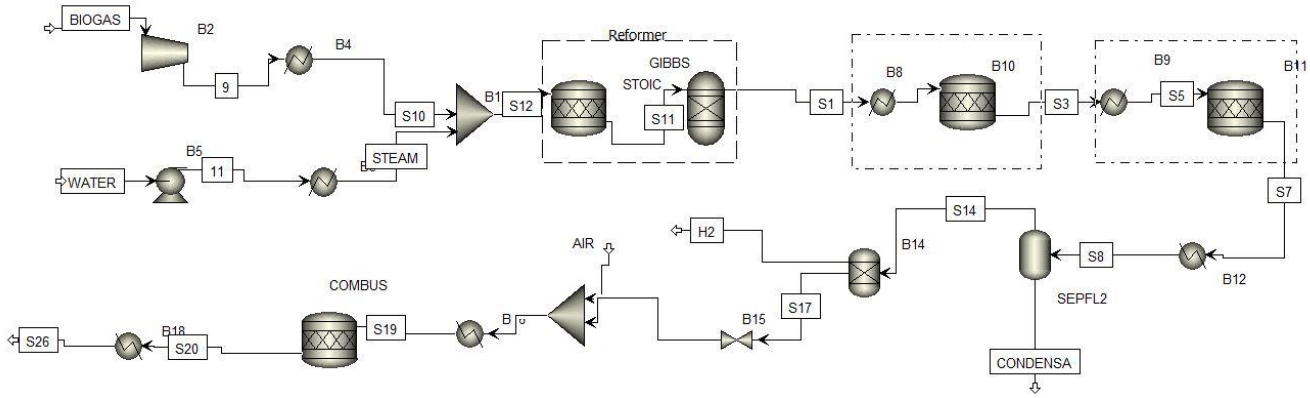



**Figure 3.1:** Global schematic of the hydrogen production station simulated by Aspen.

## 3.3 Software Aspen Plus

Click on**"Create"** button, shown at the bottom of the template window, and the main window of Aspen Plus V14 shows up as in **figure** 3.2 STARTING from the top-left corner while moving row-wise to the right horizon until we finally reach the bottom-right corner, let us familiarize ourselves with what is seen, in the

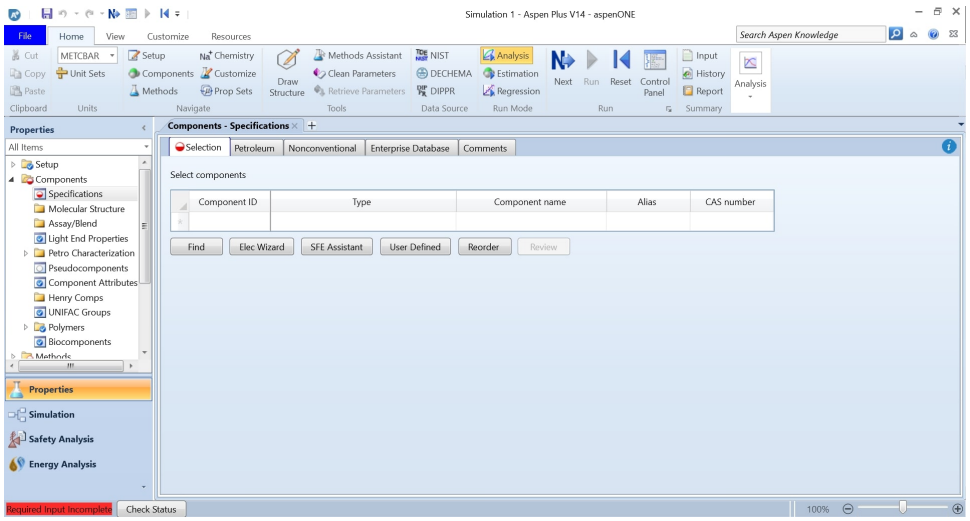



**Figure 3.2:** The main window of Aspen Plus flowsheet simulator.

form of a pane, ribbon, toolbar, status bar, input form, and tab, as shown in Figure 3.3 We briefly introduce each item with the understanding that, as the user keeps digging, he/she will become more comfortable because each item represents a shortcut key to one of the important features of Aspen Plus.

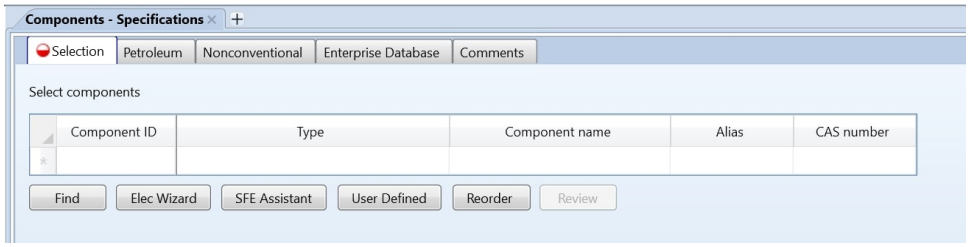



**Figure 3.3:** The top portion of Aspen Plus V14 main window contains the **"Quick Access"** toolbar **(top bar)**, the "Top" toolbar, the help-related textbox and button **(middle bar)**, and ribbon tabs associated with each **"Top"** toolbar menu (**bottom bar**).

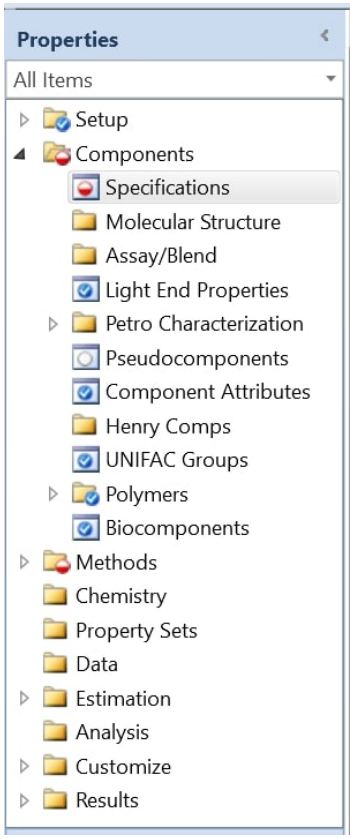



**Figure 3.4:** CaptiThe **"Navigation"** pane that acts as folder/file explorer.on

hows a sample of an input form where the user types in-process components.

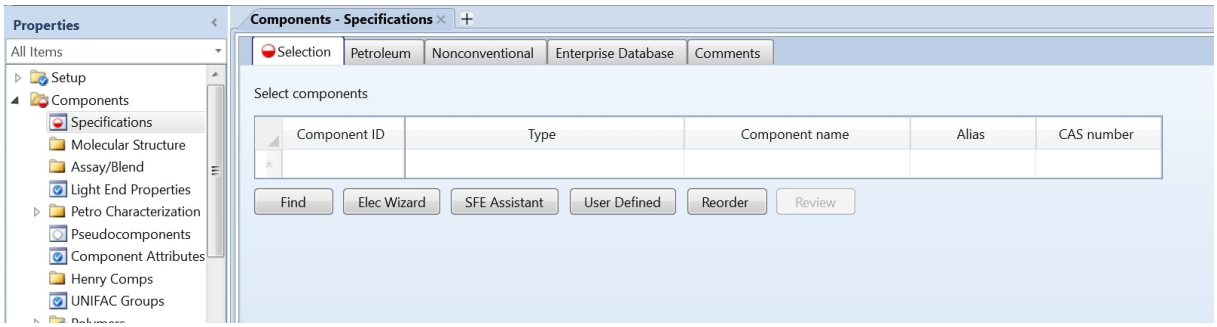



**Figure 3.5:** The input form for entering components involved in the process.

As shown in **Figures 4.2. and 3.5** Aspen Plus requires us to enter the components involved in the process. A component can be either picked up from one of **Aspen Plus** built-in component databanks or can be defined by the user and in the latter case it is considered a non-databank member.

**Figure** 3.6 shows the default (i.e., selected) databanks assigned by Aspen Plus, depending on, of course, the type of template initially chosen by the user. The user may select, however, one or more from the databanks available on the left side and add to the list of selected databanks on the right side, using the in-between arrow keys.

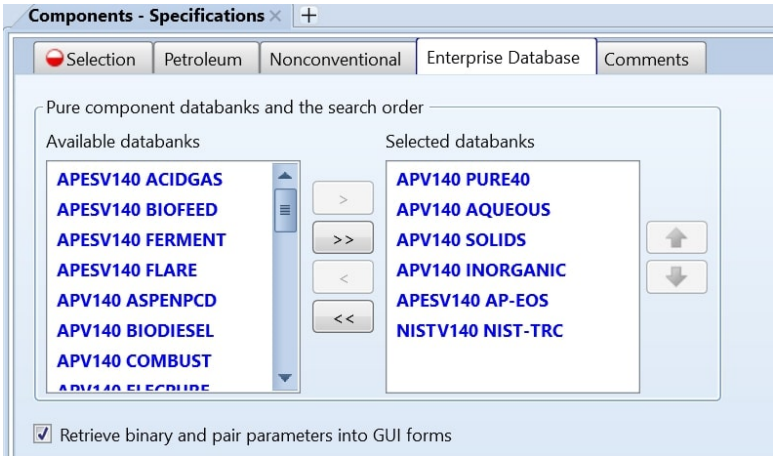



**Figure 3.6:** The selected databanks are shown on the right side under **"Enterprise Database "**or **"Databanks"** tab.

Regarding the component type, there are six major classes that can be dealt with in Aspen Plus: 1. Conventional: Single species fluids (**vapour or liquid**). Typical components that may participate in vapour–liquid-phase equilibrium.

2. Solid: Single species solids: Properties are calculated by solid-based models.

3. Non-conventional: Solids that are not pure chemical species. They are not represented as molecular components, such as coal or wood pulp. They are characterized using component attributes and do not participate in chemical or phase equilibrium.

4. Pseudo component: Assay, and Blend: Components representing petroleum fractions, characterized by boiling point, molecular weight, specific gravity, and other properties.

5. Polymer, Oligomer, and Segment: Components used in polymer models.

6. Hypothetical liquid: A component type that is mainly used in pyrometallurgical applications when modelling a component as a liquid when its properties should be extrapolated from solid properties, for example, modelling the carbon in molten steel. Afterwards, it is necessary to insert the streams involved in the process. For that, the block corresponding to Material Streams is selected from the inferior panel.

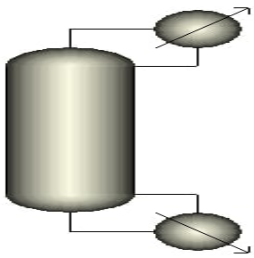
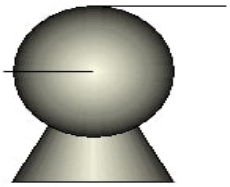
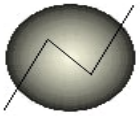
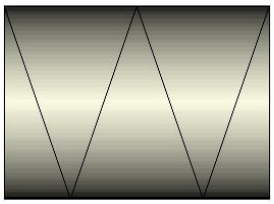
| | |
|---|---|
|  | **Absorber:** In Aspen Plus, an absorber is a unit operation used to remove a specific component from a gas stream by contacting it with a liquid solvent. The component to be removed is typically more soluble in the liquid than in the gas, and the process is driven by the difference in partial pressures between the two phases. |
|  | **Stripper:** In Aspen Plus, a stripper is a unit operation used to recover a component from a liquid stream by contacting it with a gas stream. The component to be recovered is typically more volatile than the other components in the liquid, and the process is driven by the difference in partial pressures between the two phases. |
|  | **Pump:** is designed to handle a single liquid phase. For special cases, you can specify two- or three-phase calculations to determine the outlet stream conditions and to compute the fluid density used in the pump equations. The accuracy of the results depends on several factors, such as the relative amounts of the phases present, the compressibility of the fluid, and the efficiency specified. |
|  | **Heater:** The basic heat exchanger model that performs simple energy balance calculations; it requires only one process stream. You can use "Heater" to represent heaters, coolers, valves, pumps (whenever work-related results are not needed), and compressors (whenever work-related results are not needed). This block will be initially used in this running tutorial for calculating the heat duty, which will then be used to calculate heat-transfer area requirements. |
|  | **Makeup:** provides a way to balance the circulating material flow in recycle loops. You specify one or more flow or composition specifications on Makeup's outlet stream. Makeup adjusts the flow rate of its inlet makeup streams, and purges a portion of the feed flow, as necessary, to maintain the specified specifications. |

**Table 3.1:** Main components used in the study cases

### 3.3.1 Technology of $CO_2$ capture from natural gas power plant using MEA

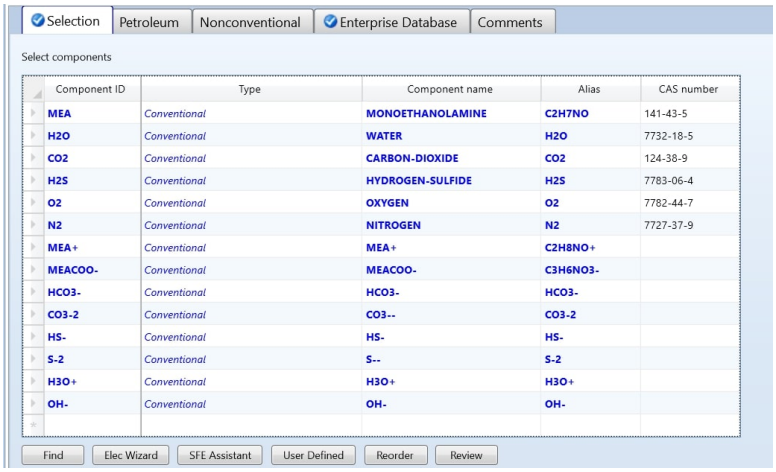



**Figure 3.7:** Components Specifications $CO_2$ capture from natural gas.

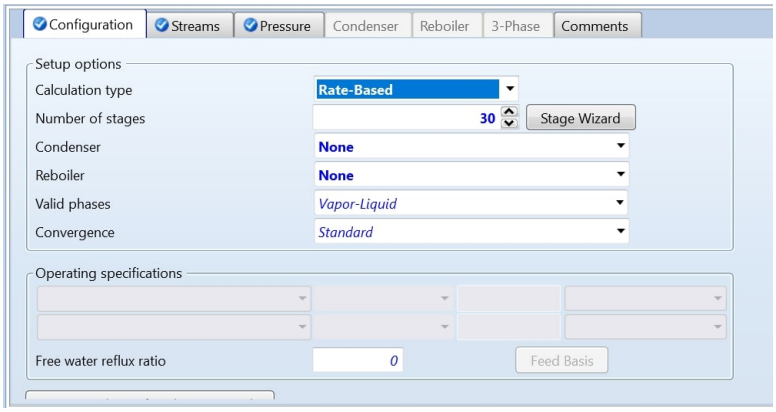



**Figure 3.8:** Configuration of ABSORBER (RedFrac) $CO_2$ capture from natural gas.

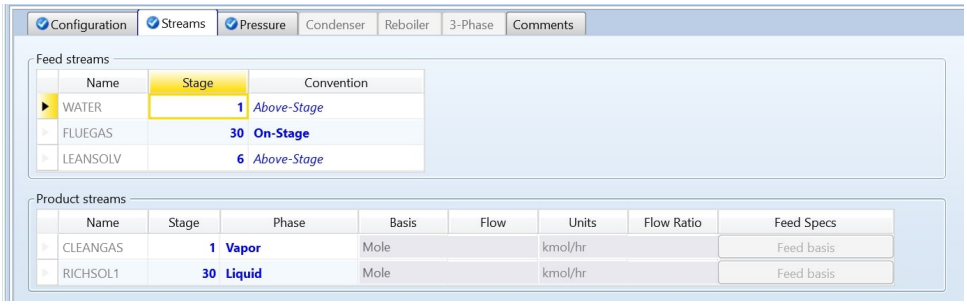



**Figure 3.9:** Streams of ABSORBER (RedFrac) $CO_2$ capture from natural gas.

for this simulation with **Aspen plus v14**. The dry flue gas, which consists of $CO_2$, $O_2$ and $N_2$, is sent to the absorber column to remove $CO_2$. The packed absorber column is divided into 30 stages in the simulation.

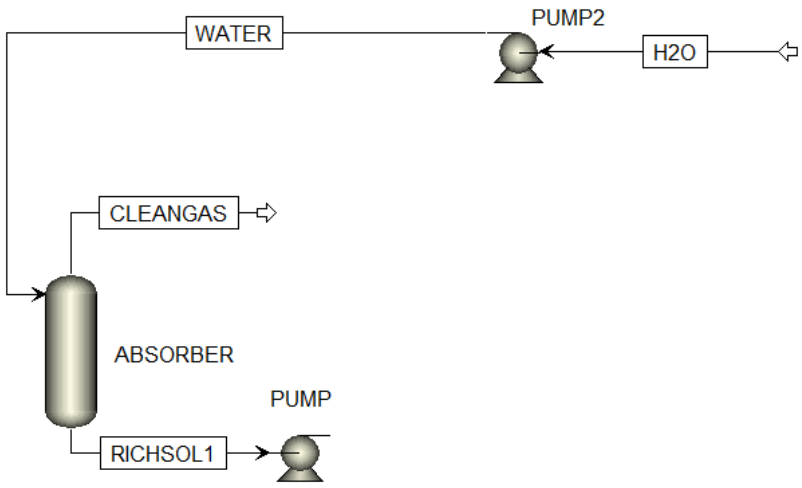



**Figure 3.10:** ABSORBER (RedFrac) of $CO_2$ capture from natural gas.

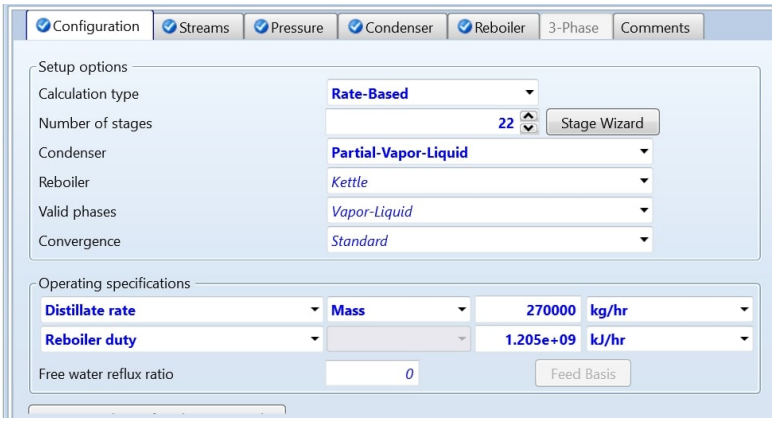



**Figure 3.11:** Configuration of STRIPPER (RedFrac) $CO_2$ capture from natural gas.

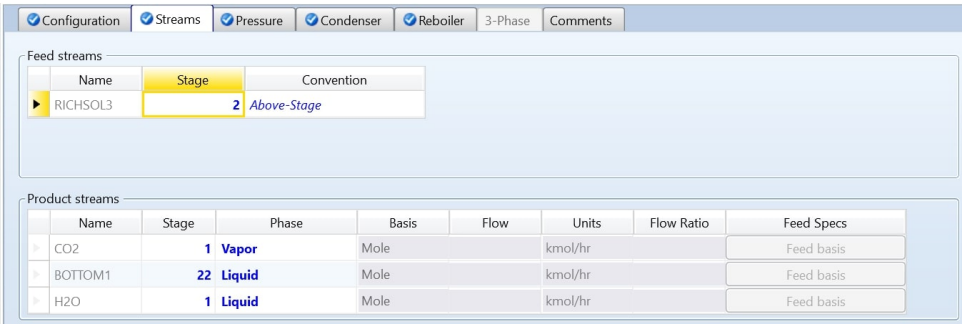



**Figure 3.12:** Streams of STRIPPER $CO_2$ capture from natural gas.

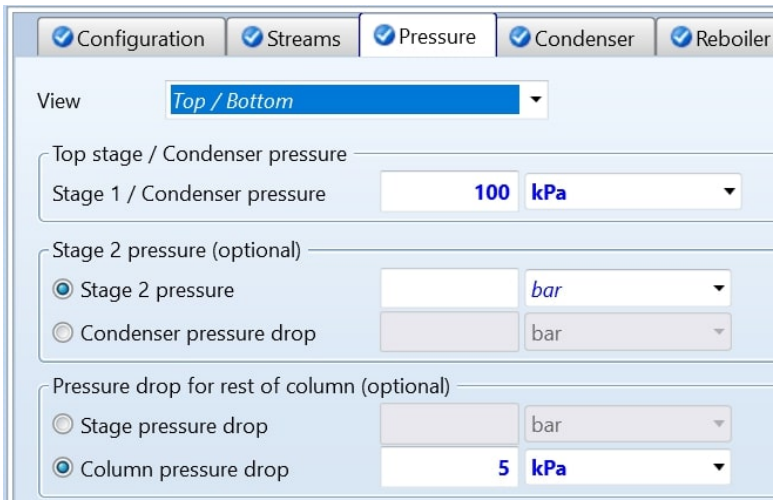



**Figure 3.13:** Pressure of STRIPPER (RedFrac) $CO_2$ capture from natural gas.

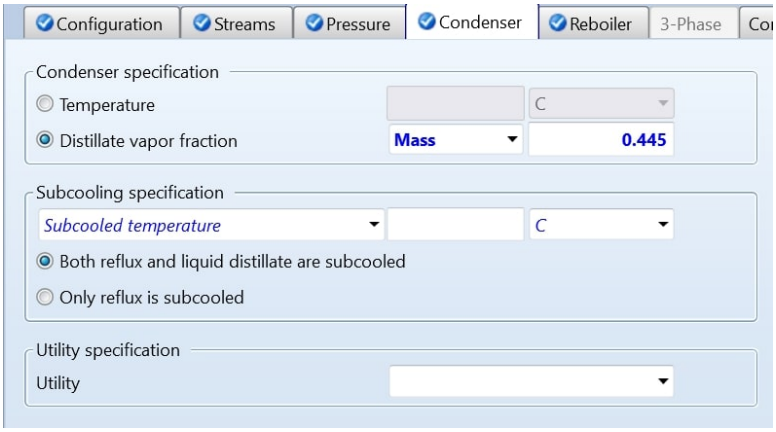



**Figure 3.14:** Condenser of STRIPPER (RedFrac) $CO_2$ capture from natural gas.

he flue gas enters the column at the bottom and the lean MEA solvent enters the column at stage 6. The solvent absorbs the $CO_2$ in the column. Water enters the absorber at the top and washes MEA from the gas stream to reduce solvent loss.

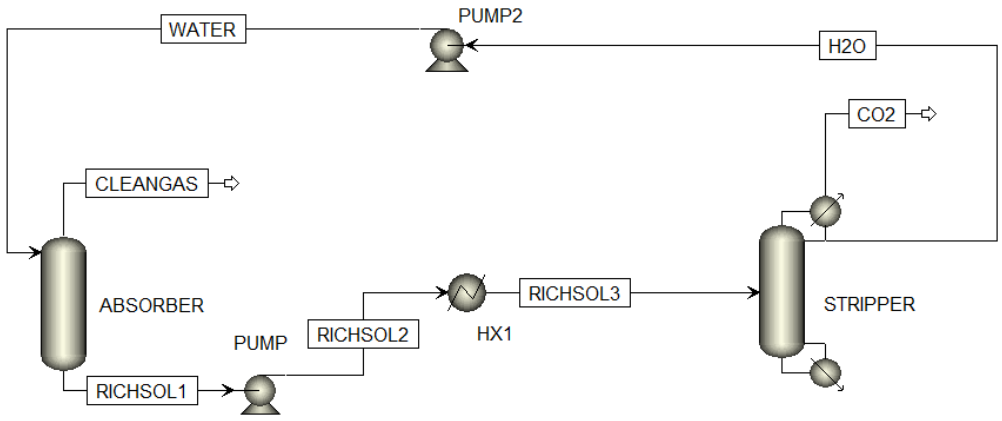



**Figure 3.15:** The flue gas enters the column at the bottom and the lean MEA solvent enters the column $CO_2$ captured from natural gas.

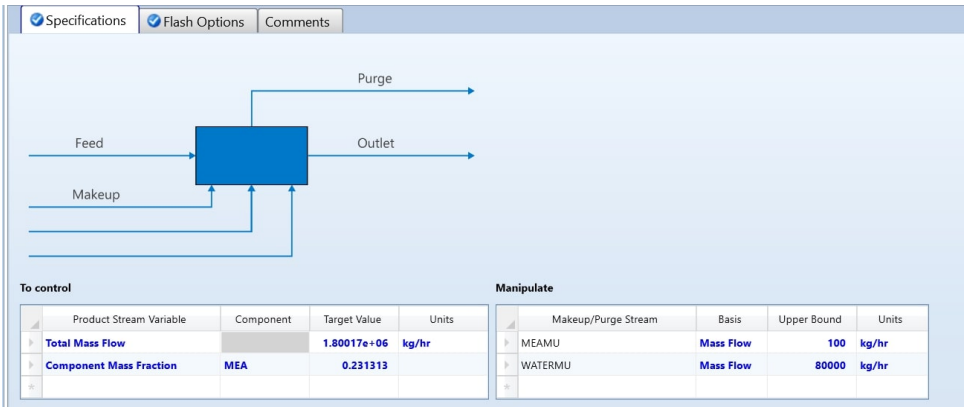



**Figure 3.16:** Spefications of MAKEUP $CO_2$ capture from natural gas.

Clean gas comes out the top of the absorber and the rich solvent leaves the absorber from the bottom and is sent to the stripper.

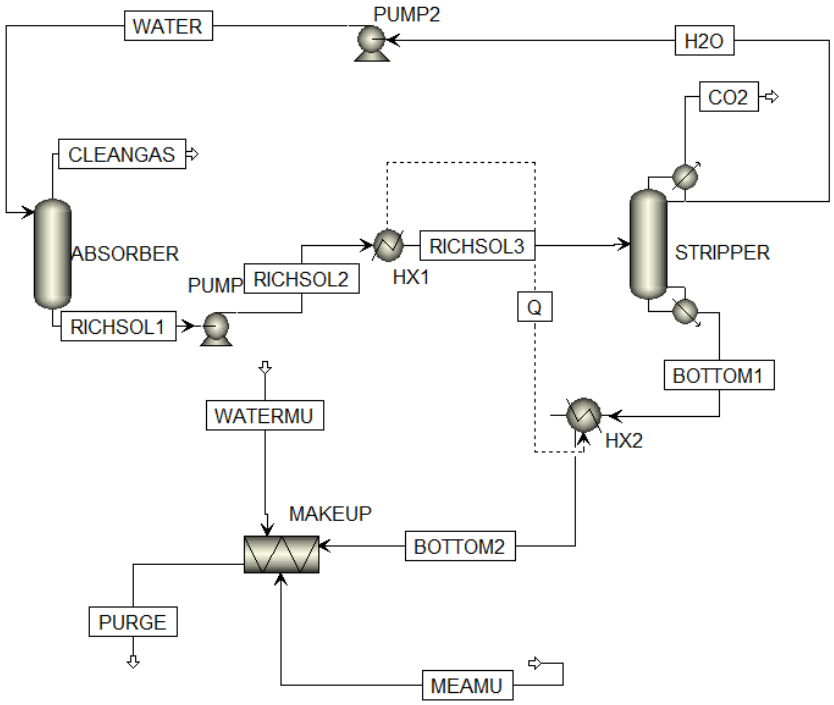



**Figure 3.17:** Clean gas comes out the top of the absorber and the rich $CO_2$ captured from natural gas.

Before entering the stripper, the rich solvent stream goes through a heat exchanger to increase the temperature to $70\,^{\circ}\mathrm{C}$. The stripper is divided into **22 stages** in the simulation. Rich solvent enters the stripper column on **stage 2**. $CO_2$ is stripped from the rich amine in the column and the MEA solvent is regenerated. The lean solvent from the bottom of the stripper is recycled with makeup back to the absorber.

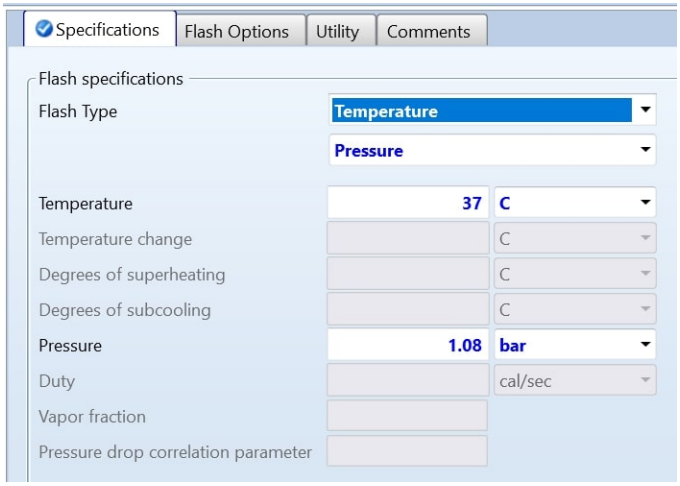



**Figure 3.18:** Spefications of COOLED (Heater) $CO_2$ capture from natural gas.

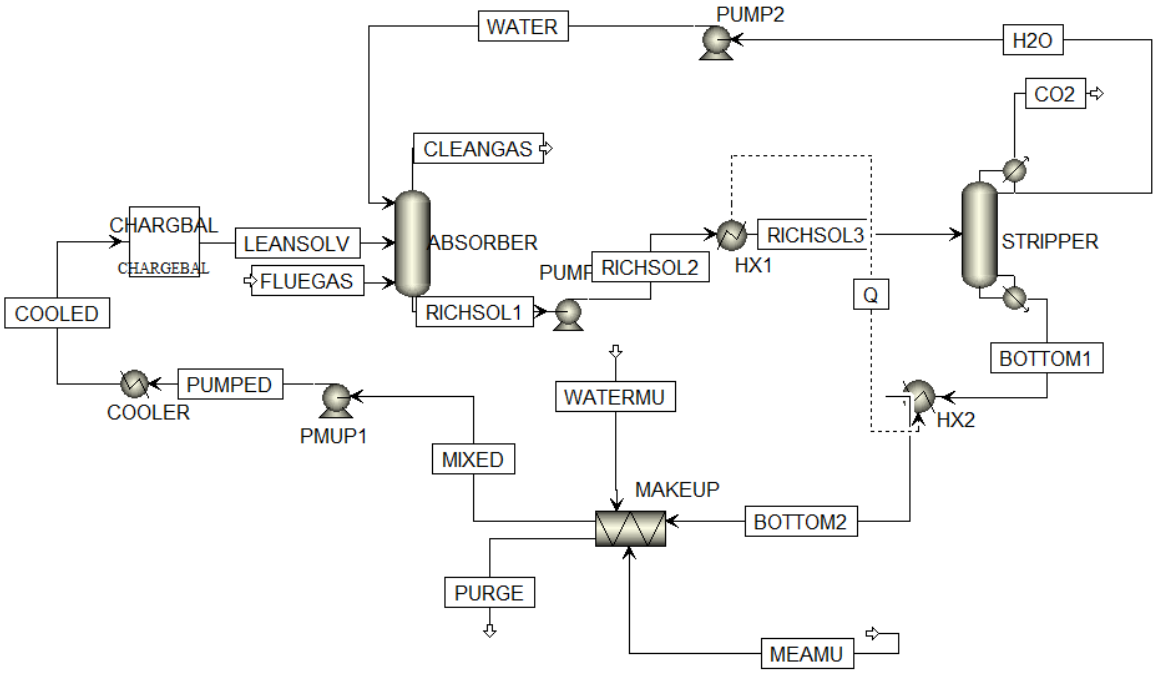



**Figure 3.19:** $CO_2$ capture using MEA flowsheet $CO_2$ capture from natural gas.

### 3.3.2 Technology of $CO_2$ capture from coal power plant using MEA

We have the same parameters as the technology of natural gas which is mentioned above for the ABSORBER in Configuration and Steams and Pressure. MEA is a commonly used solvent for $CO_2$ capture due to its high absorption capacity and relatively low energy requirements for regeneration. In the absorption process, the flue gas is brought into contact with the MEA solution in the absorber column, where $CO_2$ is absorbed into the solvent.

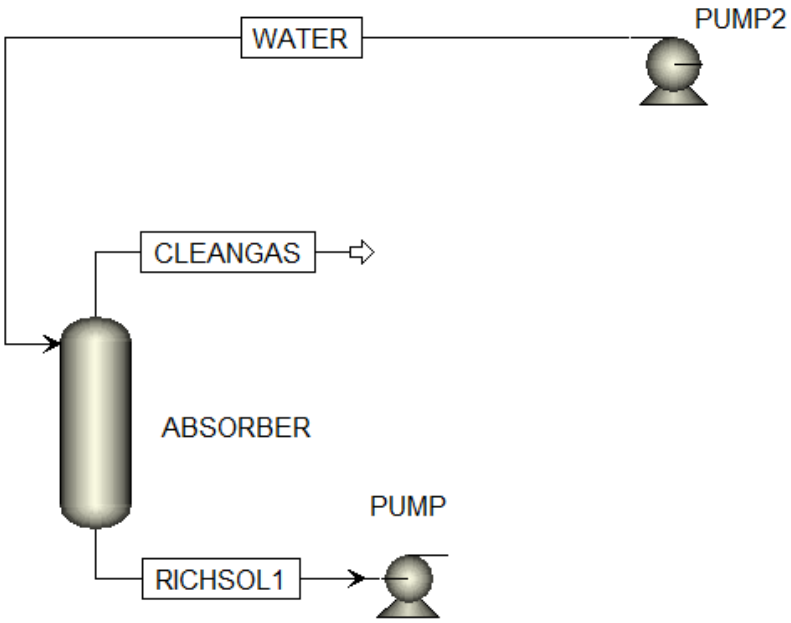



**Figure 3.20:** $CO_2$ capture due to its high absorption capacity of $CO_2$ capture from coal.

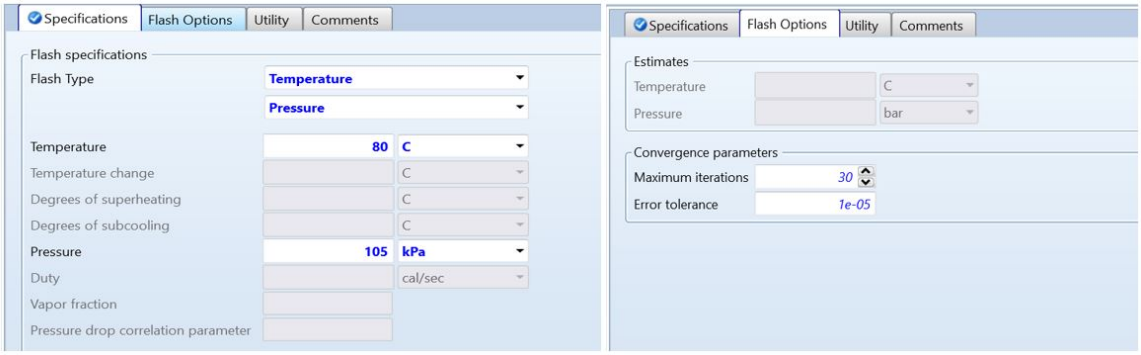



**Figure 3.21:** Specifications and Flash Options of HX1 (Heater) of $CO_2$ capture from coal.

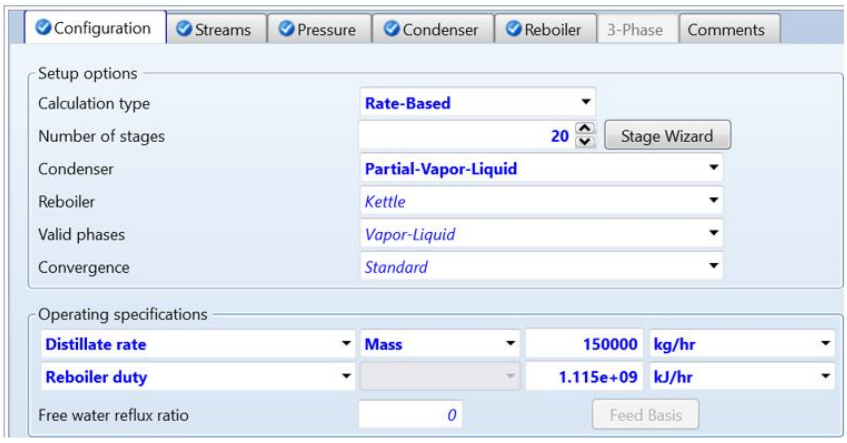



**Figure 3.22:** Configurations STRIPPER of $CO_2$ capture from coal.

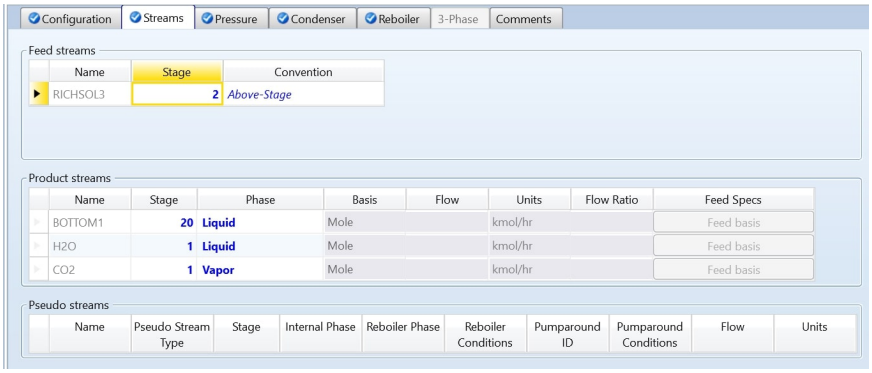



**Figure 3.23:** Stream Of STRIPPER of $CO_2$ capture from coal.

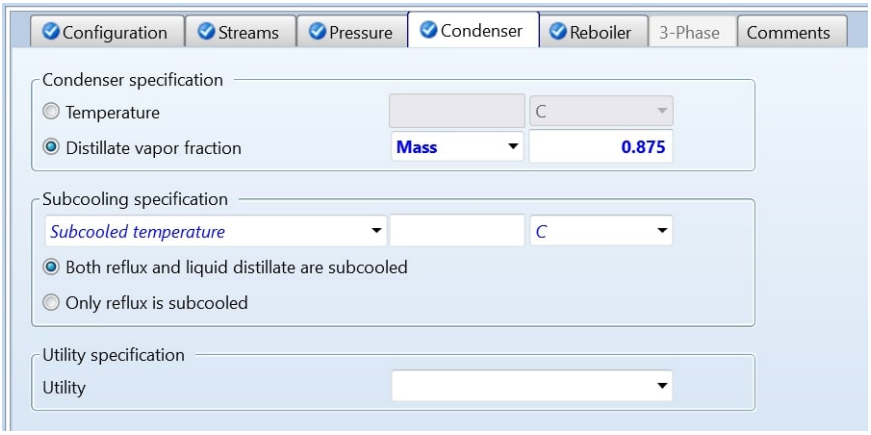



**Figure 3.24:** Condenser Of STRIPPER of $CO_2$ capture from coal.

The absorbed $CO_2$ -rich solvent is then sent to the stripper column, where the $CO_2$ is desorbed from the solvent through heating. The regenerated solvent is then recycled back to the absorber column for further $CO_2$ capture.

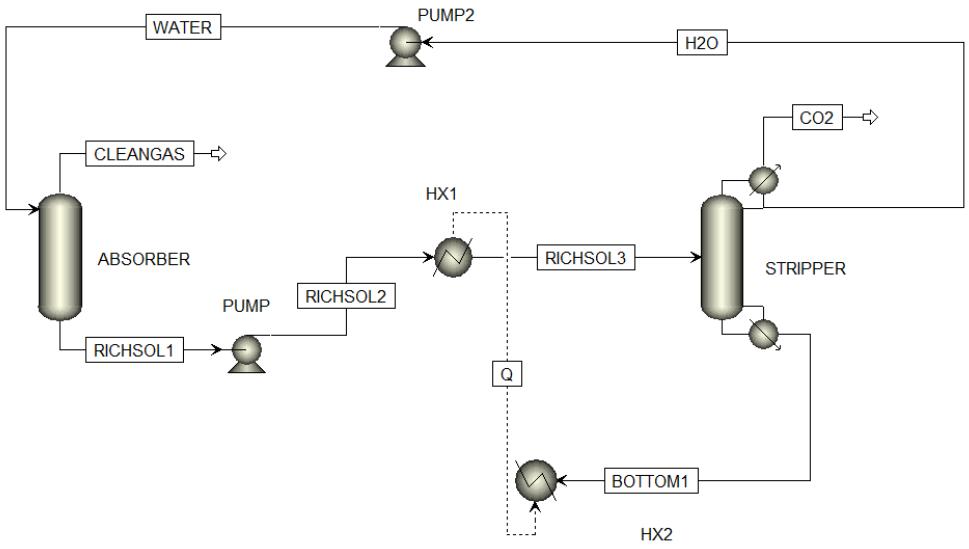



**Figure 3.25:** absorbed $CO_2$ -rich solvent is then sent to the stripper column of $CO_2$ capture from coal.

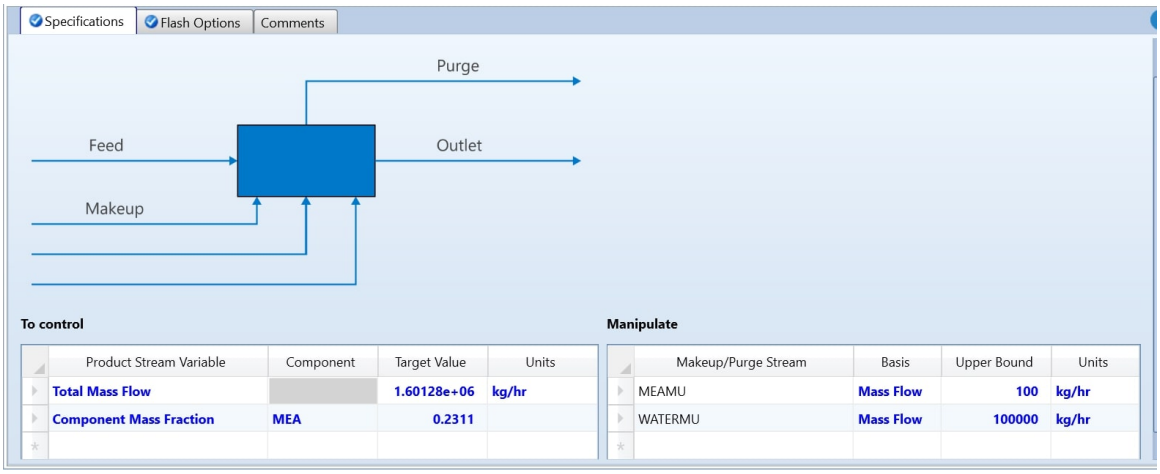



**Figure 3.26:** Spefications Of MAKEUP of $CO_2$ capture from coal.

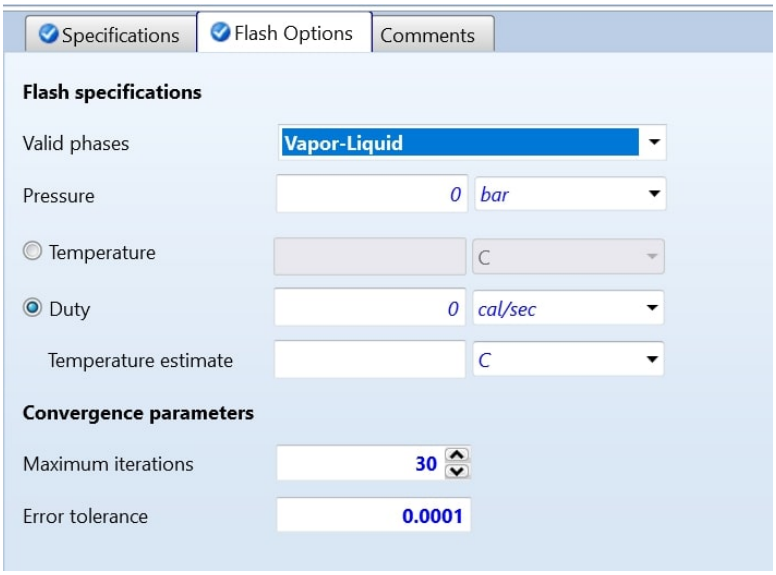



**Figure 3.27:** Flash Options of MAKEUP of $CO_2$ capture from coal.

The rate-based distillation model in Aspen Plus allows for a more detailed simulation of the mass transfer and reaction kinetics occurring in the absorber and stripper columns. This can help in optimizing the process conditions and equipment design for efficient $CO2$ capture.

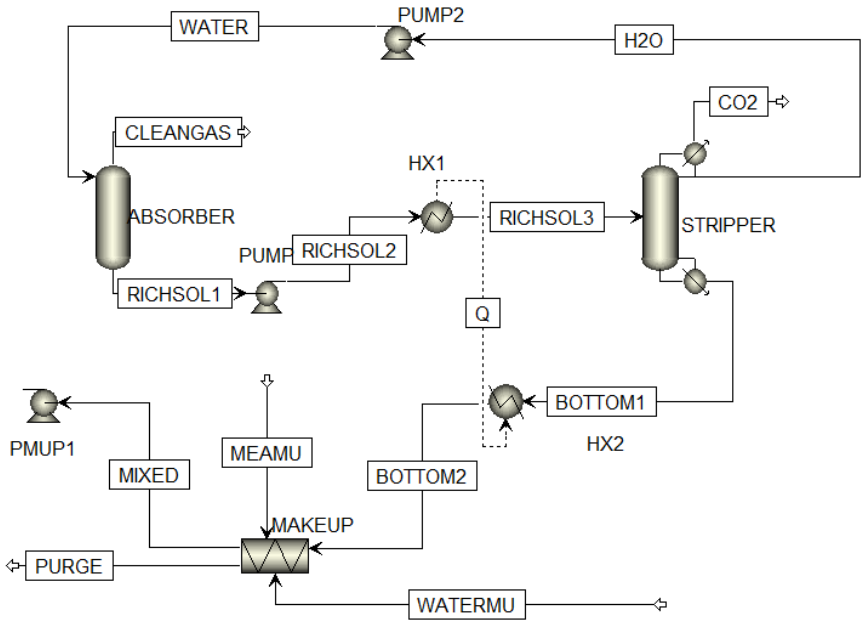



**Figure 3.28:** transfer and reaction kinetics occurring in the absorber and stripper columns of $CO_2$ capture from coal.

The solvent-based absorption technique is an important and mature solution for $CO_2$ capture. This **Aspen Plus** example models $CO_2$ capture from coal power plant flue gas at the rate of 1 million tons/year by using **MEA.** The absorber and stripper are modelled with the rate-based distillation model. It serves as a starting point for more complex models for process design and optimization, debottlenecking, and plant and equipment design.

The model includes the following key features:

• **ENRTL-RK** property method for the electrolytes system.

• ACIDGAS database for pure and binary pairs with proprietary parameters specifically for carbon capture and acid gas cleaning.

• **Kinetic** reactions for $CO_2$ and MEA.

• **Rate-based** model for distillation column simulation.

• Column Analysis for distillation column design and rating.

• Process $CO_2$ emission.

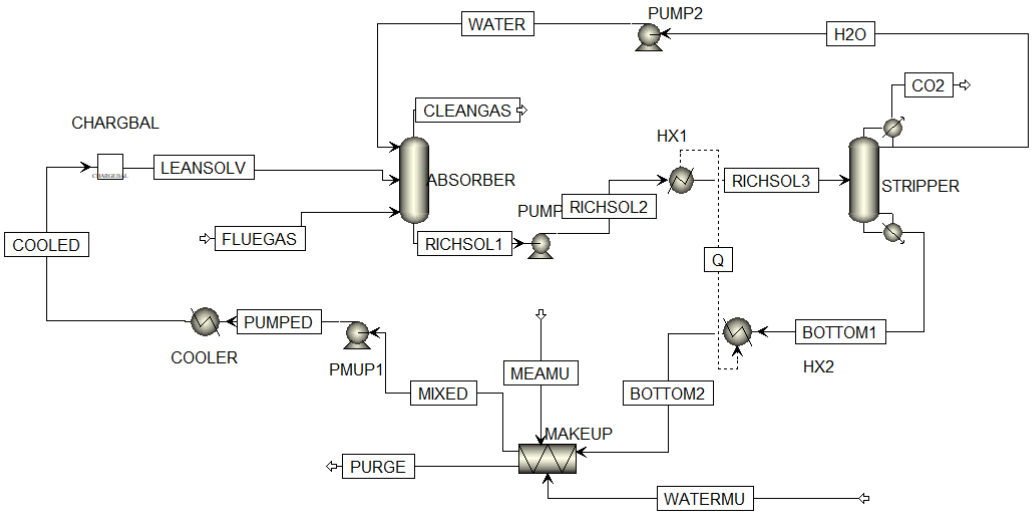



**Figure 3.29:** the rich solvent stream goes through a heat exchanger to increase the temperature to 80C of $CO_2$ capture from coal.

### 3.3.3 Technology of $CO_2$ capture from syngas for IGCC using MEA

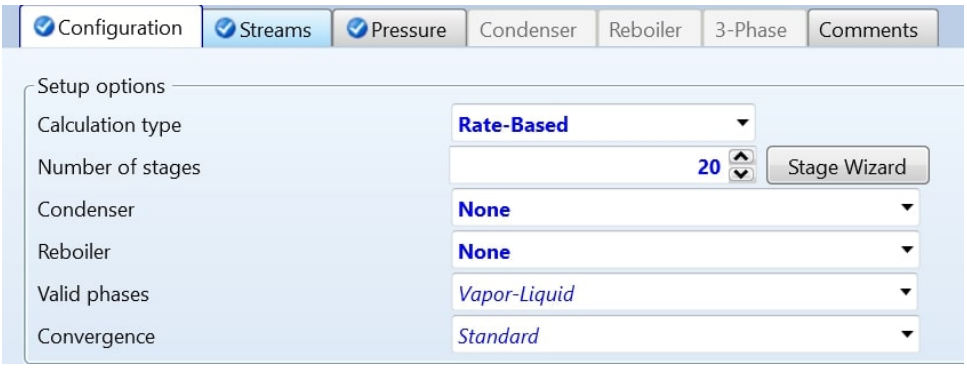



**Figure 3.30:** Configurations of ABSORBER (RedFrac) of $CO_2$ capture from syngas for IGCC.

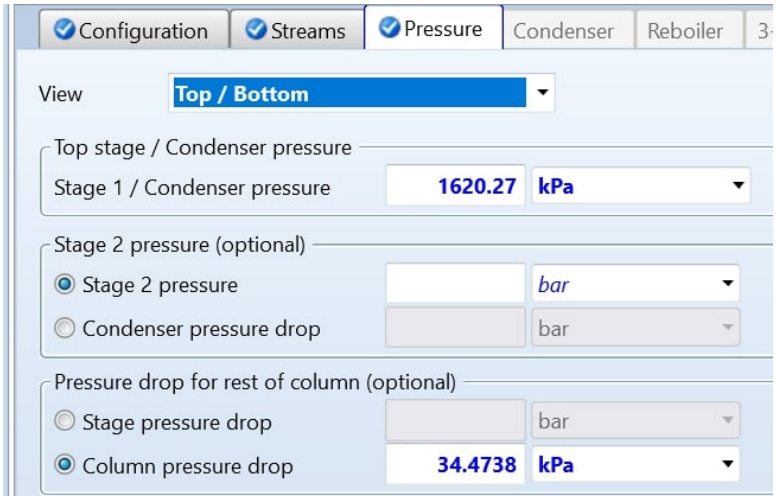



**Figure 3.31:** Pressureof ABSORBER (RedFrac) of $CO_2$ capture from syngas for IGCC.

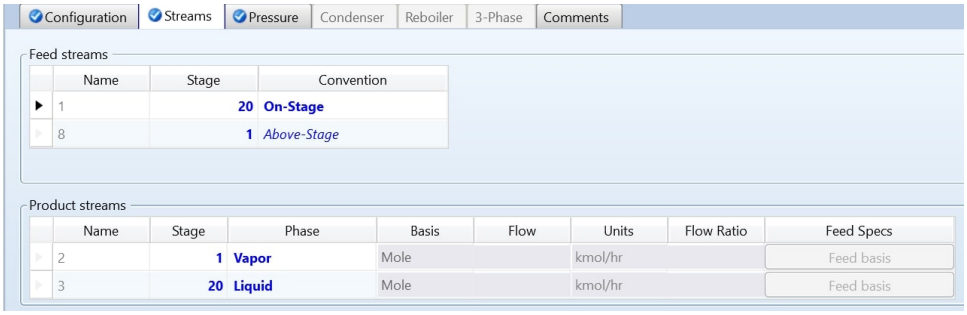



**Figure 3.32:** Streams of ABSORBER (RedFrac) of $CO_2$ capture from syngas for IGCC.

for this simulation, the dry flue gas, which consists of $CO_2$, $H_2$ and $N_2$, is sent to the absorber column to remove $CO_2$.

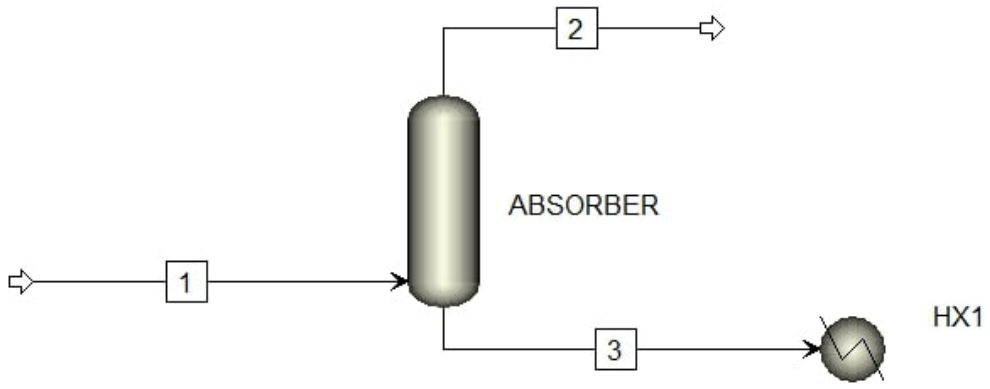



**Figure 3.33:** the dry flue gas, which consists of $CO_2$, $H_2$ and $N_2$ of $CO_2$ capture from syngas for IGCC.

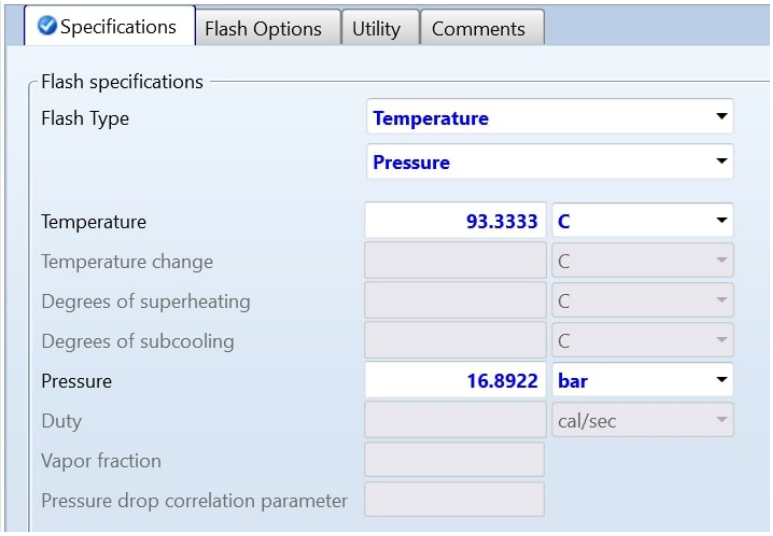



**Figure 3.34:** Specifications of HX1 (Heater) of $CO_2$ capture from syngas for IGCC.

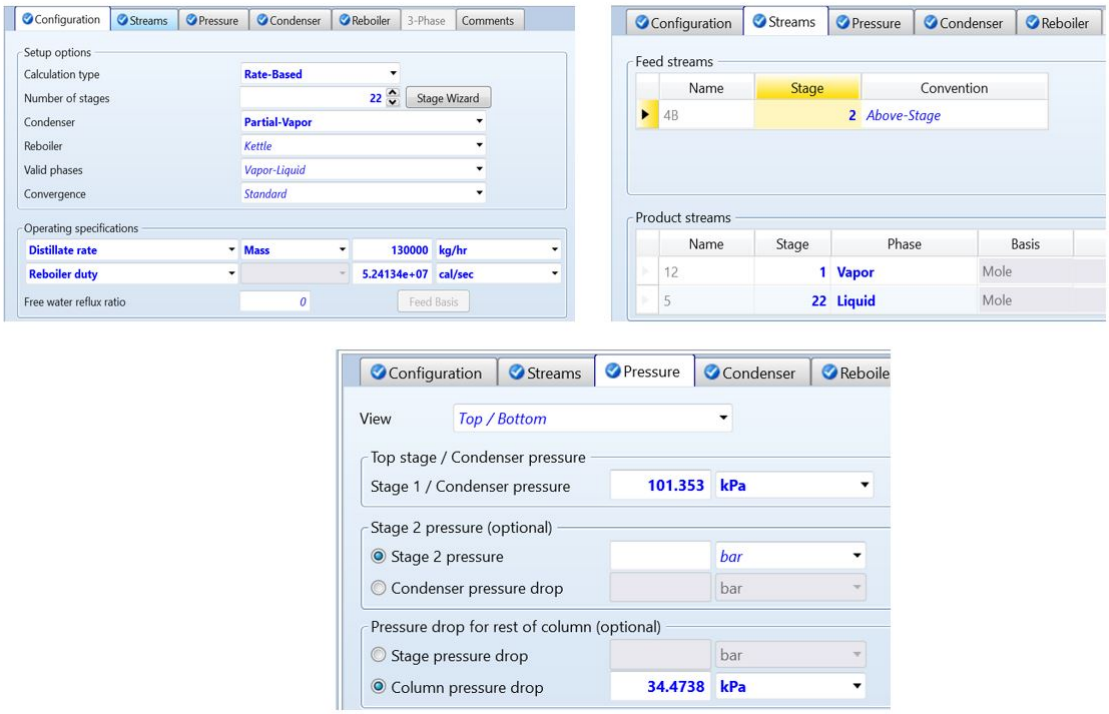



**Figure 3.35:** Configurations and Streams and Pressure of STRIPPER (RedFrac) of $CO_2$ capture from syngas for IGCC.

The packed absorber column is divided into **20 stages** in the simulation. The syngas enters the column at the bottom and the lean MEA solvent enters the column on stage 1.

$CO_2$ is absorbed by the solvent in the column.

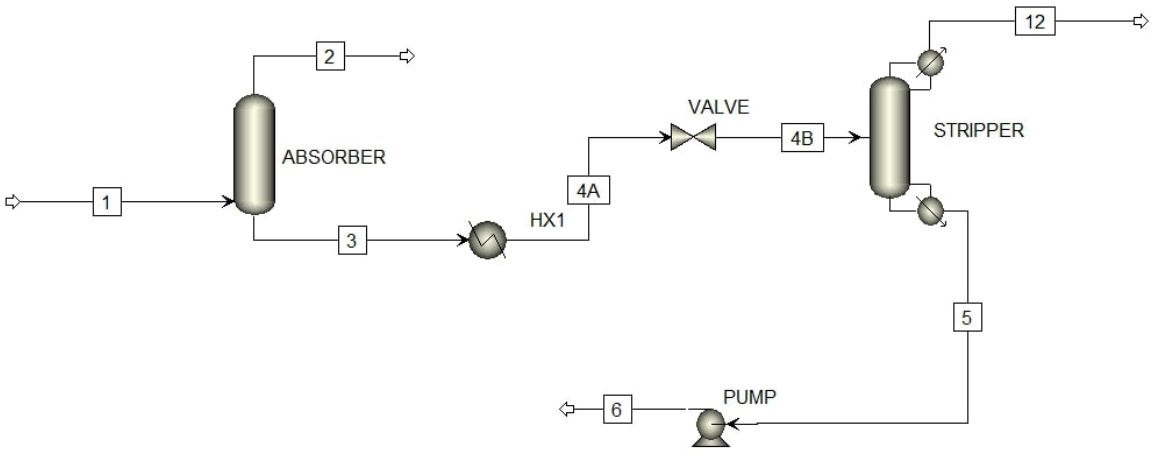



**Figure 3.36:** The packed absorber column is divided into **20 stages** in the simulation of $CO_2$ capture from syngas for IGCC.

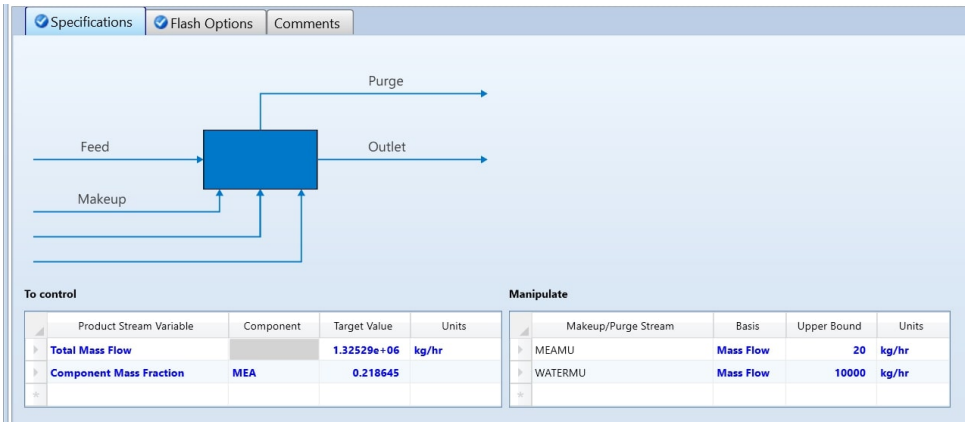



**Figure 3.37:** Specifications of MAKEUP of $CO_2$ capture from syngas for IGCC.

Clean gas comes out the top of the absorber and the rich solvent leaves the absorber from the bottom and is sent to the stripper.

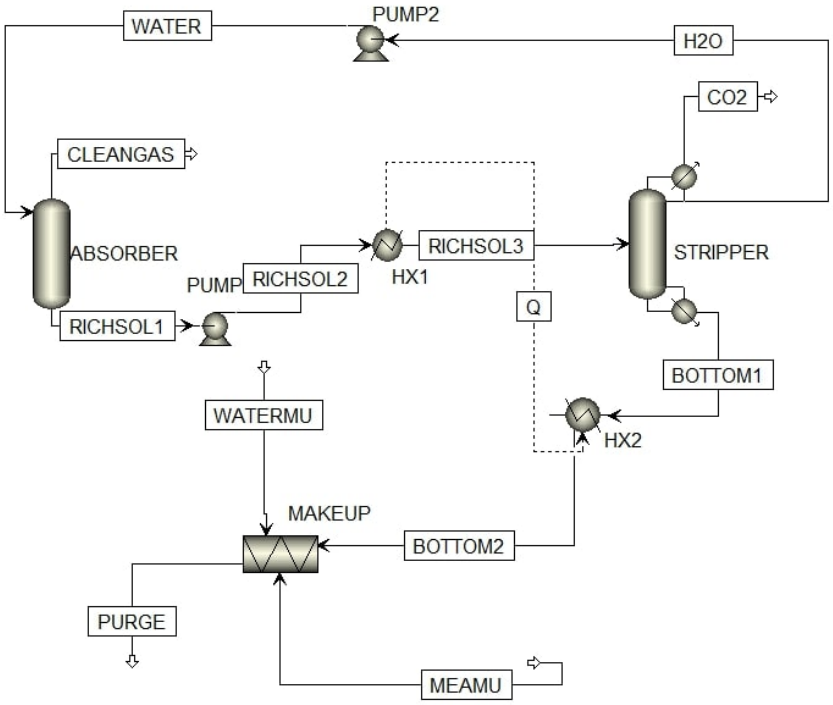



**Figure 3.38:** the absorber from the bottom and is sent to the stripper of $CO_2$ capture from syngas for IGCC.

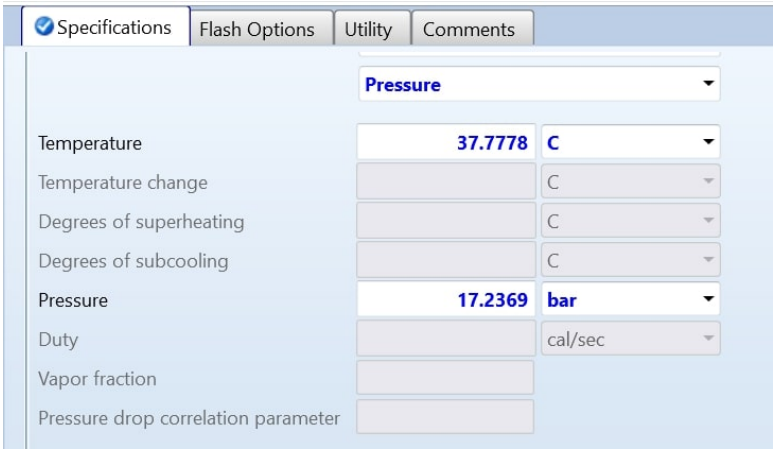



**Figure 3.39:** Specifications of COOLED (Heater) of $CO_2$ capture from syngas for IGCC.

Before entering the stripper, the rich solvent stream goes through a heat exchanger to increase the temperature to 200 F. The stripper is divided into 22 stages in the simulation. Rich solvent enters the stripper column in the first stage. $CO_2$ is stripped from the rich amine in the column and the MEA solvent is regenerated. The lean solvent from the bottom of the stripper is recycled with makeup back to the absorber.

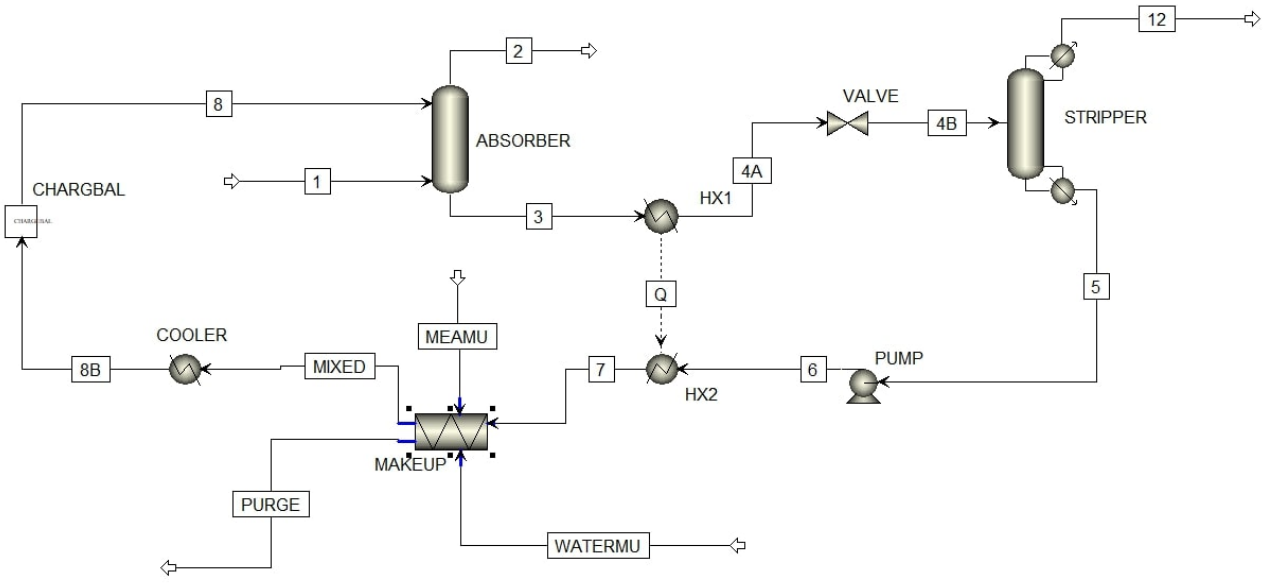



**Figure 3.40:** The lean solvent from the bottom of the stripper is recycled with makeup back to the absorber of $CO_2$ capture from syngas for IGCC.

# 4

# Result and Discussion

# 4.1 Result and Discussion

In this chapter, we analyze the data derived from our simulation to evaluate and compare the amount of carbon dioxide captured during one year of each carbon capture technique

## 4.1.1 $CO_2$ Capture from Natural Gas Power Plant Using MEA

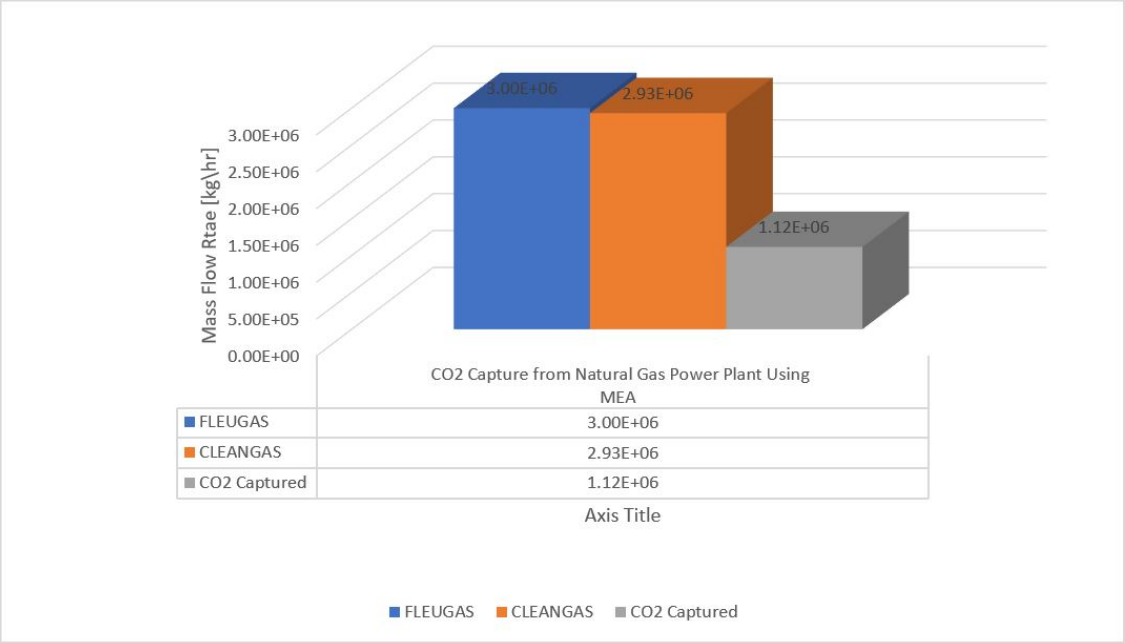



**Figure 4.1:** Quantity of Fleugas, cleangas and $CO_2$ captured during one year.

In Figure 4.2, it is evident that the quantity of CO2 captured from a natural gas power plant using monoethanolamine (MEA) is Solid. The figure illustrates the effectiveness of MEA as a solvent in the absorption of carbon dioxide, a critical process for reducing greenhouse gas emissions from natural gas combustion. The high capture rate demonstrated suggests that MEA-based carbon capture technology can play a pivotal role in mitigating climate change by significantly lowering the carbon footprint of natural gas power plants. This emphasizes the necessity of integrating such advanced capture methods in existing and future natural gas infrastructure to achieve environmental sustainability goals.

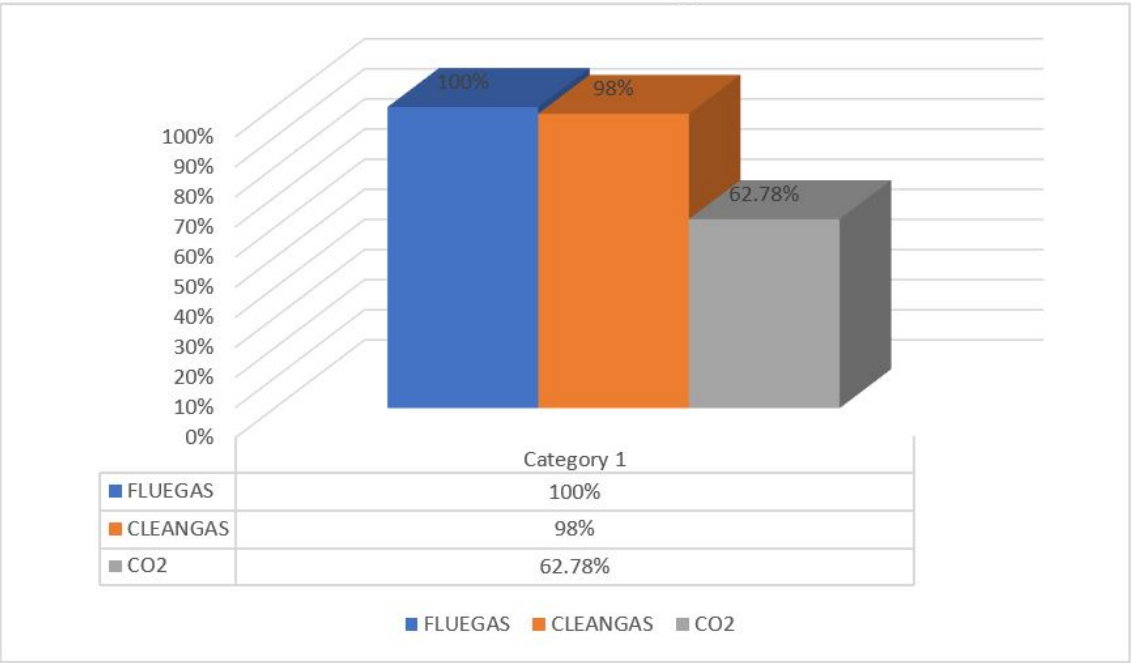



**Figure 4.2:** percentage of $CO_2$ Captured compared to the Fluegas and Cleangas

The near $99.4\%$ percentage $CO_2$ capture efficiency observed in your figure aligns with the benefits of using MEA for NG power plant decarburization.

### 4.1.2 $CO_2$ Capture from Coal Power Plant Using MEA

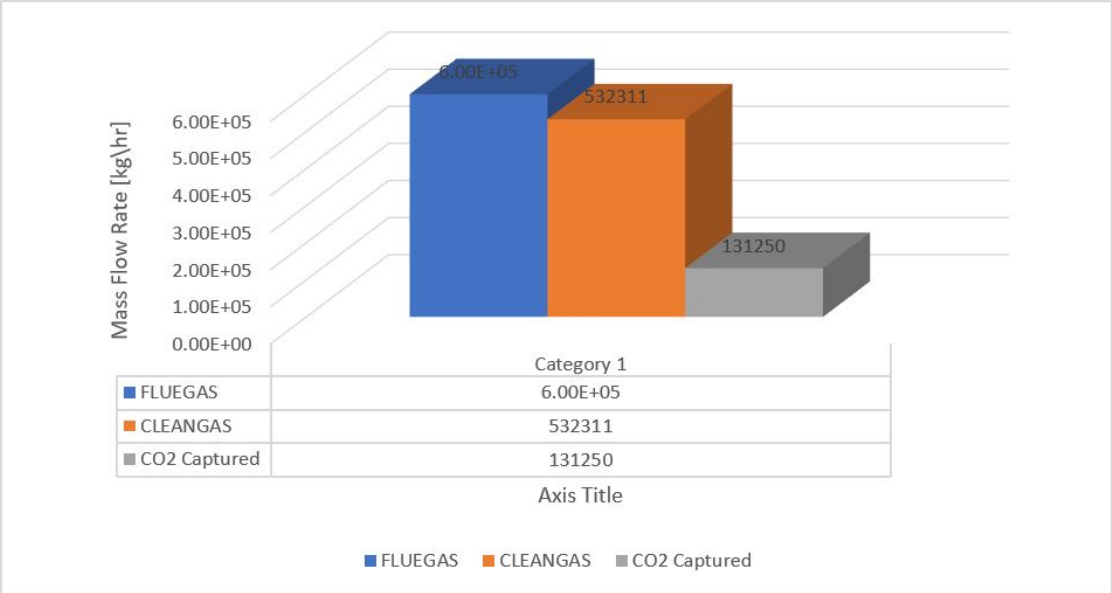



**Figure 4.3:** Quntity of Flue gas, clean gas and Carbon dioxide captured during one year.

In Figure 4.3, it is apparent that the volume of $CO_2$ captured from a coal-fired power plant using monoethanolamine (MEA) is substantial. The graph indicates that the implementation of MEA for $CO_2$ capture in coal power plants results in a notably high efficiency of carbon dioxide sequestration, highlighting the potential of MEA as an effective solvent in reducing greenhouse gas emissions from coal-based energy production. The data underscores the importance of adopting advanced carbon capture technologies to mitigate the environmental impact of fossil fuel power generation.

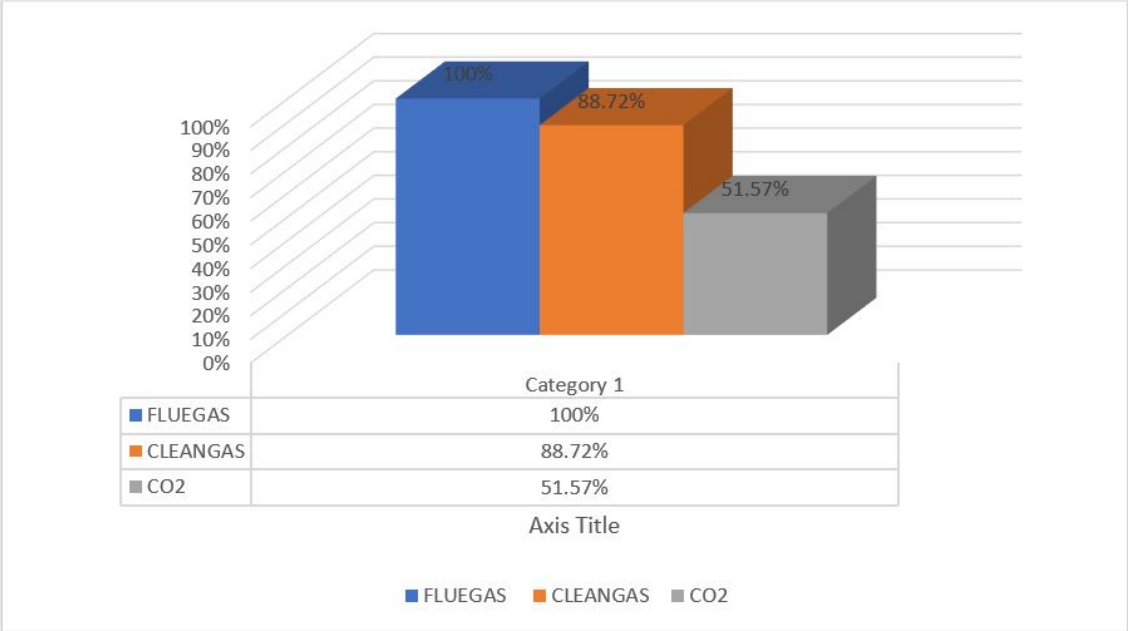



**Figure 4.4:** percentage of Co2 Captured compared to the Fluegas and Cleangas.

The efficiency of $CO_2$ capture from a coal power plant using monoethanolamine (MEA) typically depends on several factors such as MEA Concentration, Gas flow rate, and $CO_2$ concentration. In Figure 4.4, we observe a high $CO_2$ capture efficiency for CCS in coal-based power plants, attributed to the elevated concentration of $CO_2$.

### 4.1.3 $CO_2$ Capture from Syngas for IGCC Using MEA

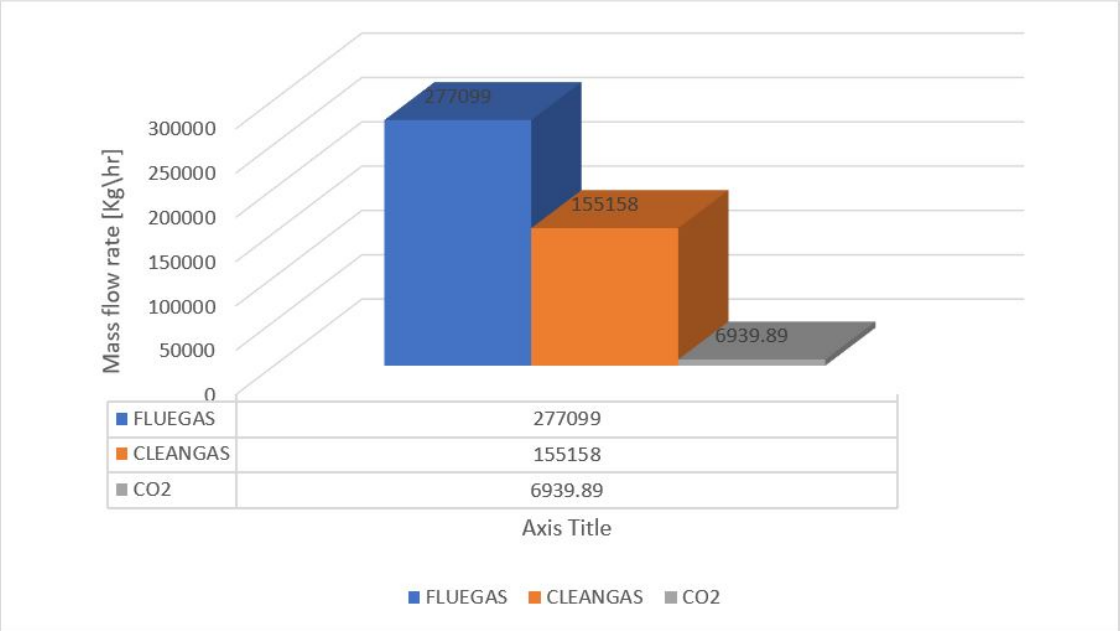



**Figure 4.5:** Quntity of Flue gas, Clean and Carbon dioxide captured during one year.

In Figure 4.5, we observe the quantity of $CO_2$ captured using the solvent-based absorption technique, which is recognized as an important and mature solution for $CO_2$ capture. This example, modeled using Aspen Plus, demonstrates the application of $CO_2$ capture from syngas in an Integrated Gasification Combined Cycle (IGCC) system. The model highlights the efficiency and reliability of solvent-based absorption in capturing significant amounts of $CO_2$, thereby enhancing the environmental performance of IGCC technology.

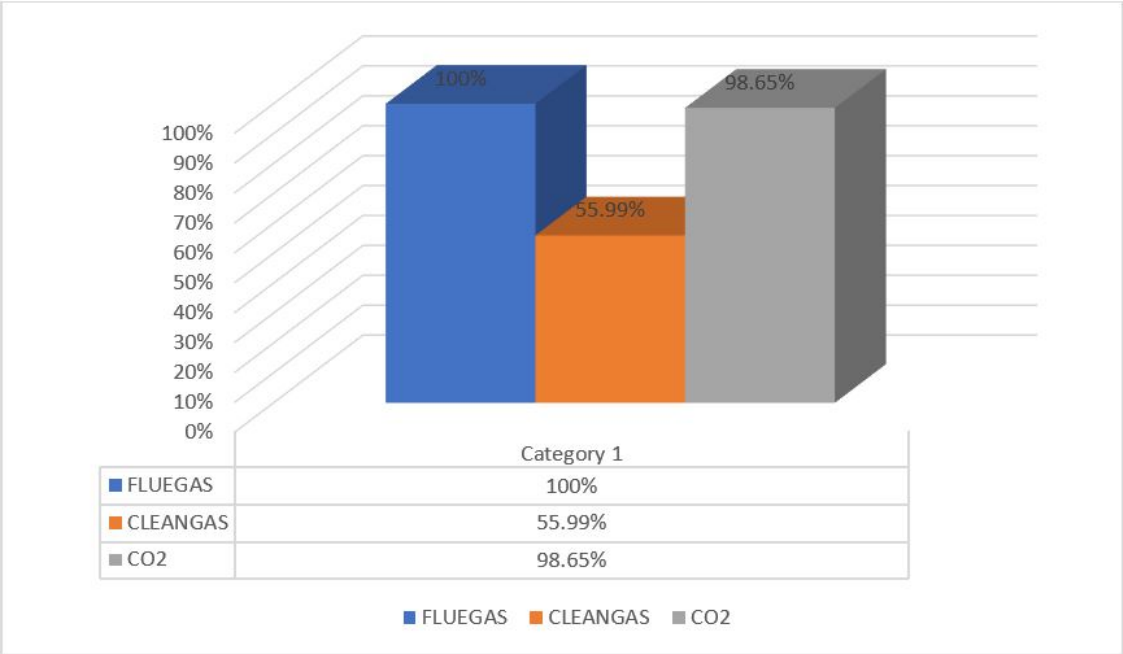



**Figure 4.6:** percentage of $CO_2$ captured compared to the Flue gas and clean gas.

Figure 4.6 represents the percentage of $CO_2$ captured by the $CO_2$ Capture from Syngas for IGCC Using the MEA technique, the efficiency depends on MEA concentration, process parameters, and economic factors. The specific efficiency value may vary based on the detailed system design and operating conditions. In our study, we utilized the default parameters in **ASPEN Plus** to achieve a high $CO_2$ capture efficiency.

# General Conclusion

In this study, we explored three distinct $CO_2$ capture technologies:

1. $CO_2$ Capture from Natural Gas Power Plant Using MEA: This method involves using monoethanolamine MEA as a solvent to selectively capture $CO_2$ emissions from natural gas power plants. It offers a promising approach to mitigate greenhouse gas emissions.

2. $CO_2$ Capture from Coal Power Plant Using MEA: Similar to the previous method, this technology employs MEA to capture $CO_2$ from coal-fired power plants. Despite the challenges associated with coal combustion, MEA -based capture remains a viable option for reducing $CO_2$ emissions.

3. $CO_2$ Capture from Syngas for IGCC Using MEA: Integrated Gasification Combined Cycle IGCC power plants produce syngas, which contains $CO_2$. By utilizing MEA, we can efficiently capture $CO_2$ from syngas streams, contributing to cleaner energy production.

Our work builds upon previous research focused on hydrogen production via methane reforming. By leveraging existing knowledge and adapting it to $CO_2$ capture, we contribute to the ongoing efforts to combat climate change.

In summary, these MEA -based technologies hold promise for achieving sustainable energy solutions while minimizing environmental impact. As we continue to refine and implement these methods, we move closer to a greener and more resilient future.

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