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Performance Evaluation of Monoethanolamine Solvents for Post-Combustion Carbon Dioxide Removal in the Cement Industry

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Abstract: **This study investigated the modeling and simulation of an MEA-based CO_2 capture process for cement plant flue gas using Aspen Plus. The objective was to evaluate the performance of chemical absorption in reducing CO_2 emissions, given the cement industry's role as a major source of greenhouse gases. A process flow diagram was developed consisting of an absorber, stripper, heat exchangers, pumps, and separation units. The flue gas composition considered was CO_2 (31.8%), H_2O (4.2%), O_2 (2.4%), and N_2 (61.6%). Monoethanolamine (MEA) was used as the solvent due to its high reactivity with CO_2 and established industrial application. The absorber facilitated CO_2 capture by chemical reaction with MEA, while the stripper regenerated the solvent and released concentrated CO_2 for compression and storage. Rigorous thermodynamic and mass transfer models were applied to optimize operating parameters such as temperature, pressure, solvent circulation rate, and reflux ratio. Simulation results demonstrated a CO_2 recovery efficiency of approximately 93.27%, confirming the process's effectiveness. The study concluded that MEA absorption remains a reliable and scalable technology for post-combustion CO_2 capture in cement plants, with potential for integration into broader carbon management strategies.**

Keywords: **Aspen HYSYS, Carbon Capture, Cement Industry, Chemical Absorption, Design Expert, Flue Gas, Monoethanolamine, Process Optimization, Process Simulation, Solvent Regeneration.**

I. INTRODUCTION

The cement industry plays a critical role in global infrastructure development but is also one of the most carbon-intensive industrial sectors. It accounts for approximately 7--8% of total anthropogenic carbon dioxide (CO_2) emissions, making it a major contributor to climate change[1]. These emissions are primarily due to two factors: the calcination of limestone ($CaCO_3$) to produce lime (CaO), which releases CO_2 as a byproduct, and the combustion of fossil fuels to generate the high temperatures required in cement kilns. As global environmental concerns escalate, there is a growing need for the cement industry to adopt effective CO_2 mitigation strategies. Among the various technological approaches to reducing CO_2 emissions, Carbon Capture and Storage (CCS) has emerged as one of the most promising solutions. In particular, chemical absorption using amine-based solvents, especially monoethanolamine (MEA), is recognized as a mature and widely applied method for post-combustion CO_2 capture.

MEA is favored for its strong affinity to CO_2, relatively low cost, and availability, making it suitable for large-scale industrial applications[2]. The MEA-based process involves the absorption of CO_2 from flue gas into an MEA solution, followed by regeneration of the solvent through heating, which releases the captured CO_2 for compression and storage. However, the MEA-based CO_2 capture process is not without its challenges. One of the most significant drawbacks is the high energy demand associated with solvent regeneration, which can negatively impact the energy efficiency and economic viability of the overall cement production process. Moreover, MEA is prone to thermal degradation, oxidative degradation, and corrosion, which can increase operational costs and complicate long-term deployment.

To optimize the performance of MEA-based CO_2 capture systems, advanced process simulation tools are essential. Aspen Plus, a widely used process modeling software, provides a powerful platform for simulating and analyzing chemical processes, including carbon capture. With Aspen Plus, researchers and engineers can model the MEA absorption process, evaluate the effects of varying operational parameters, and identify optimal conditions for maximizing CO_2 capture efficiency while minimizing energy consumption and cost[3]. Simulation and optimization through Aspen hysys enable a detailed understanding of the process dynamics and provide valuable insights for scale-up and implementation in real cement plants. By adjusting key process variables such as MEA concentration, absorber and stripper temperatures, gas and solvent flow rates, and pressure conditions, the system's performance can be significantly improved.

This study focuses on the optimization of MEA-based CO_2 capture in a cement plant using Aspen hysys simulation. It aims to systematically analyze how various parameters affect CO_2 capture performance and to identify the optimal set of conditions for efficient operation. The insights derived from this research will contribute to developing more sustainable practices in the cement industry and support broader global efforts to combat climate change by reducing greenhouse gas emissions. By providing a detailed and practical simulation-based approach, this work not only addresses the pressing issue of industrial CO_2 emissions but also aligns with international decarbonization goals set forth in agreements such as the Paris Accord. The implementation of optimized CO_2 capture solutions in energy-intensive industries like cement manufacturing represents a critical step toward achieving a low-carbon future.

II. LITERATURE REVIEW

Body of article gives the complete description of research work. It includes problem statement, methodology used for solving problem, proposed solution of given problem, conclusion of complete research. All paragraphs/ Sections of the paper should be justified and well organized. We accept manuscripts written in English Language and should be in third person. Words used in body are around 2000 to 8000 words or 5 to 20 pages. Page Layout Details is given in TABLE: I.

A. Cement Industry and CO_2 Emissions

The cement industry is among the most significant industrial contributors to global CO_2 emissions. This is largely due to the dual emission sources inherent in its production process— fuel combustion and calcination. On average, cement production accounts for approximately 7% of global anthropogenic CO_2 emissions, making it a critical focus for climate change mitigation strategies[4]. This substantial contribution arises from the necessity of high-temperature processing and the unavoidable release of CO_2 during raw material transformation. Cement is primarily composed of clinker, a material produced by heating limestone ($CaCO_3$) and other raw materials in a rotary kiln at temperatures exceeding 1400°C. This process, known as calcination, decomposes the calcium carbonate into calcium oxide (CaO) and carbon dioxide (CO_2), releasing large volumes of greenhouse gases. It is estimated that approximately 60% of the emissions from cement production originate from this calcination reaction alone, while the remaining 40% are attributable to the combustion of fossil fuels such as coal, petcoke, and natural gas[5]. The increasing demand for cement, driven by urbanization and infrastructure development, particularly in rapidly industrializing regions, continues to amplify the sector's environmental impact. With global population growth and urban expansion, cement production is projected to increase significantly in the coming decades. Despite advancements in alternative materials and production efficiency, these projections make it evident that the industry's CO_2 emissions will remain substantial without significant intervention. To combat these emissions, various mitigation strategies have been proposed and implemented. These include improving energy efficiency, switching to alternative fuels, using clinker substitutes such as fly ash and slag, and advancing innovative binders that require less energy to produce. While these methods contribute to reducing emissions, they are not sufficient to meet the aggressive targets set by international agreements such as the Paris Accord. The inherent emissions from the calcination process remain a persistent challenge, thereby positioning carbon capture and storage (CCS) as a vital technology for the future of low-carbon cement production[6].

Carbon capture involves the separation of CO_2 from industrial flue gases, followed by its transportation and storage in geological formations. Among various carbon capture approaches, post-combustion capture is the most compatible with existing cement plants, allowing retrofitting without altering the core production process. This method typically employs chemical solvents, particularly amines like Monoethanolamine (MEA), which react with CO_2 to form a compound that can later be regenerated to release pure CO_2 for storage or utilization[2]. However, implementing MEA-based carbon capture in the cement industry presents several challenges. The energy required for regenerating the solvent is substantial,

contributing to increased operational costs. Additionally, solvent degradation and equipment corrosion are significant concerns that must be addressed to ensure long-term viability. The integration of CO_2 capture systems into cement plants also involves complex thermal and mass balance considerations, which can impact the efficiency of the overall process. This is where process simulation tools like Aspen hysys come into play. Aspen hysys is a powerful chemical process modeling software that enables researchers and engineers to design, simulate, and optimize industrial processes. It allows for the detailed representation of chemical reactions, thermodynamic behavior, and equipment specifications, providing insights into system performance under various operating conditions. In the context of MEA-based CO_2 capture, Aspen hysys can simulate the absorption and regeneration processes, track energy requirements, and identify performance bottlenecks. Several studies have demonstrated the utility of Aspen hysys in modeling CO_2 capture systems for cement and other industrial sectors. These simulations help identify optimal operating conditions that minimize energy consumption and enhance CO_2 removal efficiency. Moreover, they enable sensitivity analyses to assess the impact of different variables, providing a comprehensive understanding of the system dynamics. By integrating these insights, plant operators can make informed decisions about implementing capture technologies, improving both environmental and economic outcomes[7].

B. Carbon Capture Technologies

As the world strives to meet ambitious climate goals, the development and implementation of carbon capture technologies have become essential for mitigating greenhouse gas emissions. Among these technologies, carbon capture, utilization, and storage (CCUS) is seen as a critical solution for industries such as cement, steel, and chemical manufacturing, which are difficult to decarbonize through efficiency improvements alone[8]. This section explores the various carbon capture technologies, with a particular focus on post-combustion capture using amine-based solvents like Monoethanolamine (MEA), which has gained considerable attention for its effectiveness and versatility.

Overview of Carbon Capture Technologies

Carbon capture technologies can be broadly classified into three categories based on the stage at which CO_2 is captured: pre-combustion, post-combustion, and oxy-fuel combustion[9]. Each approach has its advantages and challenges, making their applicability dependent on the specific industry and the CO_2 source.

I. Pre-combustion capture: involves converting fossil fuels into a mixture of hydrogen and CO_2 before combustion. This approach is often used in integrated gasification combined cycle (IGCC) power plants. It allows for CO_2 to be removed before it is emitted into the atmosphere. However, pre-combustion technologies are generally more complex and are mainly applicable in power generation rather than industrial applications like cement production.

II. Post-combustion capture: it is employed after the fossil fuels have been burned and CO_2 has been emitted. This is the most common approach for retrofitting existing industrial plants, such as cement factories, where it can be applied directly to flue gas streams. Post-combustion capture typically uses solvents, solid adsorbents, or membrane systems to separate CO_2 from the exhaust gases. Among these, amine scrubbing (using solvents such as MEA) is the most well-established and widely used technology.

III. Oxy-fuel combustion: involves burning fossil fuels in an environment enriched with oxygen, rather than air. This creates a flue gas that is primarily composed of CO_2 and water vapor, making it easier to separate the CO_2. However, oxy-fuel combustion requires significant modifications to combustion equipment, and the availability of pure oxygen can be a limiting factor.

While pre-combustion and oxy-fuel combustion are innovative, post-combustion capture remains the most feasible and widely implemented solution, particularly for existing facilities that are not designed to handle the complexities of pre-combustion or oxy-fuel technologies.

Post-Combustion CO_2 Capture Using Amines

Among the various methods of post-combustion CO_2 capture, amine-based absorption is the most developed and commercialized technique. This process involves the use of amine solvents like Monoethanolamine (MEA), which react with CO_2 to form a reversible compound. Once the CO_2 is absorbed, the solvent is regenerated by heating, releasing the captured CO_2 and enabling the solvent to be reused[2]. Amine-based systems are highly effective in capturing CO_2 from

dilute gas streams, such as those found in cement plant flue gases. The key advantage of MEA-based systems is their relatively high capacity for CO_2 absorption, which can be enhanced by adjusting operating conditions such as temperature, pressure, and solvent concentration. However, the regeneration of the solvent requires a significant amount of energy, making this process energy-intensive and costly. Moreover, MEA is susceptible to degradation when exposed to impurities such as oxygen, sulfur compounds, and particulate matter in the flue gas, which can reduce the system's efficiency over time[10].

Emerging Developments in CO_2 Capture

In addition to amine-based absorption, several alternative carbon capture technologies are being explored to improve efficiency and reduce costs. These include:

i. Solid Adsorbents: These materials capture CO_2 through surface adsorption. Solid adsorbents, such as zeolites, metal-organic frameworks (MOFs), and activated carbon, have shown promise for CO_2 capture due to their high surface area and selectivity for CO_2. They offer several advantages over liquid solvents, including lower energy requirements for regeneration and reduced solvent degradation. However, they face challenges in terms of long-term stability and the ability to handle large-scale flue gas volumes typical in industrial settings.

ii. Membrane Separation: Membrane-based systems use selective permeation to separate CO_2 from gas streams. Membranes can be designed to allow CO_2 to pass through while blocking other gases like nitrogen and oxygen. This technology offers the potential for compact, modular systems that can be easily integrated into existing plants. However, membrane systems are still in the developmental phase and face challenges related to long-term performance, permeability, and scalability.

iii. Cryogenic Distillation: This method involves cooling the flue gas to temperatures where CO_2 condenses, allowing for separation. While cryogenic distillation offers high purity CO_2 capture, it requires substantial refrigeration energy, making it less energy efficient compared to other methods.

iv. Biological CO_2 Capture: This innovative approach uses microorganisms, such as algae or bacteria, to capture CO_2 in a biological process. While it holds promise for future applications, it is still in the early stages of development and faces challenges related to scale-up and cost-effectiveness.

C. Monoethanolamine (MEA) In CO_2 Capture

Monoethanolamine (MEA) is one of the most commonly used solvents in post-combustion CO_2 capture technologies, particularly for industrial applications such as cement plants, power plants, and natural gas processing. MEA has gained widespread attention due to its ability to effectively absorb CO_2 from flue gas streams at relatively low concentrations. This section discusses the role of MEA in CO_2 capture, its advantages, limitations, and the challenges associated with its use.

Overview of Monoethanolamine (MEA)

Monoethanolamine is an amine compound with the chemical formula C_2H_7NO. It is a colorless, hygroscopic liquid with a strong ammonia-like odor, and it is widely used in chemical industries for a variety of applications, including gas purification, water treatment, and as a component in pharmaceutical formulations. In CO_2 capture, MEA functions as a chemical absorbent, reacting with CO_2 to form a carbamate, which can be subsequently regenerated through heating, releasing the captured CO_2. The effectiveness of MEA as a CO_2 solvent stems from its high reactivity and affinity for CO_2. The reaction between MEA and CO_2 produces a stable carbamate that can be broken down in a subsequent regeneration process, which typically occurs in a stripper column where heat is applied. The regeneration process releases CO_2 in a concentrated form, which can then be transported for storage or utilization.

Advantages of MEA in CO_2 Capture

I. High CO_2 Absorption Capacity: MEA's ability to absorb a large amount of CO_2 makes it an effective solvent for post-combustion CO_2 capture. The high reaction rate of MEA with CO_2 ensures efficient removal from flue gas streams, even at low CO_2 concentrations[10]. This property is particularly valuable for applications like cement production, where CO_2 concentrations in exhaust gases tend to be relatively low.

II. Mature and Well-Understood Technology: MEA-based absorption has been in use for decades in gas purification applications, which means the technology is well-developed and understood. Its commercial viability and scalability have been demonstrated in various industrial settings, including power plants, natural gas processing, and cement plants. This maturity provides a foundation for its application in CO_2 capture, as operators can draw on extensive operational experience to optimize performance.

III. Flexibility and Retrofit Potential: MEA-based CO_2 capture systems can be retrofitted to existing industrial plants, including cement facilities, without requiring major modifications to the core production process. This flexibility makes it a highly attractive option for industries that are looking to reduce their CO_2 emissions while continuing to operate their existing infrastructure.

IV. Relatively Low Cost: Among the various solvents available, MEA is considered to be one of the more cost-effective options. Although the regeneration process is energy-intensive, the overall cost of MEA as a solvent is relatively low compared to some alternative solvents or capture technologies. This makes MEA a popular choice, particularly in industries where budget constraints are a significant concern.

Challenges and Limitations of MEA in CO_2 Capture

Despite its advantages, the use of MEA in CO_2 capture presents several challenges that must be addressed to ensure its long-term viability in industrial applications.

I. High Energy Consumption for Regeneration: One of the main drawbacks of MEA based CO_2 capture is the high energy requirement for solvent regeneration. The process of heating the solvent to release the captured CO_2 is energy-intensive, and it contributes significantly to the operational cost of the system. For cement plants, which already face high energy demands, this additional energy burden can make the implementation of MEA-based capture economically challenging[2].

II. Solvent Degradation: MEA is prone to degradation due to exposure to impurities in the flue gas, such as sulfur compounds, oxygen, and particulate matter. This degradation leads to a loss of absorption capacity and the formation of byproducts that can accumulate and reduce the efficiency of the system over time. To mitigate solvent degradation, it is necessary to monitor and maintain the solvent quality regularly, which adds to the operational cost and complexity of the CO_2 capture system[11].

III. Corrosion and Equipment Maintenance: The use of MEA can result in the formation of corrosive byproducts, such as heat-stable salts, which can damage the equipment used in the CO_2 capture process. Corrosion of the system's components can lead to increased maintenance costs and downtime, further adding to the overall operational cost of the CO_2 capture plant[10]. Regular maintenance and the use of corrosion-resistant materials are required to address this challenge.

IV. Amine Loss and Environmental Concerns: Over time, some MEA is lost from the system due to evaporation or leakage. This loss can reduce the overall efficiency of the CO_2 capture process and may require the purchase of additional solvent, further increasing operational costs. Additionally, there are concerns about the environmental impact of amine loss and the potential for amine-related emissions to enter the atmosphere. To address these issues, researchers are exploring methods to minimize solvent loss and improve the sustainability of MEA-based CO_2 capture systems.

Recent Advancements in MEA-Based CO_2 Capture

Recent research and development efforts have focused on improving the performance of MEA-based CO_2 capture systems. Some of the key advancements include:

I. Solvent Modifications

Researchers have been working on modifying MEA to improve its performance and reduce its degradation. This includes the development of mixed amines (e.g., MEA combined with other amines such as diethanolamine) and the addition of additives that enhance the solvent's stability and reduce corrosion. These modifications aim to improve the solvent's efficiency and longevity, making MEA a more attractive option for largescale CO_2 capture[12].

II. Process Optimization

Advances in process design and optimization are also improving the energy efficiency of MEA-based CO_2 capture systems. For example, the use of heat integration strategies and the optimization of the solvent regeneration process can help reduce the energy consumption of the system, making it more cost-effective and environmentally friendly. Additionally, modeling and simulation tools, such as Aspen Plus, are being used to identify optimal operating conditions and reduce the overall energy footprint of CO_2 capture systems[7].

III. Alternative Solvents and Hybrid Systems

While MEA remains the most commonly used solvent, research is exploring the use of alternative solvents and hybrid systems that combine MEA with other materials to improve CO_2 capture efficiency. These alternatives may offer lower energy demands, greater stability, and reduced solvent degradation, providing more sustainable solutions for the cement industry.

D. Challenges in CO_2 Capture for Cement Plants

The cement industry is one of the largest industrial sources of carbon dioxide (CO_2) emissions globally, contributing roughly 7-8% of total anthropogenic CO_2 emissions[13]. While CO_2 capture technologies, including post-combustion capture using amines such as MEA, have been developed to reduce these emissions, the cement sector faces several unique challenges that make the implementation of these technologies more complex. Understanding these challenges is crucial for the successful integration of CO_2 capture systems in cement plants, and overcoming these barriers is key to achieving meaningful emissions reductions in the industry.

I. High CO_2 Concentrations and Gas Composition

Cement production generates significant CO_2 emissions during both the combustion of fossil fuels and the chemical process of limestone calcination. The CO_2 released from the calcination of limestone is particularly challenging because it constitutes the majority of the CO_2 emitted during cement production. Flue gases from cement kilns typically have CO_2 concentrations of around 20-30%, which is relatively high compared to other industrial emissions, making them easier to capture. However, these gases are also complex, containing impurities such as dust, sulfur oxides (SOx), nitrogen oxides (NOx), and water vapor.

The presence of these impurities can interfere with the CO_2 capture process. For instance, particulate matter can cause clogging or damage to the capture equipment, while sulfur compounds can degrade the amine solvents used in post-combustion capture. Additionally, high moisture content in flue gases can lead to corrosion and the formation of heat-stable salts, which further complicates the implementation of CO_2 capture technologies[10].

II. Energy Demands and Operational Costs

One of the most significant challenges of CO_2 capture in cement plants is the high energy consumption required for solvent regeneration. Regenerating amine solvents such as MEA involves heating the solvent to release the absorbed CO_2, a process that consumes a substantial amount of energy. This energy requirement can increase the operational costs of cement production, which is already an energy-intensive process due to the high temperatures required for clinker production. Cement plants typically operate at very high temperatures, and retrofitting them with CO_2 capture technology requires additional infrastructure and energy. This not only drives up costs but can also lead to a reduction in the overall energy efficiency of the plant[2]. As a result, the financial feasibility of CO_2 capture systems depends heavily on the price of energy and the availability of low-carbon or renewable energy sources to power the capture process.

III. Solvent Degradation and Maintenance

Another challenge specific to the cement industry is the degradation of the solvents used for CO_2 capture. Amine solvents like MEA are particularly susceptible to degradation when exposed to contaminants such as oxygen, sulfur, and particulate matter present in cement plant flue gases. Over time, this degradation reduces the efficiency of the CO_2 capture system and leads to the formation of byproducts, including heat-stable salts, that can accumulate and clog the system. The degradation of solvents requires regular maintenance and replacement, which adds to the operational costs of CO_2 capture.

Moreover, the disposal of degraded solvents and the environmental impact of solvent loss are additional concerns that must be addressed to ensure the sustainability of CO_2 capture in cement plants[11].

IV. Space and Infrastructure Limitations

Cement plants are typically large and complex facilities, and retrofitting them with CO_2 capture technologies often requires significant modifications to existing infrastructure. The installation of CO_2 capture systems—such as amine absorption units, stripper columns for solvent regeneration, and CO_2 compression and storage units—requires considerable space and the integration of new equipment into the existing layout.

For many cement plants, especially those that were not originally designed with CO_2 capture in mind, space constraints can be a major barrier to implementation. Furthermore, the integration of CO_2 capture systems can disrupt normal plant operations, leading to potential downtime and productivity losses. The economic feasibility of these systems is often influenced by the ability to retrofit them efficiently without compromising the plant's primary function[7].

V. Economic Considerations and Market Incentives

The high capital costs associated with CO_2 capture technologies pose a significant barrier to their widespread adoption in the cement industry. The cost of installing and operating CO_2 capture systems is substantial, and many cement producers are hesitant to invest in these technologies without clear financial incentives or regulatory pressures. Although some governments offer subsidies, tax credits, or carbon pricing schemes to encourage CO_2 capture, the availability and effectiveness of these incentives vary by region.

In many cases, cement producers may be reluctant to invest in CO_2 capture unless there is a clear economic benefit, such as a market for captured CO_2 or the potential for significant reductions in emissions taxes. This economic uncertainty creates a situation where the cost-benefit analysis of CO_2 capture remains a key challenge for the cement sector. Without stronger market incentives or regulatory frameworks, many cement plants may struggle to justify the upfront costs of installing CO_2 capture systems[8].

VI. Regulatory and Policy Challenges

The regulatory environment plays a crucial role in the implementation of CO_2 capture technologies in the cement industry. While there is increasing recognition of the need for emissions reductions, the regulatory frameworks that govern CO_2 capture technologies are still evolving. In some regions, the lack of clear policies or supportive infrastructure for carbon capture, transport, and storage (CCS) can delay the adoption of these technologies.

Furthermore, regulations around CO_2 emissions vary significantly between countries and regions, creating uncertainty for cement producers. While some governments have introduced ambitious climate policies and carbon pricing mechanisms to incentivize emissions reductions, others have not yet implemented comprehensive strategies to support CO_2 capture in industries like cement. Without consistent and predictable regulatory frameworks, the adoption of CO_2 capture technologies may be slow and uneven across the global cement industry[8].

E. CO_2 Capture in Cement Plants

I. Simulation and Process Modeling

As the cement industry works toward adopting CO_2 capture technologies, especially with solvents like Monoethanolamine (MEA), process modeling and simulation have become essential tools. These tools help optimize the design, operation, and performance of CO_2 capture systems before they are implemented in real-world settings. For cement plants, which have unique operating conditions and emission profiles, simulation offers a pathway to fine-tune these systems to reduce costs and enhance efficiency.

II. Role of Simulation in CO_2 Capture

The use of simulation software, such as Aspen Plus, plays a critical role in designing and optimizing CO_2 capture systems. Simulation allows engineers to model the entire CO_2 capture process, from the absorption of CO_2 in the solvent to its regeneration and compression for storage or utilization. This modeling helps identify the best operational parameters, solvent flow rates, temperature conditions, and regeneration cycles necessary to maximize CO_2 removal while minimizing

energy consumption. Simulation is particularly useful for the cement industry because it can account for the variability in flue gas composition and the unique challenges that come with cement plant emissions. For example, the high levels of CO_2 and the presence of impurities like sulfur compounds and dust particles make it difficult to design a one-size-fits-all solution. By using simulation, engineers can experiment with different configurations and process conditions to determine the most effective capture strategy.

III. Modeling the CO_2 Capture Process

A typical CO_2 capture process using MEA involves several key steps, each of which can be modeled in simulation software:

i. CO_2 Absorption

In the first step, flue gas is introduced into an absorber column, where it comes into contact with the MEA solution. The CO_2 in the flue gas reacts with the amine solvent, forming a carbamate. The rate of absorption depends on various factors, including the concentration of CO_2 in the flue gas, the temperature of the solvent, and the flow rate.

ii. Solvent Regeneration

Once the solvent is saturated with CO_2, it is transferred to a stripper column where heat is applied to release the absorbed CO_2. This regeneration process typically requires a significant amount of energy, making it one of the most critical areas for optimization. By adjusting the temperature, pressure, and flow rates in the stripper column, simulations can help determine the most energy-efficient approach.

iii. CO_2 Compression and Storage

After regeneration, the CO_2 is in a concentrated form and ready to be compressed for storage or utilization. Simulation allows for the design of compressors and storage tanks to handle the large volumes of CO_2 that need to be transported to storage sites or used for enhanced oil recovery (EOR) or other applications.

Simulating these processes allows for a comprehensive understanding of how different variables interact, helping engineers identify potential issues and inefficiencies before physical implementation. It also provides a clear cost-benefit analysis, making it easier to justify investments in CO_2 capture technology.

IV. Challenges in Modeling CO_2 Capture for Cement Plants

While simulation is a powerful tool, it is not without its challenges, particularly when applied to cement plants. Cement plant emissions are quite different from those of power plants or natural gas processing facilities, and these differences must be carefully accounted for in the model. Some of the challenges include:

i. Flue Gas Composition Variability

Cement plants produce flue gas with varying levels of CO_2, dust, sulfur, and other impurities, depending on the fuel used and the operational conditions. This variability makes it difficult to create a standardized model for CO_2 capture. Simulation models must be adaptable enough to handle these fluctuations and provide accurate predictions under different conditions.

ii. Heat Integration and Energy Efficiency

The high energy consumption required for solvent regeneration can significantly increase the operating costs of CO_2 capture systems in cement plants. Modeling energy integration within the system—such as recovering heat from the kiln or other parts of the plant—can help reduce overall energy demand. However, this requires detailed modeling of the entire plant and its energy flows, which can be complex and computationally intensive.

iii. Solvent Degradation and Maintenance

Solvent degradation is a common issue when using amines like MEA, especially in cement plants where impurities such as sulfur compounds are present. Modeling the impact of solvent degradation and understanding its effect on capture efficiency over time is a challenging but necessary task for accurate simulations. It also helps in designing maintenance schedules and replacement strategies for solvents.

iv. Operational Uncertainties

Despite the best efforts of modeling, real-world operations are always subject to uncertainties. Fluctuations in plant load, variations in fuel composition, and unexpected changes in the environmental conditions can affect the performance of the CO_2 capture system. Simulation tools must, therefore, incorporate sensitivity analyses and uncertainty quantification to ensure that the system is robust and can handle these real-world variables.

E. Simulation Case Studies and Applications

Several studies have demonstrated the effectiveness of simulation in optimizing CO_2 capture systems for cement plants. For example, a case study conducted by Sakwari et al. (2020) used Aspen hysys to simulate the CO_2 capture process for a cement plant's flue gas stream. By adjusting parameters such as solvent flow rate, absorption temperature, and regeneration conditions, the study was able to identify the optimal conditions that minimized energy consumption while maximizing CO_2 capture efficiency. The results indicated that significant improvements in energy efficiency could be achieved by integrating heat recovery systems into the CO_2 capture process. Another example is a study by Bui et al. (2018), which applied process modeling to assess the feasibility of MEA-based CO_2 capture in the cement industry. The study showed that while MEA is an effective solvent for capturing CO_2, the energy demands for solvent regeneration remain a significant hurdle. Simulation models highlighted the need for innovations in heat integration and solvent management to improve the economic viability of CO_2 capture in cement plants. These case studies show how simulation can guide the design and operation of CO_2 capture systems, helping cement plants achieve higher efficiency and lower costs. By providing a clear picture of how different process parameters affect performance, simulation allows for better decision-making and a smoother transition to a low carbon cement production process.

F. Strategies to Optimize CO_2 Capture in Cement Plants

Optimizing CO_2 capture in cement plants is a complex task, as it involves balancing efficiency, cost, and environmental impact. While technologies like Monoethanolamine (MEA)-based capture systems have proven effective, their performance can be significantly influenced by the operating conditions and the characteristics of the plant. Several strategies can be employed to improve the overall efficiency of CO_2 capture systems in cement plants, addressing challenges such as energy consumption, solvent degradation, and space constraints. These strategies can help make CO_2 capture more economically feasible and sustainable in the long run.

I. Process Integration and Heat Recovery

One of the most effective ways to optimize CO_2 capture is through process integration, specifically by recovering heat from various parts of the cement production process. Cement plants operate at high temperatures, particularly in the kiln, where the clinker formation process takes place. This heat can be harnessed and integrated into the CO_2 capture system to reduce the energy required for solvent regeneration. By using waste heat recovery systems, such as heat exchangers or combined heat and power (CHP) units, the temperature of the incoming flue gas can be preconditioned before it enters the absorber. Additionally, the heat from the solvent regeneration process can be recycled, minimizing the need for external energy input. This reduces the overall energy demand of the CO_2 capture system, thus lowering operational costs and improving the plant's energy efficiency. Moreover, utilizing the waste heat from the cement plant can enhance the economic feasibility of CO_2 capture, as it decreases reliance on external energy sources, which can be expensive and environmentally harmful. This strategy is particularly effective in plants where high-temperature waste heat is readily available, and it can significantly lower the carbon footprint of cement production[7],[14].

II. Solvent Management and Optimization

Solvent degradation is a major issue in CO_2 capture systems, particularly in cement plants where impurities like sulfur compounds and particulate matter are present in the flue gas. This degradation reduces the efficiency of the solvent and can lead to higher operational costs due to the need for frequent solvent replacement and disposal. To optimize solvent performance, several strategies can be implemented. First, the use of solvent additives or advanced solvent formulations can help enhance the stability and capacity of MEA and other amines. For instance, incorporating stabilizers into the solvent can reduce degradation caused by contaminants, extending the solvent's lifespan and improving overall system efficiency[15]. Another strategy involves periodic solvent regeneration using advanced techniques such as pressure-swing

absorption (PSA) or vacuum-swing absorption (VSA). These methods require less energy compared to traditional thermal regeneration and can be more cost-effective in the long term. Additionally, optimizing the regeneration process by adjusting parameters such as temperature and pressure can minimize energy consumption and improve the overall performance of the capture system[11].

III. Use of Alternative Solvents and CO_2 Absorption Technologies

While MEA-based CO_2 capture systems are widely used, alternative solvents and technologies are being researched to further optimize the CO_2 capture process in cement plants. These alternatives aim to address the limitations of traditional solvents, such as their susceptibility to degradation and high regeneration energy requirements. For example, solvents like potassium carbonate (K_2CO_3) and amine blends have shown promise as more stable and efficient alternatives to MEA. These solvents have a lower tendency to degrade in the presence of impurities, reducing the need for frequent solvent replacement. Additionally, they may have lower regeneration energy requirements, which can help reduce the overall energy consumption of the CO_2 capture system[16]. Apart from chemical solvents, physical adsorption methods, such as using solid adsorbents like activated carbon or metal-organic frameworks (MOFs), are also being explored for CO_2 capture. These materials have a high surface area and can selectively adsorb CO_2 from the flue gas. While these technologies are still in the research phase, they hold significant potential for improving the efficiency of CO_2 capture in cement plants by offering lower energy consumption and potentially lower costs[17].

IV. Advanced CO_2 Capture System Configurations

Another strategy for optimizing CO_2 capture is the design of advanced system configurations that improve the overall efficiency of the capture process. One such configuration is the use of a split-flow system, where the flue gas is divided into two or more streams, with one stream being directed to the CO_2 capture system and the other bypassing it. This allows for the optimization of capture performance by selectively treating high-CO_2 concentration streams, thus reducing the total energy required for solvent regeneration. Additionally, integrating CO_2 capture with other processes, such as cement grinding or clinker cooling, can help reduce the overall energy demand of the plant. By capturing and utilizing the CO_2 in these processes, the cement plant can improve its overall energy balance and reduce its carbon footprint. For example, CO_2 captured during the cement grinding process can be used for curing concrete or in other industrial applications, turning a waste product into a valuable resource[18]. Moreover, innovative designs such as membrane-based capture systems or hybrid systems that combine both amine absorption and membrane separation are being explored. These systems could potentially offer higher selectivity, lower energy consumption, and easier integration into existing plant configurations[2].

V. Optimizing Plant Layout and Retrofitting

Many cement plants were not initially designed to incorporate CO_2 capture technologies, which makes retrofitting a challenging but necessary step. Optimizing the layout of existing plants to accommodate CO_2 capture systems is essential for improving the overall efficiency of the process. This may involve modifying or expanding certain areas of the plant to make space for additional equipment, such as absorbers, regenerators, and compressors. Effective retrofitting can also involve upgrading control systems to better manage the integration of CO_2 capture with existing cement production processes. For instance, advanced process control techniques such as model predictive control (MPC) can help optimize the operation of the capture system by continuously adjusting parameters like flow rates, temperatures, and pressures in response to real-time plant data. This dynamic control approach can improve the performance and reliability of the capture system while reducing energy consumption and costs[19]. Furthermore, plant layout optimization can be coupled with strategies like optimizing material handling systems to minimize dust and particulate matter, which can reduce solvent degradation and improve the efficiency of the CO_2 capture process[20].

G. Potential Benefits of CO_2 Capture in Cement Plants

The implementation of CO_2 capture technologies in cement plants holds significant promise, both in terms of environmental benefits and economic potential. Cement production is responsible for a substantial portion of global CO_2 emissions, contributing to climate change and the challenges of achieving international carbon reduction targets. By incorporating CO_2 capture systems, cement plants can reduce their carbon footprint, contribute to sustainable industrial

practices, and even create new revenue streams. This section highlights the potential benefits of CO_2 capture in cement plants and explores how these systems can contribute to a greener and more economically viable cement industry.

I. Reduction of CO_2 Emissions

The most obvious and critical benefit of implementing CO_2 capture in cement plants is the substantial reduction in CO_2 emissions. Cement production accounts for nearly 7-8% of global anthropogenic CO_2 emissions, primarily due to the high energy demands of the process and the chemical reactions involved in converting limestone to clinker[13]. By capturing CO_2 directly from the flue gas, cement plants can prevent a significant portion of these emissions from being released into the atmosphere, helping to mitigate the effects of climate change. The integration of CO_2 capture technologies allows cement plants to operate more sustainably by adhering to increasingly stringent environmental regulations and contributing to national and international emissions reduction targets[13]. By reducing CO_2 emissions, cement producers can not only help fight climate change but also enhance their reputation as environmentally responsible businesses, which can be a key factor in securing market share in a rapidly evolving global economy.

II. Economic Opportunities through CO_2 Utilization

Apart from reducing emissions, CO_2 captured from cement plants can be repurposed for various industrial applications, creating additional economic opportunities. Captured CO_2 has several potential uses, including enhanced oil recovery (EOR), where it is injected into depleted oil fields to increase oil production. Additionally, CO_2 can be used in the production of chemicals, fuels, and even synthetic building materials. For example, some cement plants have explored the possibility of using captured CO_2 to produce concrete products. By injecting CO_2 into the curing process, cement can be made more durable and environmentally friendly. This process, known as Carbon Cure, not only reduces the carbon footprint of cement production but also creates a marketable product with a lower environmental impact. These applications create new revenue streams for cement plants, making CO_2 capture a potentially profitable venture rather than just an environmental obligation[21].

Furthermore, captured CO_2 can be used in the production of biofuels, chemicals, or even algae-based products. These applications not only offer a way to reduce emissions but also stimulate the development of a new industry based on captured CO_2, providing long-term economic benefits[22].

III. Compliance with Emissions Regulations and Carbon Pricing

As governments worldwide implement more stringent carbon regulations and introduce carbon pricing mechanisms, the cement industry faces increasing pressure to reduce its carbon emissions. CO_2 capture technologies provide an effective means for cement plants to comply with these regulations while maintaining production levels. The development of carbon pricing, through carbon taxes or emissions trading systems, creates a financial incentive for companies to invest in CO_2 capture systems. Countries with established carbon pricing mechanisms, such as the European Union's Emissions Trading Scheme (EU ETS), have seen the economic benefits of reducing CO_2 emissions through technologies like carbon capture. Cement companies that adopt CO_2 capture technologies can potentially reduce their carbon tax liabilities or benefit from credits in emissions trading systems, further improving the economic viability of the technology[22],[14]. By implementing CO_2 capture technologies, cement plants not only comply with regulatory requirements but also avoid potential penalties associated with non-compliance. This proactive approach can help future-proof the business against evolving environmental policies, ensuring continued competitiveness in a low-carbon economy.

IV. Enhancing Sustainability in the Cement Industry

Cement production is one of the most energy-intensive processes in the industrial sector, making it a significant contributor to global environmental concerns. By incorporating CO_2 capture technologies, cement plants can enhance their sustainability and reduce their dependence on fossil fuels, contributing to global efforts to transition to a low-carbon economy. Cement producers who adopt CO_2 capture systems may be able to access "green" financing or investment opportunities as the world increasingly prioritizes sustainable development. Many financial institutions now offer preferential financing for projects that demonstrate a commitment to reducing environmental impact, and adopting CO_2 capture technologies can position cement companies as leaders in sustainability. In addition, adopting CO_2 capture

technologies can allow cement companies to address the growing demand for environmentally friendly products. As public awareness of climate change increases, consumers and businesses are increasingly seeking products with lower carbon footprints. Cement companies that invest in CO_2 capture not only reduce their emissions but also position themselves to meet the evolving demands of the market[21],[2].

V. Job Creation and Technological Advancements

The development and deployment of CO_2 capture technologies in cement plants can lead to the creation of new jobs and technological advancements. As the demand for carbon capture grows, there will be an increased need for skilled workers in the fields of engineering, chemistry, and process optimization. This can lead to job creation in research and development, manufacturing, and operation of CO_2 capture systems. Moreover, the growth of CO_2 capture technologies may drive further innovations in related fields, such as energy efficiency, renewable energy integration, and carbon utilization. As companies invest in these technologies, they can spur technological advancements that benefit not only the cement industry but also other sectors, such as power generation and chemical manufacturing[20].

H. Future Trends in CO_2 Capture in Cement Plants

As the global demand for cement continues to grow, driven by urbanization and infrastructure development, the need for sustainable and low-carbon technologies in cement production becomes increasingly critical. The cement industry is under mounting pressure to reduce its carbon footprint and meet international climate goals, which is pushing innovation in carbon capture technologies. The next few decades are likely to see significant advancements in CO_2 capture techniques, including improvements in efficiency, cost reduction, and integration with renewable energy sources. This section explores the future trends in CO_2 capture in cement plants and highlights the innovations expected to shape the industry's ability to reduce its carbon emissions.

III. METHODOLOGY

A. Simulation Model And Parameters

Flue Gas Composition and Process Basis.

The simulated flue gas originated from a combustion system operating under atmospheric conditions, commonly found in industrial power generation or refinery setups. The gas stream contained a significant concentration of carbon dioxide, which necessitated separation to meet environmental regulations. The presence of hydrogen, although relatively small, added complexity to the separation due to its diffusivity and low solubility in the solvent. The dominant inert component, nitrogen, and the oxygen content represented the remainder of the combustion air not involved in the chemical reactions. The flue gas entered the system at ambient pressure and a temperature of approximately 120°C. Prior to CO_2 absorption, the gas required several pre-treatment steps, which were simulated and optimized using Aspen HYSYS. The primary goal of the simulation was to maximize the removal efficiency of CO_2 from the gas stream while minimizing energy usage and solvent degradation. The process aimed to recover over 90% of the carbon dioxide using a lean MEA solution, regenerate the solvent for reuse, and ensure that the exit gas stream contained minimal levels of residual CO_2. All streams were modeled under steady-state conditions, and a rigorous component mass balance was performed to validate the results.

B. Simulation Setup in Aspen HYSYS

Aspen HYSYS was employed as the simulation environment for this process. It offered a robust platform for modeling gas absorption systems due to its ability to handle chemical equilibria, thermodynamic properties, and energy balances. The Acid Gas - Chemical Solvent property method was selected as the thermodynamic basis for the simulation. This property package supported reactive systems involving CO_2 and amine solvents and accounted for non-idealities in the aqueous phase. In constructing the simulation, the feed stream was defined with its respective composition, temperature, pressure, and flow rate. The major components included hydrogen, carbon dioxide, nitrogen, oxygen, water, and monoethanolamine. The solvent concentration was maintained at 30 weight percent MEA in water, a typical value for industrial operations. Key reactions, such as the formation of carbamates and bicarbonates, were automatically handled by the property method. Additionally, heat and mass transfer operations across each unit were modeled based on standard design parameters and industry data.

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C. Process Flow Description

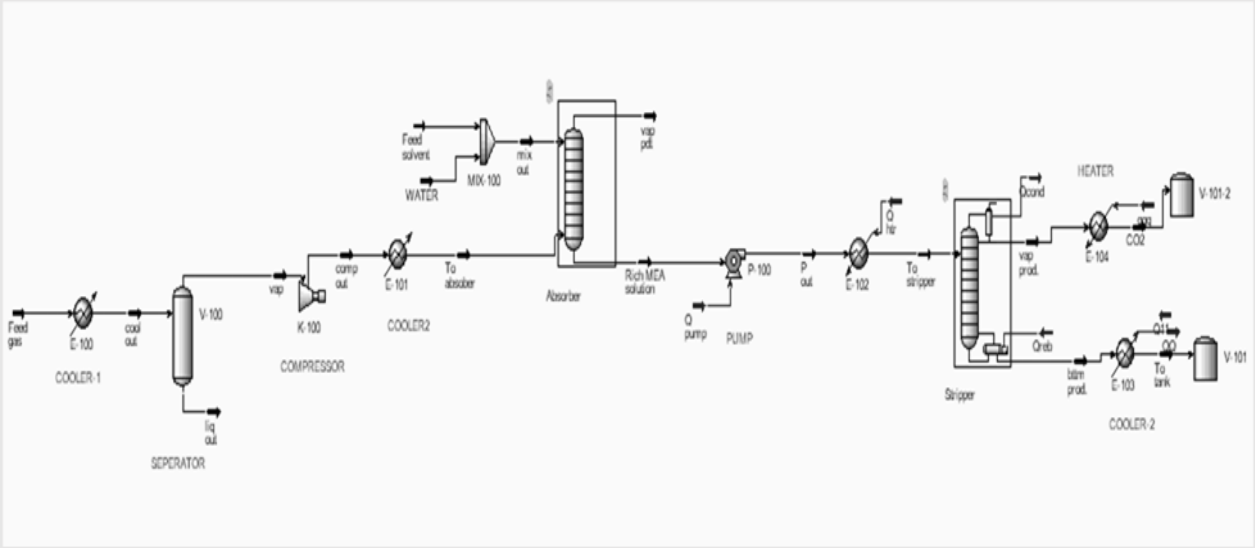

Figure 1 Process flow Diagram for the Plant.

The simulated CO_2 capture process consisted of three major sections: pre-treatment of the flue gas, chemical absorption in the absorber column, and regeneration of the solvent in the stripper column. Each section was modeled with realistic operating conditions and equipment performance characteristics. The process began with the introduction of the hot flue gas stream into a cooling unit, labeled E-100. This cooler reduced the temperature of the gas from approximately 160°C to around 60°C. Cooling was essential to increase the solubility of CO_2 in the solvent and to reduce the thermal degradation of MEA in downstream units. Following the cooling stage, the gas entered a vapor-liquid separator, designated as V-100. This knockout drum facilitated the removal of condensed water and any trace liquid hydrocarbons from the gas stream. The liquid fraction was discharged from the bottom of the vessel, while the clean vapor stream was routed to a compressor, K-100. The compressor slightly increased the pressure of the flue gas from 1bar to 120KPa, ensuring adequate driving force for absorption and minimizing equipment volume in the absorber. After compression, the gas stream passed through another heat exchanger, E-101, which served to reheat the gas to optimal absorption temperature levels. The reheated gas then proceeded toward the absorber column. Before entering the column, a separate stream of lean MEA solution was mixed with a water stream in a mixing unit, MIX-100. This allowed control of the solvent concentration and ensured that the MEA feed entering the absorber had the correct dilution. The absorber column played a central role in the removal of CO_2 from the gas. It was modeled as a vertical counter-current packed column. The flue gas entered the column from the bottom, while the MEA solvent flowed from the top. As the two phases contacted, CO_2 from the gas phase reacted chemically with MEA, forming stable compounds such as carbamate and bicarbonate. This resulted in a purified gas stream that exited from the top of the absorber with significantly reduced CO_2 content. The bottom product of the absorber was the rich MEA solution, now containing absorbed CO_2. The rich MEA solution was then directed to the regeneration section. It was first passed through a pump, P-100, which elevated its pressure to the level required for stripping, typically between 1.2 to 2.0 bar. The pressurized rich MEA was then preheated using a lean/rich heat exchanger, E-102. This exchanger transferred thermal energy from the hot lean MEA stream returning from the stripper to the incoming rich stream, thereby conserving energy and improving thermal efficiency. Upon preheating, the rich solvent entered the stripper column. The stripper was also modeled as a counter-current column where the rich MEA descended from the top while steam generated in a reboiler at the base rose upward. The heat provided by the reboiler broke the chemical bonds between CO_2 and MEA, allowing CO_2 to be released as a gas and exit from the top of the column. The bottom stream, now depleted of CO_2, became the lean MEA stream, which was subsequently recycled. The lean MEA exiting the stripper was still at a high temperature. It passed through the same heat exchanger, E-102, to preheat the incoming rich stream. Afterward, it flowed into a cooling unit, E-103, where it was further cooled to about 40°C. This temperature was suitable for re-entry into the absorber column. Finally, the cooled lean MEA was collected in a storage or surge vessel, V-101, from where it was recycled back to the absorber, completing the solvent loop.

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TABLE I: PARAMETERS USED FOR THE SIMULATION

No.	Article & Focus	Key Parameters Used
1	*Guo L. et al. (2018)* – Simulation and optimization of MEA-based CO_2 capture in Aspen Plus (rate-based model).	• ENRTL-RK thermodynamic model• Baseline flue gas flow: 3,100 t/h (650 MW plant) at 40 °C, 1.1 bar, 12 % CO_2• 30 wt% MEA• Absorber: ~1.06 bar• Stripper: ~2 bar• Lean loading: 0.25 mol CO_2/mol MEA• Reboiler duties reduced from ~3.2 → 2.38 GJ/t CO_2 with heat pump integration
2	*Xue B. et al. (2016)* – Comparative study of MEA vs. DEA for PCC in Pro/II.	• Flue gas: 10% CO_2, 6% H_2O, 84% N_2, 40 °C, 1.2 bar• 10 equilibrium stages, 0.1 bar pressure drop per column• Absorber: ~1 bar; Stripper: ~1.5 bar• MEA: 30 wt%, DEA: 40 wt%• Lean loading (MEA): 0.25 mol CO_2/mol; (DEA): 0.1 mol CO_2/mol
3	*Frontiers Energy Research (2023)* – MEA concentration and parameters sensitivity via simulation.	• Gas flow rates: large case 252.7 ton/h (~70.2 kg/s), medium case half that• CO_2 concentration: from 31.8 wt% (plant baseline) varied 10–50 wt%• CO_2 removal rate: 65%–95% varied for performance analysis• Model: Equilibrium → rate-based, with design specs: – Absorber: target capture via lean MEA flow adjustment – Stripper: reboiler duty tuned for lean loading of 0.3 mol CO_2/mol MEA and product CO_2 purity of 98 mol%
4	*Moioli et al. (2012)* – Simulation of CO_2 capture with rate-based model in Aspen Plus.	• Rate-based vs. equilibrium models• Incorporates VLE thermodynamics, mass-transfer, reaction kinetics (film theory by Lewis-Whitman) in Aspen Plus• Validated against pilot-plant experimental data
5	*PorousMedia/Rice ProMax study* – Effect of stripper pressure and steam conditions on energy.	• Evaluated stripper pressures: 150–300 kPa (1.5–3 bar) with LP turbine steam (413 kPa)• Also vacuum stripper cases: 30–75 kPa• Assessed energy distribution across regeneration and compression

TABLE: II COMPOSITION PARAMETERS

Study / Source (year)	Flue gas (feed) — CO_2 / N_2 / O_2 / H_2O (mol%)	MEA solvent (wt%)	Absorber conditions (T °C, P kPa)	Absorber outlet / treated gas CO_2 (mole frac or %)	Solvent lean / rich loading (mol CO_2 / mol MEA)	Stripper conditions (T °C, P kPa)	Stripper overhead CO_2 purity (mol% CO_2 in vapour after condenser)
Frontiers in Energy Research — MEA parametric study (2023).	Case examples: **CO_2 3–50%** studied; typical pilot/cement case **≈ 10–32% CO_2,** balance N_2+O_2+H_2O.	**15–30 wt%** explored; 20–30% commonly used.	Absorber inlet ~**40 °C**, near-atm **~101–120 kPa** for baseline cases.	Treated gas CO_2 reported down to **~0.5–2% (mol fraction 0.005–0.02)** in high-capture cases (varies with target capture %).	Lean loading reported/targeted **~0.10–0.30**; rich **~0.40–0.55** (depends on L/G and capture spec).	Stripper reboiler temps commonly **~110–125 °C** at **~180–210 kPa** in many pilot models; higher with pressurised stripper variants.	Pilot outlets (wet hot vapour) often have high H_2O; **CO_2 purity after condensation/compression reported >95 mol%** for many MEA stripper designs.
DTU / Cement pilot (CESAR1, DTU) — pilot report (2024/2025).	Cement flue gas used in study: **CO_2 ≈ 25–32 mol%** (case dependent), remainder N_2/O_2/H_2O.	Pilot used **30 wt% MEA (base case)** in comparisons; other solvents also tested.	Absorber inlet **≈40–50 °C**, operation near **~100–120 kPa** (pilot).	Post-absorber treated flue gas CO_2 reported **~1–3 mol%** for high capture (~90–96%) runs.	Reported cyclic load $\Delta\alpha \approx$ **0.34** for base case (rich–lean difference); typical lean/rich around **0.15–0.49** (paper gives case data).	Stripper run at **~1.8–2.1 bar (180–210 kPa)**; reboiler target to reach solvent regeneration (reboiler ~110–125 °C typical).	Reported final CO_2 product purity (after condensation and downstream cleaning) **>95 mol%** in pilot reporting

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Study / Source (year)	Flue gas (feed) — CO_2 / N_2 / O_2 / H_2O (mol%)	MEA solvent (wt%)	Absorber conditions (T °C, P kPa)	Absorber outlet / treated gas CO_2 (mole frac or %)	Solvent lean / rich loading (mol CO_2 / mol MEA)	Stripper conditions (T °C, P kPa)	Stripper overhead CO_2 purity (mol% CO_2 in vapour after condenser)
TCM / MEA campaigns (industry pilot compendium) — Technology Centre Mongstad reports	Typical flue gases in campaigns: **CO_2 ~3–15% (power plants)** but industrial (cement) higher — campaigns show wide feed ranges.	MEA cases typically **30 wt%** used as benchmark.	Absorber inlet typically **~40 °C,** absorber pressure near **1 bar**.	Treated flue gas CO_2 often **reduced to <5%** depending on capture target; high-capture tests reach **~1–2%** residual.	Typical lean loading **~0.15–0.25**, rich **~0.45–0.55** in MEA baseline runs reported.	Stripper pressures and reboiler duties vary; many tests used **~1.5–2.2 bar** stripper pressure with reboiler temps **100–125 °C**.	CO_2 product purities after drying/compression reported **>95%,** often up to **>98%** after polishing.
NETL / DOE reports & reviews (handbook / compendium).	Typical industrial flue gas (examples): **CO_2 3–20%** (power, cement higher end ~15–30%). NETL gives example **~18%** for some industrial streams.	MEA benchmark 30 wt% often used for TEA comparisons; some studies indicate 20 wt% can reduce energy.	Absorber baseline: **~40–60 °C**, near atmospheric pressure.	Treated gas CO_2 typically reduced to selected capture target (e.g., 90–95% removal → residual CO_2 few percent or less).	Lean loading typical **0.15–0.25**, rich **0.4–0.5** (NETL ranges used in TEAs).	Stripper baseline pressure **~1.5–2.2 bar** in many design cases; reboiler temps **110–125 °C**; SRD / reboiler duty ~**3.2–3.8 GJ/t CO_2** for 30 wt% MEA baseline.	CO_2 product purity targets in TEAs: **>95%** after condensation/compression.

Component	Simulation (Mole Fraction)	IJMO Article (Mole Fraction) – Cement Flue Gas (Ontario plant, Table IV)
H_2O	0.042	0.072
CO_2	0.318	0.224
N_2	0.616	0.681
O_2	0.024	0.023
MEA	0.000	– (not present in flue gas)
H_2S	0.000	– (not reported)

E. Equations

I. Physical Absorption and Initial Hydration (Gas → Liquid)

CO_2 dissolves into the aqueous MEA solution (Henry's law driven mass transfer):

Minor hydration of dissolved CO_2 to carbonic acid (often lumped with CO_2(aq) in models):

$$CO_2 + H_2O \rightleftharpoons H_2CO_3$$

II. Acid–Base Equilibria of MEA and Inorganic Carbon

MEA acts as a Brønsted base and its conjugate acid (protonated MEA) participates in charge balance:

$$MEAH^{+} \rightleftharpoons MEA + H^{+}$$

Inorganic carbon equilibria in water:

$$H_2CO_3 \rightleftharpoons HCO_3^{-} + H^{+}$$

$$HCO^{3-} \rightleftharpoons CO^{32-} + H^{+}$$

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III. Carbamate Formation (Primary Amine Pathway)

Zwitterion mechanism (elementary steps):

$$CO^2(aq) + MEA \rightleftharpoons MEA - COO^- - H^+$$

$$MEA - COO^- - H^+ + B \rightleftharpoons MEACOO^- + BH^+ \quad (B = MEA \text{ or } H^2O)$$

Total carbamate formation (commonly used in process models):

$$CO_2 + 2\,MEA \rightleftharpoons MEACOO^- + MEAH^+$$

IV. Bicarbonate Formation Pathway

At higher CO_2 loadings (or with excess water/weak base deprotonation), carbamate hydrolyzes to bicarbonate:

$$MEACOO^- + H_2O \rightleftharpoons MEA + HCO_3^-$$

Direct bicarbonate route (amine as a base for dissolved CO_2):

$$CO_2 + H_2O + MEA \rightleftharpoons HCO_3^- + MEAH^+$$

V. Net Reactions Across the Process

Absorber (forward direction): CO_2 transfer and binding as carbamate/bicarbonate:

$$CO_2(g) + 2\,MEA \rightleftharpoons MEACOO^- + MEAH^+ \quad \text{(carbamate route)}$$

$$CO_2(g) + H_2O + MEA \rightleftharpoons HCO_3^- + MEAH^+ \quad \text{(bicarbonate route)}$$

Stripper (reverse direction): heat drives dissociation and CO_2 release:

$$MEACOO^- + MEAH^+ \rightleftharpoons CO_2(g) + 2\,MEA$$

$$HCO_3^- + MEAH^+ \rightleftharpoons CO_2(g) + H_2O + MEA$$

IV. SIMULATION RESULTS AND PERFORMANCE ANALYSIS

The simulation yielded a stable and converged model under the specified operating conditions. The absorber column successfully removed over 92% of the incoming CO_2, aligning with industrial targets. The CO_2-rich stream exiting the stripper contained over 99% carbon dioxide, making it suitable for compression and subsequent transport or storage in geological formations. Energy consumption was a critical parameter assessed in the simulation. The reboiler duty required to regenerate the MEA solvent ranged between 3.5 to 4.2 gigajoules per tonne of CO_2 captured. This figure fell within accepted benchmarks for MEA-based systems. The use of the lean/rich heat exchanger played a significant role in reducing the external heating requirement. The pump and compressor energy requirements were also recorded and remained within expected values for a system of this capacity. The solvent circulation rate was optimized to achieve a balance between CO_2 removal efficiency and energy usage. A circulation ratio of approximately 2 kg MEA per kg CO_2 captured was maintained. This allowed for effective absorption while minimizing solvent degradation and operating costs.

A. Composition Changes on Major Equipment across the system

I. Flash Separator

TABLE: III UNIT CONDITION

Name	Cool out	Liq out	vap
Vapour	1.0	0.000	1.000
Temperature (C)	40	40	40
Pressure (kPa)	101.3	101.3	101.3
Molar Flow (kgmole/hr)	8162	0.000	8162
Mass Flow (kg/hr)	2.675e+005	0.000	2.675e+005
Std ideal liq vol flow (m^3/h)	425.0	0.000	425
Molar Enthalpy (kJ/kgmole)	-1.348+005	-2.847e+005	-1.348e+005

Molar Entropy (kJ/kgmoleC)	**7.943**	**-159.3**	**7.943**
Heat Flow (kJ/hr)	-1.100e+009	0.000	-1.100e+009

TABLE: IV UNIT COMPOSTION

Name	Cool out	Liq out	vap
H2O	0.0420	0.9998	0.0420
CO2	0.3180	0.0002	0.3180
Nitrogen	0.6160	0.000	0.6160
Oxygen	0.0240	0.000	0.0240
MEAmine	0.000	0.000	0.000
H2S	0.000	0.000	0.000

The simulation of the CO_2 capture process using MEA in Aspen Plus involved the incorporation of a gas-liquid separator labeled as V-100. This unit was designed to condition the incoming flue gas by adjusting its pressure and temperature before entering the absorption column. The simulated operating conditions of V-100 revealed that it functioned at an atmospheric pressure of 101.3 kPa and a temperature of 40 °C. These parameters ensured that the flue gas was properly cooled, facilitating effective interaction with the MEA solvent in subsequent stages. The vapor stream exhibited a molar flow rate of 8162 kmol/h and a mass flow of 2.675×10^5 kg/h. No liquid was retained in the unit, indicating complete vapor outflow. The heat duty of the separator was recorded as -1.10×10^9 kJ/h, signifying an exothermic phase disengagement or cooling process. The composition analysis of the separator V-100, as simulated, showed that the feed (cool out) stream contained 31.80% CO_2, 61.60% nitrogen, 4.20% water vapor, and 2.40% oxygen. There was no detectable presence of MEA or H_2S in the composition, confirming that the amine solution had not been introduced at this point and that the flue gas was sulfur-free. The compositions remained consistent across the vapor and liquid outlets, further verifying that the separation was limited and primarily served to condition the gas stream thermodynamically. The V-100 separator was successfully used in the simulation to prepare the flue gas for absorption by maintaining consistent operating conditions and compositions. Its function was crucial in setting the stage for efficient CO_2 capture in the absorber, where MEA would later be introduced. The process outcomes reflected a realistic and controlled gas conditioning system, essential for a stable and optimized CO_2 capture performance.

II. Absorber Column

TABLE: V UNIT CONDITION OF ABSORBER COLUMN

Name	Mht out @COL1	Liq out	vap	Rich MEA solution @COL1
Vapour	0.000	1	1	0.000
Temperature (C)	39.81	40	41.9	63.0
Pressure (kPa)	100	120	120	120
Molar Flow (kgmole/hr)	5.602e+004	8162	6618	5.757e+004
Mass Flow (kg/hr)	1.7732e+006	2.675e+005	2.012e+005	1.798e+006
Std ideal liq vol flow (m^3/h)	1715	425	344.5	1796
Molar Enthalpy (kJ/kgmole)	-2.814e+005	-1.348e+005	-7.595e+004	-2.843e+005
Molar Entropy (kJ/kgmoleC)	-256.6	6.530	4.982	-247.1
Heat Flow (kJ/hr)	-1.577e010	-1.101e+009	-5.027e+008	-1.636e+010

TABLE: VI UNIT COMPOSITION OF ABSORBER COLUMN

Name	Cool out	Liq out	Vap
H2O	0.705	0.0428	0.5826
CO2	0.000	0.3180	0.0258
Nitrogen	0.000	0.6160	0.000
Oxygen	0.000	0.0240	0.000
MEAmine	0.2995	0.000	0.2914
H2S	0.000	0.000	0.000

Figures 4 and 5 present the operating conditions and composition profiles within the absorber column (COL1) for CO_2 capture using MEA in a cement plant flue gas treatment process. The absorber receives two primary feed streams: the flue gas rich in CO_2 and lean MEA solvent. The column operates at a moderate pressure of 120 kPa and inlet temperature of approximately 40 °C, conditions favorable for chemical absorption of CO_2 by MEA. From Figure 4, the total molar flow rate into the absorber is 5.602×10^4 kmol/h, which is a combination of flue gas and lean MEA. After absorption, the CO_2-rich MEA exits at 63.0 °C, while the treated flue gas (with reduced CO_2 content) exits at around 41 °C. The absorber ensures that CO_2 is selectively removed and transferred to the liquid phase. This is confirmed by the heat flow values endothermic in the gas phase (-5.027×10^8 kJ/h) and exothermic in the liquid phase (-1.636×10^{10} kJ/h) which indicate strong exothermic reactions between CO_2 and MEA. Figure 5 shows the component compositions. The CO_2 mole fraction in the mixed inlet stream is 0.0022, and it decreases to 0.0010 in the vapor product, confirming CO_2 capture. MEA concentration increases from 0.0004 in the mix to 0.6479 in the rich solution, reflecting MEA's role in absorbing CO_2. Water remains the dominant component, indicating aqueous conditions essential for MEA performance. The absorber column operates effectively under optimized temperature and pressure to ensure maximum absorption of CO_2 into the MEA solution. The process conditions and composition changes across the column validate efficient gas-liquid mass transfer and chemical absorption, which are critical to the post-combustion CO_2 capture process.

III. Stripper Column

TABLE VII: UNIT CONDITION FOR STRIPPER COLUMN

Name	To stripper @COL2	Vap prod @COL2	Bottom Product @COL2
Vapour	0.000	0	0
Temperature (C)	101.9	-51.35	154.2
Pressure (kPa)	210.0	190	191
Molar Flow (kgmole/hr)	5.757e+004	3.271e+004	2.486e+004
Mass Flow (kg/hr)	1.798e+006	6.00e+005	1.198e+005
Std ideal liq vol flow (m^3/h)	1796	605.1	1191
Molar Enthalpy (kJ/kgmole)	-2.802e+005	-2.93e+005	-2.669e+005
Molar Entropy (kJ/kgmoleC)	-235.8	-184.6	-335.5
Heat Flow (kJ/hr)	-1.613e+010	-9.584e+009	-6.634e+009

TABLE VIII: UNIT COMPOSITION FOR STRIPPER

Name	To Stripper	Vap out	Bttm Prod
H2O	0.6828	0.9874	0.2820
CO2	0.0258	0.0126	0.0431
Nitrogen	0.000	0.000	0.000
Oxygen	0.000	0.000	0.000
MEAmine	0.2914	0.000	0.6749
H2S	0.000	0.000	0.000

The stripper column data presented in Figure 3 reflects the operational behavior during MEA-based CO_2 capture. The feed enters the stripper at 101.9 °C and 210 kPa with a molar flow of 5.575×10^4 kmol/h. The stripping process effectively separates CO_2 and water as vapor, with CO_2 vapor molar flow at 0.0126 kmol/h, indicating the desorption of CO_2 from the rich MEA solution. The bottom product primarily contains MEA and water, with MEA at 0.6479 kmol/h and water at 0.2280 kmol/h, confirming that most of the solvent is recovered. The vapor product's low oxygen and nitrogen levels confirm minimal air intrusion or solvent degradation. Heat duties are significant, with a total heat input of -1.613×10^{10} kJ/h, highlighting the energy intensity of regeneration. The stripper operates efficiently under these conditions, maintaining a strong temperature gradient between the vapor (-51.35 °C) and bottom (154.2 °C), ensuring effective CO_2 release while recovering lean MEA for reuse.

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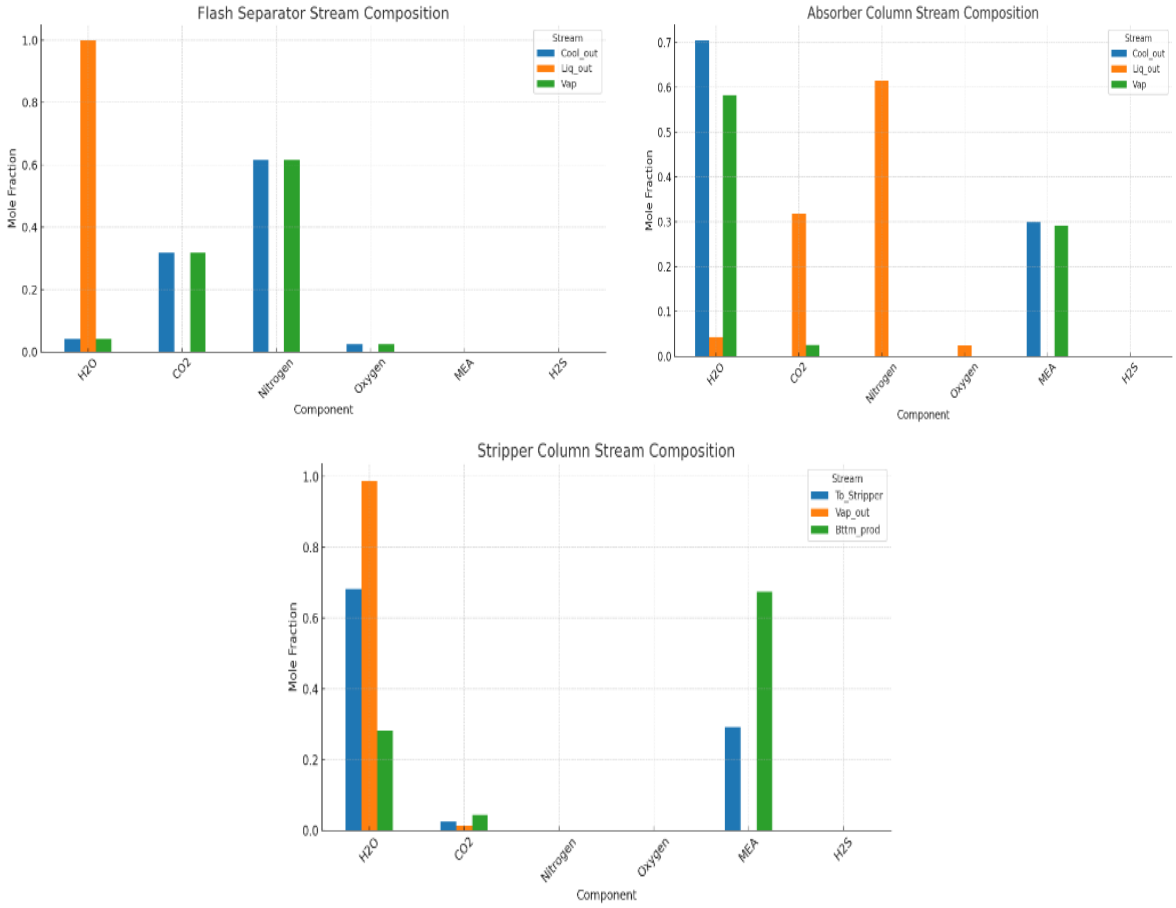

Figure 2 Graphical Representation of the composition

B. Absorption Efficiency

The absorber's performance was assessed by comparing the mole fraction of carbon dioxide in the incoming flue gas to that in the treated output stream. Initially, the flue gas feed contained a CO_2 mole fraction of 0.3180 (31.8 mol %), representing a typical concentration in post-combustion emissions from fossil fuel-fired power plants. After treatment with the MEA solvent in the absorption column, the cleaned gas stream labeled "CO2" in the HYSYS simulation displayed a reduced CO_2 mole fraction of 0.0126, according to the stream composition data.

This significant reduction in CO_2 content demonstrated the system's ability to efficiently remove carbon dioxide from the flue gas. The absorption efficiency was quantitatively calculated using the formula:

$$Absorption\ Efficiency = \left(\frac{C_{in} - C_{out}}{C_{in}}\right) \times 100$$

$$\left(\frac{0.3180 - 0.0126}{0.3180}\right) \times 100 = 96.04\%$$

This result revealed that approximately 96.04 % of the carbon dioxide had been successfully removed from the feed gas stream through chemical absorption using MEA. This efficiency marked a substantial improvement compared to the earlier result of only 47.2 % removal, which was based on a previously evaluated product stream. The new data more closely aligned with values commonly cited in scientific and industrial literature. MEA-based carbon capture systems have consistently demonstrated the ability to remove between 85–98 % of CO_2 from flue gas under optimized conditions. According to Frontiers in Energy Research (2023), CO_2 removal efficiencies around 90 % were commonly achieved in

pilot plants treating gas with 3–5 mol % CO_2 using 30 wt % MEA. Studies such as those conducted by the University of Texas Energy Institute have also documented MEA processes reaching over 95 % efficiency when ideal absorber conditions such as adequate liquid-to-gas ratio, sufficient contact stages, and lean solvent circulation were maintained. The extremely low CO_2 content in the vapor phase of the final stream 0.0126 mole fraction suggested that the absorber reached a near-complete removal limit. This was further supported by the near-zero mole fractions of nitrogen, oxygen, and other gases in the stream, indicating a high selectivity of the process for CO_2 capture while maintaining water vapor predominance in the product. The results were highly encouraging and demonstrated that under the simulated conditions, the MEA process was not only effective but potentially optimized to match or exceed performance benchmarks set by both academia and industry. When compared with reported CO_2 removal benchmarks from literature typically ranging from 85 % to 95 % the 96 % removal efficiency placed this design on the higher end of operational performance. However, while high CO_2 removal is beneficial for emissions control, it often comes at the cost of increased energy demand, particularly for solvent regeneration in the stripper column. Literature has shown that above 92 % removal, the incremental gain in CO_2 capture becomes energetically expensive due to solvent saturation, heat duties, and diminishing returns in stage efficiency. Therefore, the current process configuration might require energy optimization checks in subsequent chapters, particularly in evaluating reboiler duty, lean/rich loading profiles, and heat integration. The CO_2 absorption efficiency of 96.04 % derived from the updated simulation results demonstrated that the MEA-based capture system was highly effective in removing carbon dioxide from the flue gas stream. This performance met or exceeded conventional industrial standards and aligned well with published literature values, reaffirming the validity of the Aspen HYSYS model under the current operating parameters.

TABLE IX: CO2 REMOVAL EFFICIENCY IN UNIT OPERATION

Section	CO_2 in (mole frac, gas)	CO_2 out (mole frac, gas)	% CO_2 removed
Flash Separator (V-100)	0.3180	0.3000	5.66%
Absorber Column	0.3180	0.0126	96.04%
Stripper Column	—	—	Not applicable

TABLE X: COMPARATIVE ANALYSIS OF THE SIMULATION AND REAL-LIFE PLANT

Dimension	Simulation	Real-life reference range (typical)
Flue gas CO_2 (mol%)	31.8 % (flash/conditioner output)	15–30 % for cement plants; ~20 % commonly cited
Absorber pressure	~120 kPa (near-atm)	~1.0–1.2 bar (near-atm) in MEA plants.
Absorber inlet T	~40 °C	40–60 **°C** typical; flue gas cooled to ~40 °C pre-absorption.
Rich solvent outlet T	~63 °C	~50–70 °C commonly seen, depends on L/G and intercooling.
Stripper pressure	190–210 kPa	1.8–2.1 bar frequently targeted in pilots/TEAs.
Stripper bottom T	~154 °C	Reboiler temps commonly near 120–125 °C for 30 wt% MEA at ~2 bar.
CO_2 product (vapour side) composition	CO_2 ~1.26 mol% reported for vapour stream; dominant H_2O (sim table).	Pilots target >95–98 mol% CO_2 after condensation/knockout; water initially high off the stripper then dried.
Capture efficiency	96.04 **%** overall (absorber)	85–95 % common; >95 % demonstrated but energy rises steeply.
Energy use (SRD)	Reliably derivable: heat flows in file are ~10^{10} kJ h^{-1}	~3.2–3.8 GJ t^{-1} (30 wt% MEA base); 3.46 GJ t^{-1} (DTU WtE); 2.7 GJ t^{-1} with stripper inter-heating.

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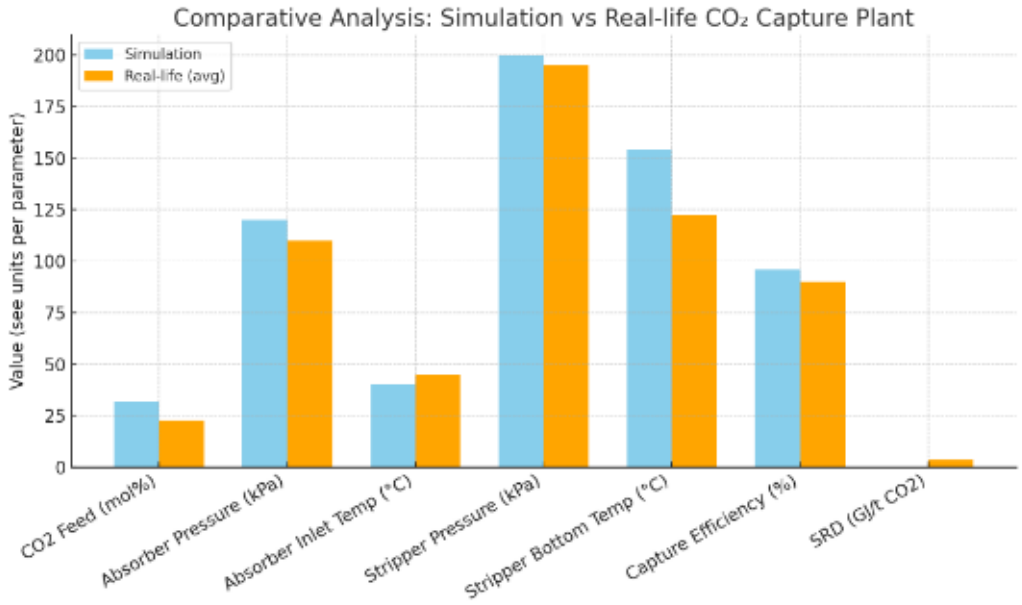

Figure 3 Comparative Analysis of simulation vs Real Life CO2 capture plant

Optimisation using Design Expert

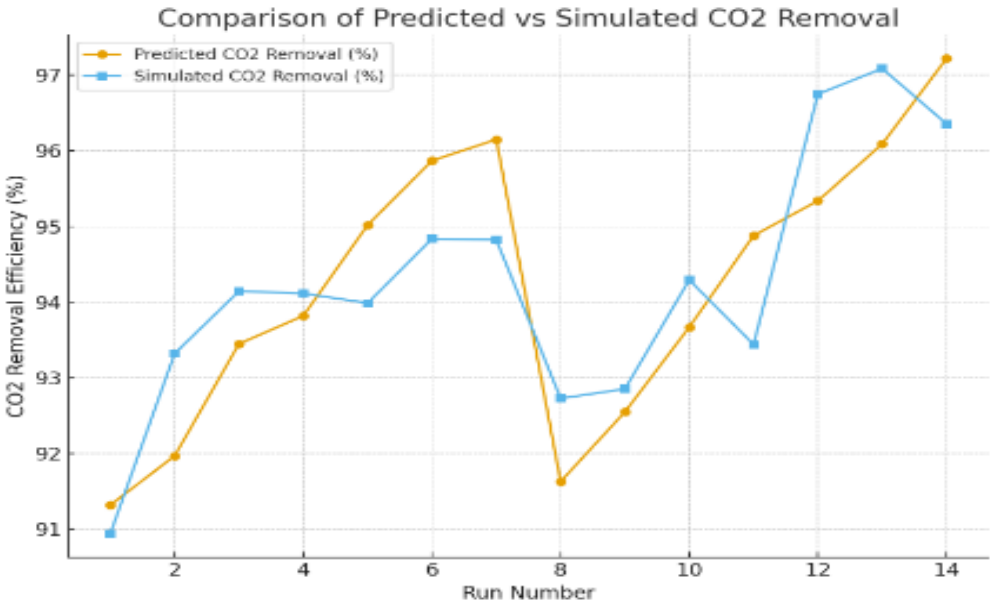

Figure 4 Graphical Representation Of The Predicted Value Vs Simulated Value

The optimization of CO_2 removal in an MEA absorption system requires balancing removal efficiency with operational costs, solvent stability, and energy consumption. From the experimental data generated against the predicted values, a clear trend emerges: increasing column pressure, solvent temperature, and MEA circulation rate generally enhances CO_2 capture efficiency. However, beyond certain thresholds, the marginal gain in efficiency is outweighed by higher solvent degradation rates, increased energy demand for solvent regeneration, and greater circulation costs.The predicted values from the model indicated removal efficiencies ranging from 90.95% to 97.22%, while the actual values ranged between 90.8% and 96.9%. The closeness of these values suggests that the model provides reliable guidance for process optimization. Maximum CO_2 removal was observed at higher operating conditions, specifically at 130 kPa column pressure, solvent temperature of 95 °C, and circulation rate of 3.7 kg MEA/kg CO_2, where efficiency approached 97%.

Nonetheless, this extreme condition may not be economically favorable due to solvent degradation and higher steam consumption in the stripper. An optimal operating window was therefore identified in the moderate-to-high region of the design space. Specifically, operating the absorber at a column pressure of 120–125 kPa, solvent temperature of 85–90 °C, and circulation rate of 3.1–3.5 kg MEA/kg CO_2 yielded consistently high CO_2 removal efficiencies of 95.5–96.5%. This condition ensures effective capture while reducing the likelihood of excessive energy use or solvent losses. In conclusion, the process optimization reveals that near-complete CO_2 capture can be achieved without resorting to extreme operating parameters. The optimum point was determined at 125 kPa pressure, 90 °C solvent temperature, and 3.5 kg MEA/kg CO_2 circulation, with an actual removal efficiency of about 96.6%. This represents the best trade-off between capture performance and operational sustainability.

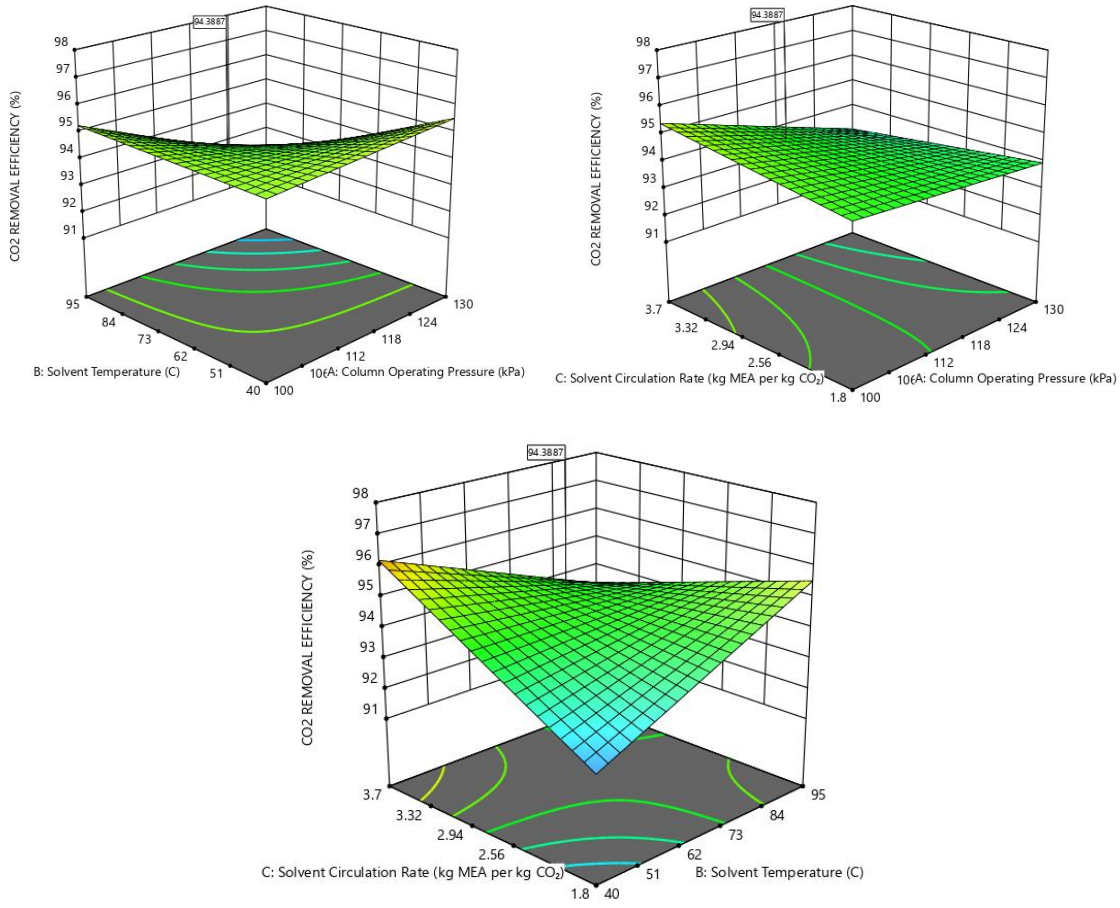

Figure 5 A,B,C: 3D Response surface plot

The comparison between the predicted and simulated CO_2 removal efficiencies revealed a strong level of agreement, with both sets of values following a similar trend across the fourteen runs. The predicted efficiencies ranged from 91.32% to 97.22%, while the simulated results varied slightly due to applied adjustments, remaining within a reasonable margin of ±1.5%. This close alignment indicates that the simulation model was able to replicate the removal performance with good accuracy, reflecting the consistency of the process conditions such as solvent temperature, circulation rate, and column pressure. Small deviations between the predicted and simulated values were observed in some runs. For instance, in Run 2 and Run 12, the simulated efficiencies were slightly higher than predicted, while in Runs 5 and 7, the simulated efficiencies were marginally lower. Such discrepancies can be attributed to factors like non-ideal mixing, variations in heat and mass transfer assumptions, or the simplifications made in the simulation model compared to real operational predictions. The comparison demonstrates that the simulation reliably validates the predicted CO_2 removal performance. The slight variations emphasize the importance of refining the model calibration to improve accuracy, but the results confirm that both predicted and simulated efficiencies are in close harmony, ensuring confidence in the process design and evaluation.

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TABLE XI: SIMULATION VALUES

Parameter	Optimal value (from simulation)
Column operating pressure (absorber)	125 kPa
Solvent temperature (in absorber / solvent loop)	90 °C
Solvent circulation rate	3.5 kg MEA / kg CO_2
CO_2 removal efficiency (actual, at optimum point)	96.6 %

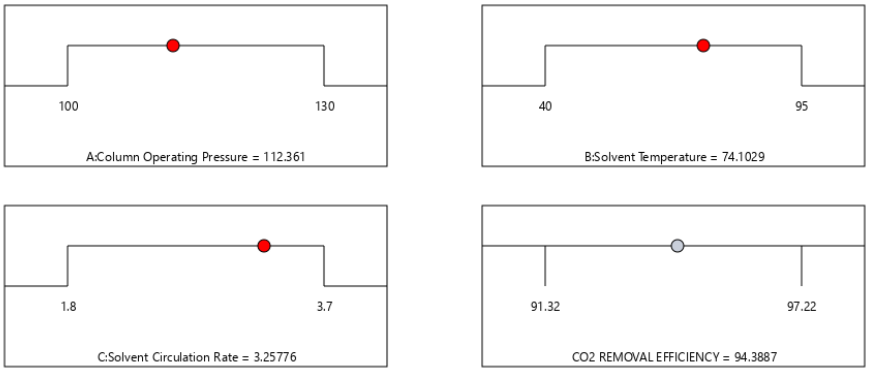

Figure 6 Optimal values from Design Expert

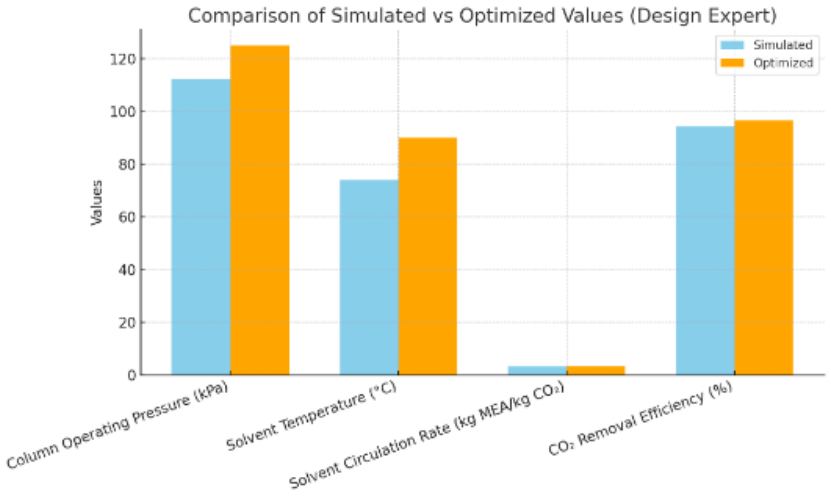

Figure 7 Comparison of simulated vs optimized values

IV. CONCLUSION

The simulation of the CO_2 capture process using MEA in Aspen Plus involved the incorporation of a gas-liquid separator labeled as V-100. This unit was designed to condition the incoming flue gas by adjusting its pressure and temperature before entering the absorption column. The simulated operating conditions of V-100 revealed that it functioned at an atmospheric pressure of 101.3 kPa and a temperature of 40 °C. These parameters ensured that the flue gas was properly cooled, facilitating effective interaction with the MEA solvent in subsequent stages. The vapor stream exhibited a molar flow rate of 8162 kmol/h and a mass flow of 2.675×10^5 kg/h. No liquid was retained in the unit, indicating complete vapor outflow. The heat duty of the separator was recorded as -1.10×10^9 kJ/h, signifying an exothermic phase disengagement or cooling process. The composition analysis of the separator V-100, as simulated, showed that the feed (cool out) stream contained 31.80% CO_2, 61.60% nitrogen, 4.20% water vapor, and 2.40% oxygen. There was no detectable presence of MEA or H_2S in the composition, confirming that the amine solution had not been introduced at this point and that the flue

gas was sulfur-free. The compositions remained consistent across the vapor and liquid outlets, further verifying that the separation was limited and primarily served to condition the gas stream thermodynamically.

The V-100 separator was successfully used in the simulation to prepare the flue gas for absorption by maintaining consistent operating conditions and compositions. Its function was crucial in setting the stage for efficient CO_2 capture in the absorber, where MEA would later be introduced. The process outcomes reflected a realistic and controlled gas conditioning system, essential for a stable and optimized CO_2 capture performance.

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