

# Process Simulation and Optimization of CO<sub>2</sub> Capture Using Amine Absorption

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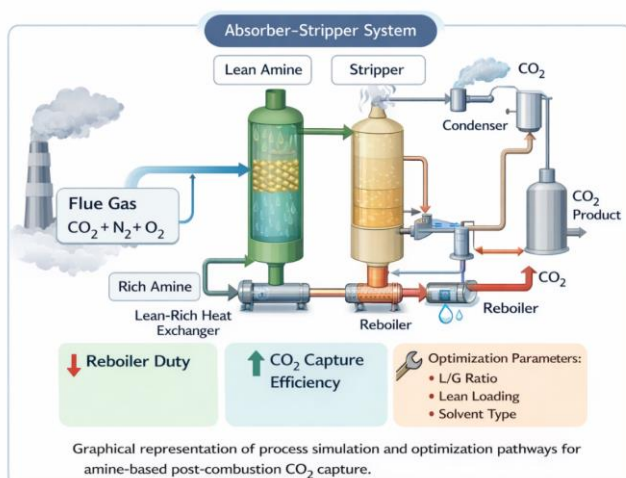
**Abstract** - The study investigates the post-combustion carbon capture using amine absorption technique and evaluates the efficiency of CO<sub>2</sub> removal and energy consumption in absorption section of the process. Carbon capture is one of the promising practices carried out from fossil-fuel based power plants and industrial sources. It targets on various amine solvents to determine the chemical absorption. However, the large energy penalty is associated with solvent regeneration. The study presents systematic reviews of published literature on the process simulation and optimization of the CO<sub>2</sub> capture using amine absorption. The data from peer-reviewed experimental, pilot-scale, and simulation studies have evaluated the solvent performance, kinetic modeling, and absorber-stripper configuration. It has strongly influenced the key operating parameters such as liquid-to-gas ratio, reboiler duty, lean solvent CO<sub>2</sub> loading and sensitivity analysis. The review compares the conventional solvents like monoethanolamine (MEA) with advanced and blended amines. The study highlights the reported energy savings and operational challenges along with potential ways to reduce regeneration energy using process integration techniques. Techno-economic assessment has revealed that approximately 60-70% of operating costs for solvent regeneration is reported. Overall, the findings provide the consolidated reference and strategic insights for development of energy-efficient and industrial viable amine-based CO<sub>2</sub> systems.

**Key Words:** Carbon Capture, Optimization, Aspen Hysys Simulation, Amine Absorption, absorber-stripper optimization, reboiler duty, thermodynamic modeling

## 1. INTRODUCTION

Despite of global climatic change, there is continuous increase in atmospheric carbon di oxide (CO<sub>2</sub>) emission. It has led to global warming and ecological imbalances where large stationary sources like coal-fired power plants, cement industries, and petrochemical units have accounted a major fraction for CO<sub>2</sub> emission anthropogenically. According to Paris Agreement, a scenario of the climatic conditions requires attention to reduce greenhouse gas emission to limit the global temperature rise to be precise to 2°C (Micari et al., 2025). In such scenario, the Carbon capture and utilization (CCU) and Carbon capture and storage (CCS) have combinedly profound a technological pathway for achieving deep decarbonization. This can allow continued use of fossil fuels during the energy transition unit through Carbon Capture Utilization and Storage (CCUS). A significant advantage of using both CCS and CCU have typically realized a closed loop comprising of CO<sub>2</sub> capture using chemical absorption in the most established way due to adaptability and existing plants and effectiveness at low CO<sub>2</sub> partial pressures (Ola et al., 2025).

In the optimization of process, the selection of aqueous amine solutions particularly mono ethanolamine (MEA) have been extensively employed for CO<sub>2</sub> Capture because of their high reactivity and absorption capacity. It has also attained maturity as post-combustion CO<sub>2</sub> capture applications reference for CO<sub>2</sub> removal, solvent degradation, high energy consumption, and operational inefficiencies. Around 60-70% of the total operating cost of amine-based capture plant is associated with solvent regeneration step. It has consequently improved the economic and environmental performance (Rubin et al., 2015). Numerous reviews have examined the CO<sub>2</sub> Capture technologies like Adsorption, Membrane Separation, Cryogenic Separation, and Calcium looping. Adsorption uses solid sorbents (MOFs, zeolites) for lower energy use and scalability but faces moisture sensitivity and adsorbent degradation. Membrane Separation being modular and efficient way for certain applications like pre-combustion with lower capital costs but faces stability issues and membrane wetting (Micari et al.,



2025). In Cryogenic Separation, a very high range of purity (>99%) and recovery to around 90-99% has been added. It remarks on complex yet energy-intensive cooling systems with high capital costs. While Calcium looping is promising pilot stage technology which has lowers regeneration of energy than amines and still requires improvement (Oyeneke & Rochelle, 2006). However, all the processes that are explored requires a significant improvement for enhancement of overall CO<sub>2</sub> removal efficiency. Among them, the technically proven technology for CO<sub>2</sub> capture from flue gas is the absorption-desorption process using amine solvent.

The amine absorption technology has commercially deployed on the principle of flue gas being passed through liquid amine solvents like MEA, tertiary methyldiethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP), and cyclic piperazine (PZ). They chemically bond with CO<sub>2</sub> and then the solvent is heated in a regenerator to release pure CO<sub>2</sub> and reuse of the solvent (Le Moulec & Neveux, 2016). The process is compatible with existing infrastructure and have high capture rates around 60-95% (Normann et al., 2017). Therefore, the process provides a direct and linear relationship between the regeneration energy and the energy efficiency penalty in power plants. Therefore, the reduction of the energy requirements of amine-based CO<sub>2</sub> capture process has attracted to meet the objectives of mitigating the CO<sub>2</sub> emission at global level.

The key problem identified in the study is that amine absorption technology hinders a large-scale challenge (Normann et al., 2017). Firstly, the stripper reboiler requires high steam demand. Secondly, the process faces corrosion and solvent degradation issues. Thirdly, the suboptimal operating conditions lead to energy loss. Lastly, the process limits on integration of rigorous simulation-based optimization in industrial practice. The challenges identified highlights the necessity for a systematic simulation and optimization of the study which captures thermodynamic behavior and evaluates key process parameters (Rochelle, 2009). In response, the extensive research that has been conducted on solvent development, kinetic modeling, thermodynamics, process simulation, and optimization strategies to attain improved efficiency and economic viability. The amine absorption technology is regarded as one of the most advanced and commercially promising technologies for post-combustion CO<sub>2</sub> capture (Rochelle, 2009).

For decades, it has provided a satisfactory result in achieving the chemical absorption using amine solutions. Advanced process simulators like ASPEN plus have become a central tool for evaluating absorber-stripper systems that enables the detailed analysis of mass transfer, vapor-liquid equilibrium, and energy integration without need for costly experimentation. The process modeling encompasses on various approaches such as steady-state modeling, dynamic

modeling, kinetic modeling (Notz et al., 2012). The process modeling serves on specific purposes that enables comprehensive analysis and optimization of chemical processes. Aspen-Hysys is a robust simulator which provide process simulation atmosphere using chemical engineering for diverse applications. The software supports environmental impact assessments with minimization of waste emission and excels in reaction engineering. The simulation tool has crucial way for designing and optimizing distillation and separation units. The simulator can provide robust thermodynamic modeling for accurate predictions and optimization to attain supply chain operations (Saeid et al.2024).

The paper focuses on the objectives where simulation and optimization of an amine-based CO<sub>2</sub> capture process using ASPEN Plus reduces energy consumption while maintaining high capture efficiency. It includes development of absorber-stripper process model, evaluation of thermodynamic and reaction behavior of MEA-CO<sub>2</sub>-H<sub>2</sub>O system and sensitivity analysis of key parameters. It also optimizes reboiler duty and solvent operating conditions outlines the review on process simulation and optimization using amine absorption, CO<sub>2</sub> Capture performance and reaction mechanism of amine solvents.

## 2. MATERIAL AND METHODS

### 2.1 Raw Materials

The raw materials considered in the review correspond to chemical solvents and gas streams which commonly employed in amine-based post-combustion CO<sub>2</sub> Capture systems (Boot-Handford et al., 2014).

**Table-1.** Raw Material Used in Amine-Based CO<sub>2</sub> Capture Systems

Category	Material	Typical Range/ Specification	Purpose
Flue Gas	Carbon-Di-Oxide (CO <sub>2</sub> )	10-15 vol%	Target gas for capture
	Nitrogen (N <sub>2</sub> )	70-75 vol%	Major inert component
	Oxygen (O <sub>2</sub> )	3-6 vol%	Excess air representation
	Water Vapor (H <sub>2</sub> O)	Saturated	Stable solvency
Solvent	Monoethanolamine (MEA)	20-30 wt%	Absorption solvent benchmark
	Diethanolamine (DEA)	20-35 wt%	Lower regeneration

			n energy
	Methyldiethanolamine (MDEA)	30-50 wt%	High selectivity, slow kinetics
	AMP	20-30 wt%	Sterically hindered amine
<b>Blends</b>	MEA-MDEA, AMP-PZ	Variable ratios	Energy-efficient solvent systems

### 2.2 Pre-treatment steps for flue gas and solvent streams

The pre-treatment steps including conditioning of flue gas and solvent streams before absorption which provide the information in the reviewed studies (Freguia & Rochelle, 2003; Abu-Zahra et al., 2007).

**Table 2: Pre-Treatment Steps for Flue Gas and Solvent Streams**

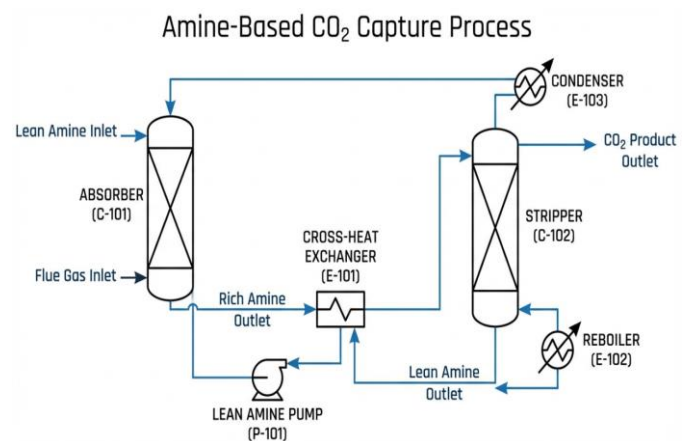
Stream	Pre-treatment Steps	Operating Conditions	Purpose
<b>Flue Gas</b>	Cooling	40-60°C	Improving Absorption efficiency
	Water Saturation	Near 100% RH	Solvent Evaporation Prevention
	SO <sub>x</sub> / NO <sub>x</sub> removal	Ppm level control	Minimizing Solvent Degradation
<b>Lean Solvent</b>	Filtration	Continuous	Removal of degraded products
	Temperature Control	30-40°C	Absorption Kinetics enhancement
	CO <sub>2</sub> loading adjustment	0.15-0.25 mol/mol	Maintaining absorption driving force

### 2.3. Aspen-Hysys Simulation

The CO<sub>2</sub> capturing process was simulated using Aspen-Hysys includes the key components like absorber and

desorbed columns which reflect on the industrial conditions. The simulation provided a baseline for understanding the process dynamics and identifying the critical operational parameters for further investigations (Freguia & Rochelle, 2003). Fig.1.Process flow diagram (PFD) for amine capturing gas treating systems and removing CO<sub>2</sub> from flue gas. The lean amine is pumped with the top of the absorber (C-101) to begin the process of absorbing CO<sub>2</sub> from treated flue gas. The treated flue gas as feed contains CO<sub>2</sub> to attain the flow in upward direction when encountering downward flowing MEA solution (Dugas, 2006).

The cooler set out to required pressure and temperature. The flue gas is pre-treated in pump (P-101) with heat exchanger (E-101) to separate pressure and temperature. The flue gas in absorption column have set clean gas as now free from CO<sub>2</sub> and exits from the top of the absorber. The rich amine is loaded with CO<sub>2</sub> have transferred from the bottom of the absorber to the regeneration section. The rich amine is heated in cross heat exchanger before it enters the desorber, while the lean amine is cooled down before it returns to the absorber. Indeed, the heat exchanger transfers the heat between rich and lean amine streams to improve efficiency of process and energy savings (Saeid et al.,2024). The rich amine process enters a distillation column as desorber and causing the process to stripped from amine solution and leaving behind lean amine. In distillation column, the reboiler (E-102) heats the bottom of desorber using steam and generates vapors. While, the condenser (E-103) cools the vapors exiting the top of the desorber. The portion of water vapor present in the gas stream with the separation from the CO<sub>2</sub> gas (Boot-Handford et al., 2014).



**Fig.1.** Process flow diagram (PFD) of carbon capturing for amine-based CO<sub>2</sub>

The recycling of lean amine ensures continuous process an operation is captured in stripper (C-102). The fresh amine and water are added to the system as makeup stream to compensate for any losses. The stream ensures the amine concentration to remain optimal for effective CO<sub>2</sub> Capture. An advanced thermodynamic model is used to predict the phase behavior of chemical solvents (Boot-

Handford et al., 2014). The models usually include non-random two-liquid (NRTL) model and electrolyte-NRTL (eNRTL) model with liquid-liquid and liquid-vapor equilibrium for systems mainly in aqueous solution.

### 2.4 Experimental Design

In the context of systematic review, the experimental design has added on the experimental and simulation process to be adopted with conventional absorber-stripped configuration. The process consists of packed absorption column operating under counter-current flow. A regeneration column equipped with reboiler and condenser and rich-lean amine heat exchanger with auxiliary units such as pumps and coolers helps in adding low CO<sub>2</sub> partial pressures designs with near-atmospheric operation.

The experimental design review on the key operating parameters have evaluated the influence on CO<sub>2</sub> capture performance. It has most frequently investigated on variables like Liquid-to-gas (L/G) ratio, amine concentration (20-30 wt% for MEA-based systems), lean solvent CO<sub>2</sub> loading (0.2), absorber inlet temperature (40–60°C), stripper pressure: (1–2 bar), column pressure-1 atm, and reboiler duty-(4.2 GJ/ton) CO<sub>2</sub>, reboiler temperature :100-120°C and packing height and type, number of stages:10-20. With those variables, the impact on absorption efficiency, mass transfer, and regeneration energy demand is high.

## 3. RESULTS AND DISCUSSION

### 3.1 Effect of Liquid-to-Gas Ratio

The liquid-to-gas (L/G) ratio is one of the most influential operating parameters through which amine-based CO<sub>2</sub> absorption systems can be maintained. It has been reported by various researchers that the upgraded solvent availability and greater gas-liquid interfacial contact within the absorber have led to increase in L/G ratio and directly linked to CO<sub>2</sub> capture efficiency improvement (Singh et al., 2025). However, at low L/G ratios, insufficient solvent flow limits absorption capacity and resulting in incomplete CO<sub>2</sub> removal and higher CO<sub>2</sub> slip in the treated gas. While, L/G ratio raises the driving force for mass transfer enrichment and leading to higher capture efficiencies.

$$\frac{L}{G} = \frac{m_L}{m_G}$$

m<sub>L</sub>= mass flow rate of liquid solvent (Kg/s or Kg/h)

m<sub>G</sub>= mass flow rate of gas stream (Kg/s or Kg/h)

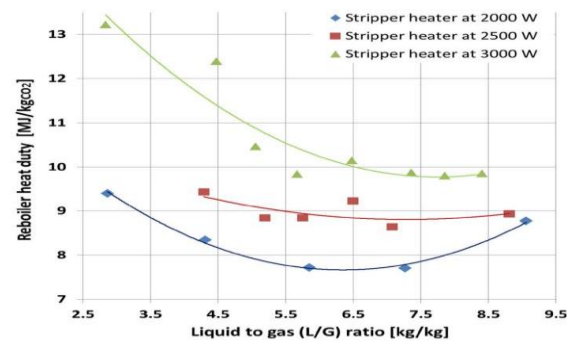
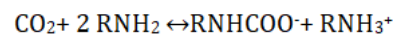


Figure 4.2: Effect of L/G ratio on reboiler heat duty

The optimal range of L/G ratio yield has certainly raised energy consumption but has diminished returns in CO<sub>2</sub> removal. Lower lean loading → higher regeneration requirement → higher energy consumption. Higher lean loading → reduced energy but lower driving force for absorption. It has also elevated the pumping power requirements and raise in thermal load on the stripper reboiler during solvent regeneration but found that it requires higher solvent circulation (Shimekit & Mukhtar, 2012).

### CO<sub>2</sub> Absorption Reaction Kinetics (MEA System)



Where, RNH<sub>2</sub> = Monoethanolamine (MEA)

### Rate Expression for CO<sub>2</sub> Absorption (Fast Reaction Regime)

$$r_{abs} = k_{MEA} C_{CO_2} C_{MEA}$$

Where, r<sub>abs</sub> = rate of CO<sub>2</sub> absorption (mol\*m<sup>-3</sup>\*s<sup>-1</sup>)

k<sub>MEA</sub> = reaction rate constant (m<sup>3</sup>\*mol<sup>-1</sup> s<sup>-1</sup>)

C<sub>CO<sub>2</sub></sub> = CO<sub>2</sub> concentration in liquid phase (mol\*m<sup>-3</sup>)

C<sub>MEA</sub> = MEA concentration (mol\*m<sup>-3</sup>)

### Temperature Dependence (Arrhenius Equation)

$$k_{MEA} = A \exp \left( - \frac{E_a}{RT} \right)$$

Where, A = pre-exponential factor

E<sub>a</sub> = activation energy (KJ\*mol<sup>-1</sup>)

R = gas constant

T = temperature (K)

Beyond this, it has been identified that optimal L/G ratio range between 1.5-2.5 kg solvent/ kg flue gas for MEA-based systems have contributed in balancing performance of absorption and energy demand. It has also contributed in L/G ratios that is excessively high with limited hydraulic practices like column flooding. It has been optimized that L/G ratio is crucial for attaining energy-efficient operation without compromising capture efficiency (Shimekit & Mukhtar, 2012).

### 3.2 Lean CO<sub>2</sub> loading and Reboiler Duty

Lean CO<sub>2</sub> loading plays a crucial role in determining both stripper energy consumption and absorber performance. There are several studies highlighting higher CO<sub>2</sub> capture efficiencies with lower lean solvent loadings driving absorption phenomenon in the absorber. This has also achieved very low lean loadings with increased thermal energy inputs in the stripper resulting in higher reboiler duty (Normann et al., 2017). The trade-off makes lean loading one of the most reliable ways to optimize variables in amine-based CO<sub>2</sub> capture process.

#### CO<sub>2</sub> loading definition

$$\alpha = \frac{n_{CO_2}}{n_{amine}}$$

$\alpha$  = CO<sub>2</sub> loading (mol CO<sub>2</sub>/ mol amine)

#### Lean CO<sub>2</sub> Loading

$$\alpha_{lean} = \frac{n_{CO_2}^{lean}}{n_{amine}}$$

Lower Lean loading= higher absorption driving force

Lower lean loading= higher regeneration energy

#### Rich CO<sub>2</sub> loading

$$\alpha_{rich} = \frac{n_{CO_2}^{rich}}{n_{amine}}$$

The studies have also shown a strong inverse relationship between lean CO<sub>2</sub> loading and reboiler energy requirement. It is typically reported values for MEA systems range from 0.15-0.25 mol CO<sub>2</sub> per mol amine. The lean loadings below 0.18 mol/mol often lead to reboiler duties exceeding 4.5 GJ per ton of CO<sub>2</sub>, whereas higher lean loadings reduce energy demand but may compromise absorption efficiency (Shimekit & Mukhtar, 2012).

#### Total Reboiler Duty

$$Q_{reb} = Q_{sens} + Q_{vap} + Q_{des}$$

$Q_{sens}$  = sensible heat

$Q_{vap}$  = latent heat (water vaporization)

$Q_{des}$  = heat of CO<sub>2</sub> desorption

#### Practical Reboiler Duty Expression

$$Q_{reb} = \dot{m}_{solv} (C_p \Delta T + \Delta H_{des})$$

$\dot{m}_{solv}$  = solvent flow rate

$C_p$  = heat capacity

$\Delta H_{des}$  = heat of desorption

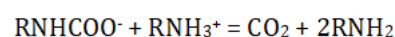
Other studies have identified the optimal lean loading window between 0.18-0.22 mol/mol which provides the balance between energy efficiency and capture performance. This can also provide essential way for minimizing the operational costs and maintaining regulatory compliance for CO<sub>2</sub> emissions.

- Lower lean loading → higher energy requirement
- Trade-off between regeneration energy and capture efficiency

### 3.3 Solvent Comparison

The solvent comparison arises directly from the absorption kinetics and regeneration energy and operational stability. The central focus of amine solvents is CO<sub>2</sub> capture research and MEA to set benchmark for solvents due to its fast kinetic reactions. This can be high when CO<sub>2</sub> capture efficiency and typically exceeding to 90% (Kim & Svendsen, 2011). However, MEA is associated with high regeneration energy, solvent degradation, and corrosion issues.

#### CO<sub>2</sub> Desorption Reaction



#### Desorption Rate Expression

$$r_{des} = K_{des} (C_{carbamate} - C_{carbamate}^{eq})$$

$r_{des}$  = CO<sub>2</sub> desorption rate

$C_{carbamate}^{eq}$  = equilibrium carbamate concentration

The DEA or tertiary amines like MDEA offers lower regeneration which is the result of slower absorption kinetics and often leading to higher solvent circulation rates in columns. Therefore, sterically hindering amines properties and need for fast kinetics with lower regeneration energy (Singh et al., 2025). The reports can indicate on optimized blends with reduced reboiler duty by 20-30% when compared to MEA while maintaining high capture efficiency (Le Moullec & Neveux, 2016).

### 3.4 Process Integration Strategies

The process integration strategies have widely recognized as effective means of reducing the energy penalty associated with amine-based CO<sub>2</sub> capture to certain extent. The most common approaches were reported in literature are use of lean-rich heat exchanger and recovers to sensible heat from hot lean solvent exiting the stripper to exothermic reactions at reduced boiler duty by 10-15% (Haaf et al., 2020). However, the integration techniques have improved absorption capacity but has result in multi-pressure operation and split-flow designs. The energy reductions may recover 30-40% of the low-grade heat (Oyeneke & Rochelle, 2006). This can improve energy efficiencies with the industrial implementation of the increased capital costs and operational complexities. This has also justified the additional investment and maintenance requirements at certain extent.

### 3.5 Techno-Economic Implications

The techno-economic implications rely on the reboiler steam consumption, solvent make-up costs, and capital expenditure for the study. The reported CO<sub>2</sub> capture costs for MEA-based systems range from USD 40-80 per ton of CO<sub>2</sub> adding uncertainty depending on fuel price, scale, and plant integration (Haaf et al., 2020).

The optimization of operating parameters and adoption of advanced solvent have reduced capture costs. This can integrate on the strategies of process integration and solvent blending at optimal rates can certainly reduce cost at 15-30% (Haaf et al., 2020). However, capital expenditure increases with careful consideration. The economic feasibility is high and specific with the fuel type, availability of waste heat and carbon pricing mechanisms. Overall, it has provided energy-efficient designs with well-supported amine-based CO<sub>2</sub> capture practices at appropriate policy incentives (Singh et al., 2025).

## 4. CONCLUSION

The study demonstrates the amine-based CO<sub>2</sub> capture remains to be most technologically mature and industrial viable option. The secondary data demonstrates solvent regeneration energy dominates both operational costs and overall process efficiency. Nearly two-thirds of total energy consumption have set out the accounting of the amine-based recovery. The liquid-to-gas ratio and lean solvent CO<sub>2</sub> loading exert on strong influence on capture efficiency and reboiler duty and making it central targets for optimization. The monoethanolamine contribution to serve as a benchmark solvent with fast kinetics and adding high capture efficiency. The advanced and blended amines offer significant potential for reducing regeneration energy and increased complexity and costing. The integration strategies have presented lean-rich heat exchange, absorber intercooling and advanced stripper configuration by

reducing energy demand. This also results in persistent challenges like limited long-term industrial validation of advanced solvents, showcasing techno-economic assessment. The gaps are addressed through integrated simulation, experimental validation, and economic analysis. Overall, the insights synthesized in the review are guiding future research on process design and policy-supported deployment of optimized amine-based CO<sub>2</sub> capture technologies.

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