

Department of Mechanical and Aerospace Engineering

Amine-Based Carbon Capture and Storage Using in Coal-Fired Power Plants

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ABSTRACT

Amine-based carbon capture and storage (CCS) is increasingly recognized as a promising technology to mitigate CO₂ emissions due to coal-fired power plant operations. While this process enhances CO₂ capture efficiency, it comes with the drawback of reducing power plant efficiency because of the energy required for regeneration. Researchers have been investigating alternative methods aimed at minimising the energy consumed by the reboiler unit such as new types of solvent development, the blending of varying amine fractions, and process modifications. This study examines the challenges associated with MEA-based CO2 capture process simulations, emphasizing the impact of process parameter variations and the integration of the vapour recompression method. The work was divided into three tasks: (a) model a system reported in the literature using the software Aspen Hysys, (b) assess the impact of changes in input parameters in the model output, and (c) include vapour recompression. The simulation of the base case was conducted using flue gas composition data gained from a 400 MW coal-fired power plant, assuming complete combustion, as illustrated in the references. After that, the parameters for the CO₂ capture process, sourced from the University of Tromsø, were employed in the simulation. Findings indicate a CO₂ capture efficiency of 74%, deviating from a reference of 85%. Furthermore, the theoretical power plant of 400 MW capacity released around 3,600 kg/h of CO₂, with approximately 970 kg/h captured. Importantly, the system consumed 184 MW, equivalent to around 46% of power plant's electricity. Energy analysis revealed that the reboiler unit, with a consumption of 127.90 MW, emerged as the predominant energy consumer, constituting 70% of the total energy consumption. When considering parameter variation, the flow rate of flue gas was found to be a noncritical parameter on CO₂ capture efficiency and reboiler duty. In contrast, a 12.5% increase in the temperature of lean amine influenced both parameters, resulting in an approximately 44% increase in CO₂ capture efficiency and a 1.19% reduction in reboiler duty. However, temperature adjustments risked MEA solvent thermal degradation and increased energy required for lean cooler. The incorporation of the vapour recompression method reduced energy consumption to 116 MW, compared to the base case's 184 MW, in line with results from previous studies. Results show that, in this configuration, carbon capture consumes 29% of the energy generated by the power plant. Despite this, there was no improvement in CO₂ capture efficiency, remaining consistent at 74%.

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LIST OF SIMBOLS

- g acceleration of gravity (m/s²)
- ρ density of liquid being pumped (kg/m³)
- η pump efficiency (-)
- Q flow rate (m^3/s)
- Q_{regen}-regeneration energy (W)
- Q_{sensible} sensible heat (W)
- Q_{latent} latent heat (W)

Q_{rxn} – heat of reaction (W)

 ΔT_{min} – minimum temperature difference (K)

 G_{in} – flow rate of the flue gas stream to the process (kgmole/h)

 G_{out} – flow rate of the gas stream outlet from the stripper (kgmole/h)

 $x_{CO_{2in}}$ – mole fraction of CO₂ in the flue gas stream to the process (-)

 $x_{CO_{2out}}$ – mole fraction of CO₂ in the gas stream outlet from the stripper (-)

mg/Nm³ – milligrams per cubic meter

wt%-weight percent

GJ – gigajoule (10⁹ Joules)

MW – megawatt (10⁶ Watts)

molCO₂ - molecular weight of carbon dioxide

GtCO₂ - gigatonnes of carbon dioxide

 $GW_e - gigawatt - Electric$

- CO₂ Carbon dioxide
- $H_2O-Water \\$
- H₂SO₄ Sulfuric Acid
- $H_3O^+ Hydronium \ ion$
- CO3²⁻-Carbonate ion
- $\mathrm{HCO}_{3}^{-}-\mathrm{Bicarbonate}$ ion
- OH⁻ Hydroxide ion
- $H_2S-Hydrogen\ Sulfide$
- $N_2\!-\!Nitrogen$
- $O_2 Oxygen$

ACRONYMS

- CCS Carbon Capture and Storage
- NETL National Energy Technology Laboratory
- PC Pulverized coal
- NGCC Natural gas combined cycle plant
- IGCC Integrated gasification combined cycle
- FTI Fusion Technology
- DEA Diethanolamine
- MEA Monoethanolamine
- AMP 2-amino-2-methylpropanol
- MDEA Methyldiethanolamine
- HEN Heat exchanger network
- IP/LP crossover Combined intermediate-pressure / low-pressure turbine
- e-NRTL Electrolyte Non-Random Two Liquid method
- PR Peng-Robinson equation
- PFD Process flow diagram
- PCC Post-combustion coal-fired power plants

1 INTRODUCTION

1.1 Problem definition

Climate change is a serious situation nowadays, and it is widely believed that carbon dioxide (CO₂) emissions heavily influence the growing disasters. These CO₂ emissions are related to electricity-generated activities in fossil-fuelled power plants [1]–[3]. Coal-fired power plants have the largest direct and indirect carbon emissions, compared to gas power systems, which are around 10 gigatonnes of carbon dioxide (GtCO₂) in 2021 [4]. Therefore, it is crucial to mitigate the amount of CO₂ emission in the coal-fired plant processes and decrease their impact on climate change through future technologies such as carbon capture and storage (CCS). The section that follows provides the latest research in coal-fired power plant with CCS technology.

Nontechnical factors such as cost, legalization, and market mechanism are also examined for the possibility of implementing the CCS on a large scale. CO₂ mineralization technology was initially adopted in several countries and faced severe regulatory problems due to inadequate political support, which could not be implemented commercially [5]. Furthermore, the CCS technology relies on regulatory frameworks and incentive schemes from the government, which is challenging to implement on a larger scale [6]. Rubin et al. (2007) suggested that the power plant cost elements, for example, capital cost and operating cost, should be significantly analysed associated with energy and policy analysis, including plant performance, such as the amount or quality of CO₂ emission, the efficiency of CCS, and the overall efficiency of power plant [7]. In spite of non-technical challenges, the efficiency of CCS and their impact on energy generation remain a central element in the feasibility of CCS deployment.

 CO_2 capture and storage technology can potentially reduce CO_2 emissions from fossil-fuelled power plants which are up to 90% efficient CO_2 capture. National Energy Technology Laboratory (NETL) investigated three main types of UK power plant; Pulverized Coal (PC), Natural Gas Combined Cycle plant (NGCC), and Integrated Gasification Combined Cycle plant (IGCC), adopting CCS technology using modelling. PC and NGCC integrated with the amine absorption process, while IGCC added the Selexol process, which is a physical process for CO_2 capture, and results indicated a reduction in CO_2 emission by up to 90%. However, the technology decreased the efficiency of the power plant by around 14 – 30% compared to the plant without CCS, leading to increase in the cost of electricity produced [8]. Cui et al. (2018) simulated six cases of PC plants with and without amine-based capture to investigate the efficiency using parameters were obtained from NETL Case 11 of 550 MWe and two Chinese coalfired power plants, which had a capacity of 600 MWe and 572 MWe. The results showed a high CO₂ capture rate by around 90% and high purity of CO₂ gas production by up to 99% in power plant with CCS; despite the net electricity decreased by around 25 - 30% [9]. Similarly, Coal-fired power plant with CCS is more expensive than conventional coal-fired power plants due to low operating efficiency. Hammond & Spargo (2014) analysed data gathering from Fusion Technology (FTI) report together with World Energy Council studies and then projected these parameters to 1 GWe coal-fired power plants with and without CCS technology with a life span of 40 years, which showed a long payback period and low energy gain ratio, accounting for 4 years and 9 times repays' energy investment, respectively [10]. Moreover, Rubin et al. (2007) results indicated that the costs of power plant having CCS was higher than in previous studies due to escalations at that time in capital and operation costs, including increases in energy requirement by around 15 - 20%; in contrast, the process could reduce the CO₂ emission typically by around 85 - 90% [7]. These previous studies stress the need for CCS technologies with current high efficiencies but with lower energy production penalties to facilitate their deployment in large scale.

Various methods were developed to increase in capture processes by using aminebased solvent and reduce energy generation penalties. Some researcher investigated different types of amines to increase capture efficiency and decrease heat consumption due to chemical reactions, which led to a decreased reboiler duty. According to Adeosun and Abu Zahra, M. (2016), evaluated amine-blend solvent system in 600 MW_e conventional coal-fired power plant using Aspen Plus[®] simulation tool. The various proportion of monoethanolamine (MEA), diethanolamine (DEA) blending with 2-amino-2-methylpropanol (AMP), and methyldiethanolamine (MDEA) were simulated and, found that 5 wt% DEA blended with 25 wt% AMP required the lowest reboiler duty accounting for 3.17 GJ/tonCO₂ [11]. As for Pourjazaieri et al. (2010), simulated different types of amine-based CO₂ recovery from flue gas in a petrochemical plant, and the results showed CO₂ in flue gas could be recovered by using MEA and DEA, which had recovery efficiency by up to 96% and 97%, respectively, whereas MDEA had efficiency about 30% [12].

Some researchers relied on process modified method for reboiler duty reduction. The conventional process mainly focused on reducing heat regeneration in the reboilerstripping units, which minimised the amount of heat consumption for steam heating, such as thermal integration, heat pump effect and absorption enhancement [13]. The intercooled absorber as an absorption enhancement was simulated to improve amine process through decrease flow rate of absorbent for increasing CO₂-rich loading. The process could reduce overall energy requirement in MEA-based coal-fired power plant by up to 8% [14]. In terms of thermal integration, rich liquid split was investigated to recover waste heat from process for decreasing of reboiler duty. The 500 MW supercritical coal-fired power plant using MEA solvent and split flow improvement were simulated by Aroonwilas & Veawab (2007), and results presented a greater overall plant efficiency in advanced MEA process from 36.8% to 40.1% as well as reduced CO₂ emission rate from 1,062 to 976 tonnes/day [15]. Lean vapour compression is one of process improvement based on heat pump effect by flashing hot lean solution from stripper then compressing the gaseous stream and feeding back to the stripper. The modelled result from Moullec & Kanniche (2011) illustrated the lean vapour compression could minimise the reboiler duty from 3.23 GJ/tCO₂ to 2.56 GJ/tCO₂ [16]. Even though it has been shown from previous research to improve overall efficiency by varied types of amine solvent, blending fraction, and process modification, but the energy penalty remained significant.

Consequently, the heat and power technique were deployed to archive the high performance of coal-fired power plant with amine-based capture. Amine-based CO_2 capture integrated with heat and power technique was investigated by S.-Y. Oh et al. (2018). The 550 MW_{net} supercritical coal-fired power plant was modelled through the Aspen Plus simulation program to analyse the energy efficiency compared to the process with and without CCS including heat and power improvement. The process was improved by back pressure turbine installation from IP/LP turbine, integrated with conventional processes, which are inter-cooling absorbent, semi-lean solvent and rich solvent splitting, could keep overall efficiency in CCS by up to 90% while reducing net energy penalty by up to 30%. (From 12.8% to 8.7%) [17].

While amine-based CO_2 capture and storage has emerged as a promising technology, there remains a limited focus on studies related to parameter variations when operating at atmospheric pressure. Most previous research has focused on variations in

amine concentration, types of amines used, and amine blending fractions. There has also been an importance on process improvement aimed at reducing reboiler duties. However, there was no attempt to explore the effects of flow rate, temperature, and column characteristics, including process enhancement, which influence energy demand and CO_2 capture efficiency within the same project.

1.2 Aims

This thesis investigates the various factors that influence the performance of CO_2 capture, such as the inlet flow rate, inlet temperature, and the characteristics of both absorber and desorber columns. Additionally, it examines process improvements aimed at increasing carbon capture efficiency and decreasing energy penalty in a base-case CO_2 capture plant.

It is complemented by detailed objectives.

- To establish and validate a detailed process model of the base case model, as reported in the literature, of a carbon capture plant employing the simulation program Aspen Hysys.
- To undertake an investigation of the heat and mass transfer within the base case carbon capture plant simulation.
- To investigate the factors, including inlet flow rate, inlet temperature, and the characteristics of columns that impact on the performance of CO_2 capture simulation.
- To evaluate the overall energy efficiency of the carbon capture plant integrated with the process improvement method for increasing carbon capture efficiency as well as decreasing energy penalty.

1.3 Overview of methodology

- Model development and validation: validate a rate-based process model with operational data from literature.
- Simulation and parameter variation: simulate multiple cases, each varying the key parameters, and compare the simulation results and energy consumption.
- High-Efficiency Simulation: simulate a base case capture plant integrated with the high-energy efficiency method for comparing the results against the base modelling to ascertain the energy demand reduction benefits.



1.4 Structure of the dissertation

This dissertation is structured in five sections, as follows:

Section 2 Literature Review

This section reviews studies relevant to the CCS technology integrated into coalfired power plants using amine absorption as well as improving their efficiency to enhance CO₂ capture efficiency and reduce energy penalties.

Section 3 Materials and Methods

The description of MEA-based CO₂ capture and its operational details are described in this section. Furthermore, this section also provides an overview of Aspen Hysys as the chosen simulation tool, detailing the input parameters and the relevant equations.

Section 4 Results and Discussion

The simulation results of the base case, as obtained through Aspen Hysys, are compared against data from base case CCS references and discussed these findings in this section. Likewise, the results coming from heat and power improvement simulation are also represented.

Section 5 Conclusions, Limitations, and Recommendation

The final section consolidates the key findings regarding the energy consumption of each scenario across parameter variation and the energy saving achieved via process modification simulation. It also highlights the limitations of MEA-based carbon capture and the recommendation to raise the potential of future research, which can be extended from this work.

2 LITERATURE REVIEW

2.1 Carbon Capture and Storage

Carbon Capture and Storage (CCS) plays a crucial role in reducing CO_2 emissions for the Net Zero target achievement. This technology could capture CO_2 from flue gas generated through coal-fired power plant activities, and then that CO_2 is compressed and stored in long-term storage or utilization [3]. However, the CCS requires energy for the operation, leading to a decrease in overall power plant efficiency; furthermore, this technology were developed slowly throughout Europe and Asia [18], [19]. Therefore, researchers investigated the process improvements aimed of reducing energy penalty as well as increasing CO_2 capture efficiency through simulation tools.

2.2 Type of Carbon Capture

 CO_2 capture technologies can be applied to coal-fired power plants in various approaches: post-combustion capture, pre-combustion capture, and oxyfuel combustion capture [7]. Post-combustion capture is the process separating CO_2 in flue gas resulting from the combustion of fuel in natural gas and pulverized coal-fired power plants, with the objective of preventing direct release into the atmosphere. In contrast, pre-combustion capture relates to a gasification reaction occurring within the power plants wherein CO_2 is removed from the syngas – mainly carbon monoxide and hydrogen, which is generated through the gasification of fuel in the presence of air and oxygen. As for Oxyfuel combustion capture, pure oxygen is used instead of air in the fuel combustion; therefore, the flue gas contains mainly CO_2 and H_2O with high temperature is produced, and CO_2 is captured in the same process as a post-combustion capture system [20].



Figure 2 Overview of CO₂ capture approaches [20]

Among these technologies, Post-combustion CO_2 capture was suitable for integrated into the existing coal-fired power plants due to its effectiveness and feasible strategy [17], [18]. Porter et al. (2015) analysed the amount of impurities in CO_2 streams after treating in the pre-combustion capture, post-combustion capture, and oxy-fuel capture technologies as well as determined the modes of operation and different technologies for reduction and removal of the impurities in the CO_2 product gas. This analysis illustrated that the efficiency could achieve up to 99% of CO_2 purity with low N_2 , Ar, and O_2 ; however, the following steps, transportation, and storage, should also be considered the level of CO_2 purity requirement [21].

Furthermore, CO₂ capture technologies can be categorized based on their underlying physical and chemical processes, such as absorption, adsorption, membrane, and cryogenics methods [7]. In the absorption process, CO₂ is absorbed by liquid solvents through chemical interaction. This CO₂-enriched solvent is then directed to a desorber unit, where it is heated to release the CO_2 . Once the CO_2 is separated, the solvent is recycled back for further absorption cycles, while the extracted CO₂ is transported toward the storage. Regarding adsorption, this process involves the selective adherence of CO₂ onto a solid adsorbent surface. The absorbed CO₂ is subsequently released through heating in the regeneration process, readying the adsorbent for the subsequent adsorption cycles. The membrane separation technique is characterized by the differential passage of CO₂ across a selective membrane material. In contrast, cryogenics separation involves decreasing the temperature of flue gas to an extremely low temperature, typically below than -56.6°C, thereby liquefying CO₂ and facilitating its separation from the gas mixture [3], [22]. However, these processes were investigated to be compared in terms of costeffectiveness, feasibility, and energy requirement. The result showed that absorption and adsorption were suggested for power plants instead of membrane and cryogenic [19].



Figure 3 Main separation processes for CO₂ capture [20]

2.3 Amine Based Carbon Capture Technology

Amine-based absorption, utilizing chemical solvents such as monoethanolamine (MEA)-based solution, is extensively employed for treating flue gas in the industrial sector. It accounts for approximately 75 - 90% of the total CO₂ capture, attributed to its low capture cost, low viscosity, and high absorption kinetics, which means it has high solubility of CO₂ at low CO₂ partial pressure [23]–[25]. In terms of capture processes, the MEA-based capture process primarily comprises two stages: scrubbing and stripping, which can be defined as an absorber and desorber. To begin with the absorber, postcombustion flue gas is directed through a scrubber, where CO_2 is selectively absorbed by MEA solvent. Subsequently, CO₂-rich amine solvent is conveyed to a stripping unit, which is heated to emit the captured CO_2 [26]. However, the process required energy, which led to the reduction of total energy efficiency by approximately 20 - 40% [17]. Nonetheless, there are concerns associated with the use of MEA solvents. Loss of the solvent can occur due to thermal degradation at 120°C as well as the emission of sulfuric acid (H_2SO_4) aerosols, leading to escalating operating costs and raising environmental concerns. In a study by Khakharia et al. (2013), the formation of H₂SO₄ particles was 2 to 4 times greater than the vapour-based emission baseline of 45 mg/Nm³ [27].



Figure 4 General schematic of an amine-based CO₂ capture process [26]

The amine capture process presents both advantages and drawbacks for coal-fired power plants. However, researchers have been investigating process configuration studies to mitigate the energy penalty and enhance capture efficiency.

2.4 Improvements of MEA-Based Carbon Capture Processes

Various methodologies have been extensively developed to overcome the energy penalty of using MEA-based Carbon Capture as well as enhance the efficiency of the carbon capture process, which are various types of amine solvents, varying blending fractions, and modifications in the process [11]–[17].

Regarding the nature of the solvents, physical properties and chemical structure were significant factors in the carbon capture process that influenced the reaction of the systems. These elements referred to the solvent's absorption capacity, which quantifies the amount of CO₂ captured throughout the process, the heat regeneration and also takes into account the rate of thermal degradation and corrosiveness [28]. According to Prachi et al. (2019), a variety of amine structures and their activities related to CO₂ capture were examined by testing in a screening apparatus operating at atmospheric pressure and 40 degrees Celsius. The results illustrated that an increase in chain length correlated with an increase in the absorption capacity of the solvents but, conversely, led to a decline in the absorption rate [29]. As for Adeosun and Abu-Zahra (2013) conducted simulations involving various amine blending fractions for CO₂ post-combustion capture, integrated into a 600 MWe coal-fired power plant, to evaluate the efficiency of carbon capture. The researchers found that the blend of 5 wt% DEA and 25 wt% AMP resulted in the lowest reboiler duty, accounting for 3.03 GJ/ton-CO₂ at lean loading of 0.07 molCO₂/mol_{blend} and they observed that the regeneration rate was faster at the lower stages of the stripper [30].





Additionally, new absorbents have been developed and integrated into postcombustion carbon capture process simulations as alternatives to conventional amines, such as MEA, with the aim of reducing regeneration energy. Kato et al. (2013) reported the development and laboratory-scale testing of Absorbent-A, comparing its properties to a 30wt% MEA aqueous solution and Toshiba-1 (TS-1). Absorbent-A revealed a larger CO_2 absorption capacity and lower CO_2 regeneration energy consumption, which was 45% less than that of 30wt% MEA and approximately 10% less than that of TS-1 [31]. Nonetheless, as previously mentioned, MEA emerges as a promising amine-based solvent in mature post-combustion carbon capture, owing to its relatively cheap and very strong reactivity to CO_2 at low CO_2 partial pressure.

Aside from the solvent used in processes, conventional absorber-stripper arrangement methods have been investigated to archive energy penalty reduction through process simulation [12], [13], [16], [17]. These methodologies aim to minimise reboiler duty thermal integration, heat pump effect, and absorption enhancement, as mentioned in the previous section. In a study by Oh et al. (2018), various scenarios of carbon capture process modifications integrated into a 550 MW supercritical coal-fired power plant were simulated and compared to a base case equipped with a conventional carbon capture plant. The amount of reboiler duty of each scenario was examined, and results in **Figure 6** showed that the improvements in the process decreased the heat consumption [17].



Figure 6 Comparison of reboiler duty from process modifications [17].

Regarding to Ahn et al. (2013) stressed the importance of heat integration within the MEA-H₂O-CO₂ processes to minimise overall heat consumption. The various improvement methods were simulated against the conventional carbon capture plant. The findings from the simulation represented a reduction in steam used in the reboiler, accounting for up to 37% through process modifications and heat integration [32].



Figure 7 Schematic diagram of process modifications by using absorber intercooling, condensate evaporation and lean amine flash [32].

Neveux et al. (2013) investigated various schemes in process modification as well as the use of two different solvents to analyse the overall heat consumption. In this simulation, methods such as lean vapour compression and stripper overhead compression were employed to improve low-quality sensible heat into high-quality latent heat. The findings indicated that a higher Coefficient of Performance (COP) led to a more efficient solvent regeneration process. It means that the stripper would need to operate at higher pressure, consequently leading to potential solvent degradation. The combination of diverse process improvement methods was thus recommended for a tackle in further research [33]. However, the energy penalty remained in the amine-based carbon capture. As a result, heat and power improvement methods can be defined as viable alternatives that should result in the reduction of the energy penalty.

Previous studies suggested heat and power strategy deployed into coal-fired power plants and CO₂ capture plants for overall efficiency improvement. As for Hanak et al. (2014), a model of post-combustion carbon capture plants using MEA aqueous were simulated to assess energy consumption. Additionally, a heat exchanger network (HEN) analysis was also conducted to improve the overall efficiency of the power plant. The results presented a reduction in energy penalty from 25% to 4.15% compared to the reference case, suggesting that the HEN method has the potential to increase heat recovery in the processes [34]. Furthermore, the installation of a back pressure turbine from the IP/LP crossover could be considered to generate high-efficiency steam at the required temperature, thereby reducing the need for additional power. Simulation findings from Oh et al. (2018) presented that improving the MEA-based capture process through

IP/LP crossover steam extraction resulted in enhanced steam quality. Subsequently, it led to an increase in net efficiency and a reduction in the net efficiency penalty [17].

Although research on amine-based CO₂ capture, including process improvements, indicates a promising technology, comprehensive studies on various large-scale coal-fired power plants still need to be explored and associated with an economic analysis.

2.5 Modelling of Carbon Capture and Storage

The capability of using MEA-based carbon capture for post-combustion in coalfired power plants has been investigating through the use of simulation tools such as Aspen Hysys, Aspen Plus, and Promax on both commercial and industrial scales [3], [13]–[17], [23], [28], [30], [32], [33], [35], [36]. However, Aspen Hysys® has been employed to evaluate methodologies aimed at overcoming the energy penalty in MAEbased post-combustion capture, due to its effectiveness [36].

2.5.1 Aspen Hysys®

Aspen Hysys serves as a robust simulation tool, facilitating both steady-state and dynamic simulations, including process design and optimization. This software allows users to create process models and conduct simulations using complex calculations, for example, thermodynamic models, mathematical calculations, and regression analysis, to predict process performance and carbon capture efficiency. Within the program, processes can be modelled using either an equilibrium or rate-based approach. In the equilibrium model, the MEA-CO₂-H₂O processes are assumed to occur at equilibrium, resulting in a composition of the vapour and liquid phases being homogeneous. Conversely, the rate-based approach is the non-equilibrium mass transfer process, which is more appropriate in modelling absorption-desorption processes since gas and liquid films are at the interface.

2.5.2 The Modelling Approach

Rate-based modelling has been adopted in MEA-based carbon capture simulation to optimize the process and increase precision for economic analyses. This methodology provides rigorous and accurate modelling results using Maxwell-Stefan formulation, process hydrodynamics, and mass transfer between vapour-liquid interfaces [37]. The simulation of the absorber and stripper columns took into consideration the mass and heat transfer processes inherent in the absorption-desorption mechanism. The rate of mass transfer within the absorber is involved several factors, such as the diffusivity of CO₂ through the amine solvent, solubility of CO_2 in the amine solvent, and the chemical reactivity between CO_2 in the vapour phase and the aqueous amine in the liquid phase, as illustrated in **Figure 8** [38].



Figure 8 Two-film theory described mass transfer of amine-based carbon capture [38].

In terms of process operating conditions, both the Electrolyte Non-Random Two Liquid (e-NRTL) method and the Peng-Robinson (PR) equation were employed. These methodologies were utilized for sizing and evaluation of the high-efficiency process conditions. PR equation was applied for vapour phase modelling under non-ideal conditions, while the e-NRTL method was applied to describe the behavior of the liquid electrolyte system. As for MEA-CO₂-H₂O processes, the related chemical reactions were considered in the simulation, which can be listed as follows [34], [39]:

$H_2O + MAEH^+ \longleftrightarrow MAE + H_3O^+$	(2.1)
$2H_2O \longleftrightarrow H_3O^+ + OH^-$	(2.2)
$HCO_3^- + H_2O \longleftrightarrow CO_3^{2-} + H_3O^+$	(2.3)
$\rm CO_2 + OH^- \rightarrow \rm HCO_3^-$	(2.4)
$HCO_3^- \rightarrow CO_2 + OH^-$	(2.5)
$MAE + CO_2 + H_2O \rightarrow MAECOO^- + H_3O^+$	(2.6)
$MAECOO^{-} + H_3O^{+} \rightarrow MAE + CO_2$	(2.7)

According to the equations, reactions (2.1) to (2.3) related to the equilibrium reactions, calculated from the standard Gibbs free energy change, while reactions (2.4) to (2.7) referred to rated-controlled reactions using power law expressions [34].

2.5.3 The main equipment used in the simulation.

Absorber Column

The absorber column can be defined as a scrubber designed to absorb CO_2 (in gaseous form) from the flue gas mixture into the MEA solution. As previously mentioned, the mass transfer occurred only at the surface where CO2 and MEA flow in a counter current. It means that flue gas is entered at the bottom of the column while MEA solvent is fed from the top. The chemical reactions occurring within are exothermic, causing an increase in temperature within the column; in contrast, the pressure decreases along the length of the column [40]. In terms of CO_2 capture efficiency, the column specifications influence the CO_2 loading in the output stream such as column height, number of stages, and type of packing. According to Alie et al. (2015), a stand-alone absorber with variations in the flow rate of a 30% wt MEA stream and the number of trays was simulated using Aspen Plus. The aim was to investigate the CO_2 loading in the rich MEA stream. The findings indicated that an increase in the number of trays directly correlated with an increase in CO_2 loading, as shown in **Figure 10** [41].



Figure 9 Diagram illustrating the stand-alone absorber with specification [41].



Figure 10 CO₂ loading versus tray number at an inlet concentration of 14%CO₂ [41].

• Rich and Lean amine pumps

Pumps are employed to elevate the pressure in both rich and lean amine streams. The rich amine stream is generated from the bottom of the absorber column and carries a high concentration of CO_2 . This CO_2 -rich amine solution is then conveyed to the stripper column, where the desorption process occurs, separating the CO_2 . The separation process required higher operational pressure, provided by the rich amine pump. Conversely, the regenerated solvent from the stripping process is recirculated to the absorber column. This stream contained low CO_2 concentration and low pressure, so the lean amine pump was applied to increase the pressure of the lean amine stream before sending it to the Rich/Lean Heat Exchanger unit. The power consumption of a pump can depend on several conditions, mainly in pressure differences. This includes factors such as friction loss within the pump, pressure losses in the Rich/Lean heat exchanger, and pressure difference between the absorber and desorber columns. Moreover, the overall pump efficiency can be relied on flow rates and hydraulic efficiency, as shown in Equation (2.8) [42],

Pump Power Input (W) =
$$\frac{\rho \times g \times H \times Q}{\eta}$$
 (2.8)

Where H is the actual total head difference between the inlet and outlet stream (m)

 ρ is the density of liquid being pumped (kg/m³)

g is the acceleration due to gravity (m/s^2)

Q is the flow rate (m^3/s)

 η is the pump efficiency

• Rich/Lean Heat Exchanger

The Rich/Lean Heat Exchanger is adopted into the process with the objective of energy recovery in the absorption-desorption process. This mechanism illustrates sensible heat transfer from the hot lean amine stream to the cold rich amine stream. Hence, these phenomena lead to a decrease in energy requirement for the reboiler in the stripper column as well as a decrease in energy consumption for the lean amine cooler, which is responsible for reducing the temperature of the lean amine stream before delivering it to the absorber unit. To assess the energy losses in heat recovery systems and ineffectiveness of a heat exchanger, the minimum temperature difference approach (ΔT_{min}) is employed. This approach is related to the smallest temperature difference between the hot and the

cold stream in the heat exchanger, which is used as a parameter to determine the minimum energy consumption, as shown in **Figure 11**.

Typically, in the modelling of Amine-based CO_2 capture systems, the setting value of ΔT_{min} at 10 K is recommended. This value aims to achieve the minimum heat duty requirement while optimizing both capital and operating costs, as cited in references [14], [17], [37], [43] and [44].



Figure 11 Composite curves illustrating the relationship between hot and cold streams in relation to ΔT_{min} [45]

• Stripper column

The stripper can broadly be defined as a desorption column where rich amine is delivered for the regeneration process. This process requires the hot utility to break the bond between the amine and CO₂, supplied by a reboiler located at the bottom of the column. Hence, the CO₂-rich amine undergoes separation, resulting in CO₂ gas and a lean amine aqueous solution due to a reverse chemical reaction. The high-temperature CO₂ gas is then sent to compression stages, preparing for the storage process. At the same time, the lean amine stream is recirculated to the absorber column, ready for the subsequent absorption cycle. As explained earlier, the energy penalty is mainly associated with the reboiler duty in the stripping process, which led to the decline in the overall efficiency of the power plant. In a study by Alie et al. (2004), the characteristics of a stand-alone stripper were investigated by varying parameters, such as number of trays and reflux ratio (L/R), using simulation. The findings of this study revealed a direct proportionality between the heat duty and the reflux ratio when feeding at an inlet concentration of 14%CO₂ and a temperature of 80°C. Conversely, an increase in the number of trays directly influenced the decrease in reboiler duty, as shown in Figure 13 [41].



Design Specifications:

- 1) Adjust Lean MEA to Rich MEA to obtain desired loading in Lean MEA stream
- 2) Adjust reflux ratio to obtain desired purity in CO2 stream





Figure 13 Reboiler Duty versus tray number at an inlet concentration of 14%CO₂ [41]

• Lean amine cooler

The lean amine cooler is the equipment purposed to reduce the temperature of lean amine before serving to the absorption unit. As a result of the looping process, the lean amine is passed through the cooler to achieve a target temperature of 40°C which is made to enhance the CO_2 absorption reaction rate within the absorber [17].

2.5.4 The advantages of using Aspen Hysys®

The various simulation tools are adopted for the MEA-CO₂-H₂O system; however, Aspen Hysys stands out as a reliable and accurate simulation software compared to other commercial process simulations [46]. It means that the Aspen Hysys's team provided an accurate calculation method, such as a rate-based approach for Absorber/Stripper columns that incorporates heat and mass transfer correlations accounting for the column's specifications and hydraulics. Furthermore, the Aspen Hysys is equipped with a suitable fluid package. The Acid Gas-Chemical Solvents properties package is recommended for rigorous calculations in the amine-based carbon capture process because this package contains both equilibrium and kinetics reactions, in addition to thermodynamic properties for electrolyte and vapour phase which are crucial to perform the heat and mass transfers of the systems [47].

2.5.5 The limitations of using Aspen Hysys®

While Aspen Hysys stands out as a promising simulation program, it is not without its limitations. A notable challenge encountered in its use is convergence problems. In the Aspen Hysys framework, there are convergence criteria and a default set of calculation models for column calculations. In the context of the carbon capture process, which is represented as a closed-loop process, the recycle block is often applied to the modelling. However, there are instances when the final lean amine stream —post makeup —does not align with the lean amine introduced to the absorber. In such a situation, the recycle block attempts to rectify discrepancies by emphasizing primary parameters, often at the expense of introducing inaccuracies in parameters deemed of lesser importance. As a result, these automated corrections might introduce errors in the simulation's process calculations [46].

2.6 Combining CCS with other industries

Although CCS technology faces challenges in large-scale implementation, such as energy penalty, high operational costs, and the need for a long-term policy framework, the industrial sector is increasingly turning its focus toward the utilization of carbon dioxide. This shift is primarily because of its vast market potential. By utilizing CO₂ in various processes, industries have the opportunity to enhance the value of end-products, for example, plastics, fuels, and platform chemicals. Regarding CO_2 use as a feedstock, around 130 million tons of CO₂ is annually used in urea, salicylic acid, and polycarbonate manufacturing industries as well as produce polymers such as mono-ethylene glycol, which is a vital substance in polyester manufacturing industries [48]. Interestingly, an incredibly sustainable avenue for CO₂ utilization is its transformation into biofuel. A study by Jacob, Xia, and Murphy (2015) investigated the potential of microalgae generated from captured CO₂ from a coal-fired power plant. The finding illustrated that a 1 GWe coal power plant operating at 35% efficiency and achieving 80% carbon capture efficiency has the potential to yield 2.65 million tons of microalgae. Once harvested, microalgae were passed through three processes: dark fermentation, photo fermentation, and anaerobic digestion. This volume of microalgae can produce bio-hydrogen and biomethane, sufficient to fuel around 600,000 cars annually [49]. Despite CCS technology's

challenges, the industrial sector is capitalizing on CO_2 's market potential, especially in biofuel production. However, CO_2 utilization still needs critical evaluation given the underlying issues of CCS and the possibility of practically scaling up to the industrial scale.

2.7 CO₂ capture plant selection for this study

To evaluate the performance of carbon capture, the operational parameters of the CO₂ capture plant were incorporated into the Aspen Hysys simulation. However, a review of the extant literature on commercial-scale CO_2 capture plant simulations showed only CO₂ loadings, solvent circulation rates, and CO₂ capture efficiency without in-depth process design parameters, which is necessary for process simulation, including energy demand evaluation [50]. Accordingly, the lab-scaled carbon capture process from the University of Tromsø was selected for investigation in this thesis, given its detailed design parameters and calculated stream results. Furthermore, the MEA-based CO₂ capture process provided the optimization parameters to achieve 85% CO₂ removal efficiency and enhanced techniques for CO₂ absorption at atmospheric exhaust gas, which is beneficial for energy demand reduction. With regard to the process description, Figure 14 presents the process flow diagram (PFD) of the standard MEA-based CO₂ capture process as simulated in Aspen Hysys. This diagram consists of several pieces of equipment: absorption column, rich amine pump, desorption column, lean/rich amine heat exchanger, lean amine pump, and water cooler as well as optimal parameters from the University of Tromsø. Additional components like MIX-100 and RCY-1 within the software to facilitate mixing and recycling, respectively [51].



Figure 14 PFD of the MEA-based CO₂ capture process from the reference [51].

2.8 Conclusions

The literature on carbon capture and storage stressed its pivotal role in climate change mitigation and its prospective integration across diverse industrial sectors. While current research provides valuable insights into the aspects of CO₂ loadings, solvent circulation rates, and capture efficiencies, there remains an evident gap concerning the granular details of process design parameters at the commercial scale, which are instrumental for energy demand evaluations and rigorous performance assessments.

From this literature review, the following pivotal conclusions have been derived:

• Post-combustion CO₂ capture using the chemical adsorption method offers a viable integration strategy for coal-fired power plants, attributed to its efficiency, feasibility, and minimal energy demands.

• Amine-based absorption remains the primary choice for flue gas treatment in industries, given its cost-effectiveness, rapid absorption kinetics, and low viscosity.

• Energy requirements for the regeneration process in the MEA-CO₂-H₂O systems can curtail power plant efficiencies.

• The use of MEA needs to be considered due to the thermal degradation mechanism of MEA at 120°C and the release of sulfuric acid aerosol.

• Optimal amine blending between 5 wt% DEA and 25 wt% AMP minimises reboiler duty. Nevertheless, 30%wt MEA stands out as an effective amine solvent for mature post-combustion carbon capture, mainly due to its cost-effectiveness and heightened reactivity to CO₂ under CO₂ partial pressures.

• Aspen Hysys has proven invaluable as a simulation tool, particularly for MEA-CO₂-H₂O processes, offering both equilibrium and rate-based modeling capabilities.

• Increasing the tray stages in capture systems augments CO₂ loading.

• A ΔT_{min} value of 10 K in amine-based CO₂ capture systems is optimal, balancing reduced heat duties with capital and operational costs.

• Reboiler duties rise with increased stripper reflux ratios and tray numbers.

• Cooler effectively mitigates lean amine temperatures – 40 degrees Celsius, enhancing CO₂ absorption rates.

• For rigorous calculations in amine-based carbon capture, the Acid Gas-Chemical Solvents properties package is preferred due to its encompassing equilibrium and kinetic reactions.

• While tools like Aspen Hysys have enriched our understanding of CCS, challenges like convergence issues indicate a need for continued exploration.

• Despite its challenges, CCS technology's market potential, especially in biofuel production, is undeniable. However, CO₂ utilization requires a more critical evaluation, especially considering CCS's inherent issues and scalability.

• The lab-scaled carbon capture process from the University of Tromsø, which offers a comprehensive set of design parameters and calculated stream results, was chosen for this thesis.

• Furthermore, the MEA-based carbon capture process from the University of Tromsø elucidates optimized parameters for achieving up to 85% CO₂ removal efficiency and operation at atmospheric absorption, which is beneficial for reducing energy demands.

3 MATERIALS and METHODS

3.1 Introduction

In order to investigate the variables impacting CO_2 capture efficiency, as well as to assess the process improvement methods for minimising the energy penalty, a comprehensive simulation was conducted using Aspen Hysys. The base case model of the CO_2 capture process was developed; moreover, to enhance the robustness of the model and ensure its accuracy, operational data were procured from the University of Tromsø. This dataset was then integrated into the simulation, serving as an initial validation to confirm the precision and reliability of the model. However, the scope of this study does not encompass the coal-fired power plant process simulation, despite its influence on the properties and conditions of the flue gas, which consequently impacts the CO_2 treatment process. Therefore, the flue gas composition and operational data have been assumed to remain constant throughout the simulation. These assumptions and corresponding details are shown in **Table 2**.

Flue Gas	Values
Conditions	
Pressure (bar)	1.01
Temperature (°C)	40.00
Flow rate (kgmole/h)	1.091x10 ⁵
Composition (mol%)	
CO ₂	3.30
H ₂ O	6.90
O ₂	13.80
N_2	76.00
MEA	-

Table 1: Flue Gas Properties and Conditions [46], [51]

Elaborating on the established base case scenario for the CO_2 capture process, **Figure 15** provides a block diagram and process flow illustrating the system under investigation. In this configuration, flue gas is introduced at the lower section of the absorber column. At the same time, a 30%wt concentration of lean amine is fed to the top of the column, moving in a counterflow direction to facilitate the efficient separation of CO_2 from the flue gas. After this process, the CO_2 -enriched amine undergoes pressurization via a rich

pump and temperature adjustment through a rich/lean heat exchanger; therefore, the hightemperature, high-temperature rich amine is conveyed to the desorber column. In this process, CO₂ is effectively separated from rich amine, simultaneously regenerating the amine solution for recirculation into the CO₂ absorption process, thereby completing the cycle. Furthermore, the CO₂ product goes through multiple compression stages, preparing it for either storage or transportation or for use as a raw material in various industrial applications. Conversely, the lean amine generated from the regeneration process is meticulously conditioned, with adjustments made to its pressure, temperature, and concentration, ensuring it meets the specifications for reuse in the absorber column.



Figure 15 Block diagram of the base case scenario for the CO₂ capture process (based on information from references [46], [51]).

In relation to parameter variation, the parameters such as flue gas flow rate, lean amine temperature, and column stages were scrutinized to evaluate their impact on CO_2 capture efficiency and reboiler duty, utilizing the base case model simulation. Accordingly, vapour recompression modification was identified and consequently integrated into the base case CO_2 capture model, as shown in **Figure 16**. This method was chosen due to its effectiveness in enhancing performance, including a minimal increase in system complexity [14], [32]. The integration of a flash tank and compressor into the process is implemented with the objective of directing an additional stream to the stripper, resulting in a reduction of reboiler duty. Nevertheless, it is crucial to note that this modification may necessitate adjustments in the operational strings of both the rich/lean heat exchanger and the stripper column. Additionally, the compressor, while vital to the process, consumes electricity during its operation.



Figure 16 Block diagram of the vapour recompression modification scenario.

Integration of MEA-based carbon capture technology into commercial-scale postcombustion coal-fired power plants (PCC) presents plenty of challenges in both technical and non-technical domains. On the non-technical issues, hurdles include economic considerations, regulatory and policy implications, as well as sociological factors. Addressing these necessitated a holistic approach from the governmental sectors and policymakers. From a technical perspective, the current research trend is geared towards increasing carbon capture efficiency and minimising the energy penalty, mainly through simulation-based studies and pilot plant experimentation. It is important to note that the reliability of these simulations might be compromised owing to the dependence on user assumptions and average data due to the lack of operation-specific data for large-scale PCCs. Hence, researchers should remain aware of potential inconsistencies, factoring in challenges such as fluctuating flue gas compositions, material degradation, and retrofitting existing infrastructures.

3.2 Input data and settings of simulations

- 3.2.1 Properties Environment
 - Component Lists and Fluid Package

The simulation begins with selecting the components involved in the MEA-based CO_2 capture — namely, carbon dioxide (CO_2), monoethanolamine (MEA), water (H_2O), hydrogen sulfide (H_2S), nitrogen (N_2), and oxygen (O_2) — were added to the component list section. In addition, the next vital step involved specifying the fluid package. Acid Gas – Chemical Solvents properties package was selected for this study owing to its comprehensive inclusion of amines and their blends' properties. Furthermore, this package provides the thermodynamics that relies on the Electrolyte-NRTL model to calculate liquid phase properties and the Peng-Robinson equation of state for vapour phase. Together, these provide a robust framework, all necessary aqueous-phase equilibrium and kinetics reactions required for rate-based calculations of the processes.

• Inlet parameters properties

The process proceeds with defining the inlet streams for both the sour gas and the lean amine, having a 30wt% concentration. These parameters were obtained from the University of Tromsø and assumed to remain constant for the base case simulation, which is made to simplify the model. Notably, the flue gas composition data in the reference gained from a 400 MW coal-fired power plant, assuming complete combustion. The details are given in **Table 2**.

Conditions	Sour gas [46], [51]		Lean Amine (30wt%MEA)	References [46], [51]
Pressure (bar)	1.01	1.01	1.01	1.01
Temperature (°C)	40.00	40.00	40.00	40.00
Flow rate (kgmole/h)	1.091x10 ⁵	1.091×10^{5}	1.600×10^5	1.600×10^5
Composition (mol%)				
CO ₂	3.30	3.30	2.95	2.95
H ₂ O	6.90	6.90	85.84	85.84
O_2	13.80	13.80	-	-
N_2	76.00	76.00	-	-
MEA	-	-	11.21	11.21

Table 2: Input parameters for the streams entering to the absorber.

However, this approach provides a foundational understanding of the process dynamics. It is essential to remember that in real-world applications, variations in these streams could occur due to coal characteristics, fluctuations in operational conditions, and other external factors.

3.3 Equipment's and measurement protocol

For the efficiency of CO_2 capture evaluation, a range of metrics were adopted. These included the capture rate, CO_2 loading, and absorption efficiency. The capture rate illustrates the percentage of total CO_2 emission captured relative to the amount of CO_2 generated at the source. In other words, a capture rate of 100% refers to all of the carbon dioxide emitted by a process captured through CCS. This relationship is expressed in Equation ((3.1).

Capture rate (%) =
$$\frac{G_{out} x_{CO_{2out}}}{G_{in} x_{CO_{2in}}}$$
. 100% (3.1)

Where G_{in} is the mass flow rate of the flue gas stream entering the process (kg/h) G_{out} is the mass flow rate of the gas stream exiting the stripper (kg/h)

 $x_{CO_{2in}}$ is the mole fraction of CO₂ in the flue gas stream.

 $x_{CO_{2out}}$ is the mole fraction of CO₂ in the gas stream at the stripper's outlet.

In assessing CO₂ loading, this particular metric is used in evaluating the performance of both the absorber and the stripper, defined as the apparent molar ratio of CO₂ to MEA within the solution. To facilitate this analysis in Aspen, a property set dubbed 'ML-LOAD' was established to obtain the results of CO₂ loading. Two specific component groups were configured for this property set: $x_{CO_2}^{app}$ and x_{MEA}^{app} , detailed parameters of which are provided in

Table 3. This property set was then added to the report page for each column to facilitate comprehensive data analysis. The rich loading is determined based on the value procured from 'ML-LOAD' at stage 14 in the absorber, whereas the lean loading is derived from the value reported at stage 10 in the stripper. The mathematical correlation between these two component groups is detailed in Equation (**3.2**).

$$CO_2 \text{ loading (molCO_2/molMEA)} = \frac{x_{CO_2}^{app}}{x_{MEA}^{app}}$$
(3.2)

$x_{CO_2}^{app}$	x_{MEA}^{app}
x_{CO_2}	<i>x_{MEA}</i>
<i>x</i> _{HCO3} ^{2–}	x _{MEAH} +
<i>x</i> _{C03} ²⁻	x _{MEACOO} -
x _{MEACOO} -	

Table 3: Component groups pivotal for calculating CO_2 loading, where *x* symbolizes the molar fraction of each respective component involved in the process.

In similar way, to gauge the performance of the absorption, the capture efficiency is also a crucial metric, which is calculated using equation (3.3).



Where G_{in} is the mass flow rate of the flue gas stream entering the process (kg/h)

 G_{out} is the mass flow rate of the gas stream exiting the stripper (kg/h)

 $x_{CO_{2in}}$ is the mole fraction of CO₂ in the flue gas stream.

 $x_{CO_{2out}}$ is the mole fraction of CO₂ in the gas stream at the stripper's outlet.

These metrics effectively illustrate how much of the CO_2 introduced into the system is captured, giving a clear indication of the CO_2 capture performance. When delving into the energy penalty analysis, the energy balance around the stripper and the rich/lean heat exchanger plays an essential role in determining the energy penalty of the system. The regeneration energy, denoted as Q_{regen} is the cumulative energy from sensible heat ($Q_{sensible}$), latent heat (Q_{latent}), and the heat of reaction (Q_{rxn}). This relationship is presented in equation (3.4), as referenced from [44]:

$Q_{regen} = Q_{sensible} + Q_{latent} + Q_{rxn}$	(3.4)
---	-------

This equation illustrates the energy components required in the regeneration process, underscoring the importance of each factor in the CO_2 capture system simulation.

3.4 List of experiments conducted.

3.4.1 Simulation of base case in Aspen Hysys



Figure 17 Schematic the Base Case of MEA-CO₂ capture modelled in Aspen Hysys.

The base case for the MEA-CO₂ capture process is illustrated in the flow diagram depicted in **Figure 17**. This schematic presents the components and flows simulated in this project. The main necessary equipment related to energy analysis and CO₂ capture efficiency is included into the simulation, which is listed as follows: Absorber Column, Rich and Lean Pumps, Rich/Lean Heat Exchanger, Stripping Column, Lean Cooler, and Lean Mixer. As for the operational parameters and equipment specifications, data gathered from the University of Tromsø was utilized for this investigation aimed to achieve an 85% CO₂ capture efficiency, the specifics of which can be found in **Table 4**.

Figures	Figures Boundary Conditions		References [46], [51]
Sweet	Absorber Unit		
Lean Main Amine 8 Tower	Top Pressure (bar)	1.01	1.01
→ 14	Bottom Pressure (bar)	1.01	1.01
Feed Rich Amine	Number of stages (stages)	14	14

Table 4	• Eai	inment	specificat	ions for	the base	case mode	el simulation
I aDIC 4	. Իս	aipment	specificat	10115 101	the base	case mout	1 Sinuanon

Figures	Boundary Conditions	Input Value	References [46], [51]
	Rich Pump		
Rich Rich Amine to	Target Pressure (bar) (Rich amine to heat exchanger)	2.00	2.00
Qrich HeatX	Adiabatic efficiency (%)	75.00	75.00
+	Rich/Lean Heat exchanger		
Lean Amine to cooler	Pressure drops in tube side (bar)	0	0
Rich Rich Amine to to Heat Desorber HeatX	Pressure drops in shell side (bar)	0	0
Lean Arbine to HeatX	Target outlet temperature (°C) (Rich amine to stripper)	104.5	104.5
	ΔT_{\min} (K)	10	10
2	Stripper Column		
	Condenser Pressure (bar)	2.00	2.00
Rich Amine to 6	Reboiler Pressure (bar)	2.00	2.00
Desorber 10 Boilup Creb Reboiler To	Number of stages (stages)	10	10
Reboiler Lean Amine from Desorber	Reflux Ratio	0.1	0.1
	Reboiler Temperature (°C)	120.0	120.0
	Lean Pump		
Lean Amine to HeatX Qlean Lean Pump Pump Amine from Desorber	Target Pressure (bar)4.00(Lean amine to heat exchanger)		4.00
	Adiabatic efficiency (%)	75.00	75.00

Figures	Boundary Conditions	Input Value	References [46], [51]
Qlean cooler	Lean Cooler		
Lean Lean amine Lean Amine to Cooler to mixer cooler	Target Temperature (°C) (Lean amine to mixer)	40.0	40.0
	Lean Mixer		
	Stream: Make up amine		
	• Pressure (bar)	2.00	2.00
	• Temperature (°C)	40.0	40.0
Lean	• Flow rate (kgmole/h)	45.0	45.0
	Composition (mol%)		
Lean Make amine to up absorber Lean amine Mixer	o MEA	100	100
Make up water	Stream: Make up water		
-	• Pressure (bar)	2.00	2.00
	• Temperature (°C)	40.0	40.0
	• Flow rate (kgmole/h)	6150.0	6150.0
	Composition (mol%)		
	0 H ₂ O	100	100
	Lean Valve		
Lean Lean	Target Pressure (bar)	1.01	1.01
amine ∟ean amine to recycle Valve absorber	(Lean amine recycle)		1.01
	Percentage open (%)	50.00	50.00

3.4.2 Parameter Study

Various parameters that influence the CO_2 capture performance were adopted into the base case model and simulated without lean amine recirculation. These adjustments were conducted using an open-loop simulation model for each scenario by specifying only two inlet streams — sour gas and lean amine with 30%wt concentration. The openloop simulation model omits the recycle stream of the lean amine from the stripper back to the absorber column. This method was implemented to avoid potential convergence issues which is usually occurred in closed-loop simulations.

List of parameters that were varied during our study are shown in **Table 5**. Among these, the inlet flow rate refers to the flow rate of the sour gas while inlet temperature indicates the temperature of the 30%wt lean amine solution. Solvent concentration defines the total weight percentage of MEA in the aqueous solution and number stage presents the column stages in both the stripper and the absorber.

 Table 5: List of parameters explored and their respective investigation intervals.

Parameters	Base case	Intervals					
Inlet flowrate (kgmole/h)							
• Sour gas (Flue gas)	1.091×10^5	$1.060 \text{ x}10^5 - 1.110 \text{ x}10^5$					
Inlet temperature (°C)							
• 30%wt MEA	40	30 - 80					
(Lean Amine)							
Solvent concentration (wt%)	20	20 - 50					
Number of stages in the absorber	14	9 – 19					
Number of stages in the desorber	10	5 – 15					

3.4.3 Process Improvement

Regarding the high-efficiency simulation, the base case of MEA-based CO₂ capture model was developed using the heat and power technique shown in Error! Reference source not found.. This modification was aimed to achieve the high performance of CO₂ capture as well as energy consumption reduction. A flash tank was introduced to the process, allowing for the separation of the lean amine exiting the stripper into its vapour and liquid phases. Then, the liquid phase underwent pressurization by pump, while the vapour phase was processed by a retrofitted compressor, both targeting a pressure of 2.00 bar preparing for regeneration process. It is important to note that prior to compression, the vapour lean amine was passed through a rich/lean heat exchanger which ensure that the stream was fully vapourized upon entering the compressor, with a target temperature set at 99.5°C. Considering, the high-pressure lean amine coming from the lean pump contained a lower amount of MEA concentration compared to the base

case, adjustments were made to the Makeup Amine and Makeup Water streams. Their molar flow rates were set at 40 kgmole/h and 5,000 kgmole/h, respectively—a reduction compared to the base case values of 45 kgmole/h and 6,150 kgmole/h. These parameters calibrated, aimed to achieve values as close as possible to 85% CO₂ capture efficiency (as reported in the literatures [51], [52]).

4 RESULTS

4.1 Simulation Results

4.1.1 Simulation Results of Base Case in Aspen Hysys

In order to validate and ensure the credibility of simulation findings, the results from this thesis are compared to the established data from the base case of the University of Tromsø, the detail is illustrated as follows:

Material Streams

Figure 18 presents a comparison between the simulated results and the base case data from the University of Tromsø, specifically examining parameters such as pressure, temperature, and flow rate. According to pressure, both the simulation outputs and reference data demonstrate consistency. Interestingly, the pressure consistently increases as the stream passes through different processes, peaking when the lean amine is released from the lean pump, which is 4.00 bar. Subsequently, there is a minor drop until it is equal to atmospheric pressure, positioning the stream appropriately for the next CO_2 capture process.



Figure 18 Comparison between the simulated results of the base case model and the data from references.

In terms of temperature, the simulation findings showed a slightly difference value when compared to references, with the largest deviation observed in the CO₂ gas stream, accounting for a 13.1 percent error. This discrepancy might arise from the specifications and calculations associated with the stripper column, which might be more complex than the simulation suggests. Regarding temperature trends, it is the same pattern as the pressure trends. The temperature initiates from 40°C, as set in the absorber column, and then progresses through various equipment. The highest temperature is shown at the outlet stream of the lean amine from the desorber column, amounting to 120°C.

Likewise, the flow rate obtained from the simulation exhibited an increase as the processes progressed, whereas the reference data presented a constant flow rate throughout. Therefore, there was a significant disparity in the percentage error between the simulated results and the reference data. It is pointed out that a considerable difference in flow rate became evident when the lean amine was experienced in the rich/lean heat exchanger. This inaccuracy might be attributed to the simulation program's attempt to adjust the flow rate to optimize heat transfer, ensuring the targeted temperature is achieved within the simulation process.



• Stream Composition

Figure 19 Comparison of process stream compositions from base case simulation.

Focusing on the CO_2 capture process, several key streams involved in the separation process were considered: sour gas feed, rich amine exiting the absorber, rich amine post the rich pump, rich amine after rich/lean heat exchanger, and the CO_2 stream exiting the stripper. Figure 19 illustrates the compositions of these abovementioned

streams. The CO₂ gas stream stands out in this figure due to containing the highest concentration of CO₂, approximately 0.212 mol%. When this parameter is compared to the CO₂ substance in the sour gas, the CO₂ capture efficiency could be calculated manually determined using Equation (3.3). This calculation yields a result of 74% capture efficiency, which shows a slight difference from the referenced value of 85%.

• Energy Streams

In the base case model simulation, the heat flow values were calculated and shown in **Table 6**. It is clearly seen that the highest heat flow, approximately 231.94 MW, occurred in the rich/lean heat exchanger. This value is different from the value gained from the references which is around 161.00 MW. A possible explanation is that this discrepancy as a result of flow rate deviation observed at the exit of the rich/lean heat exchanger, as mentioned in previous section. It means that the calculated flow rate is higher than the referenced flow rate and it has contributed to a larger increase in heat flow result.

Parameters	Simulation Results (MW)	References (MW) [46], [51]	Note
$W_{ m rich\ pump}$	0.1232	0.1345	Energy Consumer
Rich/lean heat exchanger	231.94	140.10	
Reboiler Duty	127.90	161.00	Energy Consumer
Condenser Duty	5.277	7.361	Heat Released
$W_{lean \ pump}$	0.2604	0.2744	Energy Consumer
Lean Cooler Duty	55.82	68.37	Energy Consumer
Total Energy Consumption	184.10	229.78	

Table 6: Comparison of Heat Flow from Base Case Simulation and Reference Data.

When evaluating the energy consumption as depicted in **Figure 17**, the key parameters are the energy demands of the rich pump, reboiler, lean pump and lean cooler, with simulated consumptions of 0.1232, 127.90, 0.2604 and 55.82 MW, respectively.

These calculated values are comparable to those from the reference data, with the reboiler unit accounting for the most energy consumption accounting for 69.47% of the total energy consumption. Importantly, the system consumed 184.10 MW, equivalent to around 46.02% of power plant's electricity.

4.1.2 Simulation Results of Parameter Variations

- Variation of inlet parameters
 - o Sour Gas Flow Rate

Figure 20 represents the effect of altering the sour gas flow rate on the capture efficiency and the reboiler duty. The flow rate was varied in increments of 500 kgmole/h, ranging from 1.060×10^5 to 1.110×10^5 kgmole/h.



Figure 20 Impact of sour gas flow rate variation on capture efficiency and reboiler duty.

As for **Figure 20**, the capture rate and reboiler duty follow a similar pattern when the sour gas flow rate increased as well as the CO_2 capture efficiency remains constant, consistently around 73%. Similarly, the reboiler duty also stays steady around 130 MW across the various sour gas flow rates. This uniformity indicates that varying the flow rate of sour gas does not impact in energy requirement for the reboiler. Despite adjustments in the sour gas flow rate, there is minimal fluctuation in both CO_2 capture efficiency and reboiler duty, indicating a robust and efficient system. In other word, the sour gas flow rate can be deemed a non-critical parameter concerning its influence on CO_2 capture efficiency and reboiler duty which aligns with findings from a comparable study by Morgan et al. (2018) [53].

Lean Amine with 30wt% concentration temperature

Figure 21 shows the variations in CO₂ capture efficiency and reboiler duty as the temperature of the 30%wt lean amine was adjusted between 30 and 80°C



Figure 21 CO₂ capture efficiency and reboiler duty for varying lean amine temperature.

Figure 21 provides the results into how the CO₂ capture efficiency and reboiler duty cause changes in the temperature of lean amine with a 30wt% concentration. As shown by the blue line, the reboiler duty illustrates a decreasing trend with the increasing in lean amine temperature. Starting from a temperature of 30°C, the energy consumption is around 135 MW and begins to decline as a temperature reaches 80°C, where it is around 110 MW. Regarding CO₂ capture efficiency, the orange line also represents a decline as the lean amine temperature increases. Beginning from the CO₂ capture efficiency is around 72% at a temperature of 30°C, the efficiency rises to slightly above 75% at 80°C. These findings indicate that the lean amine temperature plays a crucial role in both the CO_2 capture efficiency and the energy requirement in the reboiler. It means a 12.5% increase in the temperature of lean amine influenced both parameters, resulting in an approximately 44% increase in CO₂ capture efficiency and a 1.19% reduction in reboiler duty. It can be explained that the higher temperatures would result in faster chemical reactions, and thus also the increase in CO₂ capture efficiency. In addition, the higher temperatures lead to a lower energy demand in the reboiler to achieve the desired separation.

However, caution is required when adjusting the lean amine temperature. This is due to the thermal degradation mechanism of MEA at 120°C. Additionally, higher feed temperatures result in an increased demand for cooling in the process. This trade-off between improved absorption and the cooling requirement should be carefully considered.

• Variation of solvent concentration

Figure 22 presents the effect of varying solvent concentrations on Rich CO₂ loading. By maintain a constant inlet flow of lean amine at 1.600×10^5 kgmole/h, while the MEA concentration was varied within the range of 20 - 50 wt%.





The graph illustrates a clear inverse correlation between MEA concentration and rich CO₂ loading. As the concentration increased from 10 to 50%wt, rich CO₂ loading decreased, with a marked decline at 50%wt. The trend demonstrates that as the solvent becomes more concentrated with MEA, its capacity to absorb CO₂ reduces. These results emphasize the need for optimum MEA concentration in the solvent. While appropriate concentration provides some benefits in the CO₂ capture process, previous studies suggest a rich CO₂ loading value around 0.5 molCO₂/molMEA to achieve the 80% carbon capture efficiency [17], [46], [52]. Additionally, a higher rich CO₂ loading could contribute to a reduction in the energy consumed by the reboiler [54].

• Variation of Tray Number in Absorber

The absorber stages were adjusted between 9 and 19 stages in the base case model to investigate the effect on CO_2 capture efficiency and energy required by the reboiler which these findings are shown in the **Figure 23**.





As for **Figure 23**, the CO₂ capture efficiency is near its peak at around 80% at stage 9. As more stages were added, this efficiency began to drop, reaching just above 65% by the 19th stage. This finding suggests that increasing the number of stages does not enhance CO₂ capture efficiency; in fact, it adversely affects it. In parallel, the reboiler duty increased, growing from around 100 MW at the 9th stage to almost 160 MW at the 19th stage. This growth indicates that as more stages are introduced, more energy is required in the reboiler. The green dot provides a reference point and is optimal for balancing efficiency and energy consumption.

These findings highlight the importance of optimizing the number of absorber stages. While one might assume that more stages would lead to improved carbon capture efficiency, the results here show a trade-off: more stages lead to reduced efficiency and increased energy requirements. This trade-off underlines the need for a balanced approach in design and operation to ensure both efficient CO_2 capture and energy-efficient processes.

• Variation of Tray Number in Stripper

The desorber stages were adjusted between 5 and 15 stages in the base case model simulation to examine the correlation between the number of stripper stages and their impact on CO₂ capture efficiency and reboiler energy demand.





In **Figure 24**, It is clearly seen that as the number of desorber stages increases, the CO_2 capture efficiency remains constant, around 75%. It means that the CO_2 capture efficiency is not significantly affected by variations in the stripper stages. In contrast, the trend of reboiler consumption demonstrates a continuous decline as the number of stages grows. The energy demand started at nearly 140 MW in the 5th stage, then dropped and remained stable, approaching around 110 MW by the 15th stage. This finding indicates that as the number of stripper stages increased, the reboiler required less energy, which aligns with findings from a comparable study by Alie et al. (2004) [41].

To summarize, these findings highlight the importance of selecting the number of desorber stages. While CO_2 capture efficiency remains unaltered, the energy required by the reboiler experiences a decline with the addition of more stages, hinting at a possible increase in the overall energy efficiency of the process. As a result, a holistic approach considering both these factors is imperative when determining the appropriate stripper stages for maximum operational efficiency.

4.1.3 Results of Process Improvement Simulation

The incorporation of a flash tank and compressor into the foundational CCS process aims to channel an extra stream towards the stripper. This modification led to a decreased demand on the reboiler duty which findings from the simulation is illustrated in the **Table 7**.

As for the **Table 7**, it is evident that the vapor recompression method exhibits greater energy efficiency, resulting in substantial energy savings of approximately 36.82%, with a consumption of 116.32 MW compared to the base case simulation's consumption of 184.10 MW. Although the condenser and lean pump in the vapor recompression model may demand more energy individually, the overall system evidently benefits from a reduction in energy consumption. These results align with the findings of a similar study conducted by Ahn et al. (2013) [32].

Parameters	Vapour Recompression (MW)	Base case (MW)	Note
Wrich pump	0. 1011	0.1232	Energy Consumer
Rich/lean heat	167.75	231.94	
exchanger Duty			
Reboiler Duty	83.37	127.90	Energy Consumer
Condenser Duty	12.280	5.277	Heat Released
W _{lean pump}	0.8883	0.2604	Energy Consumer
Lean Cooler Duty	19.68	55.82	Energy Consumer
W _{compressor}	12.28	-	Energy Consumer
Total Energy Consumption	116.32	184.10	

Table 7: Comparison of heat flow between the vapour recompression-adopted

 base case and standard base case simulations.

In terms of stream properties, **Figure 25** represents the stream compositions of the vapour recompression in conjunction with the base model of CO_2 capture process simulation, with a specific focus on CO_2 capture efficiency. The CO_2 gas stream from the recompression process contained a higher concentration of CO_2 , approximately 0.2825 mol% which a marked increase when compared to the CO_2 gas product from the base case simulation, which was at around 0.212 mol%. However, this disparity in CO_2 concentrations between the two processed, the CO_2 capture efficiency remained constant at around 74% for both processes which these values were calculated manually determined using Equation (3.3).





4.1.4 The difficulties on scaled-up CO₂ capture process simulation.

For results to have practical significance and to verify their real-world applicability, it is essential to transition from a lab-scale model to a commercial scale. This simulation requires rigorous consideration, especially when inputting stream conditions of the sour gas and determining the sizing of columns. Relying on unique parameters, such as flue gas and column specifications sourced from the DOE/NETL case, provides a foundation for the base case model [17]. However, this scale-up in simulation is challenging. Some predominant issues encountered during this upscale simulation include:

Convergence Problem

One of the issues faced during the scaled-up simulation with the recirculation of lean amine is the difficulty in achieving convergence. As the scale increases, the system's complexity grows, making it harder for the simulation to find a solution that satisfies all the given equations and constraints. These findings can lead to inaccurate or unrealistic results.

Desorber Outlet Stream Errors

Another challenge was that the desorber could not solve the outlet stream due to a fatal error. This error indicated that with the current specifications provided, the simulation could not find a feasible solution. Even when modified initial specifications were applied to the simulation, the error remained.

• Extended Simulation Time

With the increase in the large amount of flow rate, the time required for the simulation to complete also increased. This longer simulation time can affect the overall efficiency of the process, especially when there are multiple iterations.

• Heat Exchanger Consistency Error

The heat exchanger unit posed its own set of challenges. When the simulation was overspecified, it led to consistency errors. Even when the target temperature setting, pressure drop, or ΔT_{min} specifications were adjusted, the error remained because the provided information was either redundant or conflicting, making it impossible for the simulator to achieve a consistent solution.

• Damping Factor Setting

Another challenge faced was in setting the appropriate damping factor. Sometimes, the default value of the damping factor cannot solve the solution in the desorber column, so the setting needs to adjust, but choosing the suitable value is essential for the simulation. An incorrect damping factor can either slow down the convergence or lead to divergence, where the simulation moves further away from a solution.

5 FINAL REMARKS

The key results gained from the simulations regarding the energy consumption of each scenario across parameter variation and the energy saving achieved via process modification simulation.

5.1 Conclusion

Based on data and analysis reported in this dissertation the following conclusions can be obtained:

• Results obtained with the base case model are in line with the literature. The CO_2 gas stream contained the highest concentration of CO_2 , with 74% capture efficiency, which shows a slight difference from the referenced value of 85%.

• The CO₂ capture system consumed 184 MW from the 400 MW coal-fired power plant, which accounted for 46% of the power plant's electricity generation. Notably, this consumption mainly came from the reboiler unit, which constituted 70% of the total energy consumption at 127.90 MW.

• Sour Gas flow rate was a non-critical parameter on CO₂ capture efficiency and reboiler duty. In contrast, a 12.5% increase in the temperature of lean amine influenced both parameters, resulting in an approximately 44% increase in CO₂ capture efficiency and a 1.19% reduction in reboiler duty. However, temperature adjustments risked MEA solvent thermal degradation and increased energy required for lean cooler.

• The variation of solvent concentration of 16% and absorber stages of 7% led to the variation of rich CO₂ loading of 7% for solvent adjustment, variation of CO₂ capture efficiency of around 1%, and variation of reboiler duty of 7% for absorber stages adjustment. However, adding desorber stages from 5 to 15 stages was beneficial for reboiler duty reduction, from 140 MW to 110 MW, while CO₂ capture efficiency at 75% remained constant, which is aligned with the literature.

• Adopting the vapour recompression method decreased energy consumption to 116 MW, as opposed to the base case's 184 MW. This outcome aligns with findings from previous studies. In this configuration, CO_2 capture consumed 29% of the energy generated by the power plant; however, there was no enhancement in CO_2 capture efficiency, which remained constant at 74%

5.2 Limitations of this study

The primary limitations of this study are rooted in challenges encountered during the scaled-up simulation processes. As detailed in earlier sections, these encompass issues like convergence problems, errors in the desorber outlet stream, prolonged simulation durations, heat exchanger consistency errors, and the intricacies of damping factor settings. A potential reason for these challenges may be attributed to the data sourced from DOE/NETL. The accessibility and comprehensiveness of the data available online from this source had certain restrictions, which could have influenced the simulation outcomes.

5.3 Direction for future investigations

Future work could aim to incorporate reality complexities, providing a more robust and comprehensive analysis of the MEA-based CO₂ capture simulation process. This means that several factors evaluation in the future research such as economic analysis, commercial scaled-up simulations, and alternative process improvement methods. The suggestions could help to develop more efficient and economically viable simulation solutions for amine-based CO₂ capture using in the coal-fired power plants, therefore contributing to mitigate the climate change as well as achieve the net zero carbon society.

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APPENDIX

- 1. Base Case Simulation Results Compared to References
- Absorber column



Boundary Conditions	Sweet Gas	References [46], [51]	%Error	Rich Amine	References [46], [51]	%Error
Pressure (bar)	1.01	1.01	0.00	1.01	1.01	0.00
Temperature (°C)	43.79	47.93	-8.64	40.76	43.45	-6.19
Flow rate	1.097×10^{5}	1.093×10^5	0.37	1.621×10^5	1.598×10^5	1 44
(kgmole/h)	1.097/110	1.095/10	0.57	1.021/10	1.590/10	
Composition						
(mol%) CO ₂ H ₂ O	2.39 8.23	n/a n/a	Qlean	1.96 91.12	n/a n/a	
O_2^{Mixer}	13.74	n/a		-	n/a	
N_2	75.64	n/a		-	n/a	
MEA	-	n/a		6.92	n/a	
CO ₂ loading				0.2840		

Table 8: Results from the base case for absorber column

• Rich Pump



Table 9: Results from the base case for rich pump

Down down Conditions	Dish Amine to Heat Fushencer	References	%Error
Boundary Conditions	Kich Amine to Heat Exchanger	[46], [51]	
Pressure (bar)	2.00	2.00	0.00
Temperature (°C)	40.78	43.49	-6.23
Flow rate (kgmole/h)	1.621x10 ⁵	1.598x10 ⁵	1.44

Doundary Conditions	Diah Amina ta Haat Evahangan	References	%Error
Boundary Conditions	Kich Annue to Heat Exchanger	[46], [51]	
Composition (mol%)			
CO_2	1.96	n/a	
H ₂ O	91.12	n/a	
O_2	-	n/a	
N_2	-	n/a	
MEA	6.92	n/a	

• Rich/lean heat exchanger



Table	10:	Results	from	the	base	case	for	Rich	/lean	heat	exchanger
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Boundary	Rich amine to	References	0/ Ennon	Lean amine	References	0/ Ennon
Conditions	Desorber	[46], [51]	70E1101	to Cooler	[46], [51]	70E1101
Pressure (bar)	2.00	2.00	0.00	4.00	4.00	0.00
Temperature (°C)	104.5	104.5	0.00	55.75	58.28	-4.34
Flow rate	$1.621 - 10^5$	1 509-105	1 4 4	$1.57(-10^5)$	1 529-105	2 47
(kgmole/h)	1.021X10	1.398810	1.44	1.3/0X10	1.558810	2.47
Composition						
(mol%)						
CO_2	1.96	n/a		1.41	n/a	
H ₂ O	91.12	n/a		91.48	n/a	
O_2	-	n/a		-	n/a	
N_2	-	n/a		-	n/a	
MEA	6.92	n/a		7.12	n/a	

• Stripper Column



|--|

Boundary Conditions	CO ₂ gas	References [46], [51]	%Error	Lean amine from desorber	References [46], [51]	%Error
Pressure (bar)	2.00	2.00	0.00	2.00	2.00	0.00
Temperature (°C)	113.2	100.0	13.20	120.0	120.0	0.00
Flow rate (kgmole/h)	4.577x10 ³	6.035x10 ³	-24.16	1.576x10 ⁵	1.538x10 ⁵	2.47
Composition (mol%) CO ₂ H ₂ O O ₂ N ₂ MEA	21.20 78.74 - 0.02 0.02	n/a n/a n/a n/a		1.41 91.48 - - 7.12	n/a n/a n/a n/a	
CO ₂ loading	0.2840			0.1975		

• Lean Pump



Table	12:	Results	from	the	base	case	for	lean	pump
1 4010		10000100			oube	•••••	101	100011	pennp

Boundary Conditions	Lean Amine to Heat Exchanger	References [46], [51]	%Error
Pressure (bar)	4.00	4.00	0.00
Temperature (°C)	55.27	58.28	-5.16

Poundamy Conditions	Loon Amino to Hoot Evolution	References	0/ Ennon	
Boundary Conditions	Lean Annue to Heat Exchanger	[46], [51]	/01/11/01	
Flow rate (kgmole/h)	1.757 x10 ⁵	1.538 x10 ⁵	14.24	
Composition				
(mol%)				
CO_2	1.16	n/a		
H_2O	92.51	n/a		
O_2	-	n/a		
N_2	-	n/a		
MEA	6.33	n/a		

• Lean Cooler



 Table 13: Results from the base case for lean pump

Boundary Conditions	Lean Amine to mixer	References	%Error	
		[46], [51]		
Pressure (bar)	4.00	4.00	0.00	
Temperature (°C)	40.0	40.0	0.00	
Flow rate (kgmole/h)	$1.757 \text{ x}10^5$	$1.538 \text{ x} 10^5$	14.24	
Composition				
(mol%)				
CO_2	1.16	n/a		
H ₂ O	92.51	n/a		
O_2	-	n/a		
N_2	-	n/a		
MEA	6.33	n/a		

• Lean mixer



Boundary Conditions	Lean Amine to absorber	References	%Error	
		[46], [51]		
Pressure (bar)	4.00	4.00	0.00	
Temperature (°C)	40.0	40.0	0.00	
Flow rate (kgmole/h)	1.757 x10 ⁵	1.602×10^5	14.24	
Composition				
(mol%)				
CO_2	1.12	n/a		
H ₂ O	92.75	n/a		
O_2	-	n/a		
N_2	-	n/a		
MEA	6.13	n/a		

Table 14: Results from the base case for lean mixer

• Lean Valve



Boundary Conditions	Lean Amine recycle	References [46], [51]	%Error
Pressure (bar)	1.01	1.01	0.00
Temperature (°C)	40.1	40.0	0.25
Flow rate (kgmole/h)	1.821×10^5	1.602×10^5	13.67
Composition (mol%)			
CO ₂ H ₂ O	1.12 92.75	n/a n/a	
O2 N2 MEA	6.13	n/a n/a n/a	

2. Vapour Recompression Simulation Results (Raw Data)

• Material Streams

			Material Streams		
		Sour Feed	Lean Amine	Sweet G	Rich Amin
Vapour Fraction		1.0000	0.0000	0.9998	0.0000
Temperature	С	40.00	40.12	43.79	40.76
Pressure	bar	1.010	1.010	1.010	1.010
Molar Flow	kamole/h	1.091e+005	1.626e+005	1.097e+005	1 621e+005
Mass Flow	ka/s	861.0	964.1	856.5	968.6
Liquid Volume Flow	LISGPM	2.456e+004	1 534e+004	2 445e+004	1 546e+004
Leat Flow		2.40001004	1.00401004	2.440C+004	1.0400-007
пеаггюм	KVV	-0.0030+003	-1.2950+007	=0.7010+005	-1.2900+007
Venner Frenking			Rich Amin to Desorb	Lean Amin Itom De	CO2 gas
vapour Fraction	-	0.0000	0.0000	0.0000	1.0000
Temperature	С	40.78	104.5	120.0	113.2
Pressure	bar	2.000	2.000	2.000	2.000
Molar Flow	kgmole/h	1.621e+005	1.621e+005	1.576e+005	4577
Mass Flow	kg/s	968.6	968.6	938.7	29.93
Liquid Volume Flow	USGPM	1.546e+004	1.546e+004	1.494e+004	515.9
Heat Flow	kW	-1.296e+007	-1.273e+007	-1.227e+007	-3.444e+005
		Lean Amin to HX	Lean Amin to cooler	Lean Amin to mix	Make up water
Vapour Fraction		0.0000	0.0000	0.0000	0.0000
Temperature	С	120.0	55.75	40.00	40.00
Pressure	bar	4.000	4.000	4.000	2.000
Molar Flow	kgmole/h	1.576e+005	1.576e+005	1.576e+005	6380
Mass Flow	ka/s	Q38.7	Q38.7	938.7	31.03
Liquid Volume Flow	USGPM	1 /10/0+00/	1 /10/0/	1 /10/0+00/	507.0
Heat Flow	kW	1.43401004	1.45467004	-1.255.007	5.0446±005
I GALLIOW	1/11	-1.227eTUU7	-1.200e+007		-0.04467000 Sour Cos
		wake up amine	Lean amine to ab	Lean amine rê	our Gas
vapour Fraction		0.0000	0.0000	0.0000	1.0000
Temperature	С	40.00	40.10	40.12	40.00
Pressure	bar	2.000	2.000	1.010	1.010
Molar Flow	kgmole/h	40.00	1.640e+005	1.640e+005	1.091e+005
Mass Flow	kg/s	0.6787	971.3	971.3	861.0
Liquid Volume Flow	USGPM	10.57	1.546e+004	1.546e+004	2.456e+004
Heat Flow	kW	-2967	-1.306e+007	-1.306e+007	-8.863e+005
		Lean Amine to absorber	Sweet Gas	Rich Amine	Rich amine to heatex
Vapour Fraction		0.0000	0.9998	0.0000	0.0000
Temperature	C	40.10	44.51	41.11	41.13
Pressure	bar	1.010	1 010	1.010	2 000
Malas Elaur	bai	1.010	1.010	1.010	2.000
Molar Flow	kgmole/n	1.2596+005	1.0966+005	1.254e+005	1.254e+005
Mass Flow	kg/s	809.5	856.1	814.4	814.4
Liquid Volume Flow	USGPM	1.291e+004	2.444e+004	1.303e+004	1.303e+004
Heat Flow	kW	-1.009e+007	-8.715e+005	-1.010e+007	-1.010e+007
		To recompression	from recompression	Rich amine to desorber	CO2gas
Vapour Fraction		0.9597	1.0000	0.0000	1.0000
Temperature	С	99.45	133.6	99.50	110.2
Pressure	bar	1.000	2.000	2.000	2.000
Molar Flow	kgmole/h	3712	3712	1.254e+005	3563
Mass Flow	kg/s	19.94	19.94	814.4	25.10
Liquid Volume Flow	USGPM	323.9	323.9	1.303e+004	440.7
Heat Flow	kW	-2 558e+005	-2 528e+005	-9 934e+006	-2 788e+005
TIGHT IOW	IXVV	Loop aming from desorbe	-2.0200 1000	Lig from flach tank	Van from flach tank
Vanour Fraction			Contramine mont valve to tiash tahi		4 0000
	6	0.0000	0.0296	0.0000	1.0000
	U	120.0	105.2	105.2	105.2
Pressure	bar	2.000	1.150	1.150	1.150
Molar Flow	кgmole/h	1.255e+005	1.255e+005	1.218e+005	3712
Mass Flow	kg/s	809.3	809.3	789.3	19.94
Liquid Volume Flow	USGPM	1.292e+004	1.292e+004	1.259e+004	323.9
Heat Flow	kW	-9.837e+006	-9.837e+006	-9.583e+006	-2.538e+005
		Lean amine to heatex	Lean amine to cooler	Lean amine to mixer	Water makeup
Vapour Fraction		0.0000	0.0000	0.0000	0.0000
Temperature	С	105.2	47.03	40.00	40.00
Pressure	bar	2.000	2.000	2.000	2.000
Molar Flow	kgmole/h	1.218e+005	1.218e+005	1.218e+005	4365
Mass Flow	ka/s	789.3	789.3	789.3	21.84
Liquid Volume Flow	USGPM	1 259e+004	1 259e+004	1 259e+004	346.0
Heat Flow	kW	0.5930±009	0.7490-000	_0 769.004	3 4510±005
I GALLIOW	1/11	-9.000eTUU0	-9.740e+000		-3.40 IETUUS
Manager Frank		Аниле такеир	wixed Lean Amine	Lean Amine to Recycle	recompressed to desorbe
vapour Fraction		0.0000	0.0000	0.0000	1.0000
I emperature	С	40.00	40.08	40.10	133.7
Pressure	bar	2.000	2.000	1.010	2.000
Molar Flow	kgmole/h	35.00	1.262e+005	1.262e+005	3713
Mass Flow	kg/s	0.5939	811.7	811.7	19.95
Liquid Volume Flow	USGPM	9.248	1.295e+004	1.295e+004	323.9
Heat Flow	kW	-2596	-1.012e+007	-1.012e+007	-2.528e+005

• Energy Streams

Energy Streams												
		WrichP	Qcond	Qreb	W LeanP	Q lean cooler	Wrich pump	Wcompressor	Qcondenser	Qreboiler	Wlean pump	Lean cooler duty
Heat Flow	kW	123.0	5277	1.279e+005	260.4	5.582e+004	101.1	2930	1.228e+004	8.337e+004	88.83	1.968e+004

