

The Potential of Amine to Feed Flowrate Ratio for Post-Combustion Carbon Capture Systems Using Aspen HYSYS

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ABSTRACT

This investigation into carbon capture systems using ASPEN HYSYS provides significant insights into optimising operational parameters, such as the solvent to feed flow rate ratio, and their impact on energy consumption and economic feasibility. The analysis of separator temperature reveals an inverse relationship with CO₂ capture efficiency, peaking at 25°C due to increased CO₂ solubility at lower temperatures. However, efficiency gains diminish beyond this threshold, indicating the necessity for optimal thermal management in the separation process. Pressure variations similarly exhibit a peak capture efficiency at approximately 220 KPa, attributed to enhanced CO₂ solubility under higher pressures, though efficiency declines at higher pressures due to solvent capacity limitations and operational challenges. Investigation into the solvent to feed flow rate ratio shows that increasing the solvent flow rate improves CO₂ capture up to a point, beyond which efficiency gains taper off, indicating diminishing returns. This finding emphasises the need to optimise solvent usage to balance capture efficiency with energy and operational costs. Achieving a 100% capture rate at a solvent-to-feed flow rate ratio of 7.0 demonstrates the potential of CCS technologies, though the economic and environmental implications of high solvent usage require careful consideration for overall process sustainability.

Keywords: Carbon, Capture, System, Aspen HYSYS, Post-Combustion.

INTRODUCTION

The relentless increase in anthropogenic greenhouse gas emissions, driven primarily by industrial processes and the combustion of fossil fuels, poses a profound threat to the global environment. This poses a huge threat to human and global security. At present, the CO₂ concentration in the atmosphere has exceeded 400 ppm, which is about 40% higher than before industrialisation, and the surface temperature has increased by about 0.8 °C [1]. The physical, biological, and human systems are changing negatively on a global scale. Sea, ice, and snow cover levels have dropped by roughly 15%, and as global temperatures rise, more diseases are spreading, droughts are occurring, and fertile soil is increasingly exposed to desertification all of which are typically linked to rising emissions of greenhouse gases, including nitrous oxide, halocarbons, carbon dioxide (CO₂), methane (CH₄), and water vapour [2].

Carbon dioxide (CO₂), a principal greenhouse gas, plays a pivotal role in the observed climate change, characterised by rising global temperatures, extreme weather events, and disruptive ecological consequences [3]. As our understanding of the implications of climate change deepens, the need for proactive measures to reduce and mitigate CO₂ emissions becomes increasingly urgent.

Historically, the scientific recognition of the link between industrial activities and climate change dates to the late 19th century, with Svante Arrhenius's ground-breaking work on the greenhouse effect [4]. However, it was in the latter half of the 20th century that the industrial-scale release of CO₂ and its impact on global climate change became evident. International consensus and regulatory efforts, including the Kyoto Protocol and subsequent climate agreements, have underscored the necessity of adopting strategies to reduce carbon emissions. According to a number of studies, CO₂ emissions will linger in the atmosphere for hundreds of years [2]. The main challenge for the entire world is how to reduce emissions even more while benefiting the economy and the environment. One of the most promising and practical strategies to address this challenge is Carbon Capture and Storage (CCS), a technology designed to capture CO₂ emissions from industrial processes and power generation, transport the captured CO₂ to suitable storage sites, and securely store it underground in geological formations. CCS has evolved from theoretical concepts to practical applications, with pioneering projects demonstrating its viability and safety. These projects, including Sleipner in Norway, In Salah in Algeria, and Petra Nova in the United States, have paved the way for the global adoption of CCS.

Aspen HYSYS, widely recognised and versatile process simulation software developed by Aspen Technology, Inc., has emerged as a fundamental tool in the field of chemical engineering and process optimisation. Its capacity to simulate complex systems, analyse thermodynamic properties, and optimise process designs makes it an invaluable asset for engineers and researchers. Its use in simulating CCS processes and assessing their feasibility has garnered significant attention in recent years, solidifying Aspen HYSYS as the major driver for the simulation and optimisation of Carbon Capture and Storage systems and positioning it as a pivotal resource in the ongoing efforts to address climate change through practical and efficient solutions [5].

The Carbon Capture Storage Framework

The CO₂ sequestration – Carbon Capture and Storage (CCS), may be subdivided into three systems:

1. CO₂ capture and compression system.
2. Transport system for taking the captured CO₂ to appropriate locations.
3. Injection and storage system for its permanent storage away from the atmosphere. The various components of CCS are depicted in Fig. 2.1.

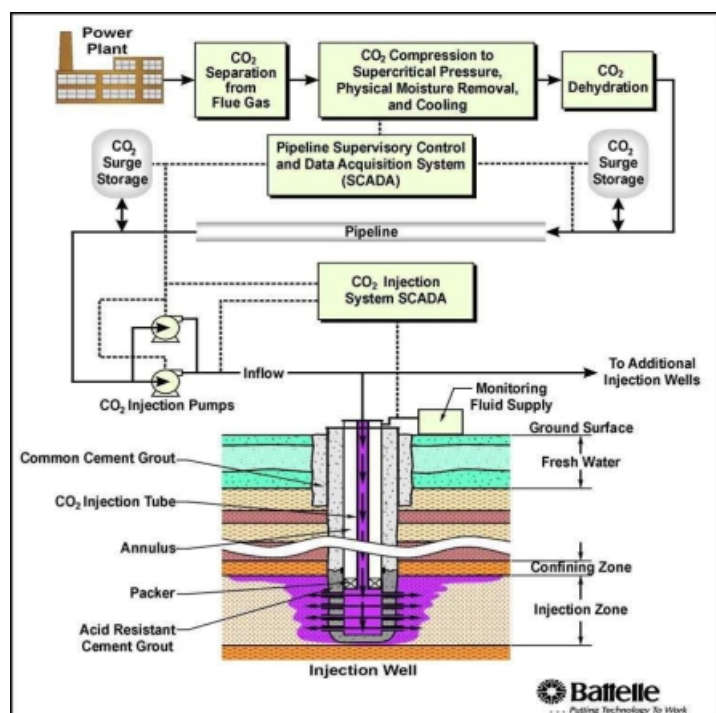


Fig. 1: Carbon Capture and Storage Technology Systems [6]

Efforts to enhance the operational dependability of carbon capture and storage (CCS) are generally organized across three interconnected phases: capture, transport, and permanent sequestration [7]. With respect to the initial capture stage, fossil-fuel-fired power stations typically rely on one of three primary technological pathways. Pre-combustion capture involves gasifying the fuel to produce a synthesis gas from which hydrogen and CO₂ are separated prior to combustion; the hydrogen is subsequently used for power generation while the CO₂ is directed toward storage. Oxy-fuel combustion, by contrast, enriches the combustion atmosphere with oxygen to generate flue gases with a substantially higher CO₂ concentration, thereby simplifying the subsequent separation process.

Post-combustion capture, the third approach, employs chemical or physical absorption to extract CO₂ directly from the flue gas stream following combustion [8]. Each of these capture routes presents distinct technical and economic trade-offs, and their relative maturity varies considerably [8], [9].

Once captured, the transportation of CO₂ to suitable geological repositories necessitates substantial infrastructure investment. Pipelines remain the most widely adopted mode of transport for both onshore and offshore routes, owing to their established technology base and cost-effectiveness over medium distances. However, shipping becomes economically viable for offshore storage sites where pipelines are absent or transport distances are prohibitively large, albeit with additional requirements for CO₂ liquefaction and specialized carrier vessels [8].

The final sequestration stage involves the selection of an appropriate storage medium, while considering storage capacity, containment security, and long-term risks. Deep saline aquifers such as porous rock formations, contains saline water, which offers the largest potential storage volume globally. Depleted oil and gas fields represent the second largest storage category and benefit from decades of geological characterization and monitoring data accumulated during hydrocarbon production, which enhances confidence in their containment integrity. Enhanced oil recovery (EOR) sites provide a comparatively smaller storage capacity but offer short-term economic incentives by improving oil extraction yields; however, this revenue stream is finite and ceases once the oil field is depleted, with some CO₂ inevitably being co-produced with the extracted oil. Emerging approaches include enhanced coal-bed methane recovery, in which CO₂ is injected to enhance methane desorption from coal seams, and CO₂ mineralization, a process that mimics natural weathering by chemically binding CO₂ into stable carbonate minerals such as calcite and limestone, although this remains at an early stage of [8], [9], [10].

Capture Technologies

The terms post-combustion, pre-combustion, and oxyfuel combustion refer to a variety of methods for capturing CO₂ [11]. Pre-combustion, which promotes the high volume at a ratio of 10:1, is a generally used and very simple method.

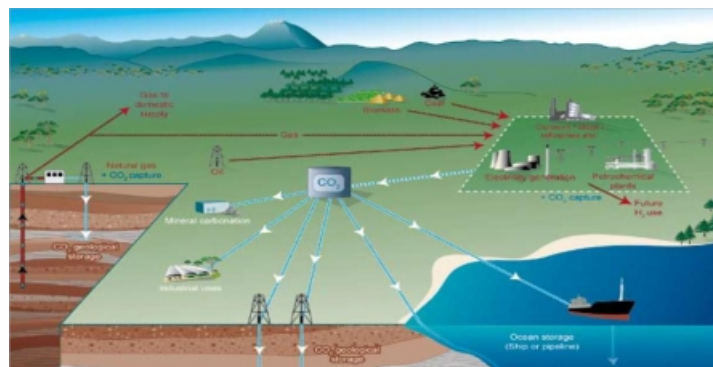


Fig. 2: Schematic diagram of possible CCS systems [12]

On the other hand, the post-combustion approach works well at lower CO₂ streams [13]. Pre-combustion CCS uses an integrated gasification combined cycle in conjunction with a shift reactor to convert carbon to CO₂ [14], [15]. Table 1 lists the various CO₂ capture classes and storage.

Table 1: Different classes of CO₂ capture and storage

Classes	Explanation
Carbon Positive	The release of a significant amount of carbon when the process of combustion takes place such as coal to liquid, refineries and natural gas processing. EOR operations are sometimes carbon positive depending on the project specifics
Carbon Neutral	Conversion of carbon into CO ₂ that can be used to produce commercial products
Carbon Negative	Removal of CO ₂ from the atmosphere directly or by this process applied to biomass combustion for generation of electricity

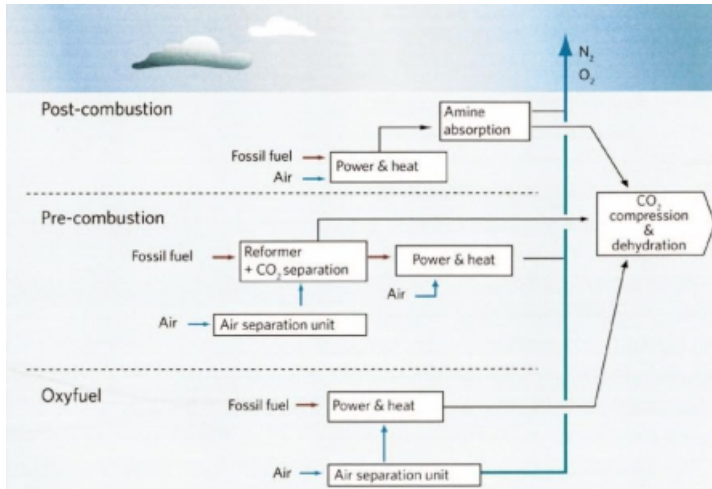


Fig. 3: Simplified diagram illustrating the three main approaches to carbon capture [16]

Review of Related Literature

The body of research on CO₂ capture using Aspen HYSYS has extensively covered various aspects of the process, including solvent efficiency, process optimisation, and economic considerations. Studies like those conducted by Ahmed *et al.* [17] delved into identifying the most efficient amine solvents for CO₂ capture, focusing on absorption capabilities and capture efficiencies, where MEA was superior to other amine-based solvents. The results obtained also demonstrated that the absorber height, solvent circulation rate and reboiler duty have the most remarkable effects on the CO₂ capture ability.

Birkelund [18] explored the technical nuances of CO₂ absorption and desorption, providing a solid technical foundation for understanding the process. In his work, three different configurations were evaluated for post-combustion CO₂ capture from a combined heat and power plant using chemical absorption. The configurations evaluated are a standard absorption process, a vapour recompression modification, and a lean split with vapour recompression modification, with the lean split with vapour recompression being too complex and having too low flexibility to achieve converged calculations in sensitivity cases.

Oluwafemi [19] demonstrated a CO₂ capture process with a CO₂-rich flue gas feed and a CO₂-free effluent using Monoethanolamine (MEA) as absorbent, which captures up to 93% from the stream.

Lars Erik *et al.* [20] focused on the cost of CO₂ capture using equipment cost data from Aspen In-plant and optimum conditions for the heat exchanger and number of plates in the absorber to maximise carbon capture.

However, despite the valuable insights into cost estimation done also by Dehghanizadeh [21] and the specific focus on coal-based power plants in studies like Eviani *et al.* [22], there remains a gap in comprehensive analysis that combines process efficiency, economic viability, and environmental sustainability with an emphasis on optimising operational parameters such as the solvent to feed flow rate ratio and energy comparison to economic value of captured CO₂.

MATERIALS AND METHOD

The model utilised was simulated using the flue gas data obtained from the Refinery Fluid Catalytic Cracking (FCC) Unit [19]. The plant was assumed to operate at steady state. The process was simulated using ASPEN HYSYS v.11 with the Acid Gas-chemical solvent fluid package. Figure 4 to 11 shows screenshots of major steps in carried out in the simulation environment. The process flow sheet is shown in figure 4.9.

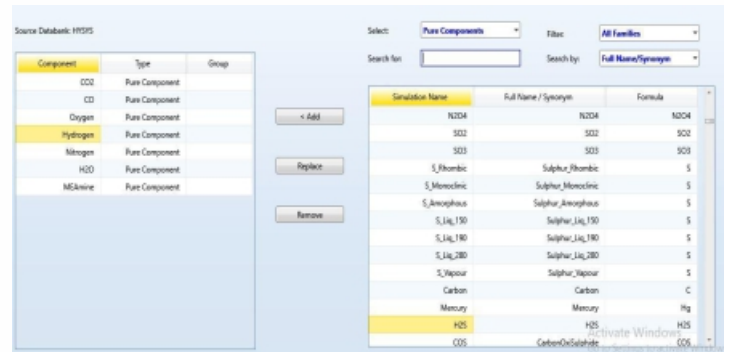


Figure 4: component Selection

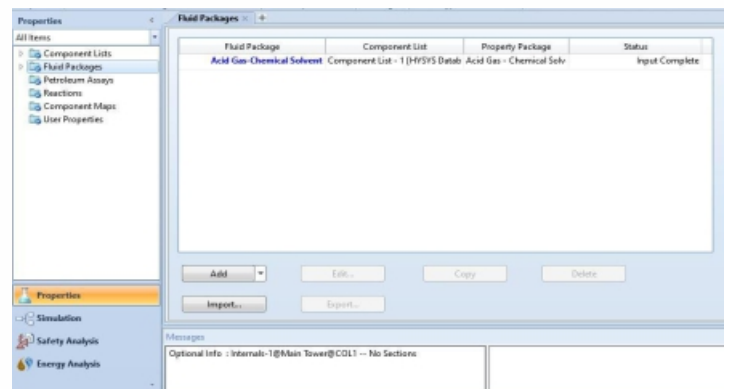


Fig. 5: Selection of fluid package

The screenshot shows the 'DCC worksheet' in Aspen HYSYS. It displays a table with columns for 'Name', 'hot flue gas', 'cool flue gas', and 'DCC duty'. The rows show various properties and composition data for the flue gas streams.

Name	hot flue gas	cool flue gas	DCC duty
Vapour	1.0000	0.9477	<empty>
Temperature [C]	180.0	40.00	<empty>
Pressure [kPa]	101.0	750.0	<empty>
Mass Flow [kg/h]	1.710e+004	1.710e+004	<empty>
Molar Flow [kgmole/h]	4.875e+005	4.875e+005	<empty>
Std Ideal Liq Vol Flow [m3/h]	878.1	878.1	<empty>
Molar Enthalpy [kJ/kgmole]	-4.699e+004	-5.361e+004	<empty>
Molar Entropy [kJ/kgmole-C]	18.18	-16.68	<empty>
Heat Flow [kJ/h]	-8.035e+008	-9.167e+008	1.131e+008

Fig. 6: DCC worksheet

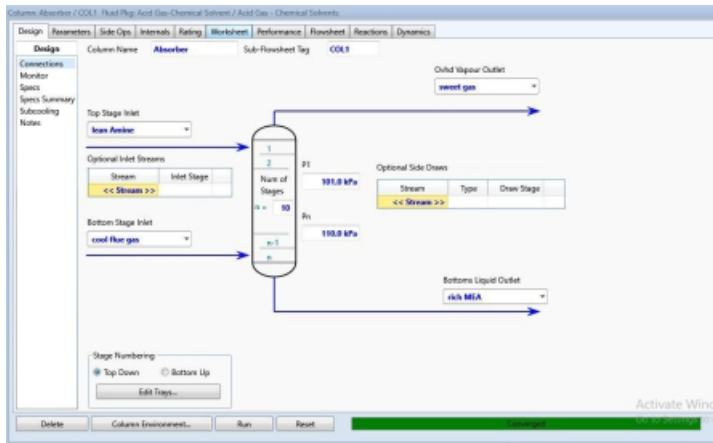


Fig. 7: Column Absorber Worksheet

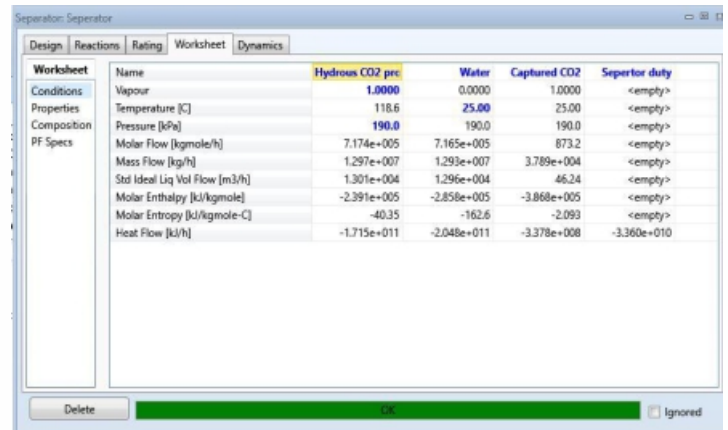


Fig. 11: Separator worksheet

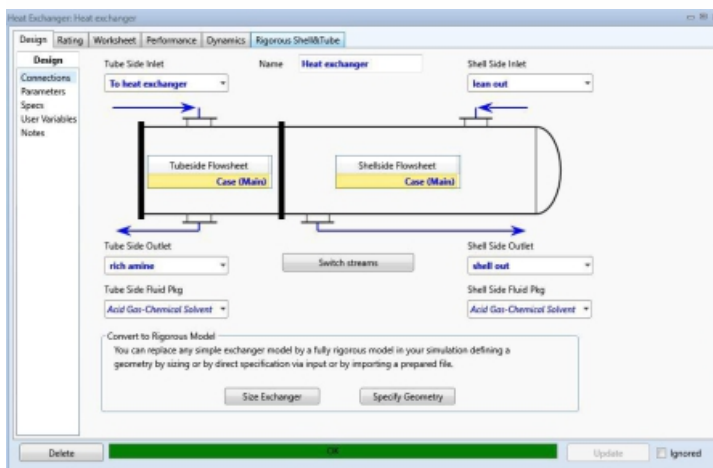


Fig. 8: Heat Exchanger fluid Specification

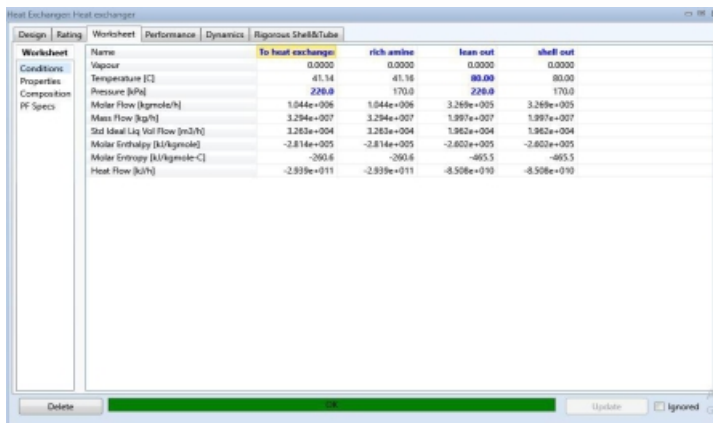


Fig. 9: Heat Exchanger Worksheet

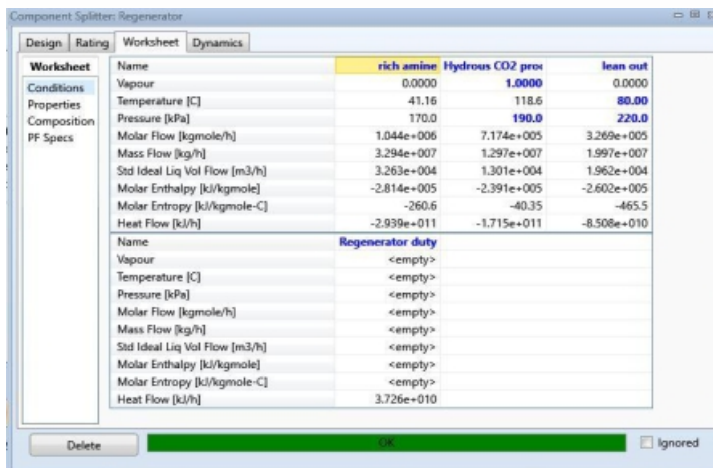


Fig. 10: Regenerator Worksheet

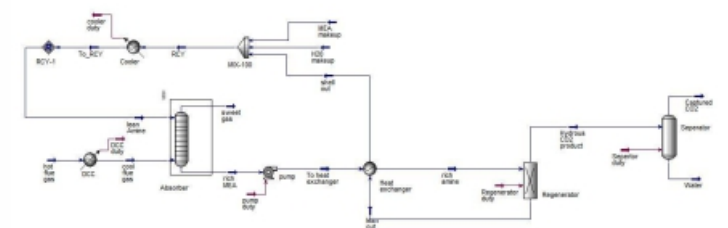


Fig. 12: Simulation Process Flow sheet

In the comprehensive analysis of the simulation outcomes facilitated by Aspen HYSYS, detailed insights into the process's operational efficiency are presented. Table 2 delineates the characteristics and compositions of the feed stream. Following this, Table 3 elucidates the properties and compositions of the product stream, illustrating the transformation achieved through the process. Table 4 presents an exhaustive account of the material streams, cataloguing the flows within the system. The intricacies of material transitions and conservation are further expounded in Table 5, where a detailed material balances is provided, offering a quantitative evaluation of input-output relationships. Lastly, Table 6 consolidates the energy balance, providing a critical assessment of energy conservation and efficiency within the system.

Table 2: Feed Stream Analysis

	H ₂ O makeup	MEA makeup	hot flue gas
Pressure [kPa]	101	101	101
Temperature [C]	30	30	180
Mass Flow [kg/h]	12888235.8	148.4334396	487535.4027
Std Ideal Liq Vol Flow [m3/h]	12913.07469	0.145839123	878.1318459
Vapor / Phase Fraction	0	0	1
Molar Enthalpy [kJ/kgmole]	-285334.0627	-268597.1479	-46990.06062

Table 3: Product Stream Analysis

	Captured CO ₂	Water	sweet gas
Pressure [kPa]	190	190	101
Temperature [C]	25	25	39.99775123
Mass Flow [kg/h]	37891.63963	12928061.41	410111.1309
Std Ideal Liq Vol Flow [m3/h]	46.24059387	12960.04557	785.2082335
Vapor / Phase Fraction	1	0	0.999999945
Molar Enthalpy [kJ/kgmole]	-386793.8379	-285809.9711	-10206.81485

Table 4: Material Stream Analysis

Stream Identifier	Pressure [kPa]	Temperature [C]	Mass Flow [kg/h]	Std Ideal Liq Vol Flow [m3/h]	Vapor / Phase Fraction	Molar Enthalpy [kJ/kgmole]
To heat exchanger	220	41.14056494	32935711.9	32627.01397	0	-281392.0589
rich amine	170	41.15730507	32935711.9	32627.01397	0	-281391.5778
lean out	220	80	19969758.85	19620.72781	0	-260236.41
shell out	170	80.00384785	19969758.85	19620.72781	0	-260237.9465
Hydrous CO2 product	190	118.5856766	12965953.05	13006.28616	1	-239099.8829
Captured CO2	190	25	37891.63963	46.24059387	1	-386793.8379
Water	190	25	12928061.41	12960.04557	0	-285809.9711
H2O makeup	101	30	12888235.8	12913.07469	0	-285334.0627
MEA makeup	101	30	148.4334396	0.145839123	0	-268597.1479
RCY	101	75.01900015	32858143.08	32533.94834	0	-277462.7077
To_RCY	101	40	32858143.08	32533.94834	0	-281206.3936
hot flue gas	101	180	487535.4027	878.1318459	1	-46990.06062
cool flue gas	750	40	487535.4027	878.1318459	0.947744154	-53606.32275
sweet gas	101	39.99775123	410111.1309	785.2082335	0.999999945	-10206.81485
rich MEA	110	41.1233353	32935711.9	32627.01397	0	-281396.6158
lean Amine	101	40	32858287.63	32534.09036	0	-281206.3699

Table 5: Material Balance Analysis

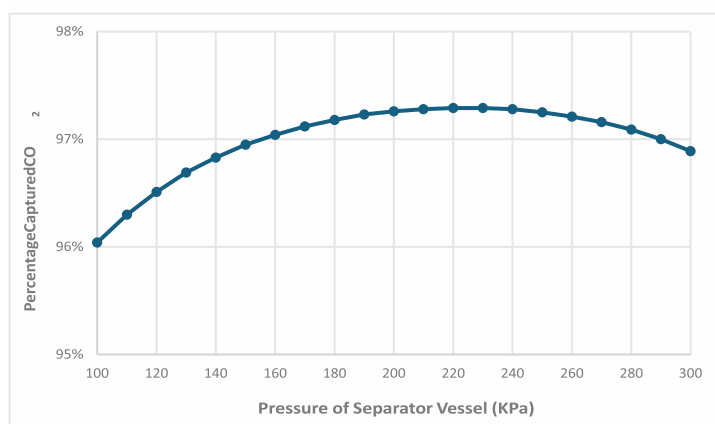
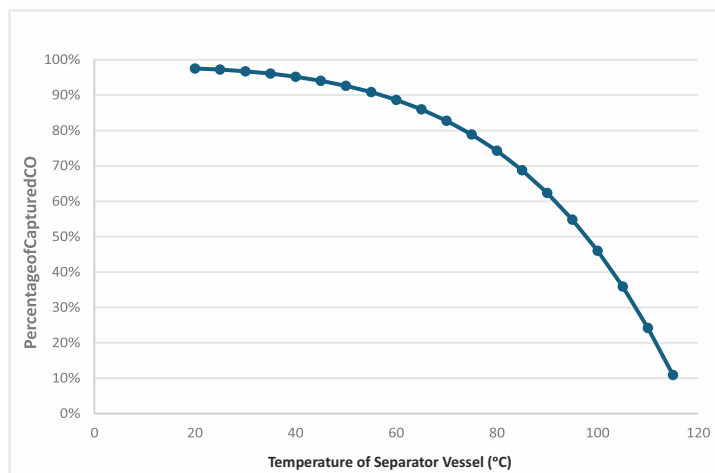
Component Identifier	Stream Identifier	Flow Rate In (kgmole/h)	Flow Rate Out (kgmole/h)
Direct Contact Cooler (DCC)	Hot Flue gas	17100	
	Cool flue gas		17100
	Total	17100	17100
Absorber	Lean Amine	1042335.002	
	Cool flue gas	17100	
	Sweet gas		15098.02335
	Rich MEA		1044336.979
	Total	1059435.002	1059435.002
MEA Pump	Rich MEA	1044336.979	
	To heat exchanger		1044336.979
	Total	1044336.979	1044336.979
Heat Exchanger	To heat exchanger	1044336.979	
	Lean out	326924.4055	
	Rich Amine		1044336.979
	Shell out		326924.4055
	Total	1371261.384	1371261.384
Regenerator	Rich Amine	1044336.979	
	Hydrous CO ₂ product		717412.573
	Lean Amine		326924.4055
Separator	Total	1044336.979	1044336.979
	Hydrous CO ₂ product	717412.573	
	Captured CO ₂		873.2385762
	Water		716539.3344
Mixer	Total	717412.573	717412.573
	MEA makeup	2.43	
	H ₂ O makeup	715405.8	
	Shell out	326924.4055	
	RCY		1042332.635
Cooler	Total	1042332.635	1042332.635
	RCY	1042332.635	
	To RCY		1042332.635
	Total	1042332.635	1042332.635

Table 6: Energy Balance Analysis

Component Identifier	Stream Identifier	Energy In (kJ/h)	Energy Out (kJ/h)
Direct Contact Cooler (DCC)	DCC Duty	-	113,138,082.376
Pump	Pump Duty	4,758,807.688	-
Regenerator	Regenerator Duty	37,256,734,278.758	-
Cooler	Cooler Duty	-	3,902,165,995.912
Separator	Separator Duty	33,598,587,522.996	-
Total		70,860,080,609.442	4,015,304,078.287
Net Energy Requirement		66,844,776,531.154 kJ/h	

RESULTS AND DISCUSSION

Analysis of the effect of temperature and pressure of the separator vessel on the percentage of captured CO₂ was also carried out. This was made possible using case studies where the percentage captured CO₂ was assigned as an independent variable while varying the temperature and pressure of the separator vessel. Figure 13 and 14 shows the graph obtained when the data obtained was plotted.

Fig. 13: Effect of Temperature of Separator on Captured CO₂Fig.14: Effect of Pressured of Separator on Captured CO₂

Furthermore, a major research gap which is the optimum feed to amine flowrate was examined using a case study. The Feed flowrate was held constant and the ratio of Amine to feed flowrate was varied from 2.8 to 7.0. The resulting mole fraction of CO₂ in sweet gas was tabulated for each ratio and is summarized in figure 15 Formula for ratio is:

$$\text{Ratio} = \frac{\text{flowrate of amine}}{\text{flowrate of feed}}$$

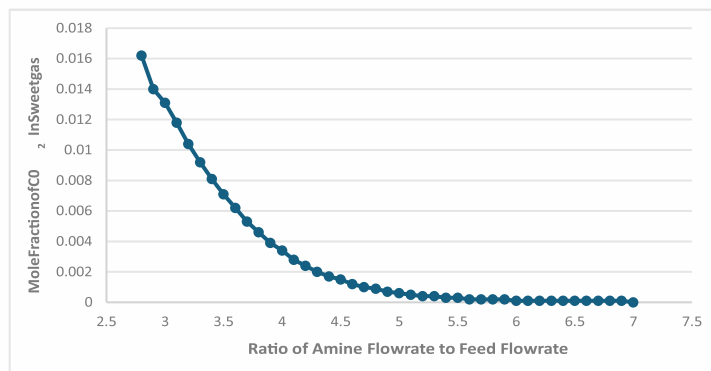


Fig. 15: Amine to feed flowrate Analysis

The outcomes of this investigation highlight significant findings that contribute to narrowing the identified research gap in optimising the solvent to feed flow rate ratio, its impact on energy consumption, and the economic implications of CO₂ capture. Notably, the variation in temperature and pressure of the separator, which is central to the separation of hydrous CO₂ from steam and CO₂, indicates a complex relationship between these operating conditions and the efficiency of CO₂ capture. The observed inverse relationship between the separator temperature and the percentage of captured CO₂, as shown in Fig 13 with an efficiency peak at 25 °C, underscores the critical role of lower operating temperatures in enhancing CO₂ capture. This phenomenon can be attributed to the increased solubility of CO₂ in the solvent at lower temperatures, which facilitates a more effective separation process. However, the concave downward curve as temperature increases suggests a diminishing return on CO₂ capture efficiency beyond a certain temperature threshold. This finding is essential for optimising the thermal management of the separation process, balancing the need for efficient CO₂ capture with the practical limitations imposed by thermal energy requirements.

Similarly, the pressure variation results, fig 14, exhibiting a peak capture efficiency at approximately 220 KPa, illuminate the pressure-dependency of CO₂ capture processes. The initial increase in capture efficiency with pressure can be explained by the enhanced physical solubility of CO₂ in the solvent under higher pressures. Nonetheless, the subsequent decline in efficiency, even if at a slower rate, points to the diminishing benefits of increased pressure, likely due to the limitations of solvent capacity and potential operational challenges at higher pressures.

The analysis of the solvent-to-feed flow rate ratio reveals a critical insight into the diminishing efficiency gains with higher ratios. The exponential decay curve in fig 15 associated with this variable indicates that while increasing the solvent flow rate relative to the feed can enhance CO₂ capture, the efficiency gains taper off, highlighting a point of diminishing returns.

This observation is pivotal for optimising solvent usage, where an excessive increase in solvent flow rate may not justify the marginal improvements in capture efficiency, especially when considering the associated energy and operational costs.

The findings related to the mole fraction of CO₂ in the sweet gas further illustrate the effectiveness of optimising the solvent to feed flow rate ratio. The achievement of a 100% capture rate at a ratio of 7.0, albeit at the cost of increased solvent usage, presents a significant milestone for CO₂ capture technologies. However, the economic and environmental implications of such high solvent usage warrant careful consideration, particularly in the context of the overall sustainability of the capture process.

CONCLUSION

This investigation provides key insights into optimising the solvent to feed flow rate ratio, impacting energy consumption and the economic feasibility of CO₂ capture systems. The study highlights the importance of operating conditions, revealing that CO₂ capture efficiency peaks at a separator temperature of 25°C and a pressure of 220 kPa. Lower temperatures enhance CO₂ solubility in the solvent, while optimal pressure levels maximise capture efficiency without significant diminishing returns.

The analysis also indicates diminishing efficiency gains with increasing solvent to feed flow rate ratios, emphasising the need to balance enhanced CO₂ capture with associated energy and operational costs. Achieving a 100% capture rate at a ratio of 7.0 underscores the potential for high efficiency, though it necessitates careful consideration of economic and environmental impacts.

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