Cover Letter:

From
Team A
Intern
The 310i technologies

To Dr . Upasana Manimegalai Sridhar The 310i technologies

23 June 2023

Sub: A plant model for CO2 capture in a chemical industry

Respected ma'am

We have done a project on the carbon capture aspect of a chemical industry plant. As almost all chemical plants are taking net zero CO2 emission as their aim Carbon Capture and Storage (CCS) is gaining popularity and use.

We have conducted a research in the same area for a chemical plant where the flue gas is treated for CO2 removal and the removed CO2 is stored and passed further for plants that use CO2 as feed for their process.

The project report is attached in this document and the entire process from the plant simulations to the criteria used for elimination.

Thanking You

Yours truly, Team A

Carbon Capture in a chemical plant using recyclable chemical solvents

Team A

The 310i technologies

Planning Memo

Tasks	Jun 21 to 29	Jun 21 to 24	Jun 24 to 30	Jun 25 to 30	Jun 25 to 30
Case 1	SreeKrishnan				
Case 2	SreeKrishnan				
Case 3	SreeKrishnan				
Case 4	Abija				
Case 5	Abija				
Case 6	Abija				
Case 7	Kannan				
Case 8	Kannan				
Case 9	Kannan				
Case 10	Ankit				
Case 11	Ankit				
Case 12	Ankit				
Report Writing		Sree Krishnan	Kannan		
PowerPoint Presentation				Abija	Ankit

Report Contribution

Tasks	Done By
Cover Letter	Sree Krishnan
Tables and Figures	Sree Krishnan
Executive Summary	Sree Krishnan
Introduction	Sree Krishnan
Project Basis	Kannan
Design Details	Kannan
Column Internals	Kannan
Process Variations	Kannan
Simulation Result	Kannan
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Objective: The objective of this project is to design a CO2 capture plant that utilizes regenerable chemical solvents to achieve a minimum CO2 capture efficiency of 90% from post-combustion flue gas. The design should consider additional details, screening options, and site-specific considerations as provided in the details below
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Executive Summary:

Carbon capture is a necessity in most of the chemical plants these days as they reduce the overall carbon footprint of the plant. In this report we have tried to build a carbon capture plant that is used to absorb CO2 from the process flue gas. The concentrated CO2 gas from the carbon capture plant can be used for other purpose where a concentrated gas of CO2 is used. The solvents screened in this process are Mono ethanol Amine and Methyl diethanol amine activated with piperazine. Both MDEA with piperazine and MEA are used as industrial solvents for acid gas removal. MEA has a relatively higher reactivity with CO2 compared to MDEA hence another amine like piperazine is added to speed up the absorption process. Both the amines are sent into an absorber column with valves or trays inside. In this report we have screened a General valve tray, Mellapakplus packing and a Raschig Super-ring packing. To reduce the emission of these amine and to reduce their circulation loss a plant with water wash section is also screened to see if it is necessary. All the cases with these screenings are simulated using protreat simulator The final outlet gas from the plant is expected to remove 90% of the CO2 from the inlet gas. The solvents have a limitation on their weight percentage in the solvent solution to reduce cost and any environmental impact they might have. These solvents are also recycled to further reduce the operational cost. Each system has a 10% variability margin for the feed and is considered for both clean and heat stable salt solutions .The safety aspect for the case reduction includes Substitution, Minimisation, Moderation and Simplification. The cases that are shortlisted based on these safety aspects are then scrutinised on performance to further reduce the number of cases.

Introduction:

CO2 is a greenhouse gas that is emitted during almost all chemical process. A large emission of CO2 to the atmosphere leads to the greenhouse effect and eventually to global warming. All chemical plants try to reduce their overall CO2 emissions and strict rules from the pollution control board has made it mandatory to process all flue gas before releasing it to the atmosphere.

CO2 removal also known as carbon capture is a techniques used by the industry to remove CO2 from tail gas, flue gas and other process gas that may contain CO2.

There are various technologies^[2] available for carbon capture. According to OpenAI's ChatGPT these are as follows:

- 1. Post combustion Capture
- 2. Pre combustion Capture
- 3. Oxyfuel combustion
- 4. Direct air capture

Post combustion capture^[3]:

It is one of the most straight forward and challenging method of CO2 removal as the CO2 concentration and pressure in the flue gas is really small. The CO2 concentration in the flue gas is nearly equal to 20% at most of the cases.

CO2 removal from flue gas follows a simple procedure of absorption of the gas in some kind of solvent. These solvents can be either physical or chemical. Chemical solvents are regenerated most of the times as to reduce the plants expenses and to avoid the release these solvents in the surrounding environment. Basic solvents are mostly used as CO2 is an acidic compound. The most used solvent is Mono ethanol amine (MEA) a primary amine that is a good absorber of CO2 at a varied temperature. MEA is widely used for its fast rate of reaction with CO2, it also cost less compared to other solvents. However the regeneration of this solvent is really hard due to its high energy consumption, ability to corrode the equipment and the vaporisation losses. These days tertiary and sterically hindered amine like 2-amino-2-methyl-1-proponal (AMP) and Methyl di-ethanol amine (MDEA) are gaining popularity in their use as solvents. Solvents like MDEA have a slow rate of reaction with CO2, this can be sped up by using another amine like piperazine that speed up the absorption process. Table 1^[4] shows the absorption ability of various solvents that are used in the industry and their absorption of CO2.

Process name	Solvent/reagent + additives	CO ₂ in treated gas (ppm)
Physical absorpt	tion systems	
Purisol (NMP)	N-methyl-2-pyrrolidone	Less than 50

Process name	Solvent/reagent + additives	CO ₂ in treated gas (ppm)
Rectisol	Methanol	Less than 10
Fluorsolv	Propylene carbonate	Function of pressure
Selexol	Polyethylene glycol dimethyl ether	Function of pressure
Processes with ch	emical reagents	
MEA	Water/monoethanolamine (20%)	Less than 50
Promoted MEA	Water/MEA (25–30%) + amine guard	Less than 50
Benfield	Water/K ₂ CO ₃ (25–30%) + DEA, etc	500-1000
Vetrocoke	Water/K ₂ CO ₃ + As ₂ O ₃ + glycine	500-1000
Catacarb	Water/ K_2CO_3 (25–30%) + additives	500-1000
Lurgi	Water/ K_2CO_3 (25–30%) + additives	500-1000
Carsol	Water/K ₂ CO ₃ + additives	500-1000
Flexsorb HP	Water/K ₂ CO ₃ amine promoted	500-1000
Alkazid	Water/K₂-methylaminopropionate	To suit
DGA	Water/diglycolamine (60%)	Less than 100
MDEA	Water/methyl diethanolamine (40%) + additives	100-500
Hybrid systems		
Sulfinol	Sulphones/DIPA	Less than 100
TEA-MEA	Triethanolamine/monoethanolamine Water/sulpholane/MDEA	Less than 50

Table 1: Overview of CO2 capture in post combustion technology

Advantages:

- 1. It's the most mature method compared to other techniques
- 2. CO2 can be captured using this technique at lower pressures
- 3. It can be placed in the existing or new chemical plants

Disadvantages:

- 1. Solvents like MEA contribute to CO2 production directly or indirectly during to their production.
- 2. The efficiency of CO2 capture is also low due to lower concentration of CO2 in the flue gas.
- 3. Energy consumption is also high due to solvents like MEA

Oxyfuel Combustion^[5]:

According to OpenAI's ChatGPT Oxyfuel combustion is a method of combustion that uses an oxygen rich environment to combust fuel. This leads to the

production of a stream of flue gas that is rich in CO2 and H2O. This leads higher efficiency in CO2 capture due to the concentration of CO2 in the flue gas.

Advantages:

- 1. Higher CO2 concentration in the flue gas
- 2. Other acid gases like NOx production can be avoided

Disadvantages:

- 1. Requirement of Oxygen and cost of Oxygen is higher
- 2. Reduced flame temperature due to the absence of Nitrogen
- 3. Higher chances of corrosion due to the higher concentration of CO2 and elevated temperature

Pre-combustion capture:

The CO2 is captured before combustion by converting the fuels into synthesis gas by gasification of the fuel under higher temperature and pressure by partial oxidation of in steam or oxygen. This method gives a concentrated stream of CO2 compared to post combustion. The CO2 concentration in this method is between 15% to 50%^[6].

According to OpenAI's ChatGPT:

Advantages:

- 1. Higher efficiency of CO2 absorption compared to post combustion.
- 2. Relatively easy capture of CO2
- 3. Lower energy demand as the CO2 is capture before combustion and therefore requires less energy.

Disadvantages:

- 1. High capital cost
- 2. Higher pressure and temperature conditions for gasification
- 3. Applicable mostly for fossil fuel like natural gas, coal, etc^[7].

Direct air capture:

Direct air capture involves removal of CO2 from air directly. The air is let to pass through chemicals that selectively remove CO2 from the air. These chemical are either liquid solvents or solid adsorbents. The absorbed or adsorbed CO2 is then removed from the solvent or adsorbent using application of heat^[8].

According to OpenAI's ChatGPT:

Advantages:

- 1. Carbon can be removed from the atmosphere that has been accumulating over the past years.
- 2. CO2 can be removed from any location regardless of the emission source.

Disadvantages:

- 1. Higher capital and operational cost due to the process energy requirement and complexity
- 2. Extensive reliance in this method can lead to distraction from the current emission reduction efforts. By focusing a lot on CO2 removal from the

- atmosphere some tend to forget to reduce the effluent treatment within the plant.
- 3. Large amount of land and resource are required to set up and run this facility. This also comes with its own environmental issues as to corroded equipment, waste management, etc^[9].

Project Basis-

Objective: The objective of this project is to design a CO2 capture plant that utilizes regenerable chemical solvents to achieve a minimum CO2 capture efficiency of 90% from post-combustion flue gas. The design should consider additional details, screening options, and site-specific considerations as provided in the details below.

Design Details:

- 1. Flue Gas Source: The design will focus on capturing CO2 emissions from a post-combustion source, such as a coal-fired power plant or an industrial process with significant CO2 emissions.
- 2. Minimum CO2 Capture Requirement: The CO2 capture plant must achieve a minimum CO2 capture efficiency of 90%. This means that at least 90% of the CO2 present in the flue gas should be captured and separated from the gas stream.
- 3. Regenerable Chemical Solvents: The CO2 capture will be accomplished using regenerable chemical solvents. These solvents will absorb CO2 from the flue gas, allowing for its subsequent release in the regenerator. The solvents which are used in this project are:
 - I. Monoethanol amine (MEA)
 - II. Methyl di-ethanol amine (MDEA)
 - III. Piperazine
- 4. Screening Options: The design considers various screening options based on the design memo. This includes evaluating solvent performance, column internal performance, and design variations. The screening process ensures that the selected option meets the project objectives and satisfies the process checklist, safety and regulatory requirements.
- 5. Site-Specific Considerations: The design considers site-specific factors that influence the CO2 capture plant's performance and feasibility. These considerations may include flue gas flow rate and composition, temperature and pressure conditions, asset integrity requirements, and utility availability.

An sample flow sheet of a CO2 capture plant with an absorber wash section developed in ProTreat® software is provided in Figure 1 below-

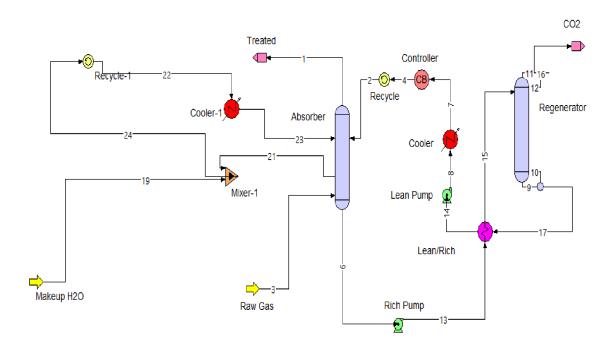


Figure 1: Sample flow sheet for CO2 capture unit with absorber wash section

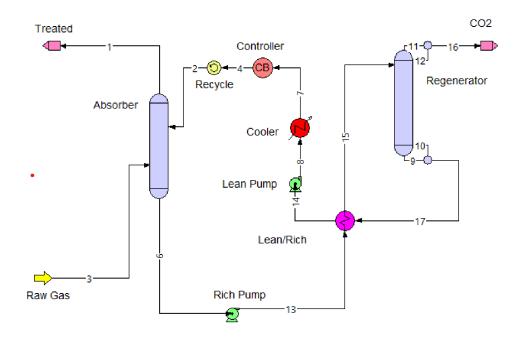


Figure 2: Sample flow sheet for CO2 capture unit without absorber wash section

Similarly, the other cases using different solvent such as MDEA and Piperazine is done accordingly with and without Water Wash Sections.

Column Internals-

Column internals are an essential component of a CO2 capture plant and play a crucial role in facilitating the separation of CO2 from the flue gas using regenerable chemical solvents. The following are the column internals that were used in this work:

- 1. Packing or Structured Packing: Packing materials, such as random packing or structured packing, are used to increase the contact area between the solvent and the flue gas. The Packing material used in this case for example in Mellapak plus Section is Metal at M352.Y packing sizes. Similarly, in the case of Raschig Super Pak section the Packing material was also Metal with packing sizes at 250Y.
- 2. Trays: Trays are another type of column internals used for CO2 capture. They consist of horizontal plates installed inside the column at regular intervals. The different trays used in our simulation are Generic Valve Trays, Mellapak Plus and Raschig Super Pak trays.

Process Variations-

Process variations in a CO2 capture plant using regenerable chemical solvents can optimize performance, enhance efficiency, or meet specific operational needs. The process variations considered in this simulation are with and without Water sections:

- 1. With Water Wash Section- A plant with a Water Wash section is ideal for it helps in Absorption of CO2 from flue gases using a solvent. Plays a role in stripping, separation of CO2 from the solvent. Helps in cooling and condensing the hot steam as well as water treatment to remove impurities. The water section also helps in regenerating the solvent for reuse in the plant. Manages water supply and usage effectively and conservatively.
- 2. Without Water Wash Section- Even though usually a Water Section is used in a plant, there are alternatives where there is no Water Section. Most widely used technology is Direct Air Capture Technology where CO2 is captured directly from air using sorbents or chemical reactions, it is then sent to be processed, purified and stored for future applications. Other sorbents such as activated carbon is also used for capturing CO2. Membrane separation technology is also utilized to selectively permeate CO2 through membranes while other gases flow through them.

It's important to carefully evaluate process variations considering project requirements, cost, constraints, and trade-offs. Use tools like process simulation, economic analysis, and pilot-scale testing to select the most effective variations for a CO2 capture plant.

Simulation Results:

Based on the process variations, solvent options, and column internals options a matrix of 12 cases were set up. The details of each of the cases and the key results from each of the case is provided in table 2 below:

Table 2: The results of each case from using ProTreat® software.

PARAMETERS	Guideline/Reference Values	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case
Solvent	MDEA-Pz/MEA	MDEA- Pz	MDEA- Pz	MDEA- Pz	MDEA- Pz	MDEA- Pz	MDEA- Pz	MEA Wash	MEA
Internals	Generic Valve Trays (GVT)/Raschig Super Ring (RSR)/Mellapak Plus (MP)	GVT	MP	RSR	GVT	МР	RSR	GVT	MP
Solvent strength total (wt %)	30-45	44	32.5	32.5	38.2	45	41.7	30	20
Blend (wt %)	MDEA 30-45/Pz 0.5- 7/MEA 20-30	MDEA 39/Pz 5	MDEA- 30/Pz- 2.5	MDEA- 30/Pz- 2.5	MDEA- 35/Pz- 3.2	MDEA 44.5/Pz 0.5	MDEA 40/Pz 1.7	MEA - 30	MEA-
CO2 removal (%)	90	90.56	92.41	94.8	90.77	91.748	90.88	91.26	91.3
CO2 in treated gas (kmol/hr)	< 27.28	25.75	20.69	14.17	24.15	22.518	24.875	2.74	23.19
CO2 capture (MT/day)	> 261	261	266	273	262.62	264.12	261.768	262	263
Rich amine loading (mol CO2/mol amine)	< 0.45	0.264	0.31	0.316	0.331	0.28	0.305	0.242	0.442
Lean amine loading (mol CO2/mol amine)	No guideline	3.85E- 03	1.66E- 02	1.40E- 02	4.52E- 03	1.06E- 03	2.24E-03	0.101	0.318

About ProTreat Simulation Software-

(According to OGTRT Official Website)

OGT Simulation Software-

Today, most simulators claim some mass transfer rate-based capabilities, but only ProTreat is fully rate-based in the true meaning of the word and allows you to simulate treating using single, multiple, and specialty amines, non-amine systems, amines mixed with a physical solvent, sour water stripping, and glycol dehydration in columns containing a vast range of trays, random packing and structured packing in absorbers, regenerators, and quench towers. The latest gas treating addition to ProTreat simulates hybrid solvent systems in which part of a standard aqueous amine is replaced with an organic nonreactive component. Currently ProTreat can simulate up to three aqueous generic amines with sulfolane as the organic additive. Other combinations are under development.

Cases where ProTreat® is used-

- 1. Acid Gas Removal AGR
- 2. Primary, secondary and tertiary amines
- 3. Amine blends
- 4. Amines with Stripping Promoters
- 5. Predict Performance of Real Solvents and effect of Heat Stable Salts
- 6. Hybrid Solvents
- 7. Accurate COS and mercaptans removal
- 8. SELEXOL™
- 9. Acid Gas Enrichment (AGE)
- 10. Tail Gas Treating
- 11. Corrosion Monitoring
- 12. CO2 Capture
- 13. MEA, Piperazine, Ammonia
- 14. AMP-Piperazine (CESAR-1)
- 15. Enzyme Catalysts
- 16. Amino Acids
- 17. CSIRO Solvents
- 18. Deep CO2 Removal
- 19. Piperazine-promoted MDEA in LNG and Ammonia
- 20. HotPot and Amine-promoted HotPot in SynGas
- 21. Selective H2S Removal
- 22. MDEA

Why ProTreat[®] is used and its Appropriateness for CO2 Capture?

Protreat is currently the most powerful tool available for simulating gas treating and processing which mainly includes our CO2 Capture as well. ProTreat is known to produce the utmost reliable and accurate values when it comes to simulation processes. ProTreat being widely used worldwide accelerates its credibility in providing maximum results. The above facts reinforces the usage of ProTreat for CO2 Capture and its appropriateness in results.

References:

- [1]: https://www.carbonclean.com/technology
- [2]: https://www.chat.openai.com/: Prompt used: Carbon capture technologies
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- [11]: https://www.chat.openai.com/: Prompt used: Process variations in co2 capture
- [12]: https://www.chat.openai.com/: Prompt used: Project basis of co2 capture process
- [13]: https://www.ogtrt.com/page/protreat
- [14]: https://www.ogtrt.com/page/protreat-details "About ProTreat" was obtained from the official website of OGTRT.