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Aspen HYSYS Simulation of CO₂ Capture for the Best Amine Solvent



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ARTICLE INFO	ABSTRACT
Article history: Received 29 December 2019 Received in revised form 25 January 2020 Accepted 25 January 2020 Available online 30 March 2020	The developing issue of the present world is a worldwide temperature alteration, which is caused by ozone-harming substance impact. Carbon dioxide has the real commitment towards a worldwide temperature alteration as it is discovered copiously in climate given anthropogenic carbon dioxide outflows and advancement of vent gasses. Businesses are additionally debilitating corrosive gasses (CO_2 and H_2S) in the earth, which prompts the perilous conditions. To control such conditions lessening of these hurtful gasses is valuable for which ingestion of corrosive gasses is for the most part favoured. Amine gas treating is an appropriate system to complete this work as it expels CO_2 and H_2S at the same time from petroleum gas streams and also modern gas streams and decontaminate them for local use and solid condition individually. For this purpose, study the best solvent selection for CO_2 capture in chemical absorption. In chemical absorption process. This research focus on the effect of various amine absorbents, their concentrations, the absorber and stripper section statures and the working conditions for carbon dioxide recuperation plant for post-combustion carbon dioxide evacuation. For every amine dissolvable, the ideal stages for the absorber and stripper segments, and the ideal absorbent concentration, the ones that give the base conditions for carbon dioxide evacuation is determined by Aspen HYSYS simulation. The results obtained showed that carbon dioxide recuperation with 50 wt. % DGA requires the best ideal conditions for removal of CO_2 with the following design and working conditions are 10-organize absorber column and 10-arrange stripper segment, 20.89 m ³ /hr circulation rate of solvent and 2545 kW of reboiler obligation and 100°C as the regenerator-delta temperature and absorbed 93.6% CO ₂ .
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Aspen HYSYS; amines; absorption; blend; carbon dioxide

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1. Introduction

In each burning response brings about the arrival of vent gasses, for example, carbon monoxide, carbon dioxide, nitrous oxides and so forth. To guarantee natural wellbeing, guidelines and directions limit the measure of these vent gasses to be depleted into the air; this can be proficient by downstream treatment of the pipe gasses emanating from the flare. Carbon dioxide is likewise a constituent of the gasses discharging from the flare. Carbon dioxide is noteworthy ozone-harming the substance. Late mechanical development has brought about intense increment in the emanations of carbon dioxide [1,2]. In this task, to have considered the above situation, the downstream treatment of pipe gasses (recuperation of carbon dioxide). Carbon dioxide catch and capacity (CCS) is the pathway that can enable the world to appreciate the advantages of fast, modern development. Fundamentally, CCS advancements in a more extensive degree discover their applications in coal-terminated power plants since they are the biggest wellspring of CO₂ discharges. In any case, it ought to be noticed that specific modern procedures (flammable gas handling, smelling salts creation, bond fabricate and the sky is the limit from there) [3,4].

The aim and objective of this research, since absorption is dependent on many parameters such as pressure, temperature, solvent circulation rate and concentration of reactants. By altering such parameters, the process can lead to optimized results. Different types of solvents MEA, DEA, MDEA and blends are used to observe which one is more efficient. Solvent and gas flowrates are varied to see their prominence on absorption.

The project leads to the ease of coal-fired plant flue gases domestic usage and capturing of greenhouse gas (CO₂) which may lead to the protection of the ozone layer, making environment-friendly. Industrial gasses that are discharged in climate contain contaminants which may consolidate delivering erosion, causing acids which may be unsafe for human and gear life. Socially, such advancements when completed in the industry they may expand the business rate because these ventures contain huge scale helpful work and specialized personalities.

The utilization of coal as a vitality source goes back to second and third century Rome, with archaeological proof proposing it was mined from outcroppings and utilized as a warming source. By the 1700s, coal was broadly utilized because it consumed cleaner and more smoking than wood charcoal, energizing the industrial revolution. Today, coal remains an essential vitality hotspot for electric power, representing 41% of worldwide power era. Creating countries, including China and India, are depending vigorously on coal to help their developing economies – to take care of rising demand for power as well as for cement and steel generation – the building squares of urbanization [5,6].

As coal turned into the fuel of decision for control era, steam turbine innovation progressed to use a greater amount of the warm vitality from combusting coal. Simultaneously, advancements were created to control the emanations from electric power era. Coal control plants today deliver 80 to 90% less particulate, sulfur oxides (SO_x) and nitrogen oxides (NO_x) discharges than only a couple of decades back.

Notwithstanding outflows control frameworks, present-day coal burning advancements create more power utilizing less coal. These high-productivity low-emanations (HELE) innovations can diminish carbon outflows by 20% for each kilowatt-hour (kWh) created. The world's most proficient coal control plants, for example, the John W. Turk plant in Arkansas and the Isogo Thermal Power Station in Japan show that taking care of developing electric demand cost-successfully can be adjusted with natural and manageability goals. These power plants depend on ultra-supercritical coal innovation, which produces high steam temperatures and weights, empowering them to be more effective at changing over warm vitality into electrical yield [7,8].



The International Panel on climate change utilizes 1750 as its pre-modern pattern to demonstrate changes in barometrical CO₂, worldwide temperature and other atmosphere markers in the post-mechanical period after 1750. The investigation of past atmospheres previously human impact moved toward becoming significant encourages us to see how extraordinary parts of the earth framework change over short and long-time scales. Specifically, it gives us a decent comprehension of the suggestions that normal changes are likely to have for humankind and the more extensive group of life [9].

Two decades prior, the worldwide group concurred on an extreme atmosphere target to balance out the centralization of CO_2 and other nursery gasses in the environment. Today, past and current readings demonstrate the proceeding, constant ascent out of sight level of CO2 in the climate. Other ozone-depleting substance levels are rising as well. Notwithstanding the present pattern, is humankind making strides now that are adequate to stop the rising pattern.

 CO_2 earth causes you to answer that inquiry by highlighting measured projections of researchers and modelers at Climate Interactive. CO_2 earth spotlights the Year 2100 projections for environmental CO_2 , barometrical GHGs (CO_2 -equivalent), GHG outflows, and worldwide temperature. It likewise joins this data into the CO_2 earth page presenting the 2015 Paris Climate Talks [10].

Physical solvents are the organic solvents which are operated at low temperature and high pressure and H₂S is removed favorably over CO₂ gas. Fluor process is a one-step process in which CO₂, C, COS, H₂S are removed from sour natural gas by using propylene carbonate. Purisol process N-methyl-2-pyrrolidone commonly known as NMP, is used as a solvent which removes H₂S, CO₂, RSH, H₂O, elastomers and hydrocarbons but this solvent is highly favorable for H₂S removal. It has a boiling point of 396 °F which is quite low, so they are not compatible with mixed amine solvents. Selexol process a blend of dimethyl ether of propylene glycols are used as a solvent. It also has not enough boiling points like NMP so that it could not be used in mixed amine preparation. This process is restricted to the high partial pressure of acid gas and the absence of heavy hydrocarbons. DIPA can be added to this formulation in order to remove CO₂ down to pipeline conditions. Sulfinol process a mixture of 40% sulfolane (tetrahydrothiophene1-1 dioxide), 40% DIPA (di-isopropanol amine), and 20% water is used as a solvent in this process which is and appreciable example of improving the amine selectivity by the addition of the physical solvent like sulfolane [11,12].

Alkanolamine is highly appreciable when H_2S and CO_2 have to be removed simultaneously from acid gas. A typical process includes an absorption column in which acid gas is fed from the bottom and the lean amine solvent from the top. The sweet gas is collected at the top and the rich solvent from the bottom. The absorption column can be either packed or tray. To regenerate the solvent, the rich solvent before sending to the stripper is flashed and filtered. It is then fed to the top of the stripper and the CO_2 and H_2S are an exit from the top. The regenerated solvent is sent back to the absorption column and the refluxed water help in steam regeneration of rich amine solvent [13].

Hot Potassium carbonate process is the process in which CO_2 and H_2S both can be treated. Since the reaction involves is reversible, so in the reversible reaction, it also removes COS and CS. The process of the optimum operating condition is the partial pressure of CO_2 , which might be in the range of 30-90 psi.

$$K_2CO_3 + CO_2 + H_2O \leftrightarrow 2KHCO_3 \tag{1}$$

$$K_2CO_3 + H_2S \leftrightarrow KHS + KHCO_3 \tag{2}$$



The reactions show that at an only high partial pressure of CO_2 , H_2S can be removed, and for this purpose, this process could not be able to produce acid gases of less concentration and to achieve better results molecular sieves could be used. This process is accomplished in absorber in which the sour gas reacts with counter-currently flowing liquid carbonate. The operating conditions of the absorber are 230 °F and 90 psi. As the absorption occurs, the rich liquid flows out from the bottom, which can further be circulated to the stripper for the regeneration of carbonate solution operating at 245 °F and 14.7 psi. The concentration of K₂CO₃ should be in the range of 20-35 wt. %.

2. Methodology

2.1 Process Selection

There are several processes available for the purification of acid gas, which all is suitable depending upon the available conditions. Our objective is to select the best solvent for CO_2 Capture it may be chemical or physical solvent so, first select that what types of solvents we must study. First, compared chemical and physical solvents. A comparison has been shown in Table 1 for physical and chemical process in which various components have been considered for the better determination of the procedure.

Table 1

Comparison between the chemical and physical process					
Properties	Chemical Process	Physical Process			
Capacity	Less sensitive to the partial pressure of the gas to be treated	More sensitive to the partial pressure of the gas to be treated			
Heat of absorption	High	Low			
Extent of acid gas removal	High	Low			
Selectivity	H ₂ S and CO ₂	H ₂ S			
Utility Cost	High	Low/Medium			

Since chemical absorption leads to chemical reactions, which may result in efficient absorption rate, increasing the absorption capacity of the respective solvent being used in the process. Furthermore, it may have the capability that when a solvent absorbs any hazardous gas, it may convert it to any harmless compound and even reacts selectively to the targeted components.

Table 2		
Comparison between amine	and carbonate pro	cess
Properties	Amine Process	Carbonate process
Utility cost	High	Medium
Efficiency	More efficient	Less efficient
Operating temperature (°F)	100-400	200-250
Selectivity	H ₂ S and CO ₂	May be selective for both

Chemisorption is often used to get complete removal of acid gases from feed gas stream because the reaction in liquid phase reduces the partial equilibrium pressure of solute in over the solution and thus, the driving force for mass transfer increases and so the increase in mass transfer coefficient occurs. This is so because the effective interfacial area is increased as the mass transfer now occurs in both static as well as a dynamic holdup. After selecting the chemical process, further is made on amine process and carbonate process, as shown in Table 2 [6,12].

The chemical process is sub divided into two methods that are amine and hot potassium carbonate process, a major technique used for the removal of CO_2 and H_2S is from synthesis gas, or



natural gas is the absorption in alkanolamine. On the point of selection, the most substantial reason to select amine process is that the hot potassium carbonate process does not give high-quality acid gas removal as it works on the high partial pressure of CO_2 and for better results molecular sieves are used to treat the exit gas further. Amine process, on the other hand, has greater compatibility when H_2S and CO_2 both must be removed at the same time. This process doesn't restrict to treat one acid gas component at a single time, also can remove the impurities according to the desired amount [14].

Based on the above discussion, we have selected amine process since its compatibility is higher for CO₂ and H₂S and remove these gases simultaneously. Now we study different amine solvents and in the last, after simulation, we conclude that which solvent gives the best results.

2.2 Alkanolamine Solvents and Reaction Mechanism

Alkanolamine removes CO₂ from a gas stream via an exothermic reaction between CO₂ and the functional amine of the alkanolamine. Different alkanolamine have different reactions with several acid gases and also in respective equilibrium absorption characteristics and have different sensitivities regarding solvent stability and corrosive factors. Alkanolamine are classified into three groups primary, secondary and tertiary. Primary amines include ethanolamine (MEA); the secondary amines include diethanolamine (DEA) and diisopropylamine (DIPA); the tertiary amines include triethanolamine (TEA) and methyl diethanolamine (MDEA). The structures of alkanol amines are also categorized on containing, at least one OH and amine group [15].

For primary amines like MEA, CO_2 is captured by chemical absorption by which CO_2 reacts with the primary amine in the form of a carbamate. Secondary and tertiary amines that do not have H⁺ atom attached to N₂ react with CO_2 in the form of bicarbonate via hydrolysis. The reactions are carried in a forward direction (for absorber) and are reversible — the captured CO_2 released at high temperatures [16]. MEA cannot be used in a pure form, only 15-20 wt. % is MEA while the other proportion is of water which gives a loading of about 0.3-0.4 moles of acid gas per moles of MEA. Due to the corrosive nature of MEA, it is used in small proportion. It can react non-selectively with CO_2 and H₂S; moreover, they can even react irreversibly with carbonyl sulfide and carbon disulfide resulting in the loss of the solution as it can form solid products in the processing solution.

Another amine solvent which can be a replacement of MEA due to its lower reactivity and less corrosive. It can be used to about 35 wt. % along with water, which gives the loading of 0.6 moles of acid gas per moles of DEA. DEA has a lower vapour pressure means it has lower losses and has a lower heat of reaction than MEA. The reactions are more or less the same as MEA. On CO₂ absorption, the lower stability of the carbamate grants a more economic regeneration step for secondary amines.

This solvent can be used up to 20-50 wt. % as it has low corrosion factor than MEA and DEA. It gives the loading up to 0.7-0.8 moles of acid gas per moles of MDEA that are practically applicable to carbon steel equipment. Low weight percent solutions are used when the low-pressure process is used. Although with a relatively lower affinity for CO₂ compared to primary amines. The carbamation reaction cannot proceed for ternary amines and leads instead to the base-catalyzed hydration of CO₂. MDEA is usually employed in natural gas treatment as it shows lower degradation rates for solvent and requires less energy for solvent regeneration in the stripper.

Di-isopropanol amine (DIPA) is mostly used in the ADIP process licensed by Shell. It is a secondary amine, which removes H2S selectively at low pressures and high pressures remove CO_2 and H_2S both. It is non-corrosive, unlike MEA/DEA and requires low heat for the regeneration of the rich amine solvent. When CO_2 is absorbed in the solution of MEA, DEA, and MDEA, the following reactions take place. For MEA, where R represents the functional group [8,12].



$$R_1 = -H, R_2 = -CH_2CH_2OH$$

$$R_{1}R_{2}NH + CO_{2} \leftrightarrow R_{1}R_{2}NH^{+}COO^{-} (Zwitter ion)$$

$$R_{1}R_{2}NH^{+}COO^{-} + R_{1}R_{2}NH \leftrightarrow R_{1}R_{2}NCOO^{-} (Carbamate)$$

$$(3)$$

$$(4)$$

The overall reaction is,

$$2R_1R_2NH + CO_2 \leftrightarrow R_1R_2NCOO^- + R_1R_2NH^+$$
(5)

For DEA, where $R_1 = R_2 = -CH_2CH_2OH$

$$R_1 R_2 NH + CO_2 \leftrightarrow R_1 R_2 NH^+ COO^- (Zwitter ion)$$
(6)

$$R_1 R_2 N H^+ COO^- + R_1 R_2 N H \leftrightarrow R_1 R_2 N COO^- (Carbamate) + R_1 R_2 N H_2^+$$
(7)

The overall reaction is,

$$2R_1R_2NH + CO_2 \leftrightarrow R_1R_2NCOO^- + R_1R_2NH_2^+$$
(8)

For MDEA, where $R_3 = CH_2CH_2OH$

$$R_3N + H_2O + CO_2 \leftrightarrow R_3NH^+ + HCO_3^-$$
(9)

Amines are also used in a mixture form, using MEA or DEA along with MDEA in order to enhance the CO_2 removal. At the lower concentrations of DEA and MEA, the total concentration of the amine can be taken up to 55 wt. % in which corrosion problems are not raised. Therefore, the addition of a small amount of alkanolamine enhances CO_2 absorption rates. When designing new acid gas removal equipment, physical properties' data such as density, viscosity, solubility and kinetic data are essential [17,18].

2.3 Process Description

The sour gas at a marginally higher than the atmospheric pressure is feed to the absorber. The gas streams countercurrent to the lean amine dissolvable. The solvent absorbed the acid gases and the sweet gas leaves the segment from the top. The rich amine is then sent to the pump and after that warmed through heat exchanger. This amine is stripped off CO_2 at low pressure in the regenerator. The acid gas and some water leave the regenerator through an overhead condenser.



Stream N	ame	flue	lean	sweet	Rich amine		Rich amine	lean amine	Acid	lean amine
		gas	amine	gas	to Heat exc	hanger	to stripper	recycle to H.E	gas	recycled
Stream N	umber	1	2	3		4	5	8	9	12
<u>~</u>			main flow	stream						
-		>	regenratio	on stream						
T-100	P-100	E-100	T-101	E-101	E-102	P-1	01	E-103	V-100	
Absorber	Pump	Shell & tul	be Strippe	Conden	ser Reboiler	pump	recycle	Cooler	Phase	
	_	heat exchna	iger			lean a	mine		separation	





(b) Fig. 1. (a) Process flow diagram (b) Simulation flow sheet of absorption



This lean amine leaving the base of the regenerator through the heat exchanger and blends with the temperament water and amine. The lean amine is additionally cooled and afterward sent back to the absorber. It is seemed that there is no cost advantage of working the absorber at high weights. Hence it is expected that the absorber works at marginally more than the atmospheric pressure equal to flue gas, 1.1 bars feed pressure. The pressure down in all equipment and the pipelines are disregarded. The stripper pressure is fixed at 1.9 bars so as to keep reboiler temperature underneath 122°C to evade the degradation of amine and to erosion in the reboiler and the stripper. Figure 1(a) demonstrates the procedure stream outline.

3. Results

3.1 Process Simulation

In this research, 10 MMSCFD of gas turbine pipe gases at 1.1 bar pressure was treated in a traditional amine-based absorption plant for carbon dioxide recuperation. The molar composition of the pipe gases like $CO_2 = 0.0922$, $H_2O = 0.0545$, $O_2 = 0.0622$ and $N_2 = 0.7872$.

Figure 1(b) shows the CO₂ catch plant for the pipe gas cleaning. The simulation is done by Aspen HYSYS Version 8.8. The CO₂ 98 mole% purity at the product stream is determined for all simulations. Typical equipment used in simulation absorber; regenerator; reboiler and condenser; pumps; preheater; cooler and mixer. For the amines, weight% used Iranian Petroleum Standards (IPS). The amines solution strength in mass % of MEA 15 to 25%, DEA 25 to 35%, DGA 50 to 70% and MDEA 40 to 50%.

3.1.1 Temperature approach rule

A 5°C (10°F) temperature approach rule (Rules of Thumb) is used in this study. During the design and operation of amine contactors, it has been exhorted for quite a while to keep up a base temperature approach of 5°C (10°F). The temperature approach is characterized as the temperature differential between the approaching corrosive gas and the lean amine feed. The explanation behind this rule is to forestall the buildup of hydrocarbons in the contactor and maintain a strategic distance from the resulting issues that a subsequent fluid stage causes an amine plant [19].

3.1.2 Fluid package

The amines property bundle is utilized as the DBR amines is chosen as the equilibrium model since it provides more dependable outcomes than empirical models, progressively reasonable for mixed amines. This study performed numbers of iterations to get optimum conditions for each solvent. From graphical representation, set solvent flowrate, absorber and stripper plates, regenerator inlet temperature, solvent wt. % and recovery of CO₂ in absorber and stripper [20,21]. Table 3 and 4 show the overall mass balance of amines and blended amines, respectively. Table 5 show the overall energy balance of amines.



Table 3

Stream Names	MEA		DGA		DEA	
	Mass Flow	Standard	Mass Flow	Standard	Mass Flow	Standard
	(kg/h)	Ideal Liquid	(kg/h)	Ideal Liquid	(kg/h)	Ideal Liquid
		Volumetric		Volumetric		Volumetric
		Flow (m³/h)		Flow (m³/h)		Flow (m³/h)
Sweet gas	13278.59	15.85	13515.41	16.05	13340.99	15.98
Rich solvent	36195.17	36.63	22480.38	22.32	52336.27	51.66
Rich solvent to desorber	36195.17	36.63	22480.38	22.32	52336.27	51.66
CO ₂	1778.41	2.15	1527.44	1.85	1366.30	1.65
Lean solvent from	34416.77	34.48	22480.38	22.32	50969.96	50.01
desorber						
Rich solvent to heat	36195.17	36.63	22480.38	22.32	52336.27	51.66
exchanger						
Flue gas	14547.03	17.49	14547.13	17.49	14547.13	17.49
Solvent solution	34926.73	34.99	21448.66	20.89	51130.13	50.16
Lean solvent to pump	34416.26	34.48	20952.39	20.47	50969.51	50.01
Lean solvent to cooler	34416.26	34.48	20952.39	20.47	50969.51	50.01
Lean solvent to mixer	34416.26	34.48	20952.39	20.47	50969.51	50.01
Make up solvent	321.09	0.32	1225.64	1.19	113.17	0.11

Table 4

Overall mass balance of MDEA and blended amines

Stream Names	MDEA		MEA-MDEA		DEA-MDEA	
	Mass Flow	Standard	Mass Flow	Standard	Mass Flow	Standard
	(kg/h)	Ideal Liquid	(kg/h)	Ideal Liquid	(kg/h)	Ideal Liquid
		Volumetric		Volumetric		Volumetric
		Flow (m³/h)		Flow (m³/h)		Flow (m³/h)
Sweet gas	13287.99	15.94	13298.99	15.90	13171.74	15.82
Rich solvent	116326.33	112.98	21824.06	21.83	39788.49	38.73
Rich solvent to desorber	116326.33	112.98	21824.06	21.83	39788.49	38.73
CO ₂	1358.73	1.64	1587.89	1.92	1371.09	1.66
Lean solvent from	114967.61	111.34	20236.16	19.91	38417.82	37.07
desorber						
Rich solvent to heat exchanger	116326.33	112.98	21824.06	21.83	39788.49	38.73
Flue gas	14547.07	17.49	14547.13	17.49	14547.13	17.49
Solvent solution	115067.24	111.43	20575.92	20.25	38413.11	37.06
Lean solvent to pump	114967.49	111.34	20235.87	19.91	38417.82	37.06
Lean solvent to cooler	114967.49	111.34	20235.87	19.91	38417.82	37.06
Lean solvent to mixer	114967.49	111.34	20235.87	19.91	38417.82	37.06
Make up solvent	122.27	0.12	274.98	0.27	-178.15	-0.17
Lean solvent to recycle	115089.77	111.45	20510.86	20.18	38239.69	36.89

Table 5

Overall energy balance of amines

Equipment	MEA Duties	DGA Duties	DEA Duties	MDEA Duties	MEA-MDEA	DEA-MDEA
Name	(kW)	(kW)	(kW)	(kW)	Duties (kW)	Duties (kW)
Cooler	820.089	563.922	860.408	3864.252	767.457	1167.988
Heat Exchanger	2463.448	1182.732	3470.739	4519.733	908.549	1973.174
Pump (P-100)	1.783	1.078	2.576	5.708	1.052	1.929
Pump (P-101)	1.384	0.822	1.830	3.729	0.801	1.498
Reboiler	4217.564	2544.947	1880.908	4136.684	1625.437	1620.998



3.1.3 Case study 1

Controlled parameter CO₂ fraction recovered by the regenerator. Figure 2(a) shows a trend between reboiler and condenser duties with CO₂ recovery in the stripper. From this figure after 80% CO₂ recovery of MEA, DGA, DEA, MEA-MDEA blend and 90% CO₂ recovery of MDEA and DEA- MDEA blend the reboiler and condenser duties goes higher suddenly. So, we set CO₂ recovery at 80% in MEA, DGA, DEA, MEA-MDEA blend and 90% in MDEA and DEA- MDEA blend.



(b)





Fig. 2. (a) Duties versus component recovery of amines (b) Duties versus solvent concentration of amines (c) CO_2 absorbed versus solvent flowrate of amines

3.1.4 Case study 2

The controlled parameter is solvent concentration. In above Figure 2(b), the trend between MEA, DGA, DEA, MDEA, MEA-MDEA and DEA-MDEA blend concentration (wt. %) versus reboiler and condenser duties. From this figure, as the increase in concentration will increase in duties. So, we set 15% MEA, 50% DGA, 25% DEA, 40% MDEA, MEA 15% and 40% MDEA (blend), DEA 25% and 40% MDEA (blend) to get minimum duties.

3.1.5 Case study 3

The controlled parameter is a solvent solution molar flow (MMSCFD). The observed parameters are CO₂ % absorbed in the solvent. In Figure 2(c), the trend between MEA, DGA, DEA, MDEA, MEA-MDEA and DEA-MDEA blend flowrate versus CO₂ absorbed in the absorber. From this figure after 35 MMSCFD (MEA), 14 MMSCFD (DGA), 45 MMSCFD (DEA), 38 MMSCFD (MDEA), 11 MMSCFD (MEA-MDEA) and 20 MMSCFD (DEA-MDEA) the effect of absorption goes linear and they are in no effect of higher flowrate on CO₂ absorption.

Monoethanolamine has strong affinity toward oxidizing agents like CS_2 , COS, SO_2 , SO_3 , and O_2 which decreases the corrosion problem in circulation system by forming soluble compounds which can easily be remove from the circulating system. Though the effective amine concentration lowers due to deactivation or degradation of MEA but these deactivated amines can recover by using a reclaimed. At the point when MEA is utilized, basically the majority of the CO_2 must be ingested to deliver gas which meets the quarter grain H_2S particular. A feed containing high concentration of carbon dioxide gas may cause either amazingly high reboiler obligation or poor corrosive gas stripping because of exceptionally high value of MEA heat reaction around 825 BTU/lb [16].

A comparison study shows that the degraded compound of DEA is much less corrosive than those of MEA. To some extend COS and CS₂ reacts with DEA irreversibly in the presence of oxygen results in formation of corrosive acids. DEA has the characteristic to decompose at atmospheric pressure below its boiling point hence the option of using reclaimed for deactivated DEA have demonstrated



operationally inconsistent. DEA is a secondary amine, so for low pressure stream it does not produce pipeline specification gas due to its low affinity towards H₂S and CO₂. Generally, a higher rate of stripping stream is required due to low pressure in the gas stream or otherwise a split low system is required. Even in some cases these measures will not be sufficient and requires another solvent. DEA remains selective towards H₂S and CO₂ when the residence time of around 2 second is provided for comparatively low pressure hence substantial fraction of the carbon dioxide are witness in sales gas [12].

As with MEA, the consumption issues with DGA avert arrangement loadings above about 0.35 mole/mole. Gas stream comprising high acids gases can be sweeten by achieving a partial pressure in absorber at temperature more than 200°F.Due to higher affinity toward CO₂ over H₂S and higher pH than MEA, Diglycolamine achieves H₂S description easily except in many cases where carbon dioxide is presents in comparative larger amount as to H₂S. Due to low freezing point DEA has sure advantages over the further amines, like the higher concentration results in lower circulation rates similarly DGA does not react irretrievably with SO₂, CS2, COS, and SO₃. In addition, DGA have a tendency to absorb COS plus methyl- and ethylmercaptans in an unquantified amount [6].

For high selectivity applications for example a SCOT tail gas cleaning unit lower weight % is use for low pressure. To reduce corrosion problem, at higher loading rate of acid gases (example 0.7 to 0.8 mole/mole) steel equipment are practically more applicable. Higher loadings of acids gases may result in few problems, like the exposure of MDEA to oxygen causes the formation of acids which ultimately results in iron sulfide build up in the system if not removed properly.

MDEA has some advantages over essential and auxiliary amines which incorporate lower vapor pressure, lower warms of response (600 BTU/lb CO₂ and 522 BTU/lb H₂S), higher protection from degradation, less erosion issues and selectivity toward H₂S within the sight of CO₂. However, the readily selective of MDEA toward H₂S in the existence of CO₂ gives it a relative edge over other amines. At high CO₂/H₂S proportions, real portions of the CO₂ can be snuck past the absorber and into the sales gas while evacuating the greater part of the H₂S. However, this enhance selectivity of MDEA, consequences in low formation of carbamate with CO₂ due to inability of tertiary amines. MDEA does not have a hydrogen appended to the nitrogen and can't respond legitimately with CO₂ to shape carbamate [13].

The mixture of DEA and MDEA or MEA are generally known as mixed amines to improve the removal of CO₂ by MDEA as ascribed by Polasek, Bullin, and Iglesias-Silva. The mixture is known as MDEA-based amines in which the secondary amines are associated with DEA or MEA. The molar distribution of secondary amines is usually around 20% of the total mixture. The alkanolamine concentration can be as higher as to 55 wt % without the application of exotic metal apparatus at low MEA and DEA concentration. MDEA-based blends are typically used to increase the CO₂ pickup in situations where the MDEA is enabling an excessive amount of CO₂ to slip overhead in the absorber. The capacity of MDEA with MEA and DEA to retain CO₂ all the more effectively when contrasted with a DEA or MEA framework since the MDEA regenerator reboiler might be undersized for the DEA or MEA framework. Anyway, at low pressure MEDA is less worthwhile over amine blends in light of the fact that at low pressure MDEA is less capable for getting adequate CO₂ to meet pipeline specifics. Blended amines are additionally helpful for situations where the CO₂ content of the feed gas is expanding after some time because of field maturing [6,21].



3.2 Manual Calculations of Amine Unit 3.2.1 Mass balance

The flowrate of feed flue gas stream = $\dot{\eta}_{total feed gas}$ = 1098 lb. mol/hr. The initial composition of the flue gas is defined in Table 3. It was assumed that the amine solvent is 50 wt. % aqueous solution of DGA. The minimum solvent flowrate (L min) for absorber is given as:

 $L_{min} = K * \dot{\eta}$ total feed gas

where K = 1.28 for DGA. So, the minimum DGA flowrate becomes L_{min} = 1405.44 lb. mol/hr. whereas the actual flowrate is given as:

 $L_{actual} = m * L_{min}$

where, m = 1.09 for DGA. Thus, the actual amine flowrate becomes $L_{actual} = F_{lean amine} = 1531.9296$ lb. mol/hr. As per standard maximum CO₂ in sweet gases must be < 3.5%, so assume that other gases will be (1-(<3.5%)) of the sweet gas. Assume that other gases will not react with an amine.

 CO_2 in sweet gas = 0.0058; other gases in sweet gas = 0.9942 $n_{other gases in sweet gas} = 0.9942 * n_{sweet gas}$ $n_{CO2 in feed} = composition of CO_2 in feed x n_{feed} = 101.2356 lb. mol/hr$ $n_{other gases in feed} = n_{feed} - n_{CO2 in feed} = 996.7644 lb. mol/hr$ $n_{other gases in feed} = n_{other gases in sweet gas}$ (assumption) $n_{sweet gas} = 1107.516 lb. mol/hr$

The overall balance on absorber is given as:

Input + Generation = Output + Consumption + Accumulation

 $\dot{\eta}_{total feedgas}$ +Flean amine^{abs}= $\dot{\eta}_{sweet gas}$ +Frich amine^{abs}

 $F_{rich amine}$ abs = 1522.4136 lb. mol/hr

Overall balance on stripper is given as;

Input + Generation = Output + Consumption + Accumulation Frich amine strip = $\eta_{absorbed}$ carbon dioxide + Flean amine strip For $\dot{\eta}$ absorbed carbon dioxide: $\dot{\eta}_{carbon}$ dioxide from stripper = $\dot{\eta}_{carbon}$ dioxide in feed - $\dot{\eta}_{carbon}$ dioxide in sweet gas $\dot{\eta}_{carbon}$ dioxide in sweet gas = 0.0058 * $\dot{\eta}_{sweet}$ gas = 6.423593 lb.mol/hr $\dot{\eta}_{carbon}$ dioxide from stripper = 94.81201 lb.mol/hr

 $\begin{array}{l} CO_2 \mbox{ recovery at 80\%.} \\ \dot{\eta}_{carbon\ dioxide\ from\ stripper} = 75.84961\ lb.mol/hr \\ Since,\ F_{rich\ amine\ }^{strip} = F_{\ rich\ amine\ }^{abs}; \\ F_{lean\ amine\ }^{strip} = 1446.564\ lb.mol/hr \end{array}$

(10)



3.2.2 Energy balance

Steam for reboiler and reboiler duty

ms* λ s = V* λ

(11)

 $P_{reboiler} = 1.9$ bar $\lambda s = 931$ btu/lb = 517.2223 cal/g @ $P_{reboiler}=1.9$ bar (T reboiler should be kept 250-300 °F)

As full reflux is assumed therefore whole liquid (rich amine) goes to the reboiler to calculate maximum heat duty.

 $\begin{array}{l} F_{\text{rich amine}} \ ^{abs} = 1522.4136 \ lb.mol/hr \\ \lambda_{\text{DGA}} = 221 \ btu/lb \\ \text{Cp} = 17 \ to \ 27 \ btu/lb.mol.^{\circ}\text{F} \ (For \ temperature \ range \ 100 \ ^{\circ}\text{F} \ to \ 300 \ ^{\circ}\text{F}) \\ ms = 361.389265 \ lb.mol/hr \\ \text{Cp}_{\text{steam}} \ at \ 1.9 \ bar = 2.15613 \ \text{KJ/kg.K} = 9.269 \ btu/lb. \ mol.^{\circ}\text{F} \\ T_{\text{B.P of water}} \ @ \ 1.9 \ bar = 239^{\circ}\text{F}; \ T_{\text{top}} = 212^{\circ}\text{F}; \ T_{\text{bottom}} = 250.2^{\circ}\text{F} \\ \text{Q}_{\text{reboiler}} = \ m^{*}\text{Cp}^{*}(239\text{-}212) + m^{*}\lambda\text{vap} + \ ms \ ^{*} \ \text{Cp}_{\text{steam}} \ ^{*}(250.2\text{-}239) = 7878098.815 \ \text{Btu/hr} \end{array}$

Cooling water for condensor $m_w = V\lambda/(T_2-T_1)$ (V is flowrate of CO₂ exiting from the top of stripper) V = n_{CO2} from stripper; T₂ = 40°C (water returning to the cooling tower must be less than 45°C); T₁=25°C (ambient temperature) $m_w = 1396.89691$ lb.mol/hr

Lean/Rich amine Exchanger Duty

 $Q = M^* Cp^* (T_2 - T_1)$ (12)

M = 1522.4136 lb.mol/hr; Cp = 17 to 27 Btu/lb.mol.°F (For temperature range 100°F to 300°F); $T_1 = 113$ °F; $T_2 = 212$ °F Q = 3767973.66 btu/hr

Cooler Duty Q = M*Cp*(T₂-T₁) M = 1446.56 lb.mol/hr; T₁ = 146.9°F; T₂ = 95°F Q = -1876916.78 btu/hr

3.2.3 Comparison simulation versus manual calculations

Table 6 represents the comparison simulation versus manual mass and energy balance.



Table 6

Comparison simulation versus manual mass balance and manual energy balance

energy balance			
Flowrates (lb.mol/hr)	HYSYS	Calculated	Error (%)
Feed	1098	1098	0
DGA	1537	1531.93	0.32989
Sweet gas	1108	1107.516	0.04368
CO ₂ in sweet gas	6.395	6.423593	0.44711
CO ₂ from stripper	76	75.84961	0.19789
Duties (Btu/hr)			
Reboiler	8684000	7878099	9.2803
Lean/Rich heat exchanger	4036000	3767974	6.64089
Cooler duty	-924000	-1876917	2.44715

3.3 Designing of Amine Unit

3.3.1 Absorber column designing

Column Diameter; V = 1098 lb.mole/hr; L = 1527 lb.mole/hr; Mv = 29.21 lb/lb.mole; ev = 0.08097 lb/ft³; ML = 32.46 lb/lb.mole; eL = 67.52 lb/ft³

Flv = 0.053517955For Tray spacing = 12 inch; Cf = 0.21 ft/sec; Ff = 0.8; Ad/A = 0.1 (because Flv< 0.1); Fha = 1 (supposed);
Fst = (surface tension/20) ^0.2; Surface tension = 53.75 dyne/cm; Fst = 1.218623909
C = Fst*Ff*Fha*Cf
(14)

C = 0.204728817 ft/s

$UI = U^{(1)} UI $	$Uf = C^*($	(el-ev)	/ev) ^0.5	
--	-------------	---------	-----	--------	--

Uf = 5.908436389 ft/s

Dt=(4*V*Mv)^0.5/(f*Uf*pie*(1-Ad/A)*&v)^0.5

```
Dt = 1.75 m = 5.74 ft = 68.88 inch
```

```
Column Height;
No of trays = 10 (assumed), tray spacing = 12 inch, space for removal of entrained liquid = 4 ft and
space for surge capacity = 10 ft. Therefore,
Total column height = 24 ft = 7.317073171 m
Pressure Drop;
\Delta P = 0.064 * Ts * SG
where, Ts = 12 ft and SG = 1.081
\Delta P = 0.083 psi/tray or 0.83 psi (10 trays)
Tray Efficiency;
KM<sub>L</sub>U<sub>L</sub>/\Phi = 1.76
Efficiency = 60%
```

(15)

(16)



3.3.2 Stripper column designing

Column Diameter; V = 77.43 lb.mole/hr, L = 1527 lb.mole/hr, Mv = 43.49 lb/lb.mole, $\text{@v} = 0.1876 \text{ lb/ft}^3$, ML = 32.46 lb/lb.mole and $\text{@L} = 18.4 \text{ lb/ft}^3$ Flv = (L*ML) *(@v/@L) ^0.5 / (V*Mv) = 1.4862655 For Tray spacing = 12 inch; Cf = 0.09 ft/s; Ff = 0.85; Ad/A = 0.2 (because Flv > 1); Fha = 1 (supposed). Fst = (surface tension/20) ^0.2 Surface tension = 44.6 dyne/cm Fst = 1.1739807 C = Fst*Ff*Fha*Cf = 0.0898095 ft/s Uf = C*((@L-@v)/@v) ^0.5 = 0.8848906 ft/s Dt = (4*V*Mv) ^0.5 / (f*Uf*pie*(1-Ad/A) *@v) ^0.5 Dt = 1.021 m = 3.34888 ft = 40.18656 in

Column Height; Number of trays = 10 (assumed); Tray spacing = 12 inch; Space for removal of entrained liquid = 4 ft; Space for surge capacity = 10 ft; Total column height = 24 ft = 7.317073171 m

Pressure Drop; $\Delta P = 0.0064 * Ts * SG$ Ts = 12 ft; SG = 0.973; $\Delta P = 0.0747264 \text{ psi/tray}$ $\Delta P = 0.74 \text{ psi} (10 \text{ trays})$ Tray Efficiency; $KM_LU_L / \mathfrak{E} = 1.03$ Efficiency = 70 Dt = 1.021 m = 3.34888 ft = 40.18656 inch

3.3.3 Heat exchanger designing

Table 7 represents the rich and lean amine in and out conditions.

Table 7						
Rich and lean amine in and out conditions						
Parameters	Rich Amine In	Rich Amine Out	Lean Amine In	Lean Amine Out		
Temperature (°F)	113	212	250	147		
Pressure (Psi)	104.5	84.7	27.7	17.7		
Flowrate	49560	49560	46190	46190		
(lb.mol/hr)						

The shell side of heat exchanger inner dia is 17.25 inch, C' is 0.25 inch, B is 5 inch and passes is 2. The tube side of heat exchanger outer dia is 0.75 inch (Heuristics), BWG is 16, pitch is 1 inch triangular (Heuristics), length is 16 ft, number of tubes 178 and passes is 4.



(17)

3.4 Heat Balance

Q = WC (T2-T1) Q = 49560x0.7578x (212-113) = 3718100.2 Btu/hr

True Temperature Difference;

LMTD=(T1-t2)-(T2-t1)/[ln(T1-t2)/(T2-t1)]

LMTD = 35.96293243R = (T1 - T2]/ (t2 - t1) = 1.040404S = (t2 - t1] / (T1 - t1) = 0.722628Ft = 0.74 Δt = LMTD * Ft = 26.61257 °FAverage Temperature ΔT = 198.5 °F; Δt = 162.5 °F

3.4.1 Heat exchanger designing

Shell side hot fluid lean amine.

as = I.D * C *B / 144 * Pt	(18)
as = 0.14974 ft ² G = W/as = 46190 / 0.14974 = 308468.9 lb/hr ft ²	
Re = De x G / μ At 198.5 °F; μ = 1.11 lb/ft.hr; Cp = 0.8742 Btu/lb.°F; K = 0.2511 BTU/hr ft ² (°F/ft); = 0.73 inch = 0.0608 ft Re = 16906 jH = 70 (Cp * μ) ^{1/3} / k = 1.569262835 ho=jH*k*(Cp* μ /k) ^{1/3} /De(20) ho = 453.42 BTU/hr ft ² °F	(19) p = 60.74 lb/ft ³ ; De
Tube side cold fluid rich amine.	
at = Nt*a't / 144*n	(21)
a't = 0.302 Inner dia = 0.62 inch	
Gt = W/at	(22)

Gt = 49560 / 0.0933264 = 531039.51 lb/hr.ft²

 $Re = D x Gt / \mu$ (23)



At 162.5 °F; μ = 6.76 lb/ft.hr; Cp = 0.7578 Btu/lb. °F; K = 0.2246 BTU/hr ft² (°F/ft); p = 67.51 lb/ft³; Inner dia = 0.0516667 ft Re = 4058 .733942 V = Gt / P = 2.1850241 fpshi = 800 hio = hi x inner dia / outer dia = 661.334 Btu / hr. ft². °F Clean Overall Coefficient; Uc = (661.3333 * 453.4) / (661.3333 + 453.4) = 268.9931 BTU/hr ft² °F Design Overall Coeeficient; $Ud = Q/A\Delta t$ (24) a" = 0.1963 A = 178 * 16 * 0.1963 = 559.0624 ft² Ud = (4E+06) / (559.0624 * 26.61) = 249.9045 BTU/hr ft² °F Rd = (Uc *Ud) / (Uc + Ud)(25) $Rd = 0.000284 hr ft^{2} oF/Btu$

Pressure Drop Calculations Shell side: Re = 16906; f = 0.0019; S = 1.024; Inner dia = 14/9 ft; N+1 = 38.4; de = 0.0608 ft; G = 308469

 $\Delta P = [fxG^2xDx(N+1)]/(5.22x10^{10}xDe x s)$

ΔP = 3.069 psi

Table 8

The optimum operating conditions for the amine-based process, blended MEA-MDEA and blended DEA-MDEA

Solvents Name	Circulation rate (m³/hr)	Concentration (wt. %)	Absorber stages	Stripper stages	Reboiler duty (kW)	Regenerator inlet temperature °C	CO2 % absorbed
MEA	34.99	15	10	10	4218	100	89.10
DGA	20.89	50	10	10	2545	100	93.60
MDEA	111.4	40	40	10	4137	100	68.97
DEA	50.16	25	10	10	1881	105	73.50
Blended 1	20.25	55	10	10	1625	90	81.56
Blended 2	37.06	65	10	10	1621	100	69.55

Tube side: Re = 4058.7339; f = 0.00035; s = 1.008; G = 531039.51 lb/hr ft²; L = 16 ft; n = 4; Inner dia = 0.0516667 ft $\Delta Pt = (f \times G^2 \times L \times n) / 5.22 \times 10^{10} \times D \times s = 2.3235938 \text{ psi}$ $\Delta Pr = (4 \times n * V^2) / (S * 2g')$

 $V^2/2g' = 0.04$

(26)



4xn/s = 15.873016 ΔPr = 0.6349206 psi ΔP_T = 2.9585144 psi

This study evaluated the impact of various amine absorbents with their concentrations, the stripper and absorber column heights, and the operating conditions on the carbon dioxide recuperation plant for post-combustion CO₂ capture. According to the above Table 8, we can easily determine which amine solvent is given more CO₂ recovery in absorber at optimum conditions. In MEA, the major disadvantage is a higher circulation rate and higher reboiler duty, but it absorbed more CO₂. In MDEA the major disadvantage is too much higher circulation rate and the absorber height and it's also absorbed least CO₂ compared to other solvents. In DEA the disadvantage is higher circulation rate and low CO₂ absorption capability, but it gives low reboiler duty. In DGA, there is no major disadvantage, but its reboiler duty is slightly higher, but it has many advantages such as lower circulation rate and more CO₂ absorption capability. Blended MEA-MDEA also gives good results but as compared to DGA almost same circulation rate but it absorbed low CO₂ than DGA. Blended DEA-MDEA gives minimum reboiler duty, but it absorbed less CO₂ and higher flowrate compared to DGA.

4. Conclusions

Amine absorption was favored for CO₂ recuperation of flue gas with low CO₂ concentration. This research displayed an optimization approach for the amine absorption process. Utilizing the proposed methodology, we investigated the effects of the stripper and absorber section statures, the grouping of amine solvents, and working condition on the carbon dioxide evacuation of amine-based CO₂ recuperation forms with different amine solvents. The results demonstrate that the absorber height, solvent circulation rate and reboiler duty have the most remarkable effects on the CO₂ retention ability however the stripper stature and the regenerator-inlet temperature does not indicate critical impacts. The primary or secondary amines addition to tertiary amines enhance the CO₂ absorption capacity of the blend. Among all the solvents examined, the 50 wt. % DGA with 93.6% CO₂ removal amount was observed to be the best solvent because of its high CO₂ absorption capacity of different solvents and ionic liquids. Also, study the effect of changing the composition of flue gasses on different solvents that which solvents behaves well at low and high acid gasses concentration in the feed and also by changing the effect of feed pressure that on high pressure which solvents give the best result.

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