



Article Simulation of Natural Gas Treatment for Acid Gas Removal Using the Ternary Blend of MDEA, AEEA, and NMP

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Abstract: Natural gas (NG) requires treatment to eliminate sulphur compounds and acid gases, including carbon dioxide (CO₂) and hydrogen sulphide (H₂S), to ensure that it meets the sale and transportation specifications. Depending on the region the gas is obtained from, the concentrations of acid gases could reach up to 90%. Different technologies are available to capture CO2 and H2S from NG and absorb them with chemical or physical solvents; occasionally, a mixture of physical and chemical solvents is employed to achieve the desired results. Nonetheless, chemical absorption is the most reliable and utilised technology worldwide. Unfortunately, the high energy demand for solvent regeneration in stripping columns presents an obstacle. Consequently, the present study proposes a novel, ternary-hybrid mixture of N-methyl diethanolamine (MDEA), amino ethyl ethanol amine (AEEA), and N-methyl 2-pyrrolidone (NMP) to overcome the issue and reduce the reboiler duty. The study employed high levels of CO_2 (45%) and H_2S (1%) as the base case, while the simulation was performed with the Aspen HYSYS® V12.1 software to evaluate different parameters that affect the reboiler duty in the acid gas removal unit (AGRU). The simulation was first validated, and the parameters recorded errors below 5%. As the temperature increased from 35 $^{\circ}$ C to 70 $^{\circ}$ C, the molar flow of the CO₂ and H₂S in sweet gas also rose. Nevertheless, the pressure demonstrated an opposite trend, where elevating the pressure from 1000 kPa to 8000 kPa diminished the molar flow of acid gases in the sweet gas. Furthermore, a lower flow rate was required to achieve the desired specification of sweet gas using a ternary-hybrid blend, due to the presence of a higher physical solvent concentration in the hybrid solvent, thus necessitating 64.2% and 76.8%, respectively, less reboiler energy than the MDEA and MDEA + AEEA.

Keywords: natural gas; absorption; simulation; Aspen HYSYS; reboiler duty

1. Introduction

Global warming has received considerable attention among significant environmental problems worldwide [1]. Commonly, carbon dioxide (CO₂) is considered a primary greenhouse gas among the sour gases, accounting for approximately 78.6% [2]. Moreover, the concentration of CO₂ in the open air has been recorded close to 400 parts per million (ppm), which is higher than the tolerated limit of 350 ppm [3].

Natural gas (NG) is one of the cleanest known fossil fuels, compared to other hydrocarbon deposits, such as coal and oil. Nevertheless, it is essential to remove all contaminants to ensure that the NG is environmentally safe, suitable for utilisation, and complies with the sale gas specifications [4]. Contaminants can affect NG applications and result in integrity issues, including corrosion, erosion, plugging, and health and environmental



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). hazards [5]. The maximum allowable amount of CO₂ and H₂S in NG is under 1% and 4 ppm, respectively [6].

Globally, 6951.8 trillion cubic feet (Tcf) of NG reserves are reported and Malaysia, with 84.5 Tcf of the NG reserves, ranks in 15th place [7]. Most of the NG reserves are sour gas fields. Sour gas refers to NG containing high amounts of CO₂ and H₂S. The NG deposits with low CO₂ and H₂S concentrations are more profitable to drill and market, as the cost of removing the gases is lower. Internationally, the concentration of CO₂ in NG varies from 0% to 90% [8]. The NG reserves in Malaysia are high in CO₂, ranging between 28% and 87%, with a relatively low H₂S content, below 1% [9].

NG reserves with low CO₂ and H₂S concentrations are declining rapidly, due to the rise in energy demand. Consequently, the 13 TcF of NG deposits which have not been drilled, due to their high CO₂ concentrations, offer an alternative option. Nevertheless, removing high CO₂ concentrations from raw NG has always been a significant challenge for oil and gas operators [10]. Accordingly, drilling CO₂-rich NG deposits, both onshore and offshore, is essential to meet future energy demands, but it requires overcoming the difficulty of removing the CO₂ at high intrinsic concentrations in high-pressure environments [11].

Various separation techniques have been established to purify NG [12]. The methods remove or reduce the acid gases (CO₂ and H₂S) from the hydrocarbon gas via absorption, adsorption, cryogenic distillation, and membrane separation techniques [13]. The primary factors to consider when selecting the appropriate process are the removal efficiency, operating costs, recovery rates, and energy demand [14]. The absorption technique, which has gained considerable attention on the industrial level, is one of the most cost-effective and reliable approaches. The qualities of the absorbent, including its reactivity, absorption capacity, and regeneration energy, are vital elements in choosing a suitable absorbent [15]. The absorption process is divided into two categories, chemical and physical, according to the type of absorbent employed [16]. Table 1 lists the absorbents commonly utilised in acid gas removal units (AGRU).

Name	Amine Abbreviation	Structural Type
MEA	Monoethanolamine	Primary amine
DEA	Diethanolamine	Secondary amine
DIPA	Diisopropanolamine	Secondary amine
MDEA	Methyl diethanol amine	Tertiary amine
AMP	2-amino-2-methyl-1-propanol	Sterically hindered amine

Table 1. Commonly employed amine solvents.

Chemical absorption, which includes primary, secondary, and tertiary amines, is the most advanced method for removing CO_2 and H_2S from NG. Chemical absorption is a reactive method, involving the mass transfer of chemical solvents with the CO_2 , and a chemical reaction that produces weakly bonded intermediate compounds [17]. By using thermal energy to break the chemical bonds, the absorbed CO_2 is removed from the solvent [18].

According to stoichiometric studies, the loading capacities of primary and secondary amines, such as monoethanolamine (MEA) and diethanolamine (DEA), are limited to 0.5 moles of CO_2 per mole of amine [19]. Aqueous amine solutions, principally MEA and DEA, are the most established solvents for CO_2 absorption, due to their strong affinity and reactivity toward CO_2 , and their low production costs. Nevertheless, the high energy required for solvent regeneration remains a substantial obstacle to deploying the method at full scale [20].

Tertiary amines, including MDEA, have recently gained popularity as a result of their higher CO₂ equilibrium loading capacity, of up to 1.0 mole of CO₂ per mol of amine, high thermal stability, minimal vapour loss, and low enthalpy of the CO₂ reaction, all of which are critical properties in the solvent regeneration process [21]. Nonetheless, despite the advantages of the tertiary amines over the other amines, MDEA reacts directly with H₂S

in the presence of CO_2 , but its loading capacity is higher than that of the primary and secondary amines [22].

The very slow reaction rate and kinetics are the main disadvantages of MDEA [23]. Consequently, various activators, such as piperazine (PZ), MEA, DEA, and amino ethyl ethanol amine (AEEA), have been employed to increase the reaction kinetics and rate of MDEA for the simultaneous capture of CO_2 and H_2S [24]. Furthermore, researchers have attempted to improve the absorption capacity of CO_2 and H_2S by incorporating activators into MDEA solvents, where primary and secondary amines are the most often utilised.

According to Lu et al. [25], adding primary and secondary amines to MDEA aqueous solutions enhances its absorption rate. The study also demonstrates the rapidity of primary and secondary amines in absorbing CO_2 molecules close to the gas-liquid interface, where the concentration of CO_2 is high. As a result, carbamate, produced as the product of the reaction, penetrates the mixture. Subsequently, the activator is regenerated and returned to the liquid interface when the carbamate has interacted with too many MDEA molecules. The process continues, increasing the absorption rate.

Dissimilar to chemical solvents, physical absorptions depend on pressure variations and the ability of the gases to dissolve in physical solvents selectively. In this technique, the absorbed CO_2 in the solvent is removed by lowering its partial pressure [26]. A physical solvent also requires less heat for regeneration than a chemical solvent. Different physical solvents are employed to absorb acid gases, such as dimethyl ether polyethylene glycols (DEPG), methanol, propylene carbonate (PC), N-methyl 2-pyrrolidone (NMP), and sulfolane [27].

Among the solvents, NMP was certified by Lurgi Germany and commercially utilised in the Purisol process. Consequently, separating high amounts of CO_2 and H_2S from NG is possible through the Purisol method [28]. Moreover, the attractive qualities of NMP, including the low vapour pressure and low viscosity, allow the substance to be completely miscible in water, and has better CO_2 solubility at high pressures, up to 9 Mpa, compared to other physical solvents [29].

Mixing physical and chemical solvents to produce a hybrid solvent is an attempt to take advantage of both methods simultaneously. The resultant solvent can remove higher acid gas contents as it takes advantage of both the chemical and physical solvents [30]. Moreover, mixed solvents do not constrain the CO₂ absorption capacity through reaction stoichiometry, particularly at a high CO₂ partial pressure. Hybrid solvents are also reported to yield a higher purity of the processed gas, require less solvent flow rate, and require less energy to regenerate than chemical solvents [31].

Foaming is one of the critical considerations when choosing amines for gas sweetening, which might occur due to corrosive inhibitors being added to the absorption solution and the amine degrading. Utilising hybrid solutions eliminates the requirement to employ anti-corrosive chemicals [32]. Moreover, it lowers the regeneration temperature, lessening the production of by-products from the degradation of amines, and slightly raises the viscosity of the solution, hence reducing the foaming [33].

The purity of the gas procured is limited by the sweetening process design, which demands a large amount of energy. The solvent circulation flow rate and reboiler duty in the stripper section are two of the most energy-consuming and cost-contributing elements in the AGRU. Accordingly, the operation and energy expense of an NG sweetening plant have been the subject of numerous research studies [34]. One of the strategies adopted to increase the efficiency of the process is by utilising different solvents to remove acid gases [35,36]. Khoshandam et al. [37] evaluated the performance of sulfinol, a mixture of sulfolane, MDEA, and water as the solvent to remove acid gases from NG, versus MDEA, DGA and a mixture of MDEA + AMP. They concluded that sulfinol required 10–25% less energy compared to aqeous chemical solvents. In another study, Boroojerdi et al. [38] compared several single amines and amine blends, and concluded that the solvent blend mixture reduced the reboiler duty more effectively than the single amine. Zoghi et al. [39] assessed the effects of MDEA kinetics with different activators, DIPA, AMP, DGA, AEEA,

and PZ. The AEEA demonstrated the highest impact on the absorption rate of MDEA. Bonenfant et al. [40] reported the CO₂ absorption and desorption of MDEA–AEEA solvents at different concentrations, and compared them to the MEA–AEEA solvent. Adding AEEA to MDEA improved the absorption performance of MDEA, but the regeneration energy was increased by 15%. Danielle et al. [41] reported that the MEDA–AEEA solution recorded a higher absorption capacity than TEA–AEEA when the absorption capacities of the tertiary amines, MDEA and TEA, with AEEA were evaluated.

Another way to enhance the performance of the AGRU process is by employing process simulation tools to assist in optimising the operating parameters. Performing simulations on either a new model or an existing gas plant can locate the areas of energy loss, and forecast the optimum conditions [42]. For example, Younas et al. [43] investigated the performance of a GASCO acid gas removal plant through a parametric sensitivity analysis. The study examined the impacts of process factors on the effectiveness of the AGRU, such as the temperature of the feed gas, the composition of the sour gas, the lean amine circulation rate, and the number of absorber stages. Banat et al. [43] conducted an NG sweetening plant exergy study by utilising MDEA, and discovered that the absorber had the most significant exergy losses. In another study, Roy et al. [44] compared and validated their model against the Bakhrabad gas processing facility with the Aspen HYSYS simulation software.

The present study aimed to investigate the simultaneous capture of CO_2 and H_2S with a novel ternary hybrid blend of MDEA, AEEA, and NMP. Aspen HYSYS[®] V12.1 software was employed to construct an AGRU simulation that was first validated with data from a plant before a valid process model was built. No simulations or experimental investigations on higher CO_2 (45%) and H_2S (1%) contents were performed prior to this study. The proposed novel solvent blend in the study was also utilised to minimise the reboiler duty. The critical variables were then subjected to a parametric sensitivity analysis to determine their effects on the process performance.

2. Process Description

The capturing stations for the sweetening of NG receive high-pressure feed gases during the removal of CO_2 and H_2S . An AGRU is an equipment unit designed to remove and reduce acid gas components, such as CO_2 and H_2S , from raw NG stream to meet the sales gas specifications. The process applies the concept of absorption, in which a hybrid solvent is employed to remove the acid gases [45].

Generally, an AGRU consists of two main pieces of equipment: an absorber, and a stripping column. A separator is employed to first separate any entrained liquid or particles from the sour feed gas before removing the acid gases. Subsequently, the sour gas is fed into the absorber column from the bottom, whereas the lean amine solvent is introduced from the top, to allow the sour gas to flow upward in a counter-current flow direction with the lean solvent [46]. Table 2 summarises the feed gas specifications and conditions.

Table 2. The sour gas specifications and conditions.

Parameters				
Methane in sour gas mol.%	47			
Ethane in sour gas mol.%	3.2			
Propane in sour gas mol.%	1.8			
CO ₂ in sour gas mol.%	45			
H_2S in sour gas mol.%	1			
Inlet gas temperature (°C)	51			
Inlet gas pressure (kPa)	7140			
Gas flowrate (kg mol/h)	3894			

The acid gas components, including the H_2S and CO_2 , are then removed by the lean solvent through absorption upon contact, while the rich solvent exits the absorber from the

bottom [47]. Subsequently, the NG, free from acid gases and commonly known as sweet gas, leaves the absorber column from the top for further processing, while the rich solvent is directed to a flash tank to allow the carried-over hydrocarbons to escape as vapours, thus preventing foaming in the stripping column.

Before entering the stripping column, rich amines from the bottom of the flash tank trade heat with a lean amine in a shell and tube heat exchanger [48]. Figure 1 illustrates the general process flow of an amine-based AGRU. The acid gases are thermally regenerated and require sufficient energy to increase the solution temperature and break the chemical bonds between the amine molecules and the acid gas components. The acid gases leave the stripper from the top, while the lean amines exit the column from the bottom. Lastly, the regenerated lean solvents are cooled and reused in the absorber column for a continuous AGRU process [49].



Figure 1. The AGRU flow sheet constructed with the Aspen HYSYS.

3. Simulation Basis

The Aspen HYSYS[®] V12.1, a commonly recognised simulation software system within the petroleum industry, was selected to perform the simulation in the present study. The UNIQUAC, which is a built-in thermodynamic package in the software, was the thermodynamic property package employed to calculate the equilibrium and kinetic reactions rigorously. Although the absorbers and stripping columns are two of the most vital components in an AGRU, a careful modelling approach is essential when utilising a process simulator [50].

The equilibrium-stage and rate-based models are the two most prominent methodologies for modelling columns. The equilibrium-based approach relies on the hypothesis that the liquids and vapours emerging from each column stage are in equilibrium. Accordingly, equilibrium-based models often necessitate empirical parameter tunings to obtain accurate results. Conversely, rate-based models analyse heat and mass transfer processes, which consider the tray shape, transport properties, and concentration gradients between the contacting phases [51]. Consequently, the outputs of the rate-based approach are closer to the original data, allowing the estimation of the processing parameters under various operating conditions [52].

Removing acid gases via the chemical absorption of amines is based on the acid–base reaction theory [53]. The CO₂ and H₂S gases are known as acid gases, since they dissociate and form weak acidic solutions in aqueous solutions, yielding Equations (1)–(3) [54]. During chemical absorptions, the amines act as weak organic bases to react with the acid gas components via exothermic reactions, thus forming soluble acid–base complexes in the treating solvent. Subsequently, the acid–base complexes are reversed to strip off the

acid gas components from the amine solvent in the stripping column through thermal regeneration [55].

The ionization of water:

 $H_2O \leftrightarrow H^+ + OH^-$ (1)

The ionisation of dissolved H₂S:

$$H_2S \leftrightarrow H^+ + HS^-$$
 (2)

The ionisation and hydrolysis of dissolved CO₂:

$$CO_2 + H_2O \leftrightarrow HCO_3^+ + H^+$$
 (3)

Based on Table 2, the feed gas, supplied at 51 °C, was admitted from the bottom of the absorber and came into contact with the lean hybrid solvent mixture at a counter-current. The columns in the current study were numbered sequentially from top to bottom and the absorber consisted of 21 trays. The lean amine solvent entered from the first tray at 57 °C, while the rich amine exited the bottom of the absorber at 64 °C. After passing through a valve and flashing with a flash drum, the high-pressure amine stream was depressurised from 7140 kPa to 551 kPa. The flow rate into the flash tank was set at 32,500 kmol/h, while the vapour phase exited from the top at 19.9 kmol/h. Consequently, the loss was only 0.05% of the input flow rate, hence negligible. The sweet gas exiting the absorber top was maintained at under 1% CO₂ and 4 ppm of H₂S.

After flowing through the flash tank, the rich amine transferred its heat to the lean amine solvent, increasing the temperature of the solvent to approximately 95 °C before it was admitted into the stripping column. The stripping column contained an overhead condenser and a reboiler at the bottom with 17 stages. Table 3 lists the absorber and stripping specifications employed for the simulation in the current study. The stripped H₂S and CO₂ gas departed from the top of the stripper at 88 °C, while the lean amine solution left from the bottom at approximately 103 °C. Subsequently, the lean amine was cooled before being returned to the absorber for an efficient process.

Table 3. The input specifications for the AGRU simulation.

Absorber	
Number of trays	21
Solvent temperature (°C)	57
Solvent pressure (kPa)	7160
Gas feed tray	1
Solvent concentration (wt.%)	55
Solvent feed tray	21
Column type	Packed
Column diameter (m)	1.219
Weir length (m)	1
Stripper	
Number of trays	17
Rich amine temperature (°C)	119
Column top pressure (kPa)	196.3
Column bottom pressure (kPa)	206.3
Inlet feed tray	1
Reboiler type	Shell & tube exchanger
Condenser type	Full reflux
Weir height (mm)	50.8
Column diameter (m)	1

4. Results and Discussion

4.1. Plant Data Validation

The initial stage in the present study was to validate the simulation model with data from a real-world plant or the literature to ensure that it could accurately anticipate the plant operation under various scenarios. In this case, the simulation results were validated against the actual plant data reported by Nasir et al. [5], in which the values from the simulation were compared to the Lekhwair plant data for validation via the built-in thermodynamic package 'acid gas'.

In the current study, hybrid solvent mixtures were employed to remove acid gases from the NG; however, the acid gas package did not support a hybrid mixture. Consequently, the actual plant data were validated against the acid gas thermodynamic package and compared to the UNIQUAC thermodynamic package. A detailed comparison between the actual plant and simulation data is demonstrated in Table 4. The comparison revealed that both thermodynamic simulation packages accurately estimated the sweet gas stream parameters and the required duties efficiently. Moreover, the standard error difference between the actual and simulated data was less than 5% [56].

Parameters	Actual Plant Data	Amine Package	Error (%)	UNIQUAC	Error (%)
Sweet gas Methane (kmol/h)	2852.21	2801.27	1.78	2761.14	3.19
Sweet gas Ethane (kmol/h)	387.19	398.39	2.89	386.02	0.3
Sweet gas Flowrate (Kmol/h)	3497.72	3499	0.03	3387.42	3.15
Sweet gas Temp (°C)	55	53.7	2.36	57.3	4.18
Sweet gas Pressure (kPa)	7140	7140	0	7143	0.04
Condenser temp (°C)	119	119.4	0.33	119	0
Reboiler Temp (°C)	124	129.1	4.11	126.4	1.93
Reboiler Duty (kW)	2170	2172	0.09	2145	1.15

4.2. Energy Analysis

The current study conducted a detailed energy analysis to identify the most intensive energy-consuming equipment in the flowsheet. As expected, the resultant values revealed that the reboiler in the AGRU was the primary energy consumer. The simulation results of the heat duty required by the main equipment for sweetening the NG are summarised in Table 5.

Table 5. The energy requirements for the various unit in an AGRU.

Equipment's	MDEA	MDEA + AEEA	MDEA + AEEA + NMP
Reboiler (kJ/h)	$7.38 imes 10^7$	$1.14 imes 10^8$	$2.64 imes10^7$
Condenser (kJ/h)	15.57	4.276	71.59
Lean Amine Pump (kJ/h)	$2.30 imes 10^6$	$2.21 imes 10^6$	$2.07 imes 10^6$
Lean amine cooler (kJ/h)	$2.67 imes 10^7$	$4.89 imes10^7$	$8.03 imes10^6$

No previous studies have reported 45% CO₂ and 1% H₂S gas being removed simultaneously from sour gas, and the amount of heat energy required to strip acid gases from reboilers is also unavailable. Consequently, the present study proposes a novel ternary-hybrid mixture of amines that could be employed as an alternative solvent to remove high acid content from NG. The simulation data of the MDEA (40 wt.%), MDEA (30 wt.%) + AEEA (10 wt.%), and MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%) solvents were then compared.

The highest energy-consuming equipment in the AGRU was the reboiler. Nevertheless, the least energy consumed was recorded when the hybrid blend was employed, necessitating 64.2% and 76.8% less energy, respectively, than the MDEA and MDEA + AEEA (see Figure 2). The reduced energy requirement by the hybrid solvent was due to the presence

of a physical solvent that could be regenerated with pressure reduction, without producing extra heat or increasing the temperature of the reboiler, thus requiring less energy for its regeneration. Furthermore, it was evident that the total regeneration energy (E_{regen}) was divided into three components: sensible heat (Q_{sens}), latent heat (Q_{latent}), and the heat of reaction (Q_{rxn}). The Q_{sens} and Q_{latent} were diminished when NMP was employed instead of some of the water in the aqueous solution, which also lowered E_{regen} [57].



Figure 2. The reboiler duty with solvents composition at MDEA (40 wt.%), MDEA (30 wt.%) + AEEA = (10 wt.%), MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%).

The second most intensive energy-requiring equipment in the AGRU is the lean amine cooler. The hybrid lean amine leaving the bottom of the stripping column exchanges heat with the lean/rich amine shell and the tube heat exchanger, and exits the exchanger at approximately 90 °C, which is still very high for utilisation as a solvent in absorbers. In the current study, the regenerator inlet temperatures for all the experiments are similar. However, the lean amine temperature with the hybrid solvent was 103 °C, less than that recorded by the MDEA and MDEA + AEEA systems, which were 124 °C and 129 °C, respectively. The data revealed that the hybrid solvent required 70% and 83% less cooling utility, respectively (see Figure 3). Conversely, for the condenser, the hybrid solvent required a higher heat duty than the other two solvents. The observation might be due to the lower boiling point of the physical solvent, NMP, compared to the MDEA and AEEA. Consequently, more vapours were moving upwards, hence the condenser required more heat energy to convert them into a liquid again.



Figure 3. The comparison of cooler duties at MDEA (40 wt.%), MDEA (30 wt.%) + AEEA = (10 wt.%), MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%).

4.3. The Effects of Solvent Temperature

The temperatures of the sour gas entering the bottom of the column and the lean amine entering the top of the column can be manipulated to regulate the temperature of the absorber column and, consequently, its reaction kinetics. In general, lowering the temperature of the absorber can enhance efficiency. Nonetheless, only the lean amine temperature was altered to obtain the desired absorber temperature, as it is typically undesirable or challenging to change the temperature of the sour gas [58].

A 5 °C temperature differential between the feed gas and amine solvent is preferably maintained to avoid hydrocarbon condensation in the absorption column [56]. In the present study, a sensitivity analysis was performed to determine the impacts of the lean amine temperature on the composition of the sweet gas and reboiler duty, while the other parameters were fixed. Figure 4a,b illustrates the effects of the temperature on the molar flow of CO₂ and H₂S in the sweet gas. The increased molar flow of H₂S and CO₂ was recorded as the temperature of the lean amine solvent was raised.



Figure 4. The effects of increased solvent temperature at MDEA (40 wt.%), MDEA (30 wt.%) + AEEA = (10 wt.%), MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%) on the (**a**) CO₂ in sweet gas (**b**) H₂S in sweet gas (**c**) reboiler duty.

Previous studies have confirmed that lower temperatures consistently enhance the absorption process, whereas higher temperatures demonstrate the opposite effect [59]. The diminished absorption results from fewer gas molecule diffusions, due to the absorption of CO_2 in the amine solution, an exothermic reaction that can change the equilibrium backward at increased temperatures. Higher lean amine temperatures that lead to increased partial pressures of H_2S and CO_2 might be another factor. The behaviour could be due to

the decreased H₂S and CO₂ solubility in alkanolamine solutions at higher temperatures, hence lowering their removal efficiency [51].

Alternatively, the hybrid blend proposed in the present study reduced the reboiler duty, compared to the MDEA and MDEA + AEEA, while increasing the temperature of the amine solvent. Figure 4c reveals that the reboiler duty decreased from the increased CO_2 and H_2S slips in the sweet gas when the temperature was higher, reducing the load on the reboiler and thus its duty.

4.4. The Effects of Absorber Pressure

It is unlikely that the absorber pressure will change much during routine operation. Furthermore, as the gas well is used up, the overall pressure of natural gas begins to fall. The plant performance will suffer if the feed gas is not delivered to the gas sweetening unit at the specified pressure [60]. Consequently, the current study performed sensitivity analyses to determine how the absorber pressure impacts the concentration of CO_2 and H_2S in the sweet gas. The impacts of altering the absorber pressures on the CO_2 and H_2S removal from the sweet gas are illustrated in Figure 5a,b respectively. In the present study, increased pressure produced positive results in the CO_2 and H_2S absorption in the system incorporated with the hybrid solvent. The loading capacity of the hybrid solvents (40 wt.%) was enhanced with increased CO_2 and H_2S partial pressures, compared to the MDEA (40 wt.%), and MDEA (30 wt.%) + AEEA (10 wt.%). The results are supported by Henry's law, which states that the solubility of a gas is theoretically improved as its pressure is elevated.



Figure 5. The results of increasing absorber pressure at MDEA (40 wt.%), MDEA (30 wt.%) + AEEA = (10 wt.%), MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%) of (**a**) CO₂ in sweet gas (**b**) H₂S in the sweet gas (**c**) the reboiler duty.

The enhanced loading capacity might be due to two reasons: the CO_2 and H_2S molar flow in sweet gas diminish as the pressure increases the solubility of acid gases, and, at higher pressures, physical diffusion occurs, hence improving the loading capacity of the hybrid solvents [61]. The findings demonstrate that, as the absorber pressure falls due to a drop in the gas reservoir pressure or other reasons, the CO_2 and H_2S concentrations in the sweet gas rise from the reduced CO_2 and H_2S partial pressure in the feed gas. Figure 5c illustrates that changes in the absorber pressure have no significant impact on the stripper reboiler duty. The solvent circulation rate must be raised in the event of low absorber pressure, which will elevate the reboiler duty to fulfil the sweet gas specification. Previous studies also report the same trends [62].

4.5. The Effects of Solvent Flow Rate

An essential variable that could be adjusted directly to obtain product purity would be the solvent circulation rate. This factor significantly affects the capital cost of the plant since it influences the size of the processing plant equipment, including the absorber, stripper, pumps, pipelines, and heat exchangers. Furthermore, the liquid flow rate has a direct impact on the reboiler duty required for the solvent regeneration. Consequently, an elevated amine circulation rate could be utilised to adjust the acid gas content of the sweet gas [58].

The effect of the solvent flow rate on the regeneration heat duty is not straightforward, as shown in Figure 6. The Q_{regen} reduces with the solvent flow rate at the low solvent flow rate because the effective interfacial area in the stripper is increased, resulting in enhancements of both the mass and heat transfer performances. At the higher solvent flow rate, the Q_{regen} increased due to the shorter residence time of the solvent in the stripping column, and more heat being required in the reboiler.



Figure 6. The results of increased solvent flow rate at MDEA (40 wt.%), MDEA (30 wt.%) + AEEA = (10 wt.%), MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%) on the (**a**) CO_2 in sweet gas (**b**) H_2S in sweet gas (**c**) reboiler duty.

An increased solvent flow rate permits more contact time between the sour gas and the solvent, thus improving the solubility. The findings of this study demonstrate that, when the circulation rate is increased, the rich amine loading decreases. Figure 6a,b illustrates that the appropriate amount of CO_2 and H_2S are eliminated in each solvent assessed. The MDEA + AEEA + NMP hybrid solvent exhibits a more significant CO_2 and H_2S removal efficiency at the low flow rates.

The CO₂ and H₂S absorption capability is constrained by the stoichiometry of the chemical reaction when chemical solvents are applied. Conversely, physical solvents record no such restrictions, and their absorption capacity is proportional to the partial pressure of the CO₂ and H₂S. Physical solvents are used where the bulk amount of acid gases needed to be removed. These solvents also have the ability to absorb mercaptans, as well as other sulphur compounds such as methyl-mercaptan, dimethyl sulfide, and ethyl-mercaptan, whereas amine solvents have weak mercaptan absorption abilities [63]. Figure 6c indicates that an increased solvent flow rate elevates the system energy consumption, especially the reboiler duty. Nevertheless, the minimum flow rate required for removing acid gas from the NG was achieved when the hybrid solution was employed. Moreover, the reboiler duty required for the solvent regeneration was less than that of the MDEA (40 wt.%), and MDEA (30 wt.%) + AEEA (10 wt.%) mixture. The observations are due to fewer chemical reactions occurring in the MDEA (15 wt.%) + AEEA (5 wt.%) + NMP (20 wt.%) hybrid solvent, hence requiring less energy.

4.6. The Effects of Solvent Concentration

Another process variable that influences the reboiler heat duty in solvent regeneration is the alkanolamine solution concentration [64]. The impacts of altered lean amine concentration on the amount of H_2S and CO_2 in the sweet gas and the reboiler duty are depicted in Figure 7a–c, respectively. The CO_2 level in the sweet gas was significantly higher than the design specification at the low solvent concentrations (MDEA = 20 wt.%), (MDEA = 15 wt.%, and AEEA = 5 wt.%), thus requiring a substantial flow rate to remove the H_2S and CO_2 contents.

A significant decrease in the reboiler duty was observed as the solvent concentration was raised, (MDEA = 40 wt.%), (MDEA = 20 wt.%, and AEEA = 20 wt.%), which resulted from the lower flow rate required to achieve the desired sweet gas specification. The MDEA = 20 wt.%, AEEA = 5 wt.%, and NMP = 25 wt.% required 1400 m³/h to obtain the preferred CO₂ and H₂S contents in the sweet gas. However, only 1200 m³/h was required by the MDEA = 20 wt.%, AEEA = 5 wt.%, and NMP = 45 wt.%, which led to a 14.2% flow rate reduction.

The results show that the presence of a physical solvent not only reduces the flow rate, but also the reduces the reboiler duty. The higher the concentration of physical solvent in the blend, the lesser the flow rate is required to achieve the allowable limits of acid gases in the sweet gas. Thus, a hybrid solvent having a higher content of NMP (45 wt.%) is considered to be the best solvent to reduce reboiler duty as compared to aqueous chemical amines.

Compared to the MDEA and MDEA + AEEA solvent requirements, the MDEA + AEEA + NMP utilises less water. The simulation findings in the present study demonstrate that replacing H_2O with NMP in the MDEA + AEEA + NMP is beneficial to the solubility of CO_2 and H_2S , in comparison to the amine-based solvents. It can be deduced that, because a physical solvent is present in the solvent combination, acidic gases are physically more soluble there than in an aqueous solution. The chemical balance between the interacting components is impacted by substituting some of the NMP with water, with the purpose of raising the level of the acidic gas concentration. Moreover, an elevated physical solvent concentration in the chemical solvent mixture further reduces the reboiler duty, because less chemical reaction takes place in the hybrid solvent as compared to the aqueous amine solvents.



Figure 7. The effects of varying solvent concentrations on the (**a**) H_2S in sweet gas (**b**) CO_2 in sweet gas (**c**) reboiler duty.

5. Conclusions

The current study evaluates and compares the CO₂ and H₂S capture performance of a novel ternary-hybrid blend (MDEA + AEEA + NMP) to that of aqueous MDEA and MDEA + AEEA mixtures. A detailed analysis was performed with Aspen HYSYS® V12.1 software post-validation, with actual plant data and different operating parameters. The simulation results reveal that the pressure and the temperature exhibit opposite trends. High pressure and low temperature increase absorption. Consequently, the lean amine temperature and absorber pressure play critical roles in removing acid gases in sweet gas. The solvent flow rate and concentration are among the most crucial factors that directly affect the reboiler duty of an AGRU. The current study observed that a lower flow rate is required for the desired sweet gas specification when the ternary-hybrid blend is applied, compared to the MDEA and MDEA + AEEA mixture. The hybrid solvent consumed 64.2% and 76.8% less energy, respectively, to regenerate the amine than the MDEA and MDEA + AEEA. In addition, as the concentration of physical solvent is increased in the ternary blend, the rate of absorption increases, compared to the aqueous amine solvents of MDEA and MDEA + AEEA. When the concentration of NMP was 25 wt.%, it required a flow rate of 1400 m³/h and, as the NMP was increased to 45 wt.%, 1200 m³/h was required to achieve the allowable limits of acid gases in the sweet gas. The trends demonstrate that the proposed ternary-hybrid blend possesses the potential as an alternative solvent to remove acid gases from NG. Accordingly, focusing on developing design options with different opportunities to reduce energy and cost consumption, and plant optimisation should be the future direction of similar projects.

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