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SIMULATION AND OPTIMIZATION OF A LIQUIFIED PETROLEUM GAS SWEETENING PROCESS USING ASPEN HYSYS

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Liquefied petroleum gas (LPG) is one of the common fossil fuels that can be derived from natural gas or crude oil. In either case, it contains impurities such as H_2S and CO_2, which should be removed to obtain sweet liquified petroleum gas with a pure concentration of hydrocarbons such as ethane, propane, and butane. The most common method of gas sweetening process is by using amine compounds, which come in various types, each designed for specific and selective removal of acidic gases. In this study, methyldiethanolamine (MDEA) (42 wt.%) was used as a solvent to extract approximately 0.8% of H_2S from sour LPG at a temperature of 40^0C. The objective of this study focuses on simulating and optimizing the LPG sweetening unit using Aspen HYSYS V11 to investigate the different parameters that affect the separation of acidic gases and to achieve high profitability. The number of trays, circulation rates, temperature, mass and molar flow rates, and other parameters were studied to reduce the H_2S concentration to 0% in the treated LPG stream. The sweetening process was proposed to produce LPG with high levels of specific preferred specifications such as calorific value and purity, in addition to being environmentally friendly.

Keywords: Aspen HYSYS, H_2S removal, liquefied petroleum gas, methyldiethanolamine, sweetening process.

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Introduction

Liquefied petroleum gas (LPG) is regarded as among the most practical and environmentally friendly fuels for household cooking, heating, commercial, and automotive sectors, especially in metropolitan regions. Generally, the request for the use of LPG is rising quickly due to rising LPG consumption [1]. LPG is a group of hydrocarbons, primarily (butane, propane, and a trace amount of pentane). It is a vapor under normal operating conditions and can be converted into a liquid form by increasing medium pressures. Raw matter after extraction from wells also contained pollutants including carbon dioxide, hydrogen sulfide, and elemental sulfur; these compounds are known to be harm people and the environment. These impurities can cause problems like corroding, refrigeration, clogging, erosion, medical conditions, and environmental threats [2]. Gas sweetening is the procedure for taking H_2S and CO_2 out of a stream of gas mixture [3]. The H_2S and CO_2 concentrations of natural gas must be reduced to 2–4 ppm and around 2%, respectively, to prevent any possible problem. Therefore, there is a great need for liquid hydrocarbon sweetening facilities to remove these impurities and obtain sweet gas without any pollutants [4–6].

Upwards fifty percent of the existing acid gas extraction techniques utilize aqueous solutions of alkanol amines, giving the amine gas sweetening procedure the much more popular approach for acid gas removal. Nevertheless, the high energy aspect of such a gas sweetening procedure, particularly for amine regenerated, carbon steel's tendency to corrode, ease of deterioration, carcinogens, and some environmental issues restrict its economic application. On the other hand, many advantages make amines suitable for sweetening operations such as rapid absorbing rates, and more suitable when there are large levels of sulfur pollutants because they can be recycled and regenerated back into the system [7].

Alkanol amines have different kinds depending on the structure of the amines group which can be classified as primary (monoethanolamine, MEA), secondary (diethanolamine, DEA), and tertiary (methyldiethanolamine, MDEA), they can all be used to sweeten LPG to varying levels in the oil and gas sector according to the concentration of CO_2, H_2S. In this study, H_2S was extracted from the liquified stream gas by using MDEA as the most effective kind of amine for this case. This is explained by a number of reasons: MDEA is more selective towards H_2S than CO_2 compared to MEA or DEA as reported by Mandal et al. [8], lower vapor pressure, with low flow rates for a solution, for that requiring minimal regeneration column, and greater resilience against deterioration and fewer corrosive issues [9,10].

Aspen HYSYS version 11 was utilized in this study to simulate and optimize the sweetening process. To minimize manufacturing costs, accelerate development times, and improve product quality, process modeling, simulation, and optimization were implemented. This study aimed to display and discuss the use of Aspen HYSYS for simulating H_2S removal from LPG by MDEA absorption. In addition, the effects of the parameters on the extraction process such as temperature, pressure, and circulation rate were studied. The investigated parameters were optimized to maximize the revenue of product according to the data collected from the South Oil Company (SOC) which is located in the south of Iraq.

Experimental

Overview of gas sweetening techniques

Amine-based H_2S extraction process

Selecting the amine in the sweetening process that will improve the investment and reduce company outgoings is the secondary goal. In addition, the circulation rate has a direct effect on regeneration requirements. For all these points, the right decision should be made before starting the sweetening process, which is applied in the amine treating unit as shown in Fig. 1.

Chemistry reaction based on amine-compounds

As is evident from Eq. (1), proton transfer is assumed to be the primary mechanism by which H_2S interacts with the amines very instantly.

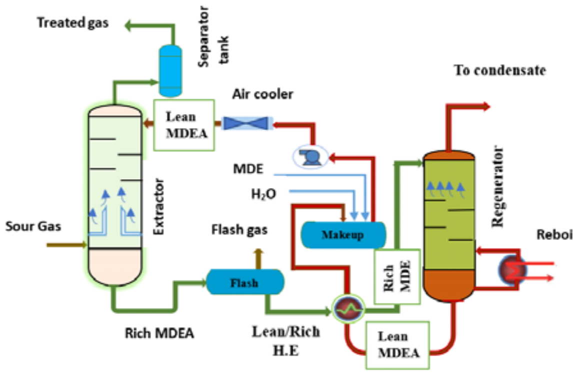


Fig. 1. Process flow diagram for a standard amine-based H_2S extraction process

$$H_2S+Amine \Leftrightarrow [Amine]H^{+}+HS^{-} \qquad (1)$$

$$R_2NCH_3+H_2S \Leftrightarrow R_2NHCH_3HS \qquad (2)$$

Here R_2 refers to the methyl group (C_2H_4OH).

Equation (2) shows the reaction of hydrogen sulfide with MDEA to produce an amine sulfide salt that is pulled down from the extractor column (rich amine stream).

In case available CO_2 in the sour gas stream, methyldiethylamine bicarbonate will be produced after absorbing water and degrades as mentioned in the reaction (Eqs. (3) and (4)).

$$CO_2+H_2O \Leftrightarrow HCO_3^{-}+H^{+} \qquad (3)$$

$$HCO_3^{-} \Leftrightarrow CO_2^{2-}+H^{+} \qquad (4)$$

The contents of various ions in the liquid phase are determined by chemical reactions, which also improve mass transfer. The quickness of equilibrium reactions allows for the maintenance of chemical equilibrium throughout the whole liquid phase [11,12].

Main sweetening process variables

Any process has some important parameters, which effect directly on the efficiency of the process, as known the familiar conditions such as pressure, temperature, the concentration of feed, and the design of equipment. All these must be examined carefully to reach for satisfying and accurate results to fully meet the requirements of the consumer.

Content of MDEA

The feed MDEA concentration has a big effect on the amine recycled to the extraction column. The solution circulating rate is reduced as MDEA concentrations increase.

Number of extractor trays

The separation efficiency is greatly affected by the number of extraction tower trays. Sweet gas is obtained due to the increased flow of lean amine in some trays, while the acid gas concentration decreases as the percentage of lean amine rises, enabling enhanced mass transfer through lean MDEA and acid LPG [13].

Rate circulation and flowrate of MDEA

Lean amine circulation rate has an impact on the sweetening process, as it mainly depends on the flow rates, the concentration of the amine solution, and the rich amine loading in the extraction unit, which is recommended to be about (0.4–0.55 mol) [14]. With increasing the circulation rate, the separation efficiency will increase but will lessen the liquid's residential duration on a tray.

Modeling of LPG sweetening unit

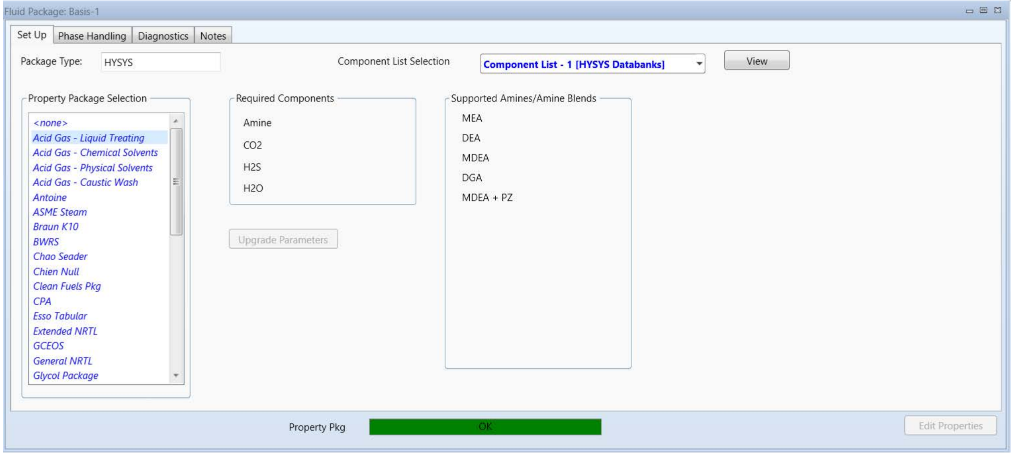
Parameters and the fluid package LPG sweetening process are simulated by Aspen HYSYS version 11 by using the fluid package special for acid gas-liquid treating which is suitable for liquefied petroleum gas as shown in Fig. 2.

Process modeling for a sweetening procedure

Figure 3 shows the process flow diagram implemented using Aspen HYSYS simulations in the case of a steady state. The purpose of the simulation LPG sweetening unit is to study the effect of variables on the concentration of hydrogen sulfide in the sweet gas and then choose the best condition for high purity of sweet LPG product. The sour gas was fed to the extraction column with ten trays at a temperature of 40–45^{0}C with a pressure gradient between 15–15.8 kg/cm^2 for the upper and the lower stage column, respectively.

The clean liquefied petroleum gas was drawn from the upper side of the tower, while the H_2S-saturated amine was collected from the external bottom extractor (rich MDEA stream), this amine was regenerated in the generation tower which consists of 20 stages, for repeated use to continue the sweetening process in the plant. The lean MDEA was recycled back to the extraction column.

To control the pressure and temperature for the inlet stream of the extractor column of lean MDEA, the cooler should be installed before the entrance of the extractor. After that, the rich amine is heated by passing through the heat exchanger, and the H_2S-rich MDEA from the extractor is fed to a stripper (regenerator) to regenerate the MDEA and then circulate back to the extractor but after being cooled



Fluid Package: Basis-1

Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

Property Package Selection:
- <none>
- Acid Gas - Liquid Treating
- Acid Gas - Chemical Solvents
- Acid Gas - Physical Solvents
- Acid Gas - Caustic Wash
- Antoine
- ASME Steam
- Braun K10
- BWRS
- Chao Seader
- Chien Null
- Clean Fuels Pkg
- CPA
- Esso Tabular
- Extended NRTL
- GCEOS
- General NRTL
- Glycol Package

Required Components:
- Amine
- CO2
- H2S
- H2O

Supported Amines/Amine Blends:
- MEA
- DEA
- MDEA
- DGA
- MDEA + PZ

Property Pkg: OK

Fig. 2. Fluid package for acid gas-liquid treating

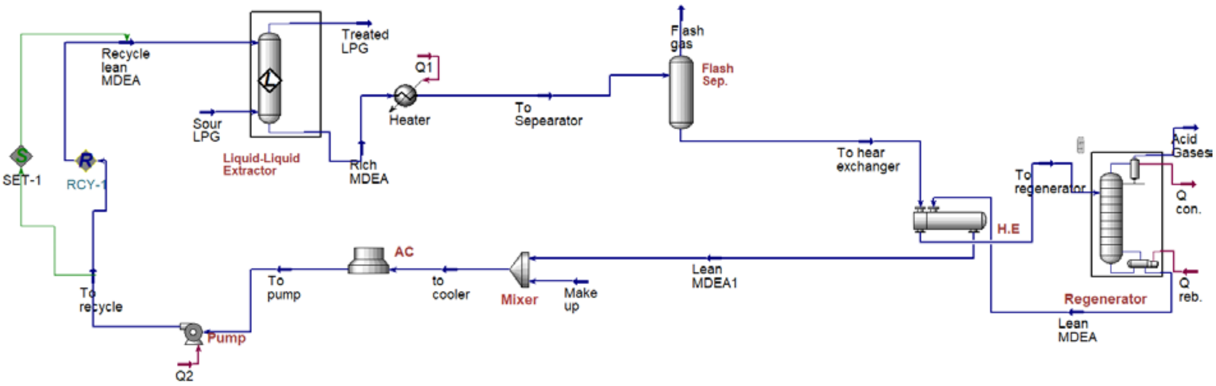


Fig. 3. Process flow diagram of LPG sweetening unit

in a cooler. The primary function of an amine cooler is to reduce lean amine temperature, which should enter the extractor at a temperature that is roughly 10^0F (5^0C) hotter than sour gas. Lower amine temperatures make the gas cooled in the extractor and cause the condensing of hydrocarbons, which frequently results in foaming. Elevated amine losses are caused by a rise in the amine vapor pressure [3].

A flash tank was used to flash some undesired heavy compounds in the rich amine stream to minimize any sudden problems that may affect the process. Finally, a water-mixing tool was used to adjust the amount of flow of the recycled back lean amine into the extraction column, as well as to compensate for the lost amount of water in the recycled rear lean amine. MDEA content may accumulate during the procedure, so the composition of the amino solution in the procedure will be maintained and supported by this tool.

Results and discussion

Table 1 shows the variables and conditions of the liquid-liquid extractor collected from the first unit of LPG sweetening/South Oil Company-Basra[1]. The different parameters were calculated such as material balance, flow rates for verity streams, the amount of removed H_2S, circulation rate, and many variables that lead to modifying the plant performance. The final results for both plant data and aspen HYSYS for sweetening LPG unit are shown in (Table 2).

Influence of MDEA concentration

The concentration of feed amine greatly influences the concentration of compounds leaving the extraction tower, especially in the sweet LPG stream. Figure 4 illustrates the effect of different feed MDEA concentrations (38–46 wt.%) on the final result of hydrogen sulfide in the sweet gas (treated gas stream). As the MDEA concentration increased, the extraction of H_2S also increased. At 42 wt.% of MDEA, it was found that the H_2S content in the treated LPG was decreased from 1.3 to 1 ppm, while the reboiler duty raised gradually due to increased extraction H_2S from sour LPG feed. The concentration of 42 wt.% appeared to be effective for the extraction process, because after increasing the amount of MDEA, the H_2S almost was stable with an simple increase in the sweet gas stream.

Liquid-liquid extractor plates

The liquid extractor and regenerator columns

Table 1

Parameters and conditions of the extractor

Parameter		Sour LPG	Recycle lean MDEA	Treated LPG	Rich MDEA
Temperature (^{0}C)		40	45	40.1	42.58
Pressure (kg/cm^2)		15.87	15	15.87	14.8
Molar flow (kmol/h)		44.94	29.18	44.58	29.54
Mass flow (kg/h)		2421	817.13	2408.5	829.6
Components (mol.%)	water	0	90.13	0.07	88.95
	hydrogen sulfide	0.82	0	0	1.25
	hydrogen	0.39	0	0.39	0.01
	MDEA	0	9.87	0	9.74
	methane	1.57	0	1.58	0.01
	ethane	5.26	0	5.29	0.01
	propane	17.02	0	17.15	0.01
	i-butane	13.62	0	13.73	0.01
	n-butane	56.45	0	56.90	0.01
	i-pentane	2.3	0	2.32	0
	n-pentane	2.57	0	2.59	0

Table 2

Comparison of plant data and aspen HYSYS for sweetening LPG unit

Data resource	Stream (mol.%)							
	recycle lean MDEA		treated gas		rich MDEA		acid gas	
	MDEA	H_2O	MDEA	H_2O	MDEA	H_2S	H_2O	H_2S
SOC	12.41	87.59	0	0.08	4.65	0.819	5.26	76.29
HYSYS	9.87	90.13	0	0.07	9.74	1.25	9.92	87.01

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[1] South Oil Refineries Company, «LPG documents for the first unit», Co. Doc., 2022.

are the two main parts of the LPG sweetening system. The principle of separation is done by passing the solvent and acid gas through several trays by counter-current flow (MDEA solvent from above and acid LPG from below) of the extractor. The separation efficiency depends on the number of trays, the interaction space between the materials, as well as other factors affecting the quality of the sweet gas. Therefore, the effect of the number of trays on different variables has been studied as shown below.

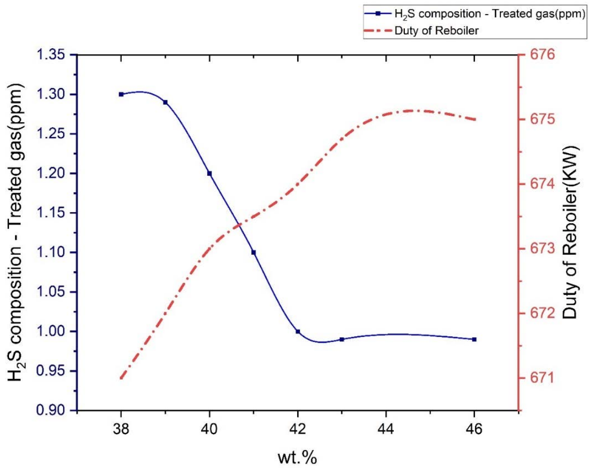

Fig. 4. Effect of the concentration of MDEA on the H_2S content of the treated LPG stream and heat flow of reboiler

Effect of number of trays on pressure and temperature in liquid–liquid extractor column

The upper (the first tray) and lower (the last tray) temperatures of the extractor column are 45 and 42^{0}C, respectively, as shown in Fig. 5. With the increase in the number of trays, the temperature decreases, at a certain tray and temperature H_2S will be extracted by MDEA solvent. In the case of studying the effect of pressure, it was observed that with reaching the last trays, the pressure was increased, this is due to the increased withdrawal of hydrogen sulfide in the lower trays and obtaining sweet gas from the upper side of the tower.

Effect of number trays on H_2S concentration

Figure 6 shows the relationship between the stage number and H_2S vapor content in the extractor. It was noted that the concentration of acidic compounds in the first stages is close to 0%, which means that this gas has been converted into sweet liquefied gas, while in the ninth stage, hydrogen sulfide was extracted by the MDEA solvent to form an MDEA-rich stream with H_2S concentration of about 0.6 mol.%, then drawn from the bottom of the tower to be sent to the flash tank. These results were consistent with the findings by Bin Sahl et al. [13], they observed that as sweet gas production increased, the acid gas content increased along with the number of feeding stages (from top to bottom).

Trays position and flow rate

Figure 7 shows the changes in the amount of liquefied petroleum gas flow over the ten trays, as the acid gases were extracted in the last stages of the tower and this explains the reason for the increase in the flow rate to 44.62 kg mol/h in the tenth plate, which means that the amine solvent is loaded with hydrogen sulfide and the separation process has been completed successfully.

MDEA circulation rate

This parameter identifies the amount of MDEA concertation and flow rate, in addition to the amount of MDEA that was recycled back to use again in the extractor. As shown in Fig. 8, with increasing the amount of circulation MDEA rate, the amount of

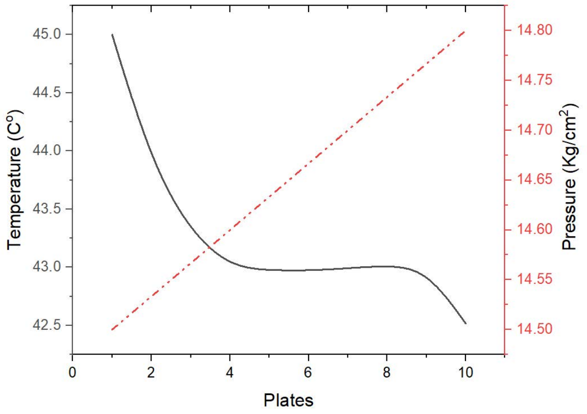

Fig. 5. Influence of liquid–liquid extractor plates on temperature and pressure

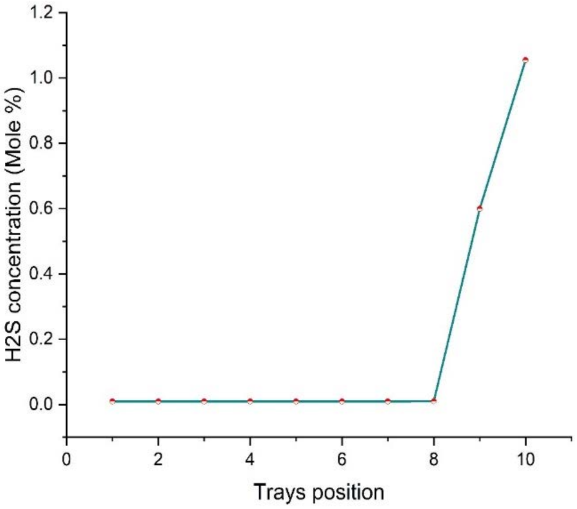

Fig. 6. Effect of trays number on the H_2S vapor content in the extractor

H_2S in the treated gas increased notably till reached the concentration of 2.4 ppm in sweet LPG and the reboiler duty is 686 kW. This means that an increase in the circulation rate leads to an increase in the concentration of H_2S in the sweet gas stream, so a lower circulation rate is preferable for extracting a large amount of acid gas. Al-Lagtah et al. [15] also concluded that the lowest circulation rate has a high acid removal efficiency.

Effect of temperature on the rate of circulation of MDEA

A case study was created to forecast the effect of a temperature-rich MDEA stream on the amine circulation rate and reboiler duty by applying gradient temperature between 41.5^{0}C and 43.5^{0}C. It can be seen that the amine circulation rate of the MDEA increased with increasing rich MDEA temperature due to the additional amine retention time inside the generating column (more boiler impacts), as illustrated in Fig. 9. Abkhiz and Heydari [16] used different kinds of amine and after some analysis, they found the MDEA has a lesser corrosive effect than DEA so it can be employed for larger quantities, which causes lower circulation and makeup.

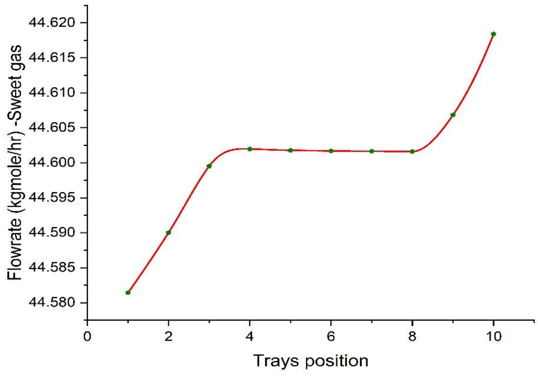

Fig. 7. Effect of increasing the extractor plates on sweet LPG flow rate

Effect of flow rate on H_2S concentration

The flow rate is one of the conditions most affecting the LPG desalination process. Whereas with the change in the mass flow amount from 2390 to 2440 kg/h of the sour LPG, the hydrogen sulfide concentration decreased from 6.4 to 2 ppm (Fig. 10). It was observed that at the value of the flow rate of 2421 kg/hour, the value used in this work led to obtaining an acceptable value of H_2S in the sweet gas mixture (2.3 ppm). The total flow rate of the sweetened LPG rises according to the rise in the mass flow rate of the sour LPG, as the amount of hydrogen sulfide decreases. Abdulrahman and Sebastine [17] showed that the extraction of hydrogen sulfide from the gas increased for all types of amine by increasing the flow rate of the amine [17].

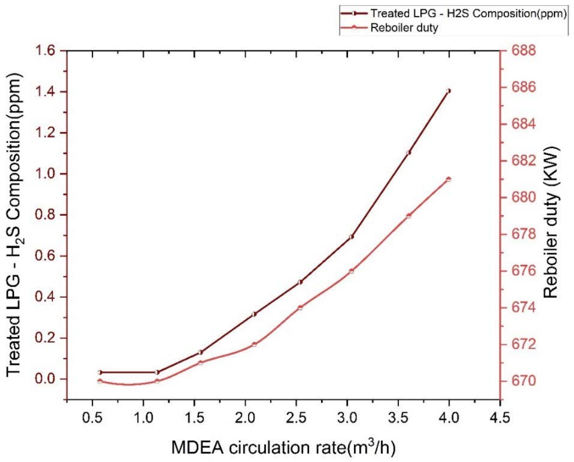

Fig. 8. Impact of lean MDEA circulation rate on the H_2S content in sweet LPG and reboiler duty

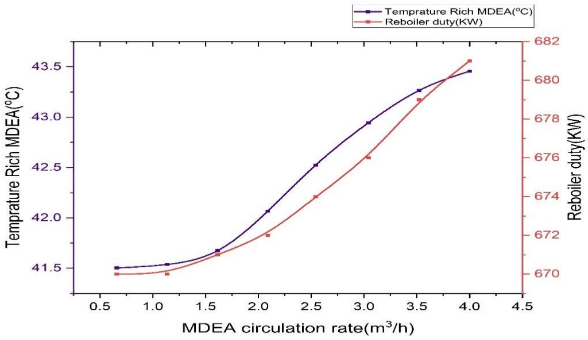

Fig. 9. Effect of change in MDEA circulation rate on the temperature and reboiler duty

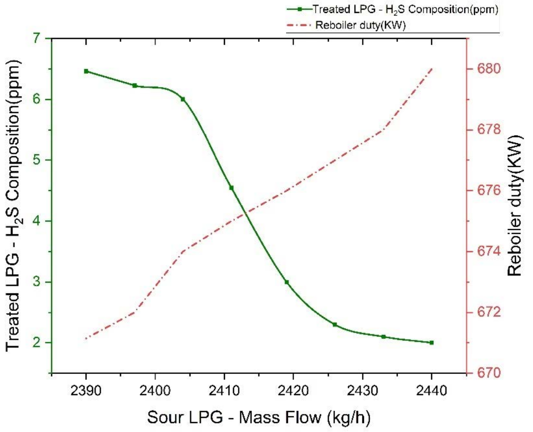

Fig. 10. Effect of sour LPG flow rate on the H_2S concentration in sweet gas stream and reboiler duty

Optimization

Profit is the most important issue in the oil and gas industry. To study the ways to get high revenue and lower cost, it is possible by using the optimizer property of Aspen HYSYS V11. To complete the optimization calculation, an objective function must be defined to calculate the required optimal values. In the spreadsheet, the required variables were imported from the sweetening process, and then the cell was selected to insert the variable that will be the main value that will change with the change of the target value.

The optimization is applied to the most active parameters that significantly affect the concentration of extracted hydrogen sulfide such as the amount of circulating amine, MDEA rate, condenser pressure, liquefied petroleum gas flow rate, and MDEA concentration to choose the ideal value of perfect condition for the variable to obtain the sweet LPG. The primary variables and their limits are summarized in Table 3.

The objective function of profit includes the amount of revenue of product streams such as treated gas, and acidic gas with their price subtracted from the cost-utility with the price. Equations (5) and (6) explain the meaning of profit and cost of sweetening process, respectively.

$$Profit = (M_{LPG}\cdot C_{LPG} + M_{H2S}\cdot C_{H2S}) - (Q_{Heater}\cdot C_{Heater}+Q_{condenser}\cdot C_{condenser}+Q_{Reboiler}\cdot C_{Reboiler}) \quad (5)$$

$$(Q_{Heater}\cdot C_{Heater}+Q_{con}\cdot C_{con}+Q_{Reb}\cdot C_{Reb}) \quad (6)$$

Here M is the flow rate (m^3/h, kg/d) and C is the cost ($).

Optimal values chosen from Table 3 are used to complete the optimal LPG profit. By applying the previous equations, and substituting the cost of one ton of liquid which is equivalent to 76.34 $ and the objective profit function was found around 4026.6 $/h.

The restriction used was the reed vapor pressure of the treated gas stream (108.5 psi<110 psi). Table 4 summarizes the final results of the operating conditions of the optimized LPG sweetening unit with a selection of optimized conditions and profit value as follows:

– In the case of the flow rate of sour LPG, the obvious effect is observed when changing the revenue rate of the LPG, as the best value that can be obtained is 5023.5$/h at 3000 kg/h.

– For the amine circulation rate, the perfect value was 1110 kg/h instead of 1000 kg/h because the profit rose to 4,068.35 $/h.

– 77.5^{0}C is the perfect temperature to obtain a high-profit value of 4033 $/h.

Conclusions

The H_2S removal model was applied by using Aspen HYSYS, which simulates the sweetening procedure to assess the results of the amine circulation rate, the tray number of the extractor, changes in temperature, and flow rates. With a concentration of 42% MDEA, a mass rate of 1000 kg/h, and a temperature of 45^{0}C, the clean LPG was obtained at a very low H_2S concentration of 0 wt.%.

The different parameters were examined carefully to improve the separation process, including the circulation MDEA rate. It was observed that by increasing the circulation rate, the separation efficiency was increased. In addition, the position of the trays was studied and it was noted that it has a clear effect on the separation efficiency.

Moreover, 87 mol.% of the H_2S compound was separated at an acidic gas stream by applying Aspen HYSYS, as it was close to the company value 76 mol.% with a slight relative difference due to the operation of the error tolerance ($1\cdot10^{-5}$) in Aspen HYSYS. In addition, 87 mol.% of the H_2S compound was separated at an acidic gas stream, which leads to an acceptable H_2S loading. All this was done by using twenty-one stages in the stripper tower to obtain a good ratio of H_2S at the top and MDEA at the bottom for recycling back again to the extraction tower.

The effect of MDEA feed flow rate on hydrogen sulfide concentration was studied, as the flow rate of both sweet and sour gas streams increased with increasing MDEA concentration. The optimization was applied to study the changes in the revenue amount and select the optimum parameter at the specific value of H_2S in sour or sweet gas.

As a result of the use of HYSYS model, the gas finally complies with gas pipeline criteria due to its significant acid extraction.

Table 3

Primary variables and main objects for optimization

Object	Variable	Low bound	Current value	High bound
amine circulation rate	mass flow	227	1000	1200
sour LPG	mass flow	1210	2421	3000
acid gas	pressure	0.5	1	2
to regenerator	temperature	45	90	120

Table 4

Operating conditions for optimized LPG sweetening units

Parameter	Original values	Optimized values	Profit, \$/h
Mass flow (kg/h)-sour LPG	2421	3000	5023.5
Amine circulation rate (kg/h)	1000	1110	4068.35
Temperature (^{0}C)	90	77.5	4033

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МОДЕЛЮВАННЯ І ОПТИМІЗАЦІЯ ПРОЦЕСУ ВИДАЛЕННЯ КИСЛОТНИХ ГАЗІВ ЗІ СКРАПЛЕНОГО НАФТОГАЗУ ЗА ДОПОМОГОЮ ASPEN HYSYS

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Скраплений нафтогаз (СНГ) є одним зі звичайних видів вуглеводневих палив, які можуть бути одержані з природного газу або нафти. У будь-якому випадку він містить домішки, такі як H_2S і CO_2, які слід видаляти для одержання очищеного від сірки скрапленого нафтогазу з високою концентрацією вуглеводнів, таких як етан, пропан і бутан. Найпоширеніший метод очищення газу від сірки включає використання амінових сполук, які мають різноманітні типи, кожен з яких призначений для конкретного та вибіркового видалення кислотних газів. У цьому дослідженні метилдіетаноламіну (42 мас.%) використовувався як розчинник для виділення кількості H_2S приблизно 0,8% з кислого СНГ за температури 40^{0}С. Мета цього дослідження полягає в моделюванні та оптимізації блоку очищення СНГ від H_2S з використанням Aspen HYSYS V11 для вивчення різних параметрів, що впливають на розділення кислотних газів та досягнення високої прибутковості. Було досліджено вплив кількості тарілок в екстракторі, швидкості циркуляції, температури, масових і мольних потоків, а також інших параметрів на зменшення концентрації H_2S до 0% в обробленому потоці СНГ. Процес очищення був запропонований для того, щоб забезпечити СНГ високим рівнем певних функціональних характеристик, таких як калорійність та чистота, крім того, він екологічно безпечний.

Ключові слова: Aspen HYSYS, видалення H_2S, скраплений нафтогаз, метилдіетаноламін, процес очищення від сірки.

SIMULATION AND OPTIMIZATION OF A LIQUIFIED PETROLEUM GAS SWEETENING PROCESS USING ASPEN HYSYS

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Liquefied petroleum gas (LPG) is one of the common fossil fuels that can be derived from natural gas or crude oil. In either case, it contains impurities such as H_2S and CO_2, which should be removed to obtain sweet liquified petroleum gas with a pure concentration of hydrocarbons such as ethane, propane, and butane. The most common method of gas sweetening process is by using amine compounds, which come in various types, each designed for specific and selective removal of acidic gases. In this study, methyldiethanolamine (42 wt.%) was used as a solvent to extract approximately 0.8% of H_2S from sour LPG at a temperature of 40^0C. The objective of this study focuses on simulating and optimizing the LPG sweetening unit using Aspen HYSYS V11 to investigate the different parameters that affect the separation of acidic gases and to achieve high profitability. The number of trays, circulation rates, temperature, mass and molar flow rates, and other parameters were studied to reduce the H_2S concentration to 0% in the treated LPG stream. The sweetening process was proposed to produce LPG with high levels of specific preferred specifications such as calorific value and purity, in addition to being environmentally friendly.

Keywords: Aspen HYSYS; H_2S removal; liquefied petroleum gas; methyldiethanolamine; sweetening process.

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