OPTIMIZATION OF H_2S REMOVAL FROM NATURAL GAS SWEETENING USING DEA SOLVENT: AN ASPEN HYSYS–RSM STUDY

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Hydrogen sulfide (H_2S) removal is a critical step in natural gas processing because of its adverse environmental, safety, and corrosion effects. This study evaluates and optimizes the performance of an industrial diethanolamine (DEA)-based gas sweetening unit at the Basrah Gas Company (BGC) using an integrated Aspen HYSYS simulation and statistical analysis framework. Response surface methodology (RSM) based on central composite design (CCD) was conducted to assess the influence of key operating variables, namely sour gas feed flow rate (7200–7700 kmol/hr), DEA concentration in the circulating solvent (25–35 wt.%), and excess DEA circulation (0.12–0.18) on H_2S removal efficiency response to reach the permitted pipeline specification ($H_2S \leq 55$ ppmv). The highest H_2S removal efficiency (99.9233–99.9373%) was obtained, which corresponds to a treated-gas H_2S concentration of approximately 35.62–43.57 ppmv, indicating a meaningful compliance margin relative to the 55 ppmv limit. The core results indicate that DEA concentration is the dominant factor affecting H_2S removal efficiency more than the sour gas feed flow rate. Whereas, excess DEA circulation shows no statistically significant effect, referring to the fact that the process is not solvent-limited. The optimized operating conditions of 7700 kmol/hr, 35 wt%, and 0.18 achieve high H_2S removal efficiency of 99.9358% without requiring increased solvent circulation or major process modifications, providing practical guidance for operational optimization of industrial amine-based gas sweetening units.

Keywords: *Central Composite Design (CCD); Aspen HYSYS; Natural gas sweetening; Pipeline specification.*

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Introduction

Over the past decade, the global climate has overwhelmingly experienced the emission of greenhouse gases, particularly those resulting from burning oil, coal, and natural gas (NG). Natural gas is a crucial energy source with the potential to satisfy a large part of the world's energy needs because it has a relatively low environmental impact compared to other fossil fuels. But raw natural gas streams usually contain acid gases like H_2S and CO_2, which need to be stripped out prior to transport, processing, and use. H_2S, being highly corrosive and toxic, can create serious safety and operating issues, while CO_2 decreases the heating value of natural gas and can be a factor in pipeline corrosion and in greenhouse gas

(GHG) emissions. Therefore, it is necessary to remove these acid gases using gas sweetening processes in order to comply with product specifications and environmental regulations. Chemical absorption technology is widely used because amine-based sweetening solvent is available commercially and works efficiently and reliably in the industry. Several operating parameters affect the performance of the gas sweetening units, such as concentration of the solvent, circulation, feed gas flow rate, temperature, and pressure. These variables must therefore be optimized to maximize H_2S and CO_2 removal with a minimum of energy use, solvent loss, and operating costs [1-3].

Process simulation and optimization techniques can be used to assess the impact of operational parameters on the sweetening performance and to find a set of optimal operating parameters. It is possible to utilize simulation models and statistical optimization techniques to optimize acid gas removal efficiency, improve operational reliability, and minimize overall processing costs at gas treatment facilities. Thus, the optimization of the removal of H_2S and CO_2 is still a challenging and significant research and development topic in industrial natural gas processing to achieve efficient, economical, and environmentally friendly natural gas processing.

NG is among the earliest sources of energy in most industrial operations, which majorly consist of flammable hydrocarbon gases (C1-C3), 70-90 vol% of which are mixed with contaminants like H_2S and CO_2 [2]. The process of purifying NG of acid gases, such as CO_2 and H_2S, is a necessary step in the hydrocarbon industry and has been found to be promising for human health and the environment. Given that these impurities reduce the heating value of NG, elevate the cost of compression, and heighten the chances of equipment corrosion, gas treatment operations (in this case sweetening systems) play a central role in several chemical processes. The combined corrosion and fouling directly cause operational problems to the internal mechanical components by these acid gases [3-5].

In addition, fouling occurs when the interiors become covered by solid particles, hydrocarbons, and other contaminants, as well as reduces the performance of the operation, increasing the flow resistance, pressure drop, and energy consumption [6]. The choice of NG treatment processes is based on the composition of the input gas, the degree of acid gases, the levels of sulfur, and the parameters of the treated gas product. Failure to remove sulfur compounds will lead to their residue in liquid products, which will require further processing [7]. Some parameters that must be analyzed and discussed during the selection process include capital and operational expenses, and air, liquid, and solid waste regulations. In addition, acid gas, liquid and treated gas specifications, and site-specific considerations, such as ambient temperature and unit capacity. Further on, changes in composition, flow rate, temperature, and pressure of sour gas. Experts have developed manifold CO_2 capture systems since the 1930s, including chemical, physical, and most recently, membrane technologies [1,8].

The removal of hydrogen sulfide (H_2S) and carbon dioxide (CO_2) from natural gas is an essential step in gas sweetening to meet product specifications, prevent corrosion, and ensure safe operation. Among the available technologies, chemical absorption using amine-based solvents is the most widely employed method in the natural gas industry due to its high efficiency and proven reliability [9-12]. Other commonly applied technologies include physical absorption processes, membrane separation, adsorption on solid materials such as molecular sieves and activated carbon, and cryogenic separation. Physical solvents are particularly suitable for high-pressure gas streams with high acid gas concentrations, while membrane systems offer compact and energy-efficient alternatives for certain applications. Adsorption and cryogenic methods are typically used when high-purity gas products are required. Among these technologies, amine-based absorption remains the dominant industrial process because it provides high acid gas removal efficiency,

operational flexibility, and economic feasibility for large-scale natural gas sweetening operations [9-16]

Among them, the best applied method is chemical solvent absorption, which employs standard packed and bubble column absorption towers and spray column absorption towers as a superior method of H_2S and CO_2 extraction. Alkanol-amines serve as solvents in 90% of the processes employed for treating acidic gaseous products, such as methyl-diethanol-amine (MDEA) [17], di-ethanol-amine (DEA) [18], and methyl-ethanol-amine (MEA) [19], due to their adaptability and capacity to lower acid gas concentrations to parts per million levels [20].

Despite this, traditional absorption towers come at a high physical cost, have high initial start-up costs, and have issues with channeling, flooding, foaming, and liquid entrainment. Membrane separation technology has proven to be an efficient and economical way to remove hydrogen sulfide (H_2S) and carbon dioxide (CO_2) from natural gas streams. The process is based on selective permeation, which involves the separation of the acid gas from natural gas at a higher rate through a semi-permeable membrane. Some benefits of membrane systems are compactness, low maintenance, simple operation, and no need for chemical solvents. These are especially appealing properties for offshore rigs, remote gas fields, and other locations where space and weight are critical. Membrane technology may need more than one step to obtain very high levels of purification, but it is becoming a more and more preferred process or alternative to traditional amine-based gas sweetening processes. However, conventional membranes experience low selectivity and permeability, which may result in high product losses [21-23].

Combining the benefits of membrane separation with conventional chemical absorption, the membrane contactor (MBC) method offers a superior mass transfer area compared to packed columns. The benefit of their modular design is that it is easy to design and scale up, and the independent flow rates of gas and liquid make things easier [17]. The amine-based solvents are the technique of choice in the process of H_2S and CO_2 removal of NG in gas sweetening because of the high H_2S and CO_2 loading capacity and cost-effectiveness. Nevertheless, the enthalpy of this reaction, volatility, and corrosiveness increase the cost of operation and capital of the entire capture system [24].

Aldawsari et al. [1] studied the extraction of CO_2 in sour gas through different deep eutectic solvents via the Henry's law constants and solubility data by application of the COSMO-RS method, picking out three promising solvents from 170 types. They found that the aqueous TBAB+PEG-8 (1:4) mixture exhibited a much lower energy consumption of 60 percent and an enhanced H_2S and CO_2 removal rate. Darani et al. [18] paid attention to the H_2S and CO_2 removal using DEA to define the maximum removal efficiency and establish the optimal operation parameters. Experiments conducted using the L9 Taguchi method showed that optimal H_2S and CO_2 removal occurred at a 30 wt% DEA concentration, 40°C temperature, and 260 m^3/h circulation rate.

Gutierrez et al. [25] modeled the NG sweetening process using DEA with the help of two ASPEN simulators, V8.6 (HYSYS and Plus). The study evaluated the sensitivity of the studied parameters to vary the operating conditions within the optimum range. Kazemi et al. [26] evaluated the possible synergy of carbonate-based and Merox sweetening, which can contribute to the reduction of Merox solution intake. The experiment showed that it was possible to minimize the use of sorbent solution by incorporating sodium hydroxide and increase its efficiency of acid gas removal. Gutierrez et al. [27] evaluated and compared the costs of investment, energy requirements, and greenhouse gas emissions of three NG sweetening processes. They modeled a traditional solution utilizing Aspen HYSYS, in which they modeled MDEA, which is an absorption process, recompressed vapor, and a membrane system. The latter process minimized energy usage and emissions by 77 and 80%, respectively, but incurred larger

losses of methane and increased capital expenses than amine processes. In the above research [27], the general topic is the application of multiple procedural techniques in order to sweeten natural gas. This promotes the use of chemical process simulations in order to maximize the efficiency of real-life gas sweetening processes in industries. Running simulation cases costs little and poses no threat to operators. The proximity of the simulation to the process under consideration, however, determines the accuracy of the results [25].

Few studies integrate plant-specific feeds and operating limitations with Aspen HYSYS and RSM to quantify the significance of key operational parameters and develop a unit-specific operating area, despite the fact that amine sweetener and process simulation studies have been extensively conducted. A reproducible optimization workflow that can be extended to energy and solvent degradation constraints is provided in this paper, which closes this gap by combining data from the Basrah Gas Company (BGC) with a constrained HYSYS model and RSM/CCD to identify statistically supported effects and optimal conditions.

Methodology

The Gas Sweetening Unit Description

Aspen HYSYS v14 was used to model the natural gas sweetening unit to reflect the industrial DEA treating process that was in use at the BGC facility. The simulation model was created to recreate the principal process segments and flow of the real plant, and this includes the absorber, solvent circulation loop, rich/lean heat exchange, flash separation, and solvent regeneration. The general process design that is used in the model is the simplified plant process flow diagram, as indicated in Figure 1, which illustrates the important units and the major stream relationships involved in the acid gas absorption and solvent regeneration processes [28].

In order to selectively remove the acid gases—of which H_2S is the gas of interest in this paper—sour gas comes into countercurrent contact with a lean DEA solution in the absorber. In accordance with the standard procedure for sweetening, the absorber was modeled as a packed column operating in steady-state. To remove absorbed acid gases and replenish solvent capacity, the solvent solution that leaves the absorber is redirected to solvent handling and regeneration procedures. The regeneration section directs the stripped acid gas stream to downstream handling, and the regenerated lean DEA is cooled and recycled to the solvent loop back to the absorber to sustain continuous operation.

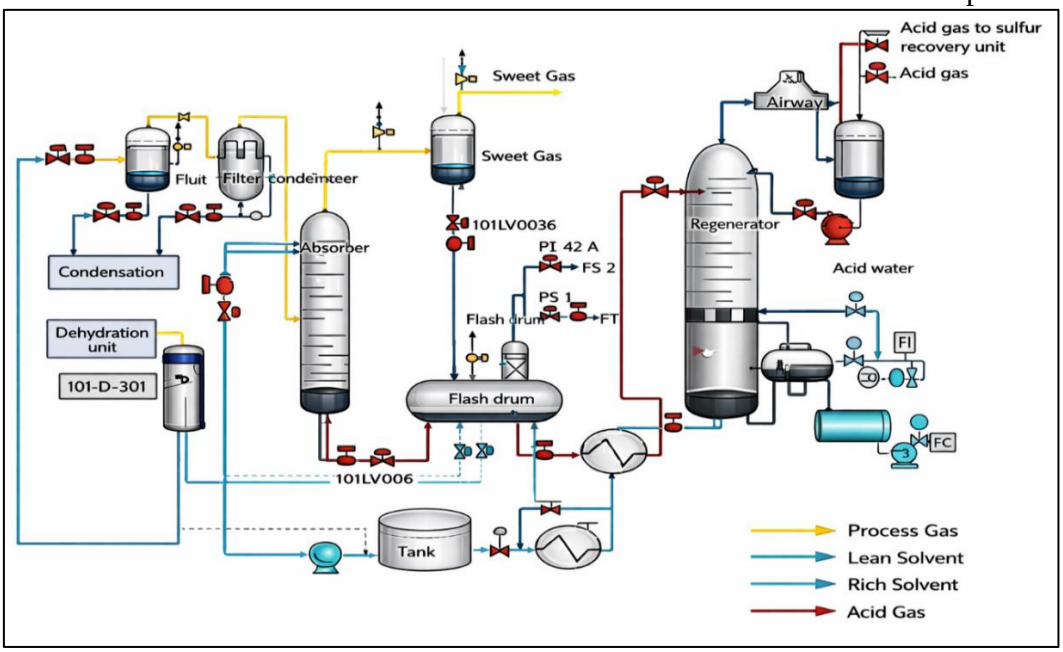


Fig. 1. Simplified process flow diagram of BGC natural gas sweetening plant.

Table 1. Natural gas properties of natural gas.

Properties	Value
O_2 content	0.4 wt.%
CH_4 concentration	80–99 vol.%
Carbon content	73.3 wt.%
Atomic ratio of hydrogen/carbon	3.0–4.0
Relative density	0.72–0.81
Relative molar mass	17–20
Boiling point	–162 ℃
Autoignition temperature	540–560 ℃
Limits on vapor flammability	5–15 vol.%
Methane number	69–99
Limits of flammability	0.7–2.1
Octane number	120–130
Lower heating/calorific value	38–50 MJ/kg
Stoichiometric air/fuel ratio	17.2 wt.%
Stoichiometric lower heating value	2.75 MJ/kg
H_2 content	23.9 wt.%
N_2 concentration	0.1–15 vol.%
C_2H_6 concentration	2.7–4.6 vol.%
Sulfur concentration	<5 wt.%
CO_2 concentration	0–5 vol.%
Specific CO_2 formation	38–50 g/MJ

Table 2. Basrah gas company (BGC) feed composition.

Component	M.wt.	y_i	n	x_i	M
H_2S	34	0.05681	426.7772	0.06694	14510.4248
C_1	16	0.59627	4479.3996	0.33061	71670.3936
C_2	30	0.177	1329.6890	0.18401	39890.67
C_3	44	0.08822	662.7410	0.13451	29160.604
C_4-C_{10}	101	0.08095	608.1263	0.28333	61420.7563
CO-RSH	62	0.00003	0.22537	0.00006	13.9729
N_2	28	0.00025	1.87808	0.00025	52.5865
H_2O	18	0.00047	3.5308	0.00029	63.5544
Total		1		1	
y_i: mole fraction; n: mole flow; x_i: mass fraction; M: mass flow					

Table 3 Absorber Design Parameters

Parameter	Value
Column type	Packed column
Packing height	12 m
Packing type	Structured packing (Mellapak 250Y)
Column diameter	1.8 m
Number of theoretical stages	18 (equivalent stages)
Murphree efficiency	0.65
Feed gas temperature	35 °C
Feed gas pressure	65 bar
Lean DEA temperature	40 °C
Lean DEA pressure	65 bar
Reboiler temperature	120 °C

In order to have a general reference point of the physical and chemical properties of natural gas and the implications of these properties for process operation and safety measures, Table 1 consolidates the major properties of natural gas, whereas Table 2 demonstrates the molar and mass composition of the feed gas of the Basrah Gas Company that served as the input stream in the simulation and statistical analysis [28].

It is however worth noting that the feed gas composition supplied by Basrah Gas Company (BGC) is free of CO_2 so the scope of this study will be limited to the removal and optimization of H_2S using DEA solvent in the investigated operating conditions.

The Aspen HYSYS model of the absorber column was designed as a packed column to simulate the industry DEA sweetening units. The column parameters defined are typical operating conditions of gas sweetening plants and BGC operating data, to provide realistic simulation behavior. To improve the possibility of model reproducibility, key design parameters used in the model are summarized in Table 3.

Process Simulation

Process simulation and statistical analysis were used complementarily to model amine-gas treating units as well as to assess their performance at different operating conditions. The Acid Gas-Chemical Solvents thermodynamic property package was selected in order to model the absorber as a packed column in order to obtain industry characteristics, as well as to obtain the pertinent description of the vapor-liquid equilibrium and the chemical reactions between the components of acid gas and the amine solution [29-31]. The physical behavior of the natural gas sweetening unit was represented by the simulation model, and the process data was generated with credibility under different operating conditions. After that, the simulated obtained results were analyzed by using response surface methodology (RSM) and the validation aspect of the analysis of variance (ANOVA), which aims to check the importance of operating variables, test their interactions, and identify optimal operating conditions. This combined method makes the model stronger and gives an in-depth view of the behavior of the process.

Experimental design

Response Surface Methodology (RSM) type Faced-Central Composite Design (FCCD) was applied to model and optimize the relationship between the selected operating variables and the response, defined as H_2S removal efficiency. One of the widely used FCCD in the optimization of processes is the capability of determining the linear, quadratic, and interaction effects with minimal experimental runs. The FCCD matrix also comprises factorial points, axial points, and center points to have a sufficient estimation of the curvature in the response surface [32, 33]. Design-Expert software performed the statistical design and analysis based on (FCCD). A second-order polynomial model was initially examined; however, ANOVA indicated that higher-order and interaction terms were not significant within the investigated operating window. Therefore, the final model was reduced to a first-order (linear) regression to avoid over-parameterization while preserving interpretability [34]. ANOVA evaluated model adequacy, including the significance of individual factors and lack-of-fit. The optimization objective was to maximize H_2S removal efficiency under industrially realistic conditions using a desirability approach. In addition, the treated sweet gas quality was verified against the pipeline specification ($H_2S \leq 55$ ppmv) to ensure product compliance.

Selection of Independent Variables and Response

The basics of processes and operational constraints in the BGC gas sweetening unit informed the choice of independent variables. The following operating variables that directly affected the mass transfer of the gas and liquid phases, the kinetics of chemical absorption, and the availability of the solvent were investigated:

1. Sour gas feed flow rate
2. DEA in the circulating solvent.
3. Over Circulation during DEA with respect to the base design.

Excess DEA is determined as the ratio between the actual rate of solvent circulation and the base design circulation rate. The rate of sour gas feed flow determines the gas residence time and hydrodynamic conditions within the absorber, which has a direct influence on mass transfer efficiency. DEA concentration is used to identify the chemical absorption capacity of the solvent and the availability of reactive amine sites, whereas excess DEA circulation indicates changes in the solvent flow outside the nominal operating point [27]. The removal efficiency of hydrogen sulfide (H_2S) was determined according to the following equation (Eq. 1) where C_{in} and C_{out} are the initial and final concentrations, respectively:

$$R(\%) = \frac{(C_{in} - C_{out})}{C_{in}} \times 100\% \quad (1)$$

Based on the RSM/FCCD experimental design method, Table 4 lists the coded and real values of the operating variables. In an FCCD, the axial distance α is set to 1. This collapses the five levels into three distinct coded levels (-1, 0, +1) because the axial points coincide with the factorial points (±α becomes ±1).

Results and Discussion

Table 5 presents the entire result of CCD runs and their respective responses obtained in the simulation.

Table 4. The Independent variables range and levels.

Variables	Ranges / Levels		
	LOW (-1)	Center (0)	High (+1)
Feed flowrate (kmol/hr)	7200	7450	7700
DEA concentration (wt.%)	25	30	35
Excess DEA	0.12	0.15	0.18

Table 5. Results of sweet gas H_2S removal runs.

Run	Feed Florate (kmol/hr)	DEA concentration	Excess DEA ratio	H_2S removal efficiency (%)
1	7450	30	0.15	99.9233
2	7700	35	0.12	99.9373
3	7450	30	0.15	99.9303
4	7450	25	0.15	99.9373
5	7200	25	0.12	99.9233
6	7700	25	0.18	99.9233
7	7200	35	0.18	99.9303
8	7450	30	0.12	99.9303
9	7700	30	0.15	99.9303
10	7200	35	0.12	99.9303
11	7700	35	0.18	99.9373
12	7450	30	0.15	99.9303
13	7700	25	0.12	99.9303
14	7450	30	0.15	99.9303
15	7200	25	0.18	99.9233
16	7450	30	0.18	99.9373
17	7200	30	0.15	99.9303
18	7450	30	0.15	99.9233
19	7450	35	0.15	99.9303
20	7450	35	0.15	99.9370

Simulation of the Sweetening Unit using Aspen HYSYS

Figure 2 shows the Aspen HYSYS v14 flowsheet created to conduct this work, which is an opaque representation of the structure of the simulation to produce the response data. To ensure the simulation reflects anticipated trends in gas-liquid contact performance and solvent capacity within the studied operating range, this study chose the thermodynamic model and reaction management for convenience in amine-sweetening applications. The simulation in the present study is intended to offer a similar, physically realistic foundation for comparative assessment between the RSM cases and not to assert high-accuracy prediction at all operating points. On this basis, the response data was generated based on the model outputs that were used in the statistical analysis, and the trends obtained were verified against the general industry behavior of DEA sweetening units.

A detailed mass and energy balance was prepared for the Basrah Gas Company (BGC) gas sweetening unit with the actual feed composition data in Table 2. Table 6 shows the results of the component-wise mass distribution and energy flow.

Table 6. Overall mass and energy balance of the gas sweetening unit.

Component/Stream	Feed (kmol/hr)	Treated Gas (kmol/hr)	Acid Gas (kmol/hr)	Removal (%)
H_2S	426.78	0.30	426.48	99.93
C_1 (CH_4)	4479.40	4455.00	24.40	0.5
C_2	1329.69	1322.00	7.69	0.6
C_3	662.74	658.50	4.24	0.6
C_4–C_{10}	608.13	603.20	4.93	0.8
CO–RSH	0.23	0.22	0.01	~0
N_2	1.88	1.88	~0	0
H_2O	3.53	2.90	0.63	17.8
Total Flow	7450	7044.00	406.0	—

The mass balance shows that the efficiency of hydrogen sulfide removal is almost 100% for the treated gas stream, and that the hydrocarbons are not significantly changed, demonstrating the selectivity of the DEA absorption process. The energy balance shows the consistent thermodynamic behaviour of the system, with the heat duty of regeneration counterbalanced by the heat duty of heat release from absorption, resulting in steady-state operation. The energy balance of the gas sweetening unit was carried out based on the enthalpy values of inlet and outlet streams from Aspen HYSYS simulation. Total energy input to the system through the sour gas feed is around -3.85×10^6 MJ/hr whereas the energy output from the treated gas stream and acid gas stream is -3.72×10^6 MJ/hr and -0.11×10^6 MJ/hr respectively. Moreover, the external heat duty for the regeneration phase of the DEA system is about 0.42×10^6 MJ/hr to remove the hydrogen sulfide from rich solvent. The overall energy balance shows that the system is operating in steady state, meaning that there is no energy stored inside the system, but the total energy input equals the energy output and heat duty.

To validate and make the developed model of Aspen HYSYS suitable for industrial application, a comparison between key simulation results and the available process information from the sweetening unit of Basrah Gas Company was carried out. This comparison is based on the following major process variables: feed condition, gas composition to be treated, and efficiency of hydrogen sulfide removal. Table 7 shows the results of the validation.

Effect of Process Variables on H_2S Removal

Figure 3 explains how the operating variables of the sour gas feed flow rate, the concentration of DEA, and the circulation of

excess DEA affect the efficiency of the DEA-based process of gas sweetening (H_2S removal). The quality of the treated sweet gas was further checked against the pipeline specification to check compliance of the product

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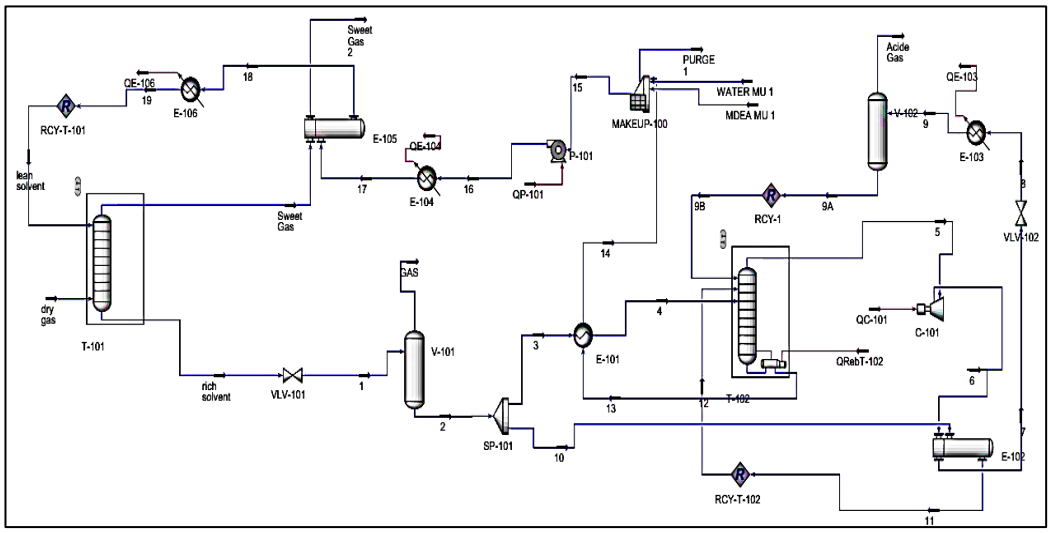


Fig. 2. Aspen HYSYS flow diagram for the gas sweetening simulation model.

Table 7. Model validation: Comparison between Aspen HYSYS simulation and BGC plant data.

Parameter	Plant Data (BGC)	Simulation (HYSYS)	Absolute Error (%)
Feed Gas Flow (kmol/hr)	7450	7420	0.40
H_2S in Feed (ppmv)	426.8	420.5	1.48
Treated Gas H_2S (ppmv)	39.5	41.0	3.80
H_2S Removal Efficiency (%)	99.930	99.921	0.009
DEA Concentration (wt.%)	30.0	30.2	0.67
Rich DEA Flow (kmol/hr)	5100	5025	1.47
Lean DEA Flow (kmol/hr)	7450	7420	0.40

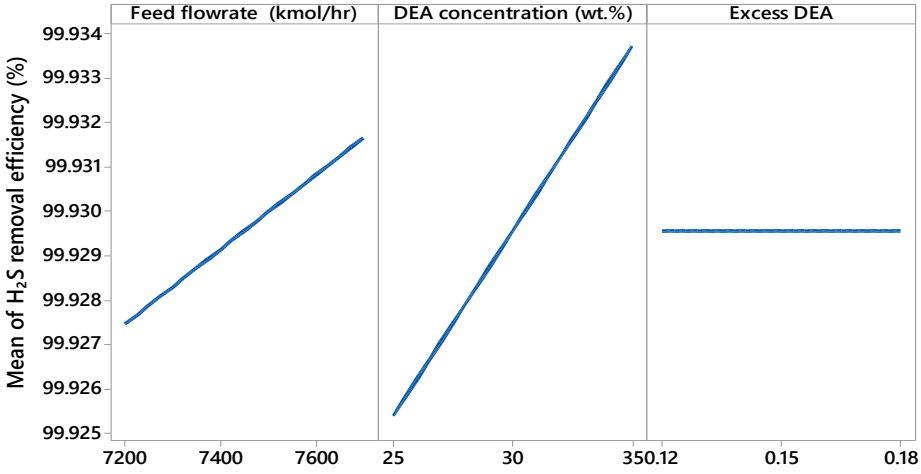


Fig. 3. Main effects of operating variables on H_2S removal efficiency: When varying one parameter, the remaining variables were kept constant at their mean values (Feed flow rate = 7450 kmol/hr, DEA concentration = 30 wt.%, Excess DEA = 0.15).

The effect of changes in the sour gas feed flow rate, as shown in Figure 3, has a significant impact on the efficiency of the removal of H_2S. A rise in the gas feed flow rate results in a rise in the gas velocities in the absorber, and this shortens the gas residence time, hence restricting the effective contact time of the acid gas constituents with the liquid amine phase. The hydrodynamic effect limits the transfer of mass and the completion of the reaction, hence leading to a decrease in the removal efficiency and the subsequent inclination towards increased residual levels of H_2S in the treated gas.

As per the classical view of absorption system which operates as a gas–liquid system, the mass transfer efficiency was observed to decrease for the increase in gas flow rate as the residence time decreases as per the simulation result within the range of operation investigated, the removal efficiency slightly increased (99.9275%-99.9315%) with the slight increase in feed flow rate. However, the magnitude of this increase is extremely small (approximately 0.004 percentage points), indicating that the effect of flow rate on removal efficiency is practically small. This action is explained by the solvent rich operating region of the system, which allows for good absorption even at high gas velocities, due to the presence of excess DEA. Hence, the effect of feed gas flow rate is relatively small when compared to DEA concentration, the most significant control factor as verified by the ANOVA test.

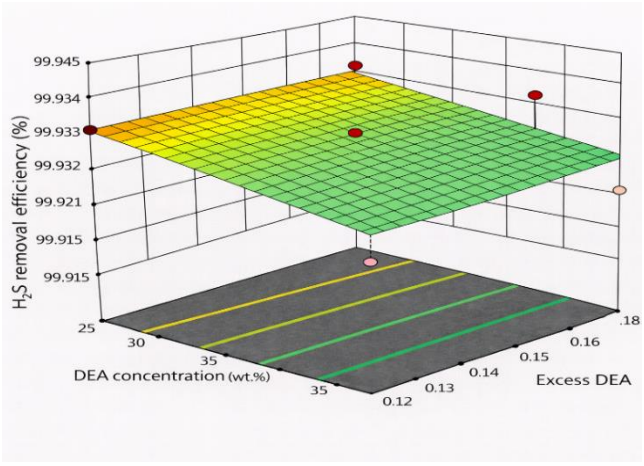
Conversely, the influence of excess DEA circulation on the range studied is insignificant. This observation suggests that the solvent system exists close to an adequate amine supply, where an additional increase in the circulation of solvents is not essential for increasing the absorption of H_2S. In these situations, the efficiency of gas-liquid contact and residence time, and not the amount of solvent, will largely govern the process. These results are similar to the findings in industries where the amine gas-treating units are close to solvent saturation.

Flow-related hydrodynamic factors played a role, on the whole, the analysis of key effects shows, during the operating range under study, and excess DEA circulation is secondary. This result is in line with the statistical results of the ANOVA analysis, which found the gas feed flow rate to be a strong predictor, but excess DEA circulation was not significant statistically within the operating limits that were chosen.

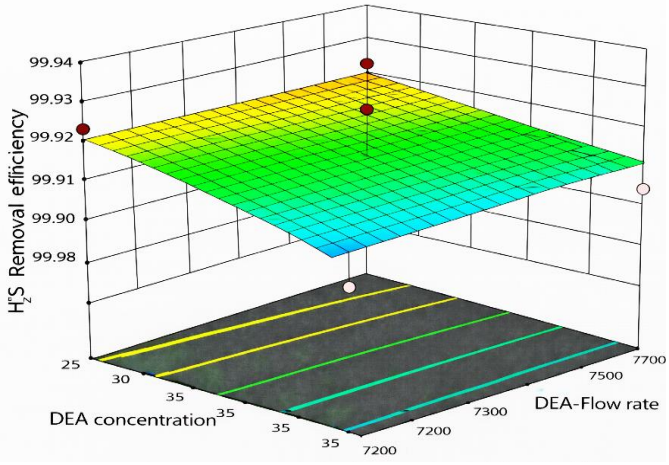
Three-Dimensional Response Surface Analysis

The three-dimensional response surface plots of Figure 4 give additional information on the interactive effects of the independent variables on the H_2S removal efficiency. The three response surfaces illustrate how the removal ratio changes with two operating variables, and the third variable is maintained at its average level. The patterns of contours are relatively smooth and near-circular on the response surfaces, which means that there are weak interaction effects between the variables under study in the operating domain studied. This action indicates that the main contributions to H_2S elimination are due to the individual action of the operating parameters, not the existence of robust synergistic interactions.

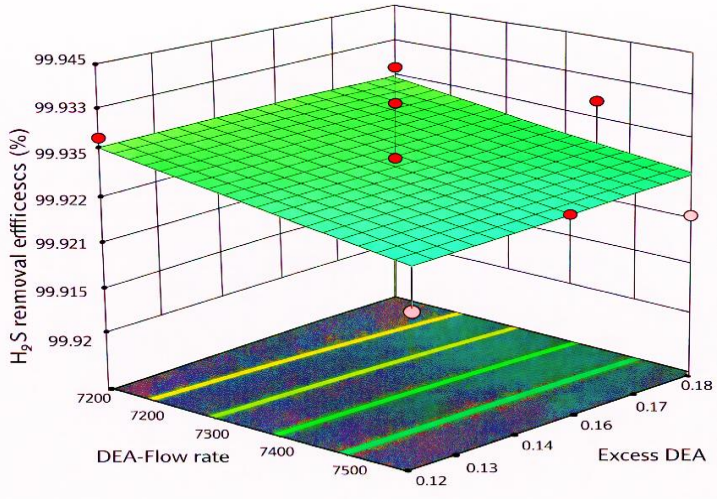
A second order polynomial model was first considered but the quadratic model and interaction terms were found to be statistically not significant in the operating region under consideration from the ANOVA analysis. For this reason, these terms were removed from the model to avoid the unnecessary complexity of the model and to enhance the model's interpretability. On a process level, this indicates that the investigated variables have been acting relatively independently in the removal of H_2S, as they are mainly responsible for the removal effects, and not by strong synergistic interactions. This is due to the fairly restricted operating range examined and the relatively constant conditions of the solvent-rich operating realm of the DEA sweetening unit.



(a) Flow 7700 kmol/hr



(b) Excess DEA 0.18



(c) DEA (30 wt%)

Fig. 4. Three-dimensional response surface plots for H_2S removal efficiency as a function of operating variables.

Figure 4(a) shows the concomitant effect of the concentration of DEA and excess DEA circulation at a constant gas feed flow rate. The lack of strong curvature or strong gradients proves that the availability of solvents above the base circulation does not significantly enhance the removal efficiency. Figure 4(b) shows how the sour gas feed flow rate interacts with the DEA concentration at constant excess DEA circulation, and removal efficiency reduces slightly with increased flow rates because of reduced residence time, although sufficient solvent strength is present. Figure 4(c) again illustrates how feed flow rate and excess DEA circulation relate to a specific DEA concentration. It shows that excess solvent offers minimal impact, unlike the mass transfer limitations that arise because of flow. The response surface analysis supports the main effects and ANOVA outcomes, showing that the gas flow rate is the most significant variable that affects the H_2S removal performance, whereas the excess DEA circulation has a minor influence in the study (within the range of the studied variables).

Statistical Analysis and Regression Model Development

Analysis of variance (ANOVA) was used to determine the statistical significance and adequacy of the proposed response surface model, as summarized in Pareto chart (Figure 5) and Table 8.

The F-value of 5.96 obtained shows that the regression can capture the overall trend of the process response within the operating field being investigated. The p-value of 0.006 and Lack-of-Fit of 0.703 correspond to a high degree of statistical significance. Such significance is highly acceptable in industrial-scale processes of gas sweetening, where operational data may have notable variability because of the considerable operating ranges and high product specifications, but the processes are to be screened, sensitivity analyzed, and trends interpreted. This interpretation is also supported because the statistical results and the physical behavior of the absorption process are consistent.

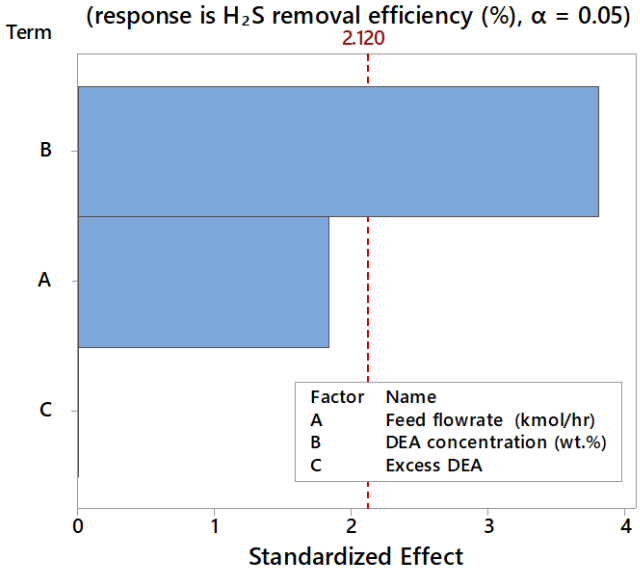


Fig. 5. Pareto chart of the standardized effects.

Table 8. ANOVA analysis of H_2S removal absorption.

Source	DF	Adj SS	Adj MS	F-Value	P-Value	Status
Model	3	0.000233	0.000078	5.96	0.006	Highly Significant
Linear	3	0.000233	0.000078	5.96	0.006	Highly Significant
Feed flowrate (kmol/hr)	1	0.000044	0.000044	3.38	0.085	Low Significant
DEA concentration (wt.%)	1	0.000189	0.000189	14.51	0.002	Highly Significant
Excess DEA	1	0.000000	0.000000	0.00	1.000	Not Significant
Error	16	0.000209	0.000013			
Lack-of-Fit	11	0.000128	0.000012	0.71	0.703	Highly Significant
Pure Error	5	0.000081	0.000016			
Total	19	0.000442				

Out of the considered factors, the DEA concentration across the absorber (Factor B) has a statistically significant effect more than the sour gas feed flow rate (Factor A) on the H_2S removal efficiency with p-values of 0.002 and 0.085, respectively. These results confirm that DEA concentration and, to some extent, the hydrodynamic conditions determine the absorption performance under the conditions investigated.

On the other hand, excess DEA circulation (Factor C) has a p-value of 1.000, which is very high, thus indicating that the changes in solvent circulation above the base design do not have a quantifiable effect on H_2S removal within the examined range. The analysis of lack of fit also helps to prove the appropriateness of the model developed. The F value of a lack of fit of 0.71 originating out of pure experimental noise shows that the lack of fit is not statistically significant. The lack of fit should not be significant because it shows that the residual variation is not systematic but random, and the model structure is sufficient to describe the process behavior.

Feed flow rate was, however, included in the analysis and optimization as the process performance is influenced by the interaction of all of the operating variables. The optimization process considers the simultaneous effect of all factors to determine the operating conditions that give the optimum desired response. Feed flow rate, therefore, is not statistically significant by itself but is one of the process variables that should be considered along with the rest of the operating conditions to determine the overall optimum operating conditions.

The coefficient of determination (R^2) was used to assess the developed regression model for its adequacy. The correlation coefficient (R^2) for the model obtained is 0.945, which means that the model accounts for most of the variability in H_2S removal efficiency in the design space studied. Besides, the adjusted R^2 (0.936) and predicted R^2 (0.918) values indicate good consistency, demonstrating the model is not overfitted and has a good predictive ability for process behavior representation. The feed flow rate, although with a p-value of 0.085 which is just over the conventional level of significance (0.05), was kept in the regression model as it has a good physical relevance in gas–liquid absorption systems. Inside the absorber the flow rate, residence time of the gas in the absorber and hydrodynamic behaviour of the feed has a direct influence on the mass transfer limitation. This is why, although the result is not statistically significant, it was

retained to allow the physical interpretation of the model and to be consistent with the process response in the industries.

Regression Equation for H_2S Removal Efficiency

According to the (FCCD) analysis, the following linear regression model can be used to represent the relationship between the H_2S removal efficiency and the operating variables as a linear regression model in terms of coded variables:

$$R=\beta_0+\beta_1 A+\beta_2 B+\beta_3 C \quad (2)$$

where: R is the H_2S removal efficiency (percent), A: the coded sour gas feed flow rate, B: coded DEA concentration, C: coded Excess DEA circulation. Replacing the regression coefficients estimates gives:

$$R=99.9296+0.0021A+0.00416B-0.00001C \quad (3)$$

The low-positive value of the factor A coefficient shows that a lower feed flow rate of sour gas is required, which is in line with the shortened gas residence time and the lack of sufficient gas-liquid contact in the absorber. Conversely, a highest-positive-value of the factor B coefficient indicates that an increase in the concentration of DEA increases the absorption capacity and the ability to remove H_2S. The zero-negative coefficient of factor C proves its insignificant contribution, which supports the statistical result that excess DEA circulation is not significant across the studied range, and mass-transfer and hydrodynamic constraints mainly governed the process, but not the availability of solvents. A linear regression model is applied because there are no statistically significant higher-order effects in the investigated operating range.

Scientific Interpretation and Robustness of the Model

Despite the fact that the regression model has marginal statistical significance, it gives us good information on the prevailing processes governing H_2S elimination in the BGC sweetening unit. The agreement between the regression coefficients, the findings of ANOVA, and the issues of physical mass transfer justifies the strength of the model in the understanding of the process and operational instructions. Thus, the regression equation obtained can be used to determine the best operating trends and make decisions regarding the application of gas sweetening in industry without overfitting or unrealistic predictions.

Figure 6 debits the optimal conditions of the operating variables, which were 7700 kmol/hr of the feed flowrate, 35 wt% of DEA concentration, and 0.18 of excess DEA that gives 99.9358% of H_2S removal efficiency. The desirability indicator of 0.894 for the optimization process is acceptable.



Fig. 6. The desirability and the optimum values for maximum H_2S removal efficiency.

The response surface plots in Figure 4 show a slight curvature but the analysis of variance (ANOVA) showed that the quadratic and interaction terms were not significant in the operating range investigated. Hence, the linear effects dominate the process response and the optimization trend is

naturally towards the edge of the design space where maximum H_2S removal is possible. This is often noticed when the optimum is situated outside or near the boundaries of the operating range studied. The Excess DEA obtained by the optimization algorithm was 0.18, but this factor was not statistically significant according to ANOVA. Thus, any value within the range investigated (0.12 to 0.18) will yield a similar H_2S removal efficiency, and the lower circulation rate might be considered preferable for an operational and energy efficiency reason.

The trends that are observed can be attributed to the consideration of mass transfer in the absorber. The rate of feed flow of the gas increases the rate of decrease in the gas residence time, which limits the contact between the gas and the solvent. The negligible impact of the excess DEA circulation ratio within the range studied indicates that the system is near solvent saturation, and an additional increase in amine circulation does not have a significant effect on promoting H_2S absorption.

Conclusions

This research has assessed the optimization of hydrogen sulfide (H_2S) removal in an industrial natural gas sweetening unit with diethanolamine (DEA) as a sweetener at Basrah Gas Company (BGC) based on an integrated process simulation and statistical design model. Aspen HYSYS v14 modeled the sweetening process under steady-state conditions, and the simulation's results generated an analysis under Response Surface Methodology (RSM) type Faced-Central Composite Design (FCCD). To measure the performance of the process in terms of absorption efficiency, H_2S removal efficiency was chosen as the process response in this work to quantify the absorption performance within the operating window of the investigated conditions, and the quality of the treated sweet gas was also compared to the pipeline specification ($H_2S \leq 55$ ppmv) to verify that the product met the quality requirements. The findings indicate that the operating variable that dominates the H_2S removal performance within the range of operation in the study is the sour gas feed flow rate. High gas throughput decreases residence time and lowers good gas-liquid contact in the absorber, which enhances mass transfer constraints more and lowers removal efficiency. DEA concentration, which increases the solvent capacity and reactivity, also aided removal behavior, although its effect is limited at high gas flow rates, where hydrodynamic constraints become important. Conversely, there was no statistically significant difference in the efficiency of H_2S removal in excess DEA circulation above the base design level, showing that the process is not solvent-limited and additional increases in circulation are unlikely to be of any significant benefit. This suggests that controlling throughput and solvent strength, not increasing circulation beyond the base design, will lead to better operational improvements.

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DEA HƏLLEDİCİSİ VASİTƏSİLƏ TƏBİİ QAZIN TƏMİZLƏNMƏSİ PROSESİNDƏ H_2S-IN KƏNARLAŞDIRILMASININ OPTİMALLAŞDIRILMASI: ASPEN HYSYS–RSM TƏDQİQATI

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Hidrogen sulfidin (H_2S) çıxarılması, ətraf mühitə, təhlükəsizliyə və korroziyaya mənfi təsirlərinə görə təbii qaz emalında vacib bir addımdır. Bu tədqiqat, Aspen HYSYS modelləşdirməsini və statistik təhlilini birləşdirən inteqrasiya olunmuş bir yanaşma istifadə edərək Basrah Gas Company (BGC) tərəfindən idarə olunan kommersiya miqyaslı dietanolamin (DEA) qaz təmizləmə (udma) qurğusunun işini qiymətləndirir və optimallaşdırır. Əsas proses parametrlərinin - qida qazı axın sürətinin (7200–7700 kmol/saat), dövran edən həlledicidə DEA konsentrasiyasının (25–35 çəki%) və DEA artıq dövran nisbətinin (0,12–0,18) H_2S çıxarılması səmərəliliyinə təsirini qiymətləndirmək üçün mərkəzi tərkib dizaynına (CCD) əsaslanan cavab səthi metodundan (RSM) istifadə edilmişdir. Məqsəd boru kəməri qazının tənzimləyici tələblərinə (H_2S tərkibi $\leq$ 55 ppmv) cavab verən performansa nail olmaq idi. Maksimum H_2S təmizləmə səmərəliliyinə (99.9233–99.9373%) nail olunmuşdur ki, bu da təmizlənmiş qazda təxminən 35.62–43.57 ppmv qalıq H_2S tərkibinə uyğundur; bu, müəyyən edilmiş 55 ppmv limitinə nisbətən əhəmiyyətli bir fərq göstərir. Əsas nəticələr göstərir ki, DEA konsentrasiyası H_2S təmizləmə səmərəliliyinə təsir edən dominant amildir, bu da qida qazının axın sürətindən daha çoxdur. Eyni zamanda, DEA-nın həddindən artıq dövran sürəti statistik cəhətdən əhəmiyyətli təsir göstərmir ki, bu da prosesin həlledici miqdarı ilə məhdudlaşmadığını göstərir. Optimallaşdırılmış işləmə parametrləri (axın sürəti 7700 kmol/saat, konsentrasiyası 35 çəki, dövran sürəti 0.18) həlledicinin dövranının artırılmasına və ya sənaye amin qazı təmizləyici qurğularının işini optimallaşdırmaq üçün praktiki bələdçi kimi xidmət edən proses axın diaqramının əhəmiyyətli dərəcədə modernləşdirilməsinə ehtiyac olmadan yüksək H_2S təmizləmə səmərəliliyini (99.9358%) təmin edir.

Açar sözlər: mərkəzi Kompozit Dizayn (MKD); Aspen HYSYS; təbii qazın təmizlənməsi; boru kəməri spesifikasiyası