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Process Modeling, Optimization and Cost Analysis of a Sulfur Recovery Unit by Applying Pinch Analysis on the Claus Process in a Gas Processing Plant

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Abstract: The Claus process is one of the promising technologies for acid gas processing and sulfur recovery. Hydrogen sulfide primarily exists as a byproduct in the gas processing unit. It must be removed from natural gas. The Environmental Protection Agency (EPA) notices that increasing SO_2 and CO_2 in the air harms the environment. Sulfur generally has an elemental content of 0.1–6 wt % in crude oil, but the value could be higher than 14% for some crude oils and asphalts. It produces SO_2 and CO_2 gases, which damage the environment and atmosphere of the earth, called primary pollutants. When SO_2 gas is reacted with water in the atmosphere, it causes sulphur and nitric acid, called a secondary pollutant. The world countries started desulphurization in 1962 to reduce the amount of sulfur in petroleum products. In this research, the Claus process was modeled in Aspen Plus software (AspenTech, Bedford, MA, USA) and industrial data validated it. The Peng–Robinson method is used for the simulation of hydrocarbon components. The influence of oxygen gas concentration, furnace temperature, the temperature of the first catalytic reactor, and temperature of the second catalytic reactor on the Claus process were studied. The first objective of the research is process modeling and simulation of a chemical process. The second objective is optimizing the process. The optimization tool in the Aspen Plus is used to obtain the best operating parameters. The optimization results show that sulfur recovery increased to 18%. Parametric analysis is studied regarding operating parameters and design parameters for increased production of sulfur. Due to pinch analysis on the Claus process, the operating cost of the heat exchangers is reduced to 40%. The third objective is the cost analysis of the process. Before optimization, it is shown that the production of sulfur recovery increased. In addition, the recovery of sulfur from hydrogen sulfide gas also increased. After optimizing the process, it is shown that the cost of heating and cooling utilities is reduced. In addition, the size of equipment is reduced. The optimization causes 2.5% of the profit on cost analysis.

Keywords: optimization; simulation; Claus process; Aspen Plus; sulfur recapture; pinch analysis

1. Introduction

Different sour gases contain different impurities such as hydrogen sulfide gas, ammonia, carbon dioxide gas, and other waste materials, including nitrogen gas. There is a high quantity of sulfur content in the petroleum product and other contaminants that must be removed for environmental pollution. The elimination of sulfur is an essential objective in petroleum products such as petrol, diesel, and LPG ETC. The removal of sulfur is a rule of the Environmental Protection Agency (EPA) because it causes environmental pollution. H_2S is found in the environment and causes harmful effects on human skin and eyes, as well as breathing problems. The H_2S gas is the raw of dangerous gases such as SO_2, CO_2, and NH_3 gases. Methane gas is the primary resource of H_2S gas. When natural gases are burned in a combustion engine, it causes SO_2 gases and CO_2 gases. Almost all the refineries in the world use the Claus process to remove sulfur, and many refineries produce sulfur at 10 tons per day. Sulfur is the raw material of sulfuric acid [1,2]. An oxygen-based modification was used in the Claus process; there was a modification reported on this process by (1) upgrading the existing systems and introducing a new system; and (2) reducing the equipment size [3,4]. The Claus process is popular engineering for retrieving sulfur and energy from gases. It is conventionally split into thermal and catalytic stages to obtain a very high conversion of acid gas. In 1993, Lurgi Company conducted an experiment on the Claus process with a capacity of 10 tons per day and an efficiency of 99.8%. According to Iranian petroleum research, the incinerator process is still used, which exhausts SO_2 into the environment for the Sulfur recovery process.

Many refineries tire out several thousand ppm of air pollution day after day, attributable to the transformation of the sulfur element to SO_2. A super Claus catalyst was introduced, whereby the reactor operates at a low temperature. A temperature reduced to 255 °C to 200 °C and saved utility decreased tail gas [5]. Researchers worked on the sulfur recovery Claus process to enhance the sulfur recovery level from the natural refinery [6]. They worked on the reaction mechanism occurring in sulfur recovery units, the reaction between H_2S, SO_2, and CO_2, and side reactions, such as hydrolysis of COS and CS_2, and sulfation of catalyst [7–9]. A simulation was performed on MATLAB in which all physical conditions and chemical characteristics were considered. The amount of sulfur entering the first bed was assumed to be 0.1 kmol/h and the amount of Sulfur present in the furnace was also assumed [10,11]. In 2015 a researcher, Nabikandi, worked on simulation of the Claus process with the kinetic and equilibrium method, and kinetic model can predict the composition, temperature, and pressure of the reactor. The reactions mechanism of this Claus process is complex rather than other processes. The modification of the Claus process to increase sulfur recovery by reduced cost is also reported in the literature [12,13]. This modification is a combination of oxygen enrichment and recycled streams. In 2016, Gupta has indicated a comparative kinetic model that can capture the consumption chemistry of H_2S gas and its along with sulfur impurities. It can be improved by changing the chemistry of chemical reactions. In 2016, Mahdipoor worked on the effect of impurities such as mercaptan on the Claus process. The author has built a reaction mechanism of sour gas by using CFD simulation of the furnace reactor and sulfur recovery process [14]. Several studies focused on the integration and simulation of Aspen Plus. The sensitivity of different processes was studied [15–17].

Analysis and thermal efficiency were attained at 45% and corresponding CO_2 and SOx emissions were 698 kg/MWh and 0.15 g/MWh. The optimum analysis of gasification cycles was according to pinch analysis [18]. In 2018, the new design of the Claus process, in which H_2S absorber is desorbed, and SO_2 absorption, the Claus reaction, separation, and recycling in which H_2S and flue gas are absorbed in MDEA. The absorbent of MDEA and sodium citrate are regenerated to reduce the cost of a process [19,20]. In 2018, the solid package of Aspen Plus was used for simulation and optimization of the Claus reactor. Variation in the change in temperature and pressure to observe the H_2S conversion into sulfur. Furthermore, to observe H_2S conversion and sulfur production, Aspen Plus model results calculated and compared the design data [21].

Another study focused on improving the performance of sulfur recovery by using an Aspen Hysys modified three-stage simulation model to study the behavior of sulfur recovery and consider a based case. The performance of the base case is 93.89%. In base case optimization, controlling air demand percent and adjusting the sulfur dew point margin. This margin changes Claus's performance to 98.60% [22]. The effectiveness of each Claus component would depend on this Claus unit's reactor stages. The two reactors must remove sulfur from sour gas capable of 90–96%, or Method Three must perform the same from sour gas capable of 95–98%. The clause process is unable to recover a 100% entered sulfur. Therefore, the total sulfur is not possible to remove from sour gases [23]. Aspen Plus takes advantage of exact fashions intended for prediction belonging to the practice performance through the proper group thermodynamic fashions and assumes an excellent design and style from a process [24,25]. These data may be provided in the iterative type to improve the design. Several studies have been reported on the increased efficiency of sulfur recovery by using numerical analysis [26]. Researchers worked on simulation and optimization of pure oxygen processes in which pure oxygen is used instead of air. It has increased the efficiency of sulfur recovery substantially [27,28]. In recent years, it has been published that the use of a catalyst increases the production efficiency. In these studies, several mechanisms have been used to multi-objective optimization of chemical reaction conditions based on a kinetic model. In multi-objective optimization, the objective function is based on the kinetic model of chemical reactions. The NSGA-II algorithm is applied on multi-objective optimization to optimize this parameter. The purpose of modeling any process is to obtain the optimal point of the process. Any optimal reaction condition is based on the kinetic model of the reactions [29]. In 2021, Anna Dell discussed the feasibility study of acid gases and economic analysis of the process [30].

In general, prior work is limited to process modeling and simulation of the Claus process. Studies on pinch and cost analysis are lacking in the literature. The main objective of this study is process modeling and simulation of the Claus process by using the Aspen Plus simulator to remove sulfur from H_2S gas. The second objective is to optimize the Claus process by using parametric and topological methods. The third objective is to use pinch analysis for the Claus process. Finally, the fourth objective is to perform an economic analysis of the Claus process. Several questions regarding pinch analysis remain to be addressed in the literature. This paper investigates several questions related to pinch and cost analysis of the Claus process. This study can be considered a significant step forward in the process modeling and simulation of the Claus process. The proposed method provides a substantial increase in sulfur recovery compared to the methods available in the literature.

2. Process Methodology

In this Claus process flow diagram, three inlet streams are entering into the process. In the first inlet stream, the temperature is 32 °C and the pressure is 10 bars. In the first stream, pure oxygen gas enters the process at 90 kmol/h, and some unwanted ammonia is also entering the process at 4.7 kmol/h. The second inlet stream enters the process at a temperature of 120 °C and the pressure is 2.4 bar. The flow rate of H_2S is 23.9 kmol/h, a flow rate of CO_2 is 16.9 kmol/h, a flow rate of CO is 2.1 kmol/h, a flow rate of H_2 is 10.2 kmol/h, and final ammonia flow rate is 31.6 kmol/h. In the third inlet stream, the temperature is 50 °C and the pressure is 2.1 bars. The flow rate of H_2S gas is 159.1 kmol/h, CO_2 is 174.1 kmol/h, and N_2 flow rate is 31.3 kmol/h. These three streams enter the flame zone section of the furnace. At the flame zone, there are two primary combustion reactions taking place.

$$H_2S + 3/2\ O_2 \rightarrow SO_2 + H_2O \quad (1)$$

$$NH_3 + \frac{3}{4}\ O_2 \rightarrow \frac{1}{2}\ N_2 + 3/2\ H_2O \quad (2)$$

These highly exothermic reactions increase the temperature substantially. Several side reactions take place. The side reaction destroys any ammonia not combusted in Reaction (2).

$$H_2S + SO_2 + H_2 \rightleftharpoons S_2 + 2H_2O \quad (3)$$

$$H_2S \rightleftharpoons \frac{1}{2}\ SO_2 + H_2 \quad (4)$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad (5)$$

$$NH_3 + \frac{3}{4}\ SO_2 \rightleftharpoons \frac{1}{2}\ N_2 + 3/2\ H_2O + 3/8\ S_2 \quad (6)$$

The flame zone temperature is 345 °C, and its pressure is 1.2 bars at anoxic section. S_2 is formed, sulfur is condensed in the condenser, and a separator separates the sulfur. Thus, in the first furnace section, 16.2 kmol/h sulfur is produced. After sulfur production, two heat exchangers are installed to decrease the temperature of the sulfur product to 195 °C, and pressure is 1.6 bars. After the separator is installed, the unreacted H_2S gas is further reheated and moved toward the reactor. In this reactor, the reaction is taking place. After the anoxic section, S_2 is formed, sulfur is condensed in the condenser, and a separator separates the sulfur. Thus, in the first furnace section, 16.2 kmol/h sulfur is produced. After sulfur production, two heat exchangers are installed to decrease the temperature of the sulfur product to 195 °C and pressure is 1.6 bars. After the separator is installed, the unreacted H_2S gas is further reheated and moved toward the reactor. In this reactor, the reaction is taking place.

After the reactor, sulfur is formed. The feed is moved toward the separator. Sulfur is separated from the bottom and other un-reacted H_2S gas is moved toward the second reactor the same reaction is taking place.

After the 2-reactor, feed is moved toward the separator and other sulfur is separated through the separator. Sulfur is a separator from the bottom and unreacted gases moved from the top of the separator.

2.1. First Stage Reaction

Figure 1 shows that hydrogen sulfide gas is reacted with oxygen at high temperatures and pressure to form sulfur dioxide and water. In the second phase, the ammonia gases containing impurities and contaminants are reacted with oxygen to form nitrogen and water.

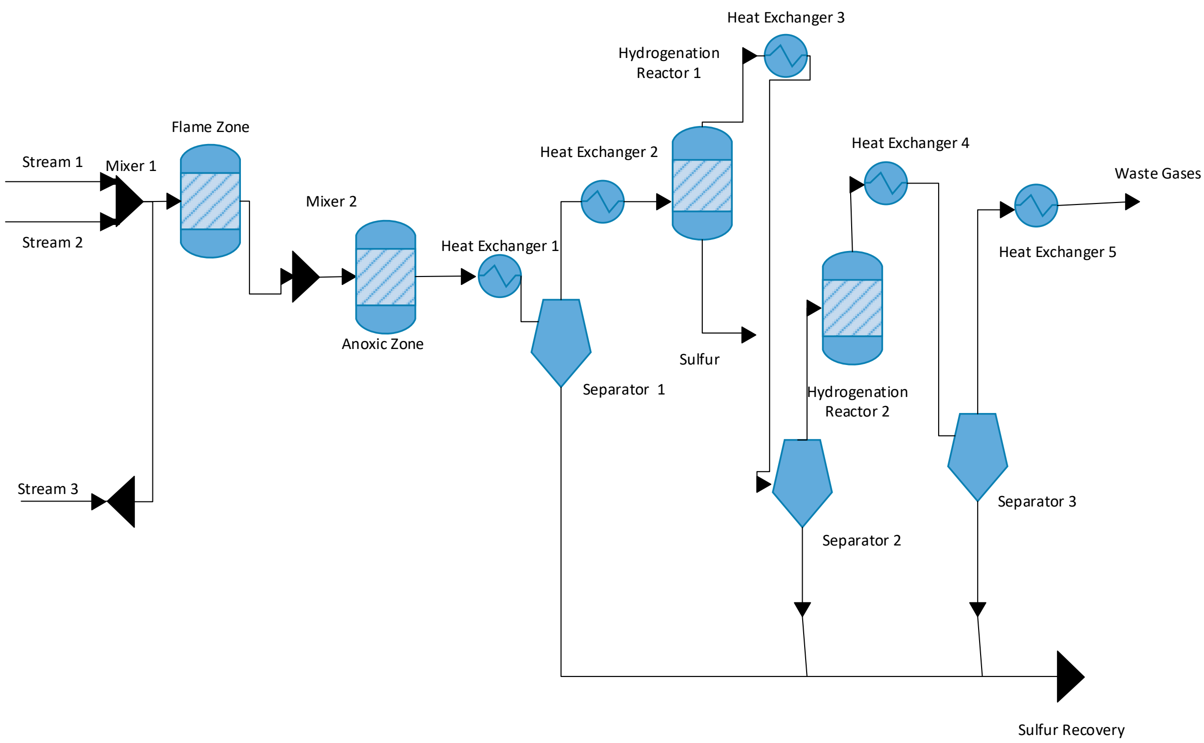

Figure 1. Block Flow diagram of the Claus process.

2.2. Second Stage Reaction

The second phase reactions consist of four different reactions taking place in the reactor. First, the hydrogen sulfide, sulfur dioxide, and hydrogen react to form sulfur and water. The second reaction is an equilibrium reaction in which hydrogen sulfide gas is converted into sulfur and hydrogen. In the third phase reaction, the CO_2 and hydrogen react to form carbon monoxide and water. Finally, in the fourth phase reaction, ammonia and sulfur dioxide react to form nitrogen, water, and sulfur.

Di-sulfur is converted into octal-sulfur at the same pressure and exact temperature in these equilibrium phase reactions. In the second stage, hydrogen sulfide gas is reacted with SO_2 to form octal-sulfur and water.

$$S_2 \rightleftharpoons \frac{1}{4}\, S_8 \tag{7}$$

$$H_2S + 1/2\ SO_2 \rightleftharpoons 3/16\ S_8 + H_2O \tag{8}$$

There is a flame zone in the Claus process in which plug flow reactors are used. Different reactions take place in the plug flow reactor. There is an exothermic reaction that takes place in the reaction furnace. Furnace reactions cause some technical problems. Due to increased reaction, the formation of ammonia gas causes corrosion in the chemical equipment. Now, the objective is to minimize the production of ammonia gas in furnace reaction because ammonia has decreased the performance of the Claus process. The exhaust gases of the furnace are sulfur dioxide gas (SO_2) and nitrogen gas (N_2), and its outlet temperature is 345 °C and 1.8 bars pressure. After the furnace reaction, these gases are cooled with waste heat boiler (WHB).

There are two catalytic reactors used in the Claus process. The two catalysts, titanium and alumina, increase the reaction rate in a plug flow reactor. In the first reactor, the reaction occurs at 330 °C, and the pressure is 10 bars. In the first reactor, the conversion of H_2S gas into sulfur is about 70%. In the first reaction, the catalyst is installed in a different layer. In the second reactor, the H_2S gas conversion to sulfur is about 92%. In the second reactor, the reaction occurs at 234 °C temperature and the pressure is 8 bars. At the final stage, the reaction conversion is 92%.

Table 1 shows the inlet composition of gas feed. Ten gases are entered into the feed composition for the sulfur recovery unit. In addition, three inlet feeds enter at the same time for chemical reactions. The oxygen flow rate is 90 kmol/h in the first stream and zero in the second and third streams. Finally, in the third stream, H_2S gas is entered into the reactor.

Table 1. Inlet composition of feed for three different inlet streams.

Composition Gases	Stream No 1	Stream No 2	Stream No 3
Hydrogen sulfide	0	23.9	159.1
Sulfur dioxide	0	0	0
Water	0	0	15.6
Carbon Monoxide	0	16.9	174.1
Carbon dioxide	0	2.1	0
Oxygen	90	0	0
Hydrogen	0	10.2	0
Nitrogen	4.7	1.3	31.3
Ammonia	0	31.6	7.9
S_2	0	0	0
S_8	0	0	0

2.3. Reactions Kinetic of Claus Process

The modeling of a flame reactor consists of two zones, including the oxygen richer zone in which exothermic reactions occur. The second reactor is slower and endothermic reactions take place.

The rate equations are:

$$-\mathrm{r}i = \mathrm{Ko}i\ \exp\left[\frac{-Ei}{RT}\right] P_{H_2S} P_{NH_3} P_{O_2} \tag{9}$$

where *i* is the equation number.

Whereas r*i* is kmol/s/m^3, p_i is atm and K_{oi} unit varies depending upon temperature and pressure.

The rate of reaction is:

$$-r_3 = 3.58 \times 10^7 \exp\left[\frac{-26.0}{RT}\right] \left(P_{H_2S}P_{NH_3}P_{O_2} - \exp\left[-0.949 - \frac{5840}{T}\right] P_{S_2}P_{H_2O}\right. \quad (10)$$

$$-r_4 = 9.17 \times 10^5 \exp\left[\frac{-45.0}{RT}\right] \left(P_{H_2S}P_{S_2} - \exp\left[-5.93 - \frac{10,880}{T}\right] P_{S_2}P_{H_2}\right. \quad (11)$$

$$-r_5 = 1.52 \times 10^{12} \exp\left[\frac{-60.3}{RT}\right] \left(C_{CO_2}C_{H_2} - \exp\left[-3.88 + \frac{4166}{T}\right] \frac{CcoCh2o}{Ch2}\right. \quad (12)$$

$$-r_6 = 2.29 \times 10^4 \exp\left[\frac{-27.5}{RT}\right] C_{NH_3}\, C_{SO_2} \quad (13)$$

Whereas r*i* is kmol/s/m^3 and pi is pressure in atm and C*i* are kmol/m^3.

$$\text{Kp} = \exp\left[-53.67 + \frac{47,800}{T(K)}\right] \quad (14)$$

In the reactor, there are two different catalysts used in each reactor. In the first reactor, alumina is used, and, in the second reactor, titanium catalysts are used. In addition, there are highly exothermic reactions in the reactor, where the coolant is used to control the reactor's temperature. Otherwise, catalyst deactivation takes place and sulfur deposits on the catalyst.

$$-7 = 5360 \exp\left[\frac{-7.35}{RT}\right]\left(\frac{P_{H_2S}P_{SO_2} - \exp\left[8.66 - \frac{5550}{T}\right] PH2O\ PS8}{\left(1 + 1.14\exp\left[\frac{-0.6}{RT}\right] PH2O\right)}\right) \quad (15)$$

The values used in Equations (9)–(15) are given in Table 2.

Table 2. Reaction kinetic values of the Claus process.

i	E*i* Kcal/kmol	K_{oi}	A	b	c
1	11,000	1.40×10^4	1	0	1.5
2	40,000	4.43×10^6	0	1	0.75

Figure 2 shows the process flow diagram of the Claus process in which sulfur recovered varies from this unit. Feed is entering into the process in three inlets. The first and second streams are mixed in a mixer and they enter the flame zone. The third stream is entering into an anoxic section for chemical reaction. After the flaming zone, some sulfur is formed that is separated at the bottom of the separator. The other unreacted gases moving toward the heat exchanger again increased the temperature at 314 °C after the heat exchanger. It is moved toward the hydrogenation reactor, in which reaction occurs at 314 °C at 1.6 atm. After passing through the hydrogenation reaction, about 10.5 kmol/h of sulfur is formed. These sulfurs are extracted separately at the bottom of the separator. After that, more unreacted gases are further moved toward another hydrogenation reactor. The reaction takes place at the same temperature and pressure, at 315 °C and 1.6 atm, respectively. After the second reactor, more sulfur is formed at a flow rate of 10.5 kmol/h. After that, all the sulfur streams are mixed at the mixer to reach the final flow rate of 25.805 kmol/h.

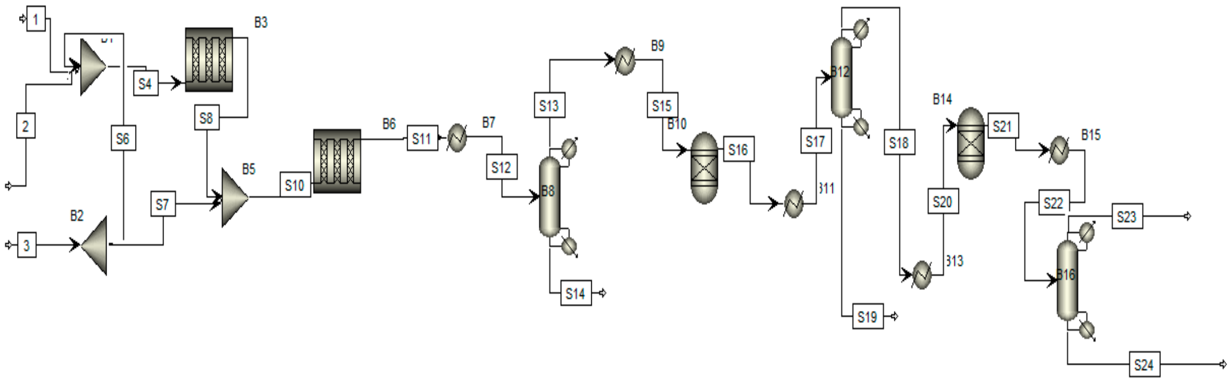

Figure 2. Process flow diagram of the Claus process.

3. Results and Discussion

3.1. Sensitivity Analysis

This parametric optimization deals with the operating variables of chemical plants, such as temperature, concentration, and the pressure of chemical equipment. The parameter is selected based on the process's nature. The critical parameters of this process are a temperature of a reactor, pressure of reaction, the composition of inlet feed, diameter, and length of the furnace. In this parametric analysis, the result shows that changing the parameter causes a significant effect on the efficiency of a chemical plant. There are four different types of parametric optimization. First, in the plug flow reactor, diameter is changed from 10 inches to 70 inches. Second, the length and diameter of the furnace are changed from 35 inches and 30 inches to 50 inches and 55 inches, respectively. Third, the oxygen flow rate changes from 90 lb/h to 170 lb/h to optimize the process. Finally, the temperature of the reactor has increased from 280 °C to 370 °C.

3.2. Effect of Changing Furnace Diameter and Length

When the length of the reactor is increased, it causes an increase in residence time of the process and has the destruction of ammonia production in a furnace (using $t = V/V_0$, t = residence time, V = volume of furnace, V_0 = flowrate of the gases). The deactivation of catalyst causes ammonia containment, and it is causes corrosion on the chemical equipment. Figure 3 shows that when the reactor's length increases, the ammonia production decreases, and the production of sulfur increases. The destruction of ammonia is decreasing due to the conversion of NO and N_2 along the length.

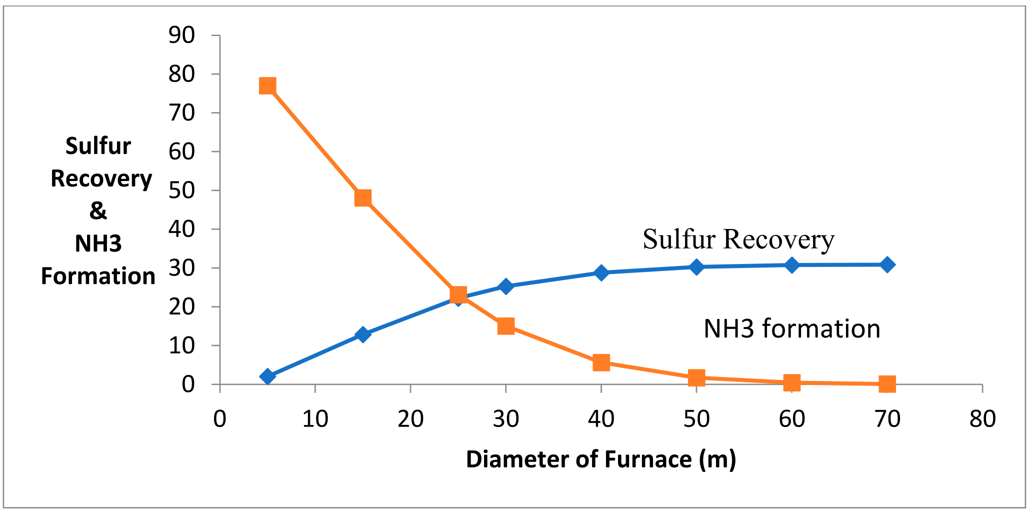

Figure 3. Effect of change in furnace diameter and length.

3.3. Effect of Increasing Oxygen Flow Rate on Sulfur Recovery

Oxygen is a limiting reactant of this Claus process. Therefore, the goal is to maximize the consumption of H_2S gas into elemental sulfur in this process. In this primary reaction of the Claus process, hydrosulfide gas is reacted with oxygen to form water and sulfur. Therefore, the oxygen flow rate varied for the maximum consumption of H_2S gas into sulfur. The target was 0% unreacted H_2S gas coming out from the product. Figure 4 shows that when the oxygen flow rate increases, the conversion of H_2S gas into sulfur increases. When the flow rate of oxygen is increasing, the unreacted H_2S is increasing. The oxygen is a limiting reactant, providing the oxygen in excess amounts.

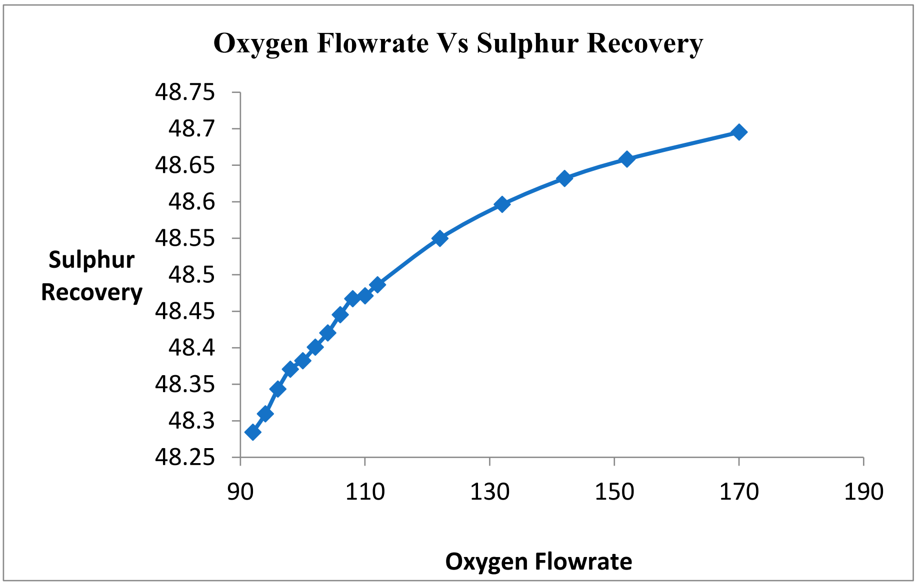

Figure 4. Effect of Oxygen on sulfur Recovery.

3.4. Effect of Changing Temperature on Sulfur Recovery

Figure 5 shows the effect of temperature on the sulfur recovery process. Due to the exothermic reaction, the temperature of the reactor is increased. Due to an increase in temperature, the deactivation of catalysts is increased. It is caused by the reduction in the sulfur recovery unit.

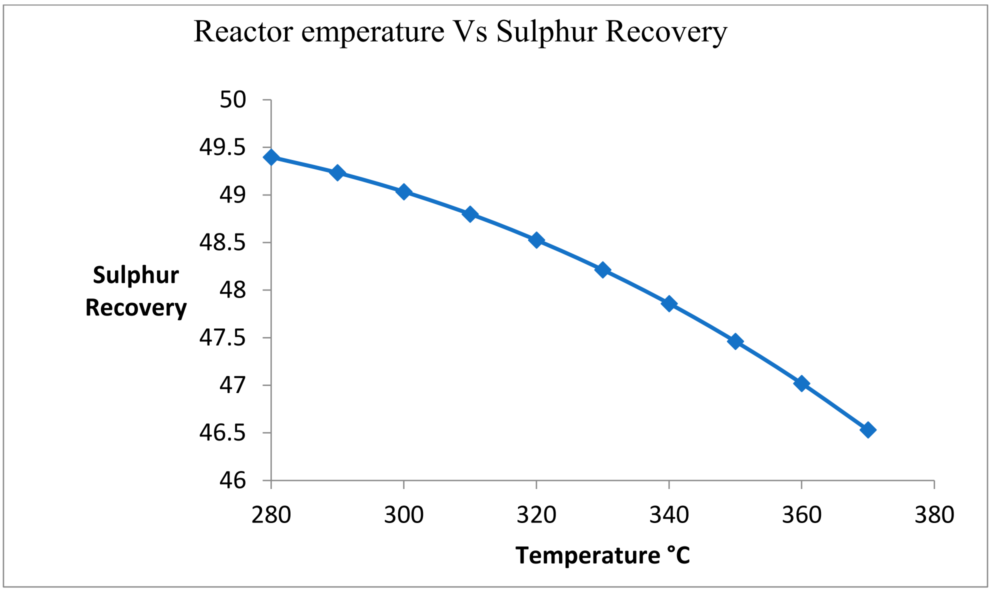

Figure 5. Effect of change in temperature on sulfur recovery.

3.5. Pinch Analysis

Pinch analysis is a method for minimizing the energy consumption of the chemical process industry. There is maximum utilization of internal utilization and minimum consumption of external utilization. The heat exchanger size is changed, and the area of the heat exchanger is also increased.

Figure 6 shows the nine pinch analysis steps followed to perform the pinch analysis of the chemical process industry. The first step is identifying cold and cold utilities to find the number of hot and cold streams. In the second step of each stream's thermal data extraction, we can find the heat duty of cold and hot streams. In the third step, the selection of ΔTmin value of the process streams in which minimum heat transfers between the two process streams. The fourth step is the construction of the grand composite curve and composite curve. It tells us about the available energy in process streams and how much energy is recovered from them. The fifth step is to estimate the energy cost of the overall chemical plant and how much cost is required to pinch analysis all over the chemical plant. The sixth step is estimating the capital cost of a heat exchanger and the utility cost of an overall chemical plant. The seventh step is used to find the optimum minimum temperature value of the chemical plant. The eighth step is to estimate the heat exchanger network design of the overall chemical plant. Finally, the ninth step is the final design of the heat exchanger network, in which we can find the optimum design of the heat exchanger and the efficient design of the heat exchanger. Figure 7 shows the process flow diagram of the sulfur recovery unit in pinch analysis on the chemical process industry. Pinch analysis is performed on five heat exchangers of the sulfur recovery unit shown in the red circle. The purpose of pinch analysis is to maximize internal utilities' utilization and minimize the consumption of external utilities. Therefore, a heat exchanger is used in pinch analysis for maximum utilization of internal utilities.

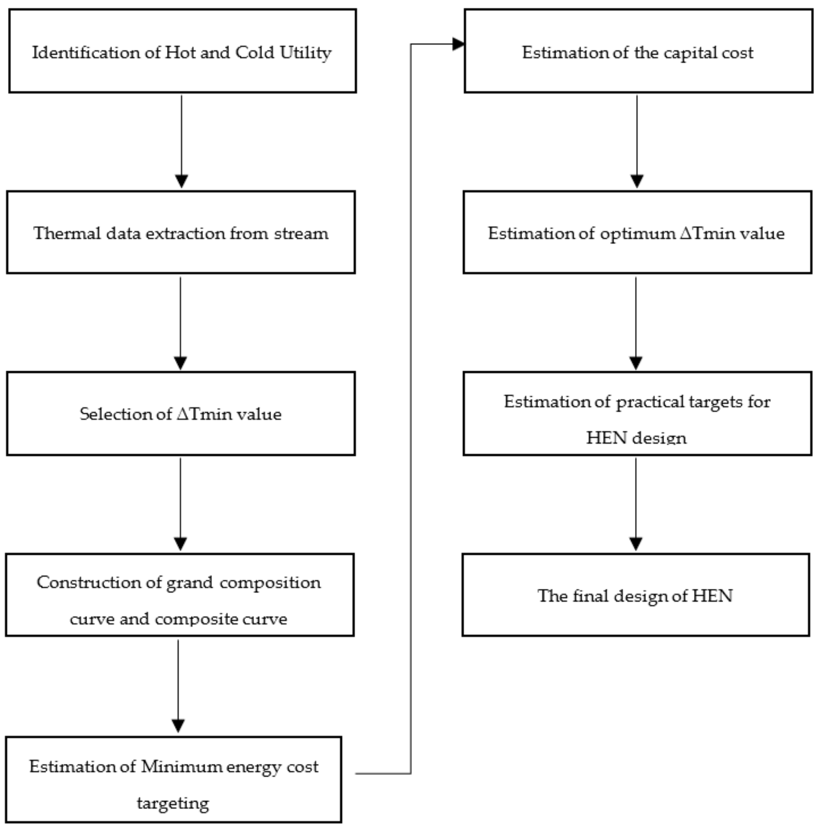

Figure 6. Steps of pinch analysis.

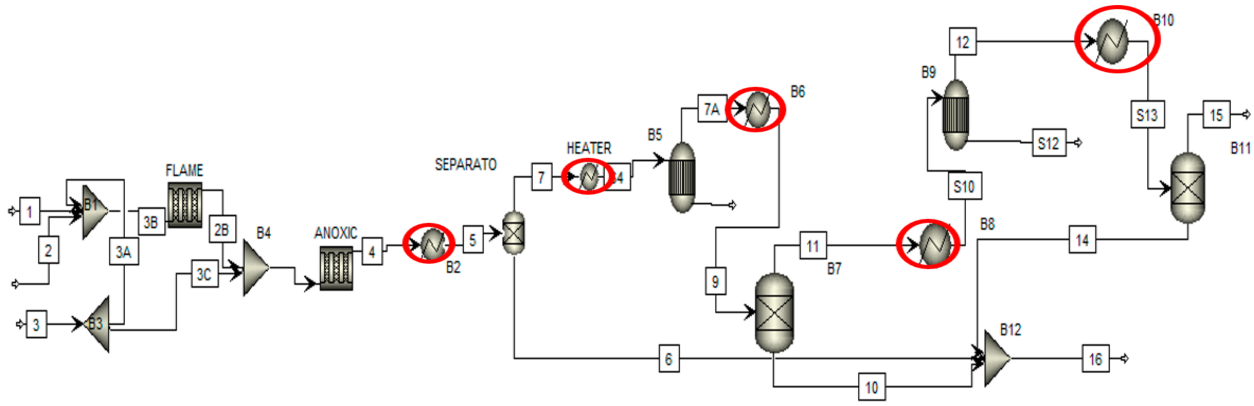

Figure 7. Pinch analysis process diagram.

Figure 8 shows the optimum heat exchanger network of the heat exchanger. There are seven heat exchangers used, which are used to process heat exchangers. The total number of areas is 5666 m^2; the total heating utilities are used at 4.12 $\times$ 10^5 kj/h. The total cooling utilities are used 3.6 $\times$ 10^7 kj/h. These diagrams show the sizes of a heat exchanger and the heat duty of each heat exchanger. The blue line shows the cold streams, and the red line shows the hot streams. The heat exchanger is shown in circles.

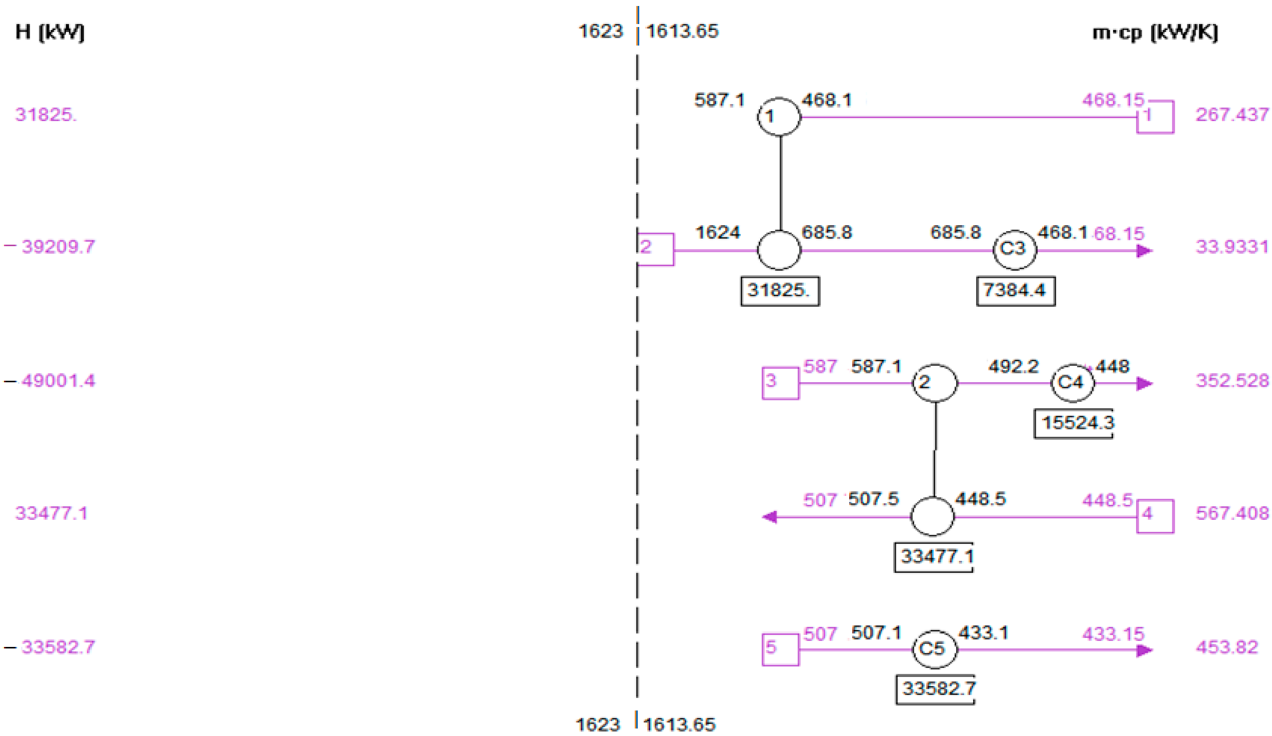

Figure 8. Heat exchanger network (HEN) design of heat exchanger.

Table 3 shows the number of heat exchangers that are used for pinch analysis. The first column shows the name of heat exchangers, and the third column shows the types of heat exchangers, such as a heater or cooler. The fourth column shows the heat duty of the heat exchanger in (cal/s). The next column shows the inlet temperature and outlet temperature of hot utility and cold utility.

Table 3. Pinch Analysis temperature interval result by using Aspen Plus.

Heat Exchanger	Types	Base Duty (cal/s)	Hot Inlet Temperature (°C)	Hot Outlet Temperature (°C)	Cold Inlet Temperature (°C)	Cold Outlet Temperature (°C)
B7	Heater	1.885×10^5	250	249	58.3	195
B9	Heater	1.701×10^5	1000	400	195	314
B13	Heater	1.553×10^5	1000	400	195	314
B14_Heat_Exchanger	Cooler	1769	314	313.5	249	250
B_10 Heat Exchanger	Cooler	2.565×10^6	314	313.5	249	250
B11	Cooler	1.73×10^6	314	195	174	175
B15	Cooler	1.566×10^5	314	194	174	175

Table 4 shows the pinch analysis result and temperature interval. It shows a detailed study of a heat exchanger. The first column shows the name of the heat exchanger. The second column shows the heat exchanger's feather-like working principle. The fourth column shows the heat duty of the heat exchanger, the fifth column shows the recoverable duty, and the other table shows the inlet and outlet temperature of hot and cold utilities.

Table 4. Pinch analysis and temperature interval result.

Heat Exchanger	Types	Recovery Duty (cal/s)	Hot Side Fluid	Cold Side Fluid
B2	Heater	1.885×10^5	HP Steam	4 to 5
Heater	Heater	1.55×10^5	Fire Heater (1000)	7 to S4
B13	Heater	1.423×10^5	Fire Heater (1000)	S18 to S20
B14 Heat Excahnger	Cooler	0	B14_Heat	HP steam generation
B5 Heat Exchanger	Cooler	0	B5_Heat	HP steam generation
B8	Cooler	0	7A to S17	MP steam generation
B10	Cooler	0	S21 to S22	MP steam generation

Table 5 shows the energy saving and utility saving during the pinch analysis of the Claus process. The table is divided into three categories; first is energy, greenhouse, and energy cost saving. In the first energy section, the total hot utilities are 5.13×10^5. The hot target utilities are 2.73×10^4 cal/s. The potential saving energy by pinch analysis is approximately 4.865×10^5 cal/s. The energy cost saving is 229,578 USD/yr by using pinch analysis. By using the pinch analysis, an energy cost saving is about 93.73%.

In Table 6, the first graph shows total utilities, the second shows heating utilities, the third shows cooling utilities, and the fourth shows carbon utilities. The actual total utilities are 3.41×10^6 cal/s and the target utilities are 2.4373×10^6 cal/s. The actual energy saving is 28.53%. The actual heating utilities are 5.13×10^5 cal/s, the target is 2.73×10^6 cal/s, and the actual saving is 94.68%. The actual cooling utilities are 2.8×10^6 (cal/s), the target is 2.4×10^6 cal/s, and the actual saving is 16.80%.

Table 5. Utilities cost and energy saving by pinch analysis with the help of Aspen Plus.

Type	Current (cal/s)	Target (cal/s)	Saving Potential (cal/s)	Energy Cost Saving (USD/yr)	Energy Cost Saving (%)	ΔTmin (°C)
HP Steam	1.884×10^5	0	1.884×10^5	62.243	100	10
Fire Heat (1000)	3.254×10^5	2.73×10^4	2.981×10^5	167.336	91.60	25
Total Hot Utilities	5.138×10^5	2.73×10^4	4.65×10^5	229.578	93.73	
HP Steam Generation	2.567×10^6	2.41×10^6	1.569×10^5	−51.618	−6.11	10
MP steam Generation	3.296×10^5	0	3.296×10^5	−95.370	−100	10
Total Cold Utilities	2.896×10^6	2.41×10^6	4.865×10^5	−146.989	−15.64	

Table 6. Total utilities, heating utilities, cooling utilities, and carbon emission.

Type	Actual	Target	Available Savings	% of Actual
Total Utilities (cal/s)	3.41×10^6	2.437×10^6	9.7025×10^5	28.53
Heating Utilities (cal/s)	51.38×10^5	2.767×10^4	4.865×10^5	94.68
Cooling Utilities	2.896×10^6	2.41×10^6	4.86×10^5	16.80
Carbon Emission (kg/h)	0	0	0	0

Table 7 shows carbon emissions into the atmosphere. The total hot utilities and cold utilities are emitted carbon compounds into the atmosphere. There is zero emission of carbon to the atmosphere by hot and cold utilities.

Table 7. Carbon Emission Details.

Type	Current (kg/h)	Target (kg/h)	Saving Potential (kg/h)	Emission Cost Saving (USD/yr)	Emission Cost Saving
HP steam	0	0	0	0	0.00
Fire Heat (1000)	0	0	0	0	0.0
Total Hot Utilities	0	0	0	0	0.00
HP Steam Generation	0	0	0	0	0.00
MP Steam Generation	0	0	0	0	0.00
Total Cold Utilities	0	0	0	0	0.00

Table 8 shows the mechanical design of the heat exchanger. Theses parameter of mechanical design plays a vital role in checking the physical stability of heat exchanger to have a safe design without any failure.

Table 9 shows the name of equipment used in a process flow diagram, the cost, and area of equipment. The type of equipment used in the process flow diagram, the material of construction of equipment, and pressure at the tube side and shell side are also shown.

Table 8. Mechanical Design of Heat Exchangers.

Heat Exchanger No	B2	HEATER	B13	B14	B5	B8	B10
Tube Length (in)	236.2	410.2	150	236.2	236.2	236.2	236.2
No of Baffles	32	58	30	34	44	38	42
Shell pass	8	8	4	4	4	4	8
No of tubes	265	400	137	203	153	155	172
Tube Pattern	Triangular	Triangular	Triangular	Triangular	Triangular	Triangular	Triangular
Baffle Type	Segmental	Segmental	Segmental	Segmental	Segmental	Triangular	Triangular
Exchanger Material	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Area (m^2)	60	559	12	32.6	70	55	82

Table 9. Equipment summary of the Claus process.

Exchanger USD	**Exchanger Types**	**Shell Pressure (bar)**	**Tube Pressure (bar)**	**MOC**	**Area m^2**	**Purchase Equipment Cost USD**	**Bare Module Cost USD**
E-101	Floating Head	1	2	Carbon Steel	113	36,500	120,000
E-102	Floating Head	1	2	Carbon Steel	103	35,100	115,000
E-103	Floating Head	1	2	Carbon Steel	105	35,300	116,000
E-104	Fixed Sheet or U-Tube	1	2	Carbon Steel	48.3	25,900	85,200
E-105	Floating Head	1	2	Carbon Steel	48.3	27,300	89,900
Heater	Types	Heat Duty (MJ/h)	Super Steam (°C)	MOC	Pressure (barg)	Purchase Equipment Cost USD	Bare Module Cost USD
H-101	Reformer furnace	28,600	-	Carbon steel	-	118,000	2,510,000
H-102	Reformer furnace	28,700	-	Carbon Steel	-	118,000	2,510,000
Reactor	**Type**	**Volume (m^3)**				**Purchase Equipment Cost USD**	**Bare Module Cost USD**
R-101	Autoclave	7.08				88,900	356,000
R-102	Autoclave	7.08				88,900	356,000
Vessel	Orientation	Length (m)	Diameter (m)	MOC	Pressure (bar)	Purchase Equipment Cost USD	Bare Module Cost USD
V-101	Horizontal	6.08	2.27	Carbon Steel	2	15,900,000	24,200,000
V-102	Horizontal	5.06	1.68	Carbon Steel	2	6,940,000	10,600,000
V-103	Horizontal	5.28	1.76	Carbon Steel	2	7,770,000	11,800,000

Table 10 shows the total model cost, grass root cost, utility cost, and actual usage cost of each piece of equipment. For example, in the heat exchanger, cooling and heating medium are used, and natural gas is used as a heating source in the furnace. Therefore, the grass-root cost of a heat exchanger, utility cost, efficiency, actual usages, and annual cost utilities are also shown.

Table 10. Utility summary of the Claus process.

Name	Total Module Cost USD	Grass Root Cost USD	Utility Cost	Efficiency	Actual Usage (MJ/h)	Annual Cost Utility USD
E-101	256,800	366,000	Cooling water		32,300	10,200
E-102	136,000	194,000	Low-pressure Steam		897	15,150
E-103	137,000	195,000	Cooling water		2900	9100
E-104	100,000	143,000	Medium pressure Steam		759	17,560
E-105	106,000	151,000	Cooling water		1430	4500
H-101	2,960,000	4,220,000	Natural gas	0.9	31,800	836,000
H-102	2,970,000	4,220,000	Natural gas	0.9	31,900	839,000
R-101	420,000	464,000	Low-pressure Steam		897	15,150
R-102	420,000	464,000	Low-pressure Steam		2900	49,000
V-101	28,600,000	28,600,000	N/A			
V-102	12,500,000	12,500,000	N/A			
V-103	14,000,000	14,000,000	N/A			
Total USD	62.5 million	65.4 million				1.89 million

Table 11 shows the material name and its classification. This table shows the price in dollars (year 2020) and the flow rate of each component. It is also described the annual cost of raw material and product cost.

Table 11. Material of construction cost summary.

Material Name	Classification	Price (USD/kg) *	Flow Rate (kg/h)	Annual Cost USD
Hydrogen Sulfide	Raw Material	-	5853	-
Oxygen	Raw Material	1.50	2880	35.95 million
Sulfur	Product	0.19	390	0.61 million
Hydrogen	Product	12	718	71.7 million
Nitrogen	Product	10	4009	333.69 million
Nitrogen	Raw Material	10	1193.73	99.9 million
Ammonia	Raw Material	9	1264	94.6 million

* All the prices are taken from https://www.alibaba.com/, accessed on 10 November 2020.

Table 12 describes the result of the heat exchanger and heating utility after the pinch analysis. This result shows that, after the pinch analysis, the size of the heat exchanger increases, and the utility consumption decreases.

Table 13 shows the revenue from the sale, raw material cost, utilities, and final profit. After the pinch analysis and parametric optimization, it takes 2.2 million USD per year. Furthermore, by comparing both tables after optimization and optimization, a difference of 2.2 million USD per year is observed.

Table 12. Cost analysis of the Claus process after pinch analysis.

Exchanger USD	Exchanger Types	Shell Pressure (bar)	Tube Pressure (bar)	MOC	Area m^2	Purchase Equipment Cost USD
E-101	Floating Head	1	2	Carbon Steel	60	28,900
E-102	Floating Head	1	2	Carbon Steel	12.8	26,000
E-103	Floating Head	1	2	Carbon Steel	559	108,000
E-104	Fixed Sheet or U-Tube	1	2	Carbon Steel	32.7	23,800
E-105	Floating Head	1	2	Carbon Steel	70.8	30,400
Heater	Types	Heat Duty (MJ/h)	Super Steam (°C)	MOC	Pressure	Purchase Equipment Cost USD
H-101	Reformer Furnace	28,600	-	Carbon Steel	-	118,000
H-102	Reformer Furnace	28,700	-	Carbon Steel	-	118,000
Reactor	**Type**	**Volume (m^3)**			**Purchase Equipment Cost USD**	**Bare Module Cost USD**
R-101	Autoclave	7.08			88,900	356,000
R-102	Autoclave	7.08			88,900	356,000
Vessel	Orientation	Length (m)	Diameter (m)	MOC	Purchase Equipment Cost USD	Bare Module Cost USD
V-101	Horizontal	6.08	2.27	Carbon Steel	15,900,000	24,200,000
V-102	Horizontal	5.06	1.68	Carbon Steel	6,940,000	10,600,000
V-103	Horizontal	5.28	1.76	Carbon Steel	7,770,000	11,800,000

Table 13. Cost comparison before and after optimization of the Claus process.

Type	Before Optimization Million USD	After Optimization Million USD
Revenue from Sale	415.7	424.5
CRM (Raw Material Cost)	229.9	237.9
CUT (Cost of Utilities)	0.144	0.042
CWT (Waste Treatment Cost)	-	-
COL (Cost of Operating Labor)	0.937	0.937
Profit	183.1	185.5

Table 14 shows the comparison between post-optimization of process and pre-optimization of a chemical process. Before optimizing the process, the direct, indirect, and utility costs are increased compared to the post-optimization column. However, after pinch analysis and parametric optimization, the production efficiency of sulfur recovery increased.

Table 15 shows the comparison between the production result obtained from the simulation of the Claus process and literature data. This table shows that the sulfur recovery increased by 18% in the proposed simulation.

Table 14. Summary of economic parameters, advantages, and disadvantages of processes for H_2S gas conversion.

Process	Before Optimization	After Optimization
Direct cost (million USD)	63.4	65.9
Indirect Cost (million USD)	1.8	1.6
Fixed Capital Cost (million USD)	65.4	67.5
Working Capital cost (million USD)	38.1	38.5
Total investment (million USD)	168.7	173.5
Raw Material Cost (million USD)	229.9	237.9
Utility Cost (million USD)	1.89	1.6
Labor Cost (million USD)	0.96	0.96
Total Product Cost (million USD)	406	425.53
Profit (million USD)	177	189.63
Payback Period (million USD)	2.9 year	1.8 year
Advantage	No Advantage.	Production efficiency is increased—also, minimum consumption of external utilities and maximum consumption of internal utilities.
Limitations	The simulation is carried out based on their Chemcad software. There is no optimization of a chemical process.	The simulation is performed on the Aspen Plus software. First, there is the optimization of a chemical process. Then, with the help of optimization, we can save external heating utilities.

Table 15. Production results compared with the literature.

	Simulation Results		Literature [31]	
Stream No	**15**	**16**	**15**	**16**
Temperature (°C)	160	187	160	187
Pressure (Bar)	0.9	0.9	0.9	0.9
Mole flow (lbmol/h)	519.3	23.18	519.3	23.18
Component's flowrate (lb/h)				
H_2S	135.811	0	4	0
SO_2	2	0.0	2	0.0
Water	148	4.738	238.7	1.2
O_2	0	0.0	0	0.0
Ammonia	89.6	0	140	0
S_2	0.03	0.3	0	0.3
S_8	0.06	**25.805**	0.4	21.7
Sulfur Recovery increased to 18% in the proposed simulation				

4. Conclusions

This study focused on the three objectives related to the Claus process: process modeling simulation, optimization, and cost analysis of the Claus process. Aspen Plus software was used for process modeling and simulation of the process. After the Claus process modeling, the result was compared with the literature result. It is shown that sulfur recovery increased by 18%. The second objective was optimization; two types of optimizations were used. The first was parametric optimization and the second was topological optimization. A parametric optimization was used for operating parameters and design parameters to increase the production of sulfur.

Furthermore, topological optimization was used to deal with the size and amount of equipment. Pinch analysis has changed the size of equipment to maximize the utilization of heating and cooling utilities. The pinch analysis on the sulfur recovery unit reduced the operating cost of a heat exchanger to 28.53%. The third objective was a cost analysis of the Claus process. It has shown that, after optimization, profit can be improved by more than 2.5% by process modeling simulation, changing operating conditions, design parameters, and pinch analysis on the Claus process.

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