DEVELOPMENT OF PROCESS SIMULATION MODEL OF SOUR GAS PROCESSING PLANT



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CERTIFICATE

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DEDICATION

This work is dedicated to our parents as an acknowledgement of their unwavering support and innumerable sacrifices they made to help us keep moving towards our destiny.

ACKNOWLEDGMENTS

In the name of the Creator who taught man with a pen.

We are thankful to Almighty who gave us courage and capability to carry out this yearlong design project.

This Final Year Project is a product obtained through cumulative efforts of group members under guidance of faculty, seniors and colleagues. The project was initiated with the cooperation of our first supervisor, Dr. Salman Raza Naqvi who showed us the roadmap to be followed. Heartly gratitude for our faculty supervisor, Dr. Asad Ullah Khan, who provided us a very detailed guidance ensuring perfection in our calculations and simulation as well as in writing the content of defense presentations, poster and thesis. The engineering knowledge applied for the completion of this project is a manifestation of the efforts of all SCME faculty who laid foundations for us to develop an understanding of chemical processes from basic to advanced level. The support and invaluable advices from our industrial supervisor, Mr. Muhammad Shehryar Khan, who always managed to provide us ample time for holding regular discussions despite his busy schedule in industry, also proved pivotal in this project. We are grateful to our parents, friends and colleagues for being supportive throughout this project.

ABSTRACT

With increasingly stringent environmental regulations, industries have to be more than ever vigilant in developing technologies for processing of raw materials. Fossil fuels processing involves several threats to the environment, sulfur emissions being the most imminent of them. Raw natural gas as obtained from wells is a mixture of various hydrocarbons in varying ratio and contains significant amounts of pollutants such as carbon dioxide, hydrogen sulfide, mercaptans and nitrogen containing organic compounds. Consequently, raw natural gas is not suitable for downstream applications. Natural gas containing sulfur impurities is called a sour gas and the removal of these impurities is a process named sweetening of sour gas. The sweetening involves amine absorption process and thus generates two streams as output; sweetened natural gas ready to be used as fuel or as a feedstock for chemical industry and a mixture of gaseous impurities which, when rich in sulfur and carbon dioxide, is called acid gas.

The scope of this project is to recover sulfur from acid gases coming from the absorption unit of a natural gas processing plant. The process chosen for sulfur recovery is a modified and a more efficient form of Claus Process, named Superclaus Process. This process introduces a specialized selective oxidation catalyst in the last of the three catalytic packed bed reactor. Focus is to bring the sulfur emissions to near zero by recovering the maximum elemental sulfur from the acid gas stream. This sulfur, in turn, will be used as a feedstock for many important and notable chemical manufacturing industries.

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INTRODUCTION

1.1. Introduction to Sour Gas

Natural gas is a fossil fuel obtained from natural gas reserves beneath the earth's surface, wells. It finds innumerable uses in chemical processing industry in addition to being used as a fuel for domestic, transportation and power plants. One prominent example of natural gas forming the foundation for chemical process lies in urea fertilizer process which uses it both as the feedstock to obtain syngas as well as for fuel in reformers. The main dominant component of natural gas is methane while it contains other hydrocarbons such as ethane, propane and butane as well. The presence of impurities like carbon dioxide, nitrogen and sulfur compounds (mercaptans and hydrogen sulfide) is what makes the utilization of natural gas in industry a complex engineering challenge. Natural gas containing hydrogen sulfide and/or mercaptans is called 'Sour Gas'. [1]

1.2. The problem with Sour Gas

Hydrogen sulfide present in raw natural gas poses a serious threat to the environment. If it burns with the gas, it releases a significant amount of sulfur dioxide into the atmosphere which is acidic in nature. Sulfur dioxide reacts with oxygen in the air and forms sulfur trioxide, which when combined with water is converted to sulfuric acid. This phenomenon is called acid rain. Acid rain severely damages the environment; natural habitat of insects near earth's surface, water bodies and soil are equally affected. It also has a deteriorating effect on buildings and architecture because of its corrosive characteristics. Moreover, sulfur dioxide causes serious respiratory problems and even, if exposure is higher than allowable limits, can prove fatal. In industry, it causes intense corrosion problems in pipelines and equipment alike. Therefore, sour natural gas is not directly used by any of the industrial sector.

1.3. Sweetening of Sour Natural Gas

To make natural gas usable as fuel or as a feedstock for many chemical industries, hazardous sulfur compounds need to be eliminated from the gas. This process of removing sulfur contents from sour natural gas is called sweetening of the sour gas [1]. There are numerous processes for sweetening of natural gas and the choice of process selection is made on the basis of concentration of various impurities. Some processes for sweetening of natural gas include:

- Amine Absorption
- Merox process
- Benfield process
- Fluor solvent process
- Membrane separation process

1.4. Sulfur Recovery Unit

The sweetening process generates a waste gaseous stream rich in H₂S and CO₂. This is called acid gas. The purpose of sulfur recovery unit is to obtain maximum of elemental sulfur from acid gas to minimize sulfur emissions to acceptable levels. [1]

1.5. Various processes for Sulfur Recovery

Upon literature review, we could analyze various processes used for sulfur recovery. A brief overview of some of those processes is discussed here.

1.5.1. Selectox Process:

Selectox Process is widely used for small capacities (less than 45tonnes/day). The gaseous mixture is first selectively oxidized by a catalyst into sulfur dioxide (SO₂) which then combines with H₂S

giving elemental sulfur. This process is followed by two claus reactors which then recover the elemental sulfur from the process stream. The efficiency of this process can be up to 97% in terms of sulfur recovered. [2]

1.5.2. Redox Process:

Redox or Liquid Redox process prevalent in the modern industry uses an iron catalysed oxidation-reduction reaction in an aqueous medium. The elemental sulfur so obtained by the reaction is in solid form and is easily separated out from the solution. This process can have a recovery efficiency as high as 99%. Nevertheless, it is sensitive to sulfur concentrations in the feed gas. Additionally, this process can produce a maximum of 20tonnes of elemental sulfur per day. [3]

1.5.3. Claus Process:

Claus process is the oldest and the most widely used technology established in the early 20th century. It involves treatment of the acid gas in a thermal section (the claus furnace) followed by a catalytic section (the typical claus reactors). The process may contain two or three reactors connected in series. The gaseous stream leaving the last of the reactors needs to be further treated in tail gas treatment unit to free it of any remaining sulfur content before releasing it into the environment. This process can be adopted for plants of large-scale production capacity. It can also provide as high an efficiency as 97%. [1] [2]

1.5.4. Superclaus Process:

Superclaus process introduces a newly developed catalyst in the conventional claus process and provides two main advantages. Firstly, it enhances the sulfur recovery efficiency to and raises it to greater than 99%. Secondly, it eliminates the need for installing a tail gas treatment unit. [4]

1.6. Selection of a Process

In this project, we designed a sulfur recovery unit on the basis of Superclaus process. This process is suitable for the concentrations of H_2S in the feed

The plant will have a production capacity of 100 metric tonnes of elemental sulfur per day. It will process the acid gas stream containing varying amounts of hydrogen sulfide and recover sulfur with a theoretical efficiency of 99%. Elemental sulfur formed is suggested to have many important industrial utilizations including the synthesis of Sulfuric acid, H₂SO₄ which is known as king of acids by chemists.

1.7. Uses of Elemental Sulfur

The elemental sulfur recovered has economical value as it finds numerous applications in chemical and processing industry. A few uses are found in the production of following marketable items:

- Sulfuric Acid
- Pharmaceuticals
- > Ointments
- > Fertilizer
- Pesticides and insecticides
- Batteries

And many other. Sulfuric acid itself is known as king of chemicals and found innumerable uses in manufacturing and production.

PROCESS DESCRIPTION

2.1. The Two Sections

The Superclaus process recovers elemental sulfur from rich acid gas stream with an efficiency greater than 99%. The process proceeds in two main stages: a *thermal section* and a *catalytic* section. It starts from Claus furnace to which feed acid gas is fed and part of H₂S is converted into SO₂. Here, some of the SO₂ formed will react with H₂S and elemental sulfur is formed. Note that only 60-70% conversion to elemental sulfur is possible in furnace (the thermal stage). High temperature of flue gases is lowered down in a waste heat boiler and then the gases go to the first sulfur condenser. After separating the sulfur out from the mixture, the liquid sulfur is sent to a sulfur pit and the remaining gases, which still contain sulfur content about 40% of the fed H₂S amount enter the catalytic section where catalytic reactions take place in three fixed bed reactors. The first two reactors are conventional Claus reactors and the third one in series with them is the Superclaus reactor containing a selective oxidation catalyst. Elemental sulfur formed in every catalytic stage is also condensed and collected in a sulfur pit. The gas leaving each condenser needs to be heated up by reheaters before entering the next reactor or else the reaction will not find sufficient activation energy to be initiated. Another reason for reheating is to prevent condensation of sulfur in the reactor which would damage the catalyst bed.

2.2. Catalysts and Selective Oxidation

The first two reactors contain the conventional claus catalyst, that is, either alumina or titania. The Superclaus reactor contains iron or chromium catalyst on alpha alumina support. [5]

2.3. Significance of Thermal Section

The thermal section, or claus furnace in particular, is a pivotal unit to be considered for a maximum process efficiency. The residence time and temperature in the furnace should be such that impurities like hydrocarbons, and, if present, ammonia and aromatics are completely broken down before process stream proceeds next to the reactors. Additional benefit of high temperature is that the formation of unwanted sulfur compounds like COS and CS₂ is impeded. [2]

The tail gas leaving the last reactor is incinerated and released into the environment through a stack.

2.4. Reactions

Combustion Reaction:

$$H_2S + 1.5O_2 \rightarrow SO_2 + H_2O$$

Claus Reaction:

$$2H_2S + SO_2 \rightleftharpoons \frac{3}{8}S_8 + 2H_2O$$

Superclaus Reaction:

$$2H_2S + O_2 \rightarrow \frac{1}{4}S_8 + 2H_2O$$

BLOCK FLOW DIAGRAM

3.1. Bounds of this Project

It is important to consider the physical boundary of this project. As natural gas comes out of the wells, it is first sent for sweetening through amine absorption. The sweetened natural gas is transported towards its downstream consumption while the gaseous waste removed goes to a sulfur recovery unit. The focus of this project is sulfur recovery unit; the harmful gaseous waste from the downstream of absorption unit becomes the feed for this plant.



Figure 1 Focus of this Project

3.2. Block Flow Diagram of Superclaus Process

For the process selected, a block diagram representing the sequence of processing steps is shown below.



Figure 2 Block Flow Diagram

PROCESS FLOW DIAGRAM

On the basis of above block flow diagram, a process flow diagram is constructed.



Figure 3 Process Flow Diagram

MASS BALANCE

5.1. Theorical foundation

Material balance has its original roots in law of conservation of mass which says that in any real process, mass can neither be created nor be destroyed and hence the quantity of matter before and after any process remains constant.

This law gives rise to the following equation:

$$Mass_{IN} - Mass_{OUT} + Generation - Consumption = Accumulation$$

In words, this equation means that sum of the material entering and leaving the system, mass generated and consumed in the system when subtracted from accumulation should count to zero. It also implies that in case of steady state process, accumulation term would be zero. [6]

In the steady state balance problem where no chemical reaction takes place, this equation simplifies to:

$$Mass_{IN} - Mass_{OUT} = 0$$

Or
 $Mass_{IN} = Mass_{OUT}$

Mass Balance is a preliminary step in plant design. The methodology is such that material entering and leaving each equipment is calculated and finally an overall material balance for the entire plant is carried out.

5.2. Feed Stream Composition

Let us first consider the feed stream composition.

Feed (1) [Acid Gas inlet for SRU]			
	Molar flowrate	Molar flowrate	Mole
Component	(lbmol/hr)	(kmol/hr)	Fraction
H ₂ S	155.44	69.95	0.49
CO ₂	93.15	41.92	0.29
H ₂ O	58.67	26.40	0.19
Methane	0.98	0.44	3.15E-03
Ethane	0.70	0.31	2.25E-03
Propane	0.40	0.18	1.28E-03
i- Butane	0.61	0.27	1.96E-03
n-Butane	0.15	0.07	4.82E-04
i-Pentane	0.40	0.18	1.28E-03
n-Pentane	0.35	0.16	1.12E-03
n-Hexane	0.55	0.25	1.77E-03
Total	311.40	140.13	1.00

Table 1 Furnace Feed Stream Composition

5.3. Calculations

Basis for calculations: 1 hour process

Conditions:

Physical State: Gas

Temperature: 65.60°C

Pressure: 135.83kPa

Assumptions: Steady state process

Now the material entering and leaving all of the remaining streams in the sequence of their processing is shown below.

Air required for the furnace is calculated on the basis of the fact in the Superclaus process one-third of the H_2S feed is to be combusted in limited

supply of oxygen. Balanced stoichiometric equation for the combustion of H₂S is as follows:

$$H_2S + 1.5O_2 \rightarrow SO_2 + H_2O$$

On the basis of this equation, oxygen required to burn 1 mole of H_2S was obtained and this value was multiplied by $1/3^{rd}$ of the total H_2S moles entering the furnace. The resulting oxygen showed the moles of air required.

$$\frac{1}{3} * Moles(H2S)_{IN} = 23.32 kmol$$

$$O_2 required = 1.5 * 23.32 = 34.98 kmol$$

Similarly, O_2 required for the combustion of hydrocarbons was calculated which sums to 10.15kmol. So the total O_2 required is as shown in the table below.

Air Feed (2) [To Furnace]			
Component	Molar flowrate (kmol/hr)	Mole Fraction	
02	45.13	0.21	
N2	169.69	0.79	
Total	214.83	1	

Table 2 Furnace Air Inlet

H₂S will burn in this limited supply of oxygen and the exhaust gases so produced will have the following moles leaving the furnace.

Furnace Exhaust (3) [WHB inlet]			
Component	Molar flowrate (kmol/hr)	Mole Fraction	
H2S	17.58	0.05	
SO2	8.16	0.02	
CO2	48.07	0.14	
H20	88.04	0.25	
N2	169.77	0.49	
S2	17.05	0.05	
Total	348.67	1.00	

Table 3 Furnace Outlet

Material Entering and leaving the waste heat boiler would be same. Gas stream leaving the first condenser would also have no change in composition and/or mass. After first condenser the process gas goes to the two phase separator to separate out the elemental sulfur formed in the furnace. The composition for both the gaseous and liquid streams at the outlet of this separator is shown in the table below

Table 4 Separator-1	Outlet
---------------------	--------

	Sep1 outlet (6,7) [(6) is RH1 inlet]			
	(6) Molar	(7) Molar	Mole	Mole
Comp	flowrate	flowrate	Fraction	Fraction
onent	(kmol/hr)	(kmol/hr)	(6)	(7)
H2S	17.58	0.00	0.05	0.00
S02	8.15	0.00	0.02	0.00
CO2	48.06	0.00	0.14	0.00
H20	88.04	0.00	0.26	0.00
N2	169.77	0.00	0.51	0.00
S6	0.0042	0.62	1.28E-9	0.04
S8	0.0588	14.85	1.17E-4	0.96
Total	331.68	15.47	1.00	1.00

Now the stream is reheated and sent to the first reactor which contains the conventional Claus catalyst. The material change in heater inlet and outlet is zero. The change in reactor is depicted through the composition of the exit stream of the reactor.

Stoichiometry is brought into use for these calculations. The reaction taking place in the reactor is the conventional Claus reaction. Conversion for this reactor is taken to be 73%.

$$2H_2S + SO_s \ \rightleftharpoons \ \frac{3}{8}S_8 + 2H_2O$$

Reactor-1 outlet (9) [Condenser-2 inlet]			
Component	Molar flowrate (kmol/hr)	Mole Fraction	
H ₂ S	4.75	0.01	
SO ₂	1.74	0.01	
CO ₂	48.07	0.15	
H ₂ O	100.88	0.31	
N2	169.77	0.52	
S6	0.01	0.00	
S ₈	2.46	0.01	
Total	327.67	1.00	

Table 5 Reactor-1 Outlet

Elemental sulfur so formed is to be condensed in second condenser and then separated from the main process stream. Remaining gaseous stream still contains appreciable amounts of H₂S and is sent to the reheater and the second reactor for further processing. The conversion based on H₂S is 63%. The exit stream of the second reactor is of the following composition.

Reactor 2 outlet (14) [inlet of condenser-3]			
Component	Molar flowrate (kmol/hr) Mole Fraction		
H ₂ S	1.76	0.01	
SO ₂	0.24	7.53E-04	
CO ₂	48.07	0.15	
H ₂ O	103.87	0.32	
N2	169.77	0.52	
S6	4.90E-03	1.51E-05	
S8	0.59	1.81E-03	
Total	324.30	1.00	

Table 6 Reactor-2 Outlet

In the last reactor, remaining H_2S is selectively oxidized by a Superclaus catalyst directly into sulfur. This requires an Air stream. On the basis of stoichiometry, Air required for the last of the reactors has been calculated.

Table 7 Reactor-3 Air Inlet

Reactor-3 Air (19) [inlet]			
Component	Molar flowrate (kmol/hr)	Mole Fraction	
02	0.77	0.21	
N2	2.91	0.79	
Total Air	3.68	1.00	

Finally, gases coming out from the last reactor are of the following composition as shown in the table. The reaction taking place is the selective oxidation of H₂S into elemental sulfur on Fe or Cr on alpha-alumina catalysts. The chemical equation foe this reaction is:

$$2H_2S + O_2 \rightarrow \frac{1}{4}S_8 + 2H_2O$$

Reactor 3 outlet (20) [inlet of con4]			
Component	Molar flowrate (kmol/hr)	Mole Fraction	
H ₂ S	0.02	1.07E-03	
SO ₂	0.07	7.47E-04	
CO ₂	48.07	0.15	
H ₂ O	105.27	0.32	
S6	2.18E-03	6.67E-06	
S8	0.19	5.91E-04	
02	0.07	2.15E-04	
N2	172.68	0.53	
Total	326.88	1.00	

Table 8 Reactor-3 Outlet

5.4. Overall Material Balance

Based upon these calculations, we found that the overall mass remains conserved in the system. For this, a summary of overall mass balance is shown in tabulated form.

Components	IN (kg/hr)	OUT (kg/hr)
Elemental Sulfur	-	4291.66
H ₂ S	4313.23	-
SO ₂	-	2.23
CO2	1183.60	1515.04
H ₂ O	295.20	1438.80
02	1440.00	1.70
N ₂	4732.00	4732.00
Methane	7.06	-
Ethane	9.45	-
Propane	7.92	-
Total	11981	11981

Table 9 Overall Material Balance

The elemental Sulfur obtained from this plant in the unit of metric tons per day is found as summarized below.

Elemental Sulfur Recovered		
Molar Flowrate (kmol/hr) 134.32		
MTPD	103.16	

Table 10 Elemental Sulfur Recovered

ENERGY BALANCE

6.1. Theoretical Foundation

After material balance we then moved to the energy balance. All the calculations were based on the fundamental idea of conversation of energy which states that the total amount of energy in a system never changes. Using the data calculated from the material balance along with the required enthalpy data from relevant sources we were able to carry out the energy balance. [6]

Energy IN + Energy Generated = Energy OUT + Energy Consumed

6.2. Feed Stream Enthalpies

The following table shows the component wise enthalpies of the feed stream. Using molar flowrates and molar enthalpies we were able to work out the enthalpies of each component present and the total enthalpy of the Acid gas feed stream into the furnace. [6] [7]

Feed (1) [Acid Gas inlet for SRU]			
Component	Molar	Molar Enthalpies	Enthalpies
	flowrate	(kJ/kmol)	(kJ/hr)
	(kmol/hr)		
H ₂ S	69.95	2230.13	155993.45
CO2	41.92	2480.34	103969.46
H ₂ O	26.40	2194.09	57927.27
Methane	0.44	2395.89	1056.59
Ethane	0.32	3642.24	1147.31
Propane	0.18	8881.15	1598.61
i- Butane	0.27	6757.03	1854.81
n-Butane	0.07	6857.55	462.88
i-Pentane	0.18	8619.51	1551.51
n-Pentane	0.16	8519.51	1341.82
n-Hexane	0.25	10192.81	2522.72
Total	140.13	62770.25	329426.42

Table 11 Feed Gas Energy Inlet

6.3. Calculations

Following are the basis we took for the calculations:

Basis		
Ambient T (Ref) C	25.00	
Ambient P (kPa)	101.33	
Time (hr)	1.00	

In the similar manner as discussed above, interpolating enthalpies values data table to find the enthalpies at the desired air inlet temperature of 85°C.

Air Feed (2) [To Furnace]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
02	45.13	2507.96	113191.13
N2	169.70	2473.22	419703.31
Total	214.83	4981.18	532894.44

Table 13 Feed Air Energy Inlet

The temperature in the furnace is raised to 1100°C. There are multiple hydrocarbons combustion reactions along with the claus reaction that takes place inside the furnace. To work out the heat involved with each of these reactions we used the Hess's law.

Furnace Exhaust (3) [WHB inlet]						
	Component	Molar flowrate	Molar Enthalpies	Enthalpies		
		(kmol/hr)	(kJ/kmol)	(kJ/hr)		
	H ₂ S	17.58	46413.42	815947.84		
	SO ₂	8.16	55814.79	455225.42		
	CO ₂	48.07	55310.76	2658732.68		
	H ₂ O	88.04	43024.72	3787982.62		
	N_2	169.77	34719.92	5894401.58		
	S2	17.05	39627.96	675649.75		
	Total	348.67		14287939.90		

Table 14 Furnace Energy Outlet

To determine the duty of the waste heat boiler, we incorporated the enthalpies of the inlet and outlet stream to the waste heat boiler.

Table 15 WHB Energy Outlet

WHB outlet (4) [Inlet of condender-1]					
Component	Molar flowrate	Molar Enthalpies	Enthalpies		
	(kmol/hr)	(kJ/kmol)	(kJ/hr)		
H ₂ S	17.58	13254.52	233014.46		
SO ₂	8.16	16409.06	133832.29		
CO2	48.07	15649.62	752261.58		
H ₂ O	88.04	12728.20	1120616.18		
N2	169.77	10776.50	1829526.41		
S6	7.16	32022.80	229312.92		
S ₈	9.89	41676.15	412131.17		
Total	348.67	142516.85	4710695.01		

Table 16 WHB Duty

Duty	(kJ/hr)
Q	-15308032.06

Using the latent heat and the moles of sulphur condensed we were able to work out the latent heat of condensation of sulphur condensed. We then used this value along with the inlet and outlet enthalpies to determine the duty of the condenser.
Condenser-1 outlet (5) [Separator-1 inlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	17.58	5021.08	88270.59
SO ₂	8.16	6045.80	49309.54
CO2	48.07	5677.18	272896.37
H ₂ O	88.04	4908.24	432121.45
N ₂	169.77	4225.82	717417.46
S6	0.62	12670.00	7871.31
S8	14.91	16490.00	245868.16
Total	347.15	55038.12	1813754.88

Table 17 Condenser-1 Energy Outlet

Table 18 Condenser-1 Duty

Duty Q [Condenser-1]		
Duty	kJ/hr	
Q	-2754835.22	

In the reheater the temperature is increased from 145°C to 222°C. Using the sensible heat of the inlet and outlet stream we calculated the duty of the reheater.

	RH1 outlet (8) [Reactor1 inlet]				
Component	Molar flowrate	Molar Enthalpies	Enthalpies		
	(kmol/hr)	(kJ/kmol)	(kJ/hr)		
H ₂ S	17.58	7803.11	137178.66		
SO ₂	8.16	9525.27	77688.06		
CO2	48.07	8997.30	432491.43		
H ₂ O	88.04	7583.80	667693.10		
N ₂	169.77	6500.97	1103669.68		
S ₆	4.25E-03	19152.57	81.37		
S ₈	0.06	24915.85	1466.90		
Total	331.68	84478.87	2420269.19		

Table 19 RH1 Energy Outlet

Table 20 RH1 Duty

Duty	(kJ/hr)
Q	859217.47

As there is a claus reaction taking place in this reactor, we used Hess's law to calculate the heat of reaction.

Reactor1 outlet (9) [Condenser-2 inlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	4.75	10808.50	51303.63
SO ₂	1.74	13321.50	23170.08
CO2	48.07	12656.25	608373.28
H ₂ O	100.88	10432.50	1052382.61
N2	169.77	8881.25	1507769.81
S6	0.01	27273.00	394.04
S ₈	2.46	35081.00	86211.11
Total	327.67		3329604.57

Table 21 Reactor-1 Energy Outlet

Table 22 Reactor-1 Heat of Reaction

Heat of reaction (kJ/hr)	-1394840.50

In the similar manner as discussed before we calculated the duty of this condenser.

Table 23 Condenser-2 Energy Outlet

Condenser-2 outlet (10) [Separator-2 inlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	4.75	4660.48	22121.43
SO ₂	1.74	5594.80	9731.04
CO2	48.07	5247.08	252221.89
H ₂ O	100.88	4561.44	460137.08
N ₂	169.77	3935.34	668103.27
S6	0.01	11501.00	166.17
S ₈	2.46	14959.00	36761.55
Total	327.67	50459.14	1449242.43

Table 24 Condenser-2 Duty

Duty	(kJ/hr)
Q	-1857626.14

Table 25 Reactor-2 Energy Outlet

Reactor-2 outlet (14) [Condenser-3 inlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	1.76	8468.62	14872.95
SO ₂	0.24	10364.10	2530.09
CO2	48.07	9802.39	471191.08
H ₂ O	103.87	8216.62	853425.46
N ₂	169.77	7031.79	1193786.99
S6	4.90E-03	20739.14	101.57
S8	0.59	26980.71	15821.62
Total	324.30	91603.37	2551729.77

Table 26 Reactor-2 Heat of Reaction

Heat of reaction (kJ/hr)	-326589.16	

Condenser-3 (15) [outlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	1.76	4407.31	7740.30
SO ₂	0.24	5302.72	1294.51
CO2	48.07	4911.00	236066.86
H ₂ O	103.87	4306.40	447287.50
N ₂	169.77	3750.00	636637.50
S6	0.02	14401.81	300.06
S ₈	0.57	14401.86	8273.17
Total	324.30	51481.09	1337599.90

Table 27 Condenser-3 Energy Outlet

Table 28 Condenser-3 Duty

Duty	(kJ/hr)
Q	-1208839.25

After going through the same sequence of equipment's, the process stream now enters the third reactor where superclaus reaction takes place. Here again using Hess's law we calculated the heat of reaction for the superclaus reaction. Interpolating between various temperatures helped us finding the enthalpy of the inlet and outlet streams.

Table 29 Reactor-3 Air Inlet

Reactor-3 Air (19) [inlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
02	0.77	2507.96	1938.02
N2	2.91	2473.22	7189.65
Total Air	3.68	4981.18	9127.66

Reactor-3 outlet (20) [SuperClaus Reactor]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	0.35	8104.32	2846.63
SO ₂	0.24	9815.17	2396.09
CO2	48.07	14100.23	677783.96
H ₂ O	105.27	11930.40	1255922.17
S ₆	2.18E-03	19857.71	43.30
S ₈	0.19	25833.57	4992.73
02	0.07	6822.00	479.24
N2	172.68	6650.00	1148302.04
Total	326.88	103113.40	3092766.16

Table 30 Reactor-3 Energy Outlet

Table 31 Reactor-3 Heat of Reaction

Heat of reaction (kJ/hr)	-244569.61
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Table 32 Conderser-4 Energy Outlet

Condenser-4 (21) [outlet]			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	0.35	4129.59	1450.51
SO ₂	0.24	4942.10	1206.47
CO2	48.07	4628.81	222502.27
H ₂ O	105.27	4047.47	426080.21
S6	0.01	10216.36	60.19
S ₈	0.19	13287.57	2531.04
02	0.07	3561.18	250.17
N2	172.68	3504.00	605060.20
Total	326.88	48317.08	1259141.06

Table 33 Condenser-4 Duty

Duty	(kJ/hr)
Q	-1831919.34

Table 34 Incinerator Energy Outlet

Incinerator outlet (24)			
Component	Molar flowrate	Molar Enthalpies	Enthalpies
	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	0.00	5561.98	0.00
SO ₂	0.60	11318.10	6738.45
CO ₂	48.07	10722.99	515443.41
H ₂ O	105.62	8931.42	943354.44
S ₆	0.00	22502.00	0.00
S8	0.00	29275.00	0.00
02	0.05	7628.39	401.92
N2	2.18	7853.47	17122.52
Total	156.52	103793.35	1483060.74

Table 35 Inlet to Sulphur Pit

Sulfur Pit inlet			
Sulfur Pit	Molar flowrate	Molar enthalpy	Enthalpy
inlet	(kmol/hr)	(kJ/kmol)	(kJ)
S ₆	4.75	11329.71	53769.84
S8	143.32	14736.14	2111960.54
Total	148.06	26065.86	2165730.38

In Gas-Gas heat exchanger, waste heat recovery is taking place. Some of the heat from the exiting gas stream is being extracted and that heat is being used to preheat the air used in the plant. Using the enthalpies of the inlet and outlet gas stream to the heat exchangers we calculated the heat recovered.

Gas-Gas Heat Exchanger outlet (25)			
Compone	Molar flowrate	Molar Enthalpies	Enthalpies
nt	(kmol/hr)	(kJ/kmol)	(kJ/hr)
H ₂ S	0.00	0.00	0.00
SO ₂	0.60	8345.90	4968.89
CO ₂	48.07	7870.69	378336.20
H ₂ O	105.62	6676.92	705229.64
S6	0.00	0.00	0.00
S8	0.00	0.00	0.00
02	0.05	5862.71	308.89
N2	2.18	5729.81	12492.41
Total	156.52	34486.03	1101336.04

Table 36 Gas-Gas Heat Exchanger Energy Outlet

Table 37 Gas-Gas Heat Exchanger Air Inlet

Gas-Gas Heat Exchanger (Cold Air in 26)			
Componen	Molar flowrate	Molar Enthalpies	Enthalpies
ts	(kmol/hr)	(kJ/kmol)	(kJ/hr)
02	45.13	732.00	33035.16
N2	169.69	728.00	123534.32
Total	214.82	1460.00	156569.48

Air balance on Gas-Gas Heat Exchanger (Hot air out 27)			
Componen	Molar flowrate	Molar Enthalpies	Enthalpies
ts	(kmol/hr)	(kJ/kmol)	(kJ/hr)
02	45.13	2507.96	113184.23
N2	169.69	2473.22	419680.70
Total	214.82	4981.18	532864.94

Table 38 Gas-Gas Heat Exchanger Air Outlet

Table 39 Heat Recovery

	-
Heat Recovered (kJ/hr)	-376295.46

6.4. Overall Energy Balance

Table 40 Overall Energy Balance

IN (MJ/hr)	OUT (MJ/hr)
23353.00	23353.00

Following are some of the tables used in the calculations [6]:

к	CI	C2	C3	n-C4	i-C4	n-C5	n-C ₆
273	0						
291	630	912	1,264	1,709	1,658	2,125	2,545
298	879	1,277	1,771	2,394	2,328	2,976	3,563
300	950	1,383	1,919	2,592	2,522	3,222	3,858
400	4,740	7,305	10,292	13,773	13,623	17,108	20,463
500	9,100	14,476	20,685	27,442	27,325	34,020	40,622
600	14,054	22,869	32,777	43,362	43,312	53,638	64,011
700	19,585	32,342	46,417	61,186	61,220	75,604	90,123
800	25,652	42,718	61,337	80,600	80,767	99,495	118,532
900	32,204	53,931	77,404	101,378	101,754	125,101	148,866
1,000	39,204	65,814	94,432	123,428	123,971	152,213	181,041
1,100	46,567	78,408	112,340	146,607	147,234	180,665	214,764
1,200	54,308	91,504	131,042	170,707	171,418	210,246	249,868
1,300	62,383	105,143	150,331	195,727	196,480	240,872	286,143
1,400	70,709	119,202	170,205	221,375	222,212	272,378	323,465
1,500	79,244	133,678	190,581	247,650	248,571	304,595	361,539
1,600	88,031						
1,800	106,064						
2,000	124,725						
2,200	143,804						
2,500	173,050						

Figure 4 Enthalpies of Hydrocarbon Vapors

ĸ	N ₂	NO	N ₂ O	NO ₂	N204
273	0	0	0	0	0
291	524	537	686	658	1,384
298	728	746	957	917	1,937
300	786	686	1,034	985	2,083
400	3.695	3,785	5,121	4,865	10,543
500	6,644	6,811	9,582	9.070	19,915
600	9,627	9,895	14,386	13,564	30,124
700	12.652	13,054	19,513	18,305	
800	15,756	16,292	24,950	23,242	
900	18,961	19,597	30,693	28,334	
,000,	22,171	22,970	36,748	33,551	
.100	25,472	26,392	43,129	38,869	
.200	28,819	29,861	49,862	44,266	
,300	32.216	33,371		49,731	
.400	35,639	36,915		55,258	
.500	39,145	40,488		60,826	
,750	47,940	49,505	(a.)		
000,5	56,902	58,634			
2,250	65,981	67,856			
2,500	75,060	77,127			

Figure 5 Enthalpies of Nitrogen and some of its Oxides

к	S ₂ (g)	SO ₂	SO3	H ₂ S	CS2
273	0	0	0	0	0
291	579	706	899	607	807
298	805	984	1,255	845	1,125
300	869	1,064	1,338	909	1,217
400	4,196	5,234	6,861	4,372	5,995
500	7,652	9,744	13,033	7,978	11,108
600	11,192	14,514	19,832	11,752	16,455
700	14,790	19,501	27,154	15,706	21,974
800	18,426	24,647	34,748	19,840	27,631
900	22,087	29,915	42,676	24,145	33,388
1.000	25,769	35.275	50,835	28,610	39,220
1.100	29,463	40,706	59,203	33,216	45,103
1,200	33,174	46,191	67,738	37,953	51,044
1,300	36,898	51,714	76,399	42,802	57,027
1.400	40,630	57,320		47,739	63,052
1,500	44,371	62,927		52,802	69,119
1,600	48,116	68,533		57,906	75,186
1,700	51,881	74,182		63,094	81,295
1,800	55,605	79,872		68,324	87,361
1,900	59,370	85,520		ANY 7187330222	
2,000	63,136	91,253			
2,500	82,006	119.871			
3,000	100,959	148,657			

Figure 6	Enthalpies	of Sulphur	Compounds	(vapor)
	r			(

(1) $C_p^\circ = a + b(T) + c(T)^2 + d(T)^3$; (2) $C_p^\circ = a + b(T) + c(T)^{-2}$. Units of C^o_p are J/(g mol)(K or °C). To convert to cal/(g mol)(K or °C) = Btu/(lb mol)(°R or °F), multiply by 0.2390. Note: $b \cdot 10^2$ means the value of b is to be multiplied by 10^{-2} , e.g., 20.10×10^{-2} for acetone. Temp. Range Mol Formula Wt. State $b \cdot 10^2$ $c \cdot 10^5$ $d \cdot 10^9$ (in T) Compound Form Τ а Acetone CH₃COCH₃ 58.08 °C 71.96 20.10 -12.7834.76 0-1200 g 1 Acetylene C_2H_2 26.04 °C 42.43 6.053 -5.033 18.20 0-1200 g Air 29.0 °C 28.94 0.4147 0.3191 -1.965 0-1500 g K 28.09 0.1965 0.4799 -1.965 273-1800 1 g NH₃ 17.03 °C 35.15 2.954 0.4421 -6.686 0-1200 Ammonia g 1 Ammonium sulfate $(NH_4)_2SO_4$ K 275-328 132.15 215.9 с 1 ĸ -7.27329 1,897.9 279-350 Benzene 78.11 77.054 -164.82 C₆H₆ ۱ 1 °C 74.06 32.95 -25.2077.57 0-1200 g 1 °C ℃ ℃ $C_{4}H_{10}$ 0-1200 -18.9149.87 Isobutane 58.12 89.46 30.13 g 1 0-1200 58.12 92.30 -15.4734.98 n-Butane $C_{4}H_{10}$ g 1 27.88 Isobutene 56.10 82.88 -17.2750.50 0-1200 C_4H_8 g 1 25.64 -8.66×10^{10} K 298-720 Calcium carbide CaC₂ 64.10 с 2 68.62 1.19 -12.87×10^{10} _ Calcium carbonate CaCO₃ 100.09 с 2 ĸ 82.34 4.975 273-1033 Calcium hydroxide Ca(OH)2 74.10 с 1 K 89.5 276-373 Calcium oxide CaO 56.08 2 ĸ 41.84 2.03 -4.52×10^{10} 10273-1173 с Carbon 12.01 c† 2 к 1.095 -4.891×10^{10} 273-1373 С 11.18 CO₂ Carbon dioxide 44.01 °C 4.233 -2.887 7.464 0-1500 1 36.11 g 28.01 °C 0.3548 -2.2200-1500 Carbon monoxide co 28.95 0.4110 1 g CCI4 ĸ -318.26 273-343 Carbon tetrachloride 153.84 12.285 0.01095 3,425.2 1 1 °C -1.607 6.473 0-1200 Chlorine 70.91 1.367 Cl_2 33.60 g 1 ĸ Cu 63.54 22.76 0.06117 273-1357 Copper с 1

[†]Graphite. [‡]Rhombic. [§]Moinoclinic. ^{*}(at 1 atm)

Forms:



CHAPTER 7

EQUIPMENT DESIGN

Three type of equipment is employed in this process: furnace, heat exchangers and reactors. Heat exchangers include waste heat boiler, sulfur condensers and reheaters. In addition to these are separators, sulfur pit and incinerator. Design of the former equipment is shown here.

7.1. Furnace Design

7.1.1. Claus Furnace:

This is also called Claus furnace or reaction furnace. Surprisingly, the main purpose of this equipment is not to heat up a fluid using a fuel. Rather this furnace is better called a combustion chamber. Process stream is flammable; it is burnt in limited supply of oxygen in this equipment. Only $1/3^{rd}$ of H₂S is oxidized to SO₂ and the remaining H₂S goes to the catalytic section to react with this SO₂ to give elemental sulfur. [2]

7.1.2. Main Reactions:

The two main reactions taking place in the furnace are:

$$H_2S + 1.5O_2 \rightarrow SO_2 + H_2O$$
$$2H_2S + SO_s \rightarrow \frac{3}{2}S_2 + 2H_2O$$

In addition to these, there are various side reactions such as formation of unwanted sulfur compounds like carbon disulfide (CS₂) and carbonyl sulfide (COS) and combustion of hydrocarbon impurities. A high temperature and sufficient residence time ensures break down of these impurities which, when otherwise pass to the reactors, severely damage the catalyst. [2]

For this plant, the furnace will be Direct Fired type box furnace with the burner which ensures that oxygen supply is way below the stoichiometric amount so only $1/3^{rd}$ of the H₂S is burnt here. [4] [1]

7.1.3. Design Calculations:

For design, the reaction furnace is treated just like a plug flow reactor. So the following design equations were employed. [8]

$$F_A = F_{A_o}(1 - \varepsilon X_A)$$
$$\dot{V}_A = \dot{V}_{Ao}(1 - \varepsilon X_A)$$

Where,

F represents molar flowrate and \dot{V}_A represents volumetric flowrate of acid gases. X denotes the conversion of H₂S both to SO₂ and sulfur. ε is the expansivity factor. It is a numeric depiction of the expansion of gases in the furnace. That is, it is a relative increase in the volume of the exit gases leaving the furnace as compared to the inlet acid gas stream. Mathematically,

$$\varepsilon = \frac{\dot{V}_{out} - \dot{V}_{in}}{\dot{V}_{in}}$$

To obtain entering volume, V_{in}, feed gas composition and the air inlet is taken into consideration. Average molecular weight of the mixed stream is found to find volumetric flowrate. Then to obtain volume of the claus reactor, as assumption for the residence time is to be made. This assumption is needed because of the lack of information regarding reaction kinetics. Literature suggests the residence time for furnace is in the range of 0.5s to 4s [9]. Assumption for residence time for this calculation is 3.5s.

	Mixed Streams (1) and (2) [Furnace feed]						
Component	Mole Fraction	Molar Mass (kg/kmol)	Mole frac x Mw				
H ₂ S	0.32	34.00	10.74				
CO ₂	0.07	44.00	3.12				
H2O	0.04	18.00	0.78				
Methane	1.16E-03	16.00	0.02				
Ethane	8.30E-04	30.00	0.02				
Propane	4.74E-04	44.00	0.02				
i- Butane	7.23E-04	58.00	0.04				
n-Butane	1.78E-04	58.00	0.01				
i-Pentane	4.74E-04	72.00	0.03				
n-Pentane	4.15E-04	72.00	0.03				
n-Hexane	6.52E-04	86.00	0.06				
02	0.12	32.00	3.80				
N2	0.45	28.00	12.51				

Table 41 Mixer Feed Stream Composition

Thus,

 $MW_{avg} = 10.74 + 3.12 + 0.78 + 0.02 + 0.02 + 0.02 + 0.04 + 0.01 + 0.03 + 0.03 + 0.06 + 3.8 + 12.51$

 $MW_{avg} = 31.19 \text{kg/kmol}$

mass flow rate = 11981.69 kg/hr

 $density = 0.87kg/m^3$

volumetric flowrate $= \frac{mass flowrate}{density} = 12989.76 \text{m}^3/\text{hr}$

Now we incorporate the expansivity to find the maximum volume of gaseous mixture in the furnace.

$$V_A = V_{Ao}(1 - \varepsilon X_A)$$

 $\dot{V}_A = 13668.12 \text{m}^3/\text{hr} = 3.92 m^3/s$
 $\tau = 3.5s$

.

.

volume of the reactor = $\dot{V}_A \times \tau = 13.72m^3$

A general rule of thumb for L/D ratio is; L/D = 4/1. Using this assumption and the formula for volume of a cylinder, length and diameter of the reaction furnace is obtained. Volume of the reactor's shell is given by this formula.

$$V_s = \frac{\pi D^2 L}{4}$$

To obtain thickness, e, this formula is used. (Coulson volume 6)

$$e = \frac{P_i \times D_i}{2Jf}$$

Where, Pi is the design pressure, Di is the internal diameter of the vessel, f is design stress and j is joint factor.

$$e = 6.50mm$$

This thickness when added to the inner diameter of the furnace will determine outer diameter of it.

$$D_{out} = 1.21m$$

Lastly, mass of steel required will be calculated on the basis of its volume and density.

$$V_{s} = \frac{\pi (D_{o}^{2} - D_{1}^{2})L}{4}$$

Density_{steel} = 7850kg/m³
Mass_{steel} = 2235.99kg

7.1.4. Overall Summary of the Design Specifications

In order to summarize the design specifications for the claus reactor (or reaction furnace), here is constructed a table.

Design Specifications				
Туре	Direct Fired			
Volume (m ³)	13.72			
Diameter (m)	1.63			
Length (m)	4.38			
Shell Thickness (mm)	6.5			
Shell Material	Carbon Steel			
Refractory material	High Alumina			
Design Pressure (kPa)	165			
Design Temperature (°C)	1200			
H ₂ S Conversion (%)	88			

Table 42 Furnace Design Specifications

7.1.5. Material of Construction:

Now for the material of construction, carbon steel will be used for shell construction. As there are very high temperatures in the furnace (>1100°C) and the process stream is both acidic and corrosive in nature, this situation calls for a strong refractory material providing a significant resistance to corrosive action of acid gases and to large amounts of heat released in the furnace. Therefore, high alumina is chosen as refractory material.

7.2. Heat Exchanger Design

There are four heat exchangers in this sulphur recovery unit and the purpose of each of them is to condense the sulphur that is being produced in the furnace and the reactors through the claus reaction.

Considering the economics, efficiency, and the ease of maintenance, we choose shell and tube as our type for the heat exchanger. Cooling water in the shell side is being used to cool the hot acid gas stream in the tube side. Acid gas being the more corrosive fluid is selected as a tube side fluid.

The type of tube layout chosen for this design is triangular pitch. Triangle pitch helps in creating greater turbulence flow in the shell side as compared to other layouts, which is an important factor in achieving efficient heat transfer.

We have followed the Kern's method for the calculations. [10] [10]

Heat Load

$$Q = ((4.7 * 10^{6}) - (1.4 * 10^{6})) + (1.4 * 10^{5})$$
$$Q = 3.4 * 10^{6} kJ/hr$$

Log Mean Temperature Difference:

Table 43 LMTD Calculations

HOT FLUID		COLD FLUID	DIFFERENCE
365	Hight Temperature (°C)	120	245
145	Low Temperature (°C)	30	115
220		90	130

$$LMTD = \frac{245 - 115}{\ln(\frac{245}{115})}$$

$$LMTD = 171.80^{\circ}C$$

True Log Mean Temperature Difference:

$$R = \frac{220}{90} = 2.40$$

$$S = \frac{90}{365 - 30} = 0.27$$

Using values of R and S to find Temperature Difference Factor from figure 4:



Figure 8 LMTD Correction Factor

From figure 4:

$$F_T = 0.97$$

Assuming the Design Coefficient for further calculations based on literature data of similar Sulphur Recovery Systems:

$$U_D = 140W/m^2k$$

Total heat transfer Area:

$$Area = \frac{Q}{U_D * \Delta t}$$

$$Area = \frac{933922}{(140)(171.80)}$$

 $Area = 38.83m^2$

7.2.1. Tube Section Calculations:

Assuming Tube sizing:

Tube	BWG	Wall	ID in	Flow area	Surface pe	er lin ft, ft²	Weight
OD, in.	Bird	ness, in.	12, 11.	in. ²	Outside	Inside	lb steel
35	$12 \\ 14 \\ 16 \\ 18 \\ 20$	0.109 0.083 0.065 0.049 0.035	0.282 0.334 0.370 0.402 0.430	$\begin{array}{c} 0.0625\\ 0.0876\\ 0.1076\\ 0.127\\ 0.145\end{array}$	0.1309	$\begin{array}{c} 0.0748 \\ 0.0874 \\ 0.0969 \\ 0.1052 \\ 0.1125 \end{array}$	0.493 0.403 0.329 0.258 0.190
34	10 11 12 13 14 15 16 17 18	$\begin{array}{c} 0.134\\ 0.120\\ 0.095\\ 0.083\\ 0.072\\ 0.065\\ 0.058\\ 0.058\\ 0.049 \end{array}$	$\begin{array}{c} 0.482 \\ 0.510 \\ 0.532 \\ 0.560 \\ 0.584 \\ 0.606 \\ 0.620 \\ 0.634 \\ 0.652 \end{array}$	$\begin{array}{c} 0.182\\ 0.204\\ 0.223\\ 0.247\\ 0.268\\ 0.289\\ 0.302\\ 0.314\\ 0.334 \end{array}$	0.1963	$\begin{array}{c} 0.1263\\ 0.1335\\ 0.1393\\ 0.1466\\ 0.1529\\ 0.1587\\ 0.1623\\ 0.1660\\ 0.1707 \end{array}$	$\begin{array}{c} 0.965 \\ 0.884 \\ 0.817 \\ 0.727 \\ 0.647 \\ 0.571 \\ 0.520 \\ 0.469 \\ 0.401 \end{array}$
1	8 9 10 11 12 13 14 15 16 17 18	$\begin{array}{c} 0.165\\ 0.148\\ 0.134\\ 0.120\\ 0.095\\ 0.095\\ 0.083\\ 0.072\\ 0.065\\ 0.058\\ 0.049 \end{array}$	$\begin{array}{c} 0.670\\ 0.704\\ 0.732\\ 0.760\\ 0.782\\ 0.810\\ 0.834\\ 0.856\\ 0.870\\ 0.884\\ 0.902 \end{array}$	$\begin{array}{c} 0.355\\ 0.389\\ 0.421\\ 0.455\\ 0.479\\ 0.515\\ 0.546\\ 0.576\\ 0.594\\ 0.613\\ 0.639 \end{array}$	0.2618	$\begin{array}{c} 0.1754\\ 0.1843\\ 0.1916\\ 0.1990\\ 0.2048\\ 0.2121\\ 0.2183\\ 0.2241\\ 0.2277\\ 0.2314\\ 0.2361\\ \end{array}$	1.61 1.47 1.36 1.23 1.14 1.00 0.890 0.781 0.710 0.639 0.545
11/4	8 9 10 11 12 13 14 15 16 17 18	$\begin{array}{c} 0.165\\ 0.148\\ 0.134\\ 0.120\\ 0.095\\ 0.095\\ 0.083\\ 0.072\\ 0.065\\ 0.058\\ 0.058\\ 0.049 \end{array}$	$\begin{array}{c} 0.920\\ 0.954\\ 0.982\\ 1.01\\ 1.03\\ 1.06\\ 1.08\\ 1.11\\ 1.12\\ 1.13\\ 1.15\\ \end{array}$	$\begin{array}{c} 0.665\\ 0.714\\ 0.757\\ 0.800\\ 0.836\\ 0.884\\ 0.923\\ 0.960\\ 0.985\\ 1.01\\ 1.04 \end{array}$	0.3271	$\begin{array}{c} 0.2409\\ 0.2572\\ 0.2674\\ 0.2701\\ 0.2701\\ 0.2775\\ 0.2839\\ 0.2839\\ 0.2896\\ 0.2932\\ 0.2969\\ 0.3015 \end{array}$	2.09 1.91 1.75 1.58 1.45 1.28 1.13 0.991 0.900 0.808 0.688
135	8 9 10 11 12	0.165 0.148 0.134 0.120 0.109	1.17 1.20 1.23 1.26 1.28	1.075 1.14 1.19 1.25 1.29	0.3925	$\begin{array}{c} 0.3063 \\ 0.3152 \\ 0.3225 \\ 0.3299 \\ 0.3356 \\ 0.3456 \end{array}$	2.57 2.34 2.14 1.98 1.77
	14	0.083	1.33	1.40		0.3492	1.37
	16	0.072	1.30	1.47		0.3587	1.09

Figure 9 Heat Exchanger and Condenser Tube Data

Table 44 Tube Sizing Data

Outer	BWG	Wall	Internal	Flow area per
Diameter (m)		Thickness (m)	Diameter (m)	tube (<i>m</i> ²)
0.038	14	0.002	0.03	0.04

Flow area:

$$Flow Area = \frac{N_t a_t}{144n} = 0.12m^2$$

Mass flowrate:

From the material balance, total mass flowrate is $1.05 * 10^4 kg/hr$

Mass velocity:

$$G_t = \frac{w}{a_t} = 1.76 * 10^4 \frac{kg}{hr.\,m^2}$$

Number of tubes:

$$N_t = Mass \frac{flow rate}{Mass \ velocity \ * \ Flow \ area \ per \ tube} = 135$$

Length of a single tube:

$$Length = \frac{Area}{\pi * 0D} = \frac{38.83}{(\pi)(0.038)}$$
$$length = 2.40m$$

Reynolds Number:

$$Re_t = \frac{DG_t}{\mu} = 4.6 \times 10^3$$

Determining Chiltern-Colburn Factor (j_H) :

Using our calculated Reynolds Number and figure 6 we were able to calculate the j_H factor.

$$j_{H} = 20$$



Calculating hi:

$$h_{i} = j_{H} \left(\frac{k}{D}\right) * \left(\frac{c\mu}{k}\right)^{\frac{1}{3}} * \varphi_{t} = \frac{20}{0.125} (0.76)^{\frac{2}{3}} (1941 * 0.968)^{\frac{1}{3}}$$
$$h_{i} = 1644.23 W/m^{2}k$$
$$h_{io} = (1644.23) \left(\frac{1.33}{1.5}\right) = 1457.89 W/m^{2}k$$



Figure 11 Tube Side Friction Factor

Friction factor using figure 7:

$$f = 0.0002 \frac{ft^2}{m^2} = 0.00002 \frac{m^2}{m^2}$$

Pressure Drop:

$$\Delta P_t = \frac{f G_t^2 L n}{5.22 * 10^{10} D_S \varphi_t} = 1.79 \ kpa$$

7.2.2. Shell Side calculations:

Assumed the Internal Diameter of the shell using relevant data from literature:

$$ID = 0.85m$$

Determining Clearance:

$$C = P_T - OD(Tube)$$

$$C = (1.25 * 0.0381) - (0.0381) = 9.15 * 10^{-3}m$$

7.2.3. Baffles Calculations:

$$Baffle \ spacing = 1.0m$$

 $Baffle \ thickness = (tube \ thickness)(2.5) = (4.32 * 10^{-3})(2.5) = 0.01m$

Baffle Height = (0.75)(Internal shell diameter) = (0.75)(0.85) = 0.64m

Number of Baffles:

$$B = \frac{\text{length of the tube}}{(Baffle spacing)(Baffle thickness)} = 3$$

Flow area:

$$a_s = \frac{ID * CB}{P_T} = 0.33m^2$$

Mass Flowrate:

Mass flow rate (W) from the material balance is $8.9 * 10^3 kg/hr$

Mass Velocity:

$$G_s = \frac{W}{a_s} = 2.71 * 10^4 \frac{kg}{hr.m^2}$$

Equivalent Diameter:

The Equivalent Diameter was found using figure 8:



Figure 12 j_H vs Re curve for Shell Side

$$d_e = 0.03m$$

Reynolds Number:

$$Re_s = \frac{D_e G_s}{\mu} = 3.87 * 10^4$$

Determining Chiltern-Colburn Factor (j_H) :

Using the Reynolds number and figure 9 we were able to find the j_H .

$$j_{H} = 120$$

Calculating the h_o factor:

$$h_o = j_H \left(\frac{k}{D_e}\right) \left(\frac{c\mu}{k}\right)^{\frac{1}{3}} = 614 W/m^2 k$$



Figure 13 Shell Side Friction Factor

Friction factor from figure 9:

$$f = 0.003 \frac{ft^2}{m^2} = \frac{0.0003m^2}{m^2}$$

Number of crosses:

$$N+1 = \frac{L}{B} = \frac{2.4}{1} = 2.4$$

Pressure Drop:

$$\Delta P_s = \frac{f G_s^2 D_e (N+1)}{5.22 * 10^{10} D_e s \varphi_t} = 9.10 \ kpa$$

Design Overall Coefficient:

$$U_C = \frac{h_{io}h_o}{h_{io} + h_o} = 431.96 \, W/m^2 k$$

Dirt Factor:

$$R_d = \frac{U_C - U_D}{U_C U_D} = 4.8 * 10^{-3}$$

7.2.4. Overall Summary of the Design Specifications:

TUBE SIDE					
Inlet Temperature (°C)	365.00				
Outlet Temperature (°C)	145.00				
Outer Diameter (m)	0.038				
Inner Diameter (m)	0.034				
Mass flow rate (kg/hr)	$1.05 * 10^4$				
Mass Velocity (kg/hr. m^2)	$1.76 * 10^4$				
Flow area (m^2)	0.12				
Tube Pattern	Triangular Pitch				
Number of Tubes	135				
Length of Tubes (m)	2.40				
Passes	1				
hi (W/ m^2 .k)	1644.23				
hio (W/ m^2 .k)	1457.89				

Table 45 Tube Side Specifications

SHELL SIDE					
Inlet Temperature (°C)	30.00				
Outlet Temperature (°C)	120.00				
Internal Diameter (m)	0.85				
Clearance (m)	9.15 * 10 ⁻³				
Pitch (m)	0.05				
Flow Area (m ²)	0.33				
Mass Flowrate (kg/hr)	8.9 * 10 ³				
Mass Velocity (kg/hr. m^2)	2.71 * 10 ⁴				
Number of Baffles	3				
Baffle Height (m)	0.64				
Baffle Spacing (m)	1.00				
Baffle Thickness (m)	0.01				
ho (W/m².k)	614.00				

Table 46 Shell Side Specifications

Table 47 Overall Heat Exchanger Design Specifications

Design Specifications				
Heat Duty (kJ/hr)	3.40 * 10 ⁶			
LMTD (°C)	171.80			
True LMTD (°C)	165.79			
Area (m²)	38.82			
Reynolds Number (Tube Side)	$4.60 * 10^3$			
Reynolds Number (Shell Side)	$3.87 * 10^4$			
j _h (Tube Side)	20			

j _h (Shell Side)	120
Clean Overall Coefficient U_c (W/m ² .k)	431.96
Design Overall Coefficient U_D (W/m ² .k)	140.00
Dirt Factor Rd	0.0048
Pressure Drop (kPa) Tube Side	1.79
Pressure Drop (kPa) Shell Side	9.10

From the above calculations, we can conclude that our heat exchanger design is satisfactory for the required service. The pressure drops on both the shell and tube side is less than 10psi and the dirt factor is lower than the threshold limit of $5 * 10^{-3}$. It is evident from these values that our calculations have met the criteria of the kern's method.

7.3. Design of Superclaus Reactor

A reactor is a device or vessel which is used to carry out the reactions. It is a very important component in the process industry and convert the raw material into useful products.

7.3.1. Theory of Reactors:

Following are the prominent reactor types used in industry.

- ➢ Batch Reactor
- Continuous stirred tank reactor
- Fluidized bed reactor
- Fixed Bed Reactor

7.3.1.1. Batch eactor:

In batch reactor a fixed number of reactants is processed, and the reaction proceeds under controlled conditions. In a batch reactor, once the reaction initiated, it proceeds until completion before products are removed.

7.3.1.2. Continuous Stirred- Tank Reactors (CSTR):

A well-mixed reactor where from reactants and products are fed and withdrawn continuously. It is used in industry for steady states process and where continuous flow involved. It suitable in the reactions where efficient mixing is required such as homogenous reactions. Catalytic reactions, and enzymatic processes.

7.3.1.3. Fluidized bed reactor:

In fluidized bed reactor solid particles are suspended and fluidized by a gas or liquid flowing through it. When the fluid passing through the granular solid material, causing the particles to behave like a fluid. The created bed provides the properties of both liquids and fluids.

> FBR offers enhanced heat and mass transfer and that is why it is more suitable for catalytic reactions.

7.3.1.4. Fixed Bed Reactor:

A fixed bed type of a reactor in in which solid particles fixed configuration and solid particles are packed to form a bed. The solid particles remain stationary and allow the reactants to pass through it. In this way desired chemical reaction take place.

7.3.2. Reasons to Choose Fixed Bed Reactor for Superclaus Process:

These are some important reasons that we chose fixed bed reactor for our process.

7.3.2.1. Efficient Utilization of Catalyst:

Fixed bed reactor has effective utilization of catalyst and provide greater surface are for the interaction of catalyst and reactants. It gives the higher conversion rate and selectivity.

7.3.2.2. Continuous Operation:

Fixed bed reactor is used for the continuous and steady state operations. These properties make this reactor industrially more suitable. The feed is fed into the reactor continuously and products are withdrawn simultaneously.

7.3.2.3. Hear Management:

Solid catalyst is used in fixed bed reactor. These catalyst act as a sink that is why heat transfer phenomenon occurs efficiently both in endothermic and exothermic reactions. In this way the temperature can be controlled effectively during reactions.

7.3.2.4. Scalability:

The size of the fixed bed reactor can easily be modified just by loading the catalyst. In this way we can make them adaptable to different production requirement.

7.3.2.5. Long Life Span of Catalyst:

In fixed bed catalyst are fixed and there is no iteration between the particles. So, that is why the life span of the catalyst in fixed bed reactor is long. And one more thing there is no entrainment of the catalysts in Fixed Bed Reactor.

Due to all the above-mentioned advantages, we preferred fixed bed reactor for our process.

7.3.3. Design Calculations:

Reactor designs can vary depending on the specific application and the nature of the reactions involved. There will be following steps involved in designing of our superclaus reactor.

Step 1: Calculation of Volumetric flow rate

Step 2: Calculation of volume of catalytic bed

Step 3: Calculation of diameter and length of Bed

Step 4: Calculation of internal diameter and length of reactor

Step 5: Calculation of volume of reactor

Step 6: Calculation of wall thickness of reactor

Step 7: Calculation of outer diameter of reactor

Step 8: Calculation of volume of steel required.

Step 9: Calculation of mass of steel required.

Step 10: Calculation of weight of Catalyst

Step 11: Pressure Drop Calculation

Inlet Stream of Reactor:

Table 48 Reactor Inlet Stream Composition

Component	Molar flowrate (kmol/hr)	Mole Fraction
H ₂ S	1.76	0.005
SO ₂	0.24	0.00075
CO2	48.06	0.14
H ₂ O	103.86	0.32
N2	169.77	0.52
S6	0.0021	6.73E-06
S8	0.017	5.44E-05
Total	323.72	1

As for selective oxidation reaction, air is a requirement, hence:

Component	Molar flowrate	Mole Fraction
	(kmol/hr)	
02	0.77	0.21
N2	2.90	0.79

Table 49 Air Inlet to Reactor

Step 1: Calculation of Volumetric flow rate

Temperature of entering stream = 170 °C = 443.15 K

Pressure of entering stream = 112.33 kPa = 1.10 atm

Flow rate of entering stream = Air + Feed = 3.67 kmol/hr

Flow rate of entering stream = 327.40kmol/hr

Molar Density = $\frac{P}{T \times R}$ Molar Density = $\frac{1.108}{0.0821 \times 443.15}$ Molar Density = $0.0304kmol/m^3$ Average Density = $\frac{P \times M}{T \times R}$ Put value of $\frac{P}{T \times R} = 0.0304kmol/m^3$ Average Density = 0.03×18.48 Average Density = $0.56kmol/m^3$ Average Molecular Weight of Inlet Stream = 28.21kg/kmolVolumetric Flow Rate = $\frac{Molar Rate of stream \times Average molecular weight}{Density}$ Volumetric Flow Rate = $\frac{327.90 \times 18.48}{0.56}$ Volumetric Flow Rate = $10766.42m^3/hr$ Step 2: Calculation of volume of catalytic bed

As we Know that

$$V_B = (1 + \varepsilon)V_b$$

 $\varepsilon = \text{Void fraction}$
 $V_B = rac{\text{Volumetric flow rate}}{\text{Space Velocity}}$

For 80% Conversion and at Temperature 512 K, Space velocity is taken to be $\frac{1800}{hr}$

Space time
$$= \frac{1}{\text{Space Velocity}}$$

Space time $= \frac{1 \times 3600}{1800} = 2 \sec V_b$
 $V_b = \frac{10766}{1800}$
 $V_b = 5.98m^3$
And,
 $V_B = 5.98(1 + 0.4)$
 $V_B = 8.37m^3$

Step 3: Calculation of diameter and length of Bed

Suppose

$$\frac{L}{D} = 3$$

$$L = 3D$$

$$V_B = \pi r^2 L$$

$$V_B = \frac{\pi \times L \times D_B^2}{4}$$

$$V_B = (\frac{4 \times 8.37}{3\pi})^2$$

$$D_B = 1.52m$$
Now,

 $L_B = 3(1.52)$ $L_B = 4.57 \mathrm{m}$

Step 4: Calculation of internal diameter and length of reactor

Provide 10% free space above and below the catalyst bed for support, so

Length of reactor = 0.45m + 4.57m

Length of reactor = 5.02m

Internal Diameter of Reactor $=\frac{L}{3}=1.6733$ m

Step 5: Calculation of volume of reactor

$$V = \frac{\pi \times L \times D_B^2}{4}$$
$$V = 11.039m^3$$

Step 6: Calculation of wall thickness of reactor

$$\mathbf{e} = \left(\frac{P_i D_i}{4Jf - 1.2P_i}\right) + C_c$$

$$e = 0.004248m$$

Step 7: Calculation of outer diameter of reactor

$$D_o = D_i + 2T$$

 $D_o = 1.67 + 2(0.004)$
 $D_o = 1.68m$

Step 8: Calculation of volume of steel required.

Volume of Steel Required:

$$V_{s} = \frac{\pi (D_{o}^{2} - D_{1}^{2})L}{4}$$
$$V_{s} = 0.1524m^{3}$$

Step 9: Calculation of mass of steel required.

Density of Steel = $8000 \frac{\text{Kg}}{m^3}$

Volume of steel required = $0.15m^3$

So,

Mass =
$$(8000 \frac{\text{Kg}}{m^3}) \times 0.15m^3$$

Mass = 5607.9kg

Step 10: Calculation of weight of Catalyst

Bulk Density of Catalyst =
$$670 \frac{\text{Kg}}{m^3}$$

Volume of Catalyst Bed = $8.37m^3$

Weight of Catalyst = 8.37×670

Weight of Catalyst = 5607.9kg

Step 11: Pressure Drop Calculation

 $\frac{P}{L} = \left(\frac{150\varepsilon^2 \mu v_s}{(1-\varepsilon)3D_p^2} + \frac{1.75\rho\varepsilon v_s^2}{(1-\varepsilon)3D_p}\right)$

P =pressure drops across the bed

 $D_p =$ equivalent spherical diameter of the packing

 $\mu = dynamic viscosity of the fluid$

 v_s = superficial velocity

 $\varepsilon = \text{void fraction of the bed}$

L = length of the bed (not the column)

P = 11.22kPa

7.4. Overall Summary of Design Calculations:

Reactor Category	Fixed Bed Reactor
Mode of Operation	Adiabatic Process
Space Time (s)	2.00
Void fraction	0.40
Volume of reactor (m^3)	11.04
Length of reactor (m)	1.67
Diameter of reactor (m)	5.02
Reactor wall thickness (mm)	4.20
Catalyst	Iron and chromium oxides on α -
	alumina
Weight of catalyst (kg)	5607.90
Weight of steel (kg)	1219.20
Pressure Drop (kPa)	11.22

Table 50 Overall Design Specifications of Reactor
CHAPTER 8

SIMULATION

Our Project involves the utilization of Aspen HYSYS, a leading process simulation software, to model and analyse the system's behaviour. With the aim of efficiently processing sour gas, a critical aspect of the project is to ensure the effective removal and recovery of sulphur compounds. To accurately simulate the sulphur recovery process, the Sulsim (Sulphur Recovery) fluid package was selected. This fluid package is renowned for its comprehensive representation of sulphur chemistry and thermodynamics, making it an ideal choice for accurately predicting the behaviour of sulphur compounds within the gas processing system. By incorporating the Sulsim fluid package into the Aspen HYSYS simulation, the project aims to optimize the acid gas processing system's performance, improve efficiency, and ensure the successful recovery of valuable sulphur as a resource for downstream chemical process industries.



8.1. Complete Flowsheet

Figure 14 Flowsheet on ASPEN HYSYS

8.2. Equipment-wise details

Here we include the details for the simulation of some main equipment on the plant.

8.2.1. Furnace

Claus furnace is a combustion chamber to burn part of H₂S and other hydrocarbon which are coming in the feed acid gas in the form of impurities. Sulsim fluid package has a provision to use Claus reaction furnace which is different than fire heaters in that it does not require fuel stream. As detailed in process description, here the fuel is acid gas itself.







Figure 16 Connections of Furnace

8.2.2. Waste Heat Boiler

The simulation of a Waste Heat Boiler (WHB) was conducted using Aspen HYSYS. The WHB plays a crucial role in recovering and utilizing waste heat generated in industrial processes. By simulating the behaviour of the WHB in Aspen HYSYS, we aimed to optimize its design and performance, ensuring efficient heat transfer and energy recovery. The outlet stream from the Waste Heat Exchanger was then utilized to validate the accuracy of the simulation results. By comparing the simulated outlet conditions with the manually calculated results, we could assess the reliability of calculations and ensure that the simulated model accurately represents them. This validation step is vital for building confidence in the simulation and enabling the project to make informed decisions regarding system optimization and energy efficiency improvements.



Figure 17 Waste Heat Boiler Simulation



Figure 18 Waste Heat Boiler Connections

8.2.3. Condenser

The use of a condenser in the Sulphur Recovery Claus process is essential for efficient operation and the recovery of valuable sulfur compounds. The condenser is responsible for cooling down the hot gas stream exiting the WHB (in this case) and reactor, allowing the condensation of sulfur compounds. This condensation process facilitates the separation and collection of elemental sulfur, which can then be further processed or utilized.

To optimize the design and performance of the condenser in the Sulphur Recovery Claus process, simulating its behaviour in Aspen HYSYS becomes imperative. By utilizing Aspen HYSYS, we aimed to model the heat transfer and mass transfer phenomena occurring within the condenser accurately. The simulation enabled us to evaluate various operating conditions, design parameters, and process configurations, ensuring optimal performance of the condenser.

Through Aspen HYSYS, we studied factors such as cooling water flow rate, temperature, and pressure, as well as the overall heat transfer area and effectiveness of the condenser. By simulating different scenarios, we were able to determine the most efficient operating conditions and optimize the design of the condenser for maximum sulfur recovery.

Furthermore, the simulation in Aspen HYSYS allows for the evaluation of different control strategies and their impact on the overall process performance. By incorporating the condenser simulation into the larger Sulphur Recovery Claus process model, we gained valuable insights into the process's overall efficiency, energy consumption, and sulfur recovery rates.



Figure 19 Condenser Simulation



Figure 20 Condenser Connections

8.2.4. Reheater

The utilization of a heater before the Claus reactor inlet is crucial in the Sulphur Recovery Claus process to ensure optimal operating conditions and facilitate the desired reactions. The heater is responsible for preheating the gas stream entering the reactor, which helps to initiate and maintain the necessary chemical reactions for sulfur recovery. Simulating the behavior of the heater in Aspen HYSYS is necessary to accurately model the heat transfer and energy requirements of the process. By using Aspen HYSYS, we can assess various design parameters and operating conditions of the heater, such as the fuel type, flow rate, and temperature, as well as the overall heat transfer efficiency.

Simulating the heater in Aspen HYSYS allows us to optimize the heater's design and performance. Furthermore, by simulating the heater on Aspen HYSYS, we can assess the energy consumption of the heater and identify opportunities for energy optimization. The simulation can provide insights into the heat recovery potential, identify potential heat integration opportunities within the process, and help determine the overall energy efficiency of the Sulphur Recovery Claus system.

In summary, simulating the heater on Aspen HYSYS enables us to understand and optimize the heating requirements of the Claus reactor inlet, ensuring optimal temperature conditions for sulfur recovery while considering energy efficiency and process integration opportunities.



Figure 21 Reheater Simulation

Conditions:

We are Heating our Stream 5 to 220 °C to obtain optimal operating conditions and facilitate the desired reactions.

worksheet	Nama	5	0	O PH	
Canalitiana	Vapour	1 0000	1 0000	Q-Kn	
Conditions	Vapour Tarra anti-an (C)	10000	1.0000	<empty></empty>	
Properties	Temperature [C]	125.0	222.0	<empty></empty>	
Composition	Pressure [kPa]	125.5	123.8	<empty></empty>	
PF Specs	Molar Flow [kgmole/h]	307.9	307.9	<empty></empty>	
	Mass Flow [kg/h]	8775	8775	<empty></empty>	
	Std Ideal Liq Vol Flow [m3/h]	10.34	10.34	<empty></empty>	
	Molar Enthalpy [kJ/kgmole]	-1.261e+005	-1.228e+005	<empty></empty>	
	Molar Entropy [kJ/kgmole-C]	216.2	223.5	<empty></empty>	
	Heat Flow [kJ/h]	-3.883e+007	-3.783e+007	1.002e+006	

Figure 22 Reheater Conditions

8.2.5. Claus Reactor

Sulphur Recovery Claus process offers the conditions required for the desired chemical reactions, which includes the Claus reaction. To improve the design and operation of the Claus reactor, the way it operates must be simulated. We may precisely analyze the reactor's behaviour and assess many factors that impact its performance by using simulation software like Aspen HYSYS. We may examine different operating conditions by simulating the Claus reactor using Aspen HYSYS and studying the reaction kinetics and evaluating the efficiency of sulfur compound conversion.

The simulation also aids in troubleshooting and locating any problems inside the Claus reactor. We can locate regions where the reactor performance might be suboptimal or where undesirable side reactions might take place by examining the simulated data. The performance of the reactor can be improved, and modifications can be made based on this information to maximize sulfur recovery. Claus reactor can be simulated, and various reactor designs or changes can be assessed. In summary, simulating the Claus reactor on Aspen HYSYS is crucial to optimize its design, assess performance parameters, determine optimal operating conditions, troubleshoot potential issues, and explore potential process improvements. It provides valuable insights into the behavior of the reactor, enabling us to make informed decisions and maximize the efficiency of the Sulphur Recovery Claus process.







Figure 24 Claus Reactor Connections

19.57
74.47
124.9
235.5
97.06
50.59
71.81
36.81
72.35
1.645e+004
<empty></empty>
<empty></empty>

Figure 25 Reactor Performance Data

8.2.6. Superclaus Reactor

The Super Claus reactor is an advanced version of the conventional Claus reactor used in the Sulphur Recovery Claus process. It is employed to achieve higher sulfur recovery efficiencies and reduce sulfur emissions by further promoting the conversion of sulfur-containing compounds.

Simulating the Super Claus reactor on Aspen HYSYS is essential to optimize its design and operation. By utilizing the simulation software, we can accurately model the behavior of the Super Claus reactor and evaluate various factors that impact its performance. These factors include temperature, pressure, residence time, catalyst activity, and reactant feed composition.

Simulating the Super Claus reactor on Aspen HYSYS allows us to study the reaction kinetics and assess the conversion efficiency of sulfur compounds. We can explore different operating conditions and process configurations to determine the optimal reactor conditions for achieving higher sulfur recovery rates and reducing sulfur emissions.

Additionally, the simulation helps in troubleshooting and identifying potential issues within the Super Claus reactor. By analyzing the simulated results, we can identify areas where the reactor performance may be suboptimal or where undesired side reactions may occur. This information can guide process improvements and modifications to enhance the reactor's performance and maximize sulfur recovery while minimizing emissions. Furthermore, simulating the Super Claus reactor on Aspen HYSYS enables the evaluation of different reactor designs or modifications. By testing various scenarios and configurations, we can assess the impact of changes such as reactor size, catalyst selection, or reactor internals on process efficiency, sulfur recovery, and emissions reduction.

In summary, simulating the Super Claus reactor on Aspen HYSYS is crucial to optimize its design, assess performance parameters, determine optimal operating conditions, troubleshoot potential issues, and explore potential process improvements. It provides valuable insights into the behavior of the reactor, enabling us to make informed decisions and maximize the efficiency of the Sulphur Recovery Claus process while minimizing environmental impacts.



Figure 26 Superclaus Reactor Simulation



Figure 27 Superclaus Reactor Connections

Vapour 1.000 1.0000 roperties omposition F Specs Temperature [C] 85.00 170.0 Molar Flow [kgmole/h] 135.8 112.3 Molar Flow [kgmole/h] 5.000 299.9 Mass Flow [kg/h] 144.3 8006 Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 Molar Enthalpy [kJ/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kJ/kgmole-C] 204.0 215.5 - Heat Flow [kJ/h] 8768 -3.964e+007 -3.96	1.0000 204.8 108.9	1.0000	1 0000			
Peroperties Composition PF Specs Temperature [C] 85.00 170.0 Molar Flow [kPa] 135.8 112.3 100 Molar Flow [kgmole/h] 5.000 299.9 144.3 8006 Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 1.302e+005 -1.30 Molar Entralpy [kl/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kl/kgmole-C] 204.0 215.5 1.442 Heat Flow [kl/h] 8768 -3.964e+007 -3.96	204.8 108.9	204.8	1.0000	1.0000	Vapour	Conditions
Composition PF Specs Pressure [kPa] 135.8 112.3 Molar Flow [kgmole/h] 5.000 299.9 Mass Flow [kg/h] 144.3 8006 Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 Molar Enthalpy [kl/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kl/kgmole-C] 204.0 215.5 - Heat Flow [kl/h] 8768 -3.964e+007 -3.96	108.9		170.0	85.00	Temperature [C]	Properties
Molar Flow [kgmole/h] 5.000 299.9 Mass Flow [kg/h] 144.3 8006 Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 Molar Enthalpy [kl/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kl/kgmole-C] 204.0 215.5 -1.306 Heat Flow [kl/h] 8768 -3.964e+007 -3.96	10012	108.9	112.3	135.8	Pressure [kPa]	Composition
Mass Flow [kg/h] 144.3 8006 Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 Molar Enthalpy [kJ/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kJ/kgmole-C] 204.0 215.5 - Heat Flow [kJ/h] 8768 -3.964e+007 -3.96	304.3	304.3	299.9	5.000	Molar Flow [kgmole/h]	PF Specs
Std Ideal Liq Vol Flow [m3/h] 0.1668 9.594 Molar Enthalpy [kJ/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kJ/kgmole-C] 204.0 215.5 - Heat Flow [kJ/h] 8768 -3.964e+007 -3.96	8150	8150	8006	144.3	Mass Flow [kg/h]	
Molar Enthalpy [kJ/kgmole] 1754 -1.322e+005 -1.30 Molar Entropy [kJ/kgmole-C] 204.0 215.5 - Heat Flow [kJ/h] 8768 -3.964e+007 -3.96	9.728	9.728	9.594	0.1668	Std Ideal Liq Vol Flow [m3/h]	
Molar Entropy [kl/kgmole-C] 204.0 215.5 Heat Flow [kl/h] 8768 -3.964e+007 -3.96	2e+005	-1.302e+005	-1.322e+005	1754	Molar Enthalpy [kJ/kgmole]	
Heat Flow [kl/h] 8768 -3.964e+007 -3.96	217.9	217.9	215.5	204.0	Molar Entropy [kJ/kgmole-C]	
	3e+007	-3.963e+007	-3.964e+007	8768	Heat Flow [kJ/h]	

Figure 28 Superclaus Reactor Conditions

Sulfur conversion [kgmole/h]	1.383
Sulfur conversion efficiency [%]	61.63
Inlet sulfur dewpoint temperature [C]	130.1
Outlet sulfur dewpoint temperature [C]	169.8
Inlet sulfur dewpoint margin [C]	39.95
Outlet sulfur dewpoint margin [C]	35.07
Conversion [%]	98.00
Selectivity [%]	90.00
COS + CS2 + H2S at outlet [ppmmol]	1606
Space velocity [1/hours]	<empty></empty>
Catalyst bed volume [m3]	<empty></empty>

Figure 29 Superclaus Reactor Performance

Design	Reaction Model		
Connections	Legacy	16	
Parameters			
Jser Variables	Delta P	3.447 kPa	
Votes			
	Conversion (H2S reacted)	98.00 %	
	Calantivity (and start 1120 to 10)	00.00 %	
	Selectivity (reacted H2S to S)	90.00 %	
	Air availability		
	Current air flow rate [kgmole/h]		5.000
	Approximate O2 at outlet [mol %]]	4.217e-002
	Minimum air flow rate needed for	r specified conversion [kgmole/h]	4.389
	Conversion with current air flow [%]	98.00

Figure 30 Design Parameters of Superclaus

8.2.7. Incinerator

The use of an incinerator in the Super Claus process is integral for the effective treatment and disposal of the off-gas stream. The incinerator is responsible for the combustion of residual sulfur compounds, converting them into less harmful by-products such as sulfur dioxide.

Simulating the behavior of the incinerator on Aspen HYSYS is crucial to optimize its design and operation. By utilizing the simulation software, we

can accurately model the combustion process and evaluate various factors that affect the incinerator's performance. This includes parameters such as temperature, residence time, fuel composition, and air supply.

Simulating the incinerator on Aspen HYSYS allows us to study combustion kinetics and assess the efficiency of sulfur compound combustion. We can explore different operating conditions, such as air-to-fuel ratio and temperature, to determine the optimal combustion conditions for maximizing the destruction of sulfur compounds and minimizing emissions.

Additionally, the simulation helps in troubleshooting and identifying potential issues within the incinerator. By analysing the simulated results, we can identify areas where the combustion performance may be suboptimal or where the emission levels may not meet regulatory standards. This information can guide process improvements and modifications to enhance the incinerator's performance and ensure compliance with environmental regulations.

Simulation allows for the evaluation of emissions control and compliance with environmental regulations. By simulating the incinerator, we can estimate pollutant emissions, such as sulfur dioxide (SO2), nitrogen oxides (NOx), and particulate matter, and assess their impact on air quality. This information is valuable for implementing appropriate emission control measures and ensuring compliance with regulatory standards.

Simulating the incinerator on Aspen HYSYS also enables the evaluation of different design options and modifications. By testing various scenarios and configurations can assess the impact of changes such as combustion chamber design, air distribution, or fuel injection strategy on combustion efficiency and emission control.

In summary, simulating the incinerator on Aspen HYSYS is essential to optimize its design, assess performance parameters, determine optimal operating conditions, troubleshoot potential issues, and explore process improvements. It provides valuable insights into the behavior of the incinerator, enabling the project team to make informed decisions and maximize the efficiency of the Super Claus process while ensuring effective combustion and emissions control.



Figure 31 Incinerator Simulation



Figure 32 Incinerator Conditions

Design Rating	g Worksheet Performance					
Worksheet		21	Air	Fuel Gas	24	
Conditions	Hydrogen	0.0188	0.0000	0.0000	0.0094	
Properties	Argon	0.0000	0.0000	0.0000	0.0000	
Composition	Oxygen	0.0004	0.2100	0.0000	0.0300	
PF Specs	Nitrogen	0.4972	0.7900	0.0000	0.5893	
	Methane	0.0000	0.0000	0.9586	0.0000	
	CO	0.0152	0.0000	0.0000	0.0097	
	CO2	0.1413	0.0000	0.0000	0.1110	=
	Ethane	0.0000	0.0000	0.0404	0.0000	
	H2S	0.0001	0.0000	0.0000	0.0000	
	COS	0.0015	0.0000	0.0000	0.0002	
	SO2	0.0012	0.0000	0.0000	0.0018	
	CS2	0.0000	0.0000	0.0000	0.0000	
	H2O	0.3241	0.0000	0.0000	0.2487	

Figure 33 Incinerator Stream Composition

Design Rating	Worksheet Performance					
Worksheet	Name	21	Air	Fuel Gas	24	
Conditions	Vapour	1.0000	1.0000	1.0000	1.0000	
Properties	Temperature [C]	120.0	40.00	25.00	600.0	
Composition	Pressure [kPa]	105.4	100.0	95.00	98.54	
PF Specs	Molar Flow [kgmole/h]	304.1	164.8	9.275	477.6	
	Mass Flow [kg/h]	8104	4755	154.3	1.301e+004	
	Std Ideal Liq Vol Flow [m3/h]	9.702	5.497	0.5089	15.49	
	Molar Enthalpy [kJ/kgmole]	-1.332e+005	437.8	-7.527e+004	-8.612e+004	
	Molar Entropy [kJ/kgmole-C]	211.3	200.0	189.5	238.1	
	Heat Flow [kJ/h]	-4.051e+007	7.216e+004	-6.981e+005	-4.113e+007	

Figure 34 Incinerator Conditions

Design	Rating	Worksheet Perfo	ormance			
Desi	gn	Incinerator Delta	P [kPa]		3.448	
Connec	tions	Stack Delta P [kF	Pa]		3.448	
Parame User Va	ters riabler	Stack Delta T [C]			0.0000	Include Stack
Notes	lables	Target Incinerato	or Exit T [C]		600.0	
		Kinetic Value			4	Use Kinetic Correlations
		Target Outlet O2	2 Mole Fraction		0.0300	
		Breakthrough CO Hydrogen H2S COS CS2 Methane Ethane	100.00 % 78.57 % 2.97 % 23.43 % 29.16 % 0.00 % 0.00 %	* III		
		Propane	0.00 %			
		n-Butane	0.00 %	-		

Figure 35 Incinerator Design Parameters

Duty [kJ/h]	5.537e+006
Sulfur Emission as S1 [kgmole/h]	0.9518
Calculated Outlet O2 Mole Fraction	0.0300
Calculated Incinerator Exit Temperature [C]	600.0
Exit H2S Concentration [ppmmol]	1.949
Exit SO2 Concentration [ppmmol]	1764
Exit COS Concentration [ppmmol]	223.9
Exit CS2 Concentration [ppmmol]	0.5128
Exit Hydrogen Concentration [ppmmol]	9412
Exit CO Concentration [ppmmol]	9676
COS + CS2 + H2S at Exit [ppmmol]	226.3
Heat Release at Complete Burn (HHV) [kJ/h]	8.521e+006
Heat Release at Complete Burn (LHV) [kJ/h]	7.687e+006
Heat Release at Burner Stoichiometry (HHV) [kJ/h]	8.521e+006
Heat Release at Burner Stoichiometry (LHV) [kJ/h]	7.687e+006

Figure 36 Incinerator Performance

8.2.8. Gas-Gas Heat Exchanger

In the Super Claus process, the Gas-Gas heat exchanger is positioned after the incinerator and offers a few benefits.

Firstly, it allows for efficient heat recovery from the hot gas stream exiting the incinerator. By preheating the incoming feed gas and transferring heat from the high-temperature gas to it, the heat exchanger lowers the energy requirement for following processes.

Additionally, the Gas-Gas heat exchanger helps to reduce the temperature of the gas stream before it enters equipment farther downstream. The safety of downstream equipment from excessive heat and potential damage depends on this temperature reduction.

The effectiveness of the Gas-Gas heat exchanger's heat transfer can be assessed through simulation. We can evaluate variables like the heat transfer coefficient, temperature profiles, and other factors by modelling the heat exchanger in Aspen





Design Rating	Worksheet Performance Rigor	ous Shell&Tube			
Design	Tube Side Inlet	Name	Gas-Gas HE	Shell Side Inlet	
Parameters	Cold Air 🔻			24	•
Specs User Variables					
Notes	Tubeside Flows SRU-	heet I (SRU1)	Shellside Flows SRU-	heet I (SRU1))
	Tube Side Outlet			Shell Side Outlet	
	PreHeated Air		Switch streams	25	•
Delete			ОК		Update 🔲 Ignored

Figure 38 Gas-Gas Heat Exchanger Connections

Worksheet Name Cold Air PreHeated Air 24 25 Conditions Properties Composition PF Specs Vapour 1.0000 1.0000 1.0000 1.0000 1.0000 Molar Flow [kgmole/h] 25.00 85.00 660.0 581.1 Molar Flow [kgmole/h] 136.1 135.8 98.54 98.04 Molar Flow [kgmole/h] 186.4 186.4 477.6 477.6 Molar Flow [kg/h] 5378 5378 1.301e+004 1.301e+004 Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 15.49 Molar Entrapy [kl/kgmole] -2.375e-004 -8.612e+004 -8.680e+004 Molar Entrapy [kl/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Conditions Properties Composition PF Specs Vapour 1.0000 1.0000 1.0000 1.0000 Molar Flow [kg/h] 25.00 85.00 660.0 581.1 Molar Flow [kg/h] 136.1 135.8 98.54 98.04 Molar Flow [kg/h] 5378 5378 1.301e+004 1.301e+004 Molar Findapy [kl/kgmole] -2.375e-004 754 -8.612e+004 -8.680e+004 Molar Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Properties Composition PF Specs Temperature [C] 25.00 85.00 600.0 581.1 Molar Flow [kpa] 136.1 135.8 98.54 98.04 Molar Flow [kgmole/h] 186.4 186.4 477.6 477.6 Molar Flow [kg/h] 5378 5378 1.301e+004 1.301e+004 Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 15.49 Molar Entropy [kl/kgmole] -2.375e-004 1754 -8.612e+004 -8.680e+004 Molar Entropy [kl/kgmole-C] 199.6 204.0 28.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Composition PF Specs Pressure [kPa] 136.1 135.8 98.54 98.04 Molar Flow [kgmole/h] 186.4 186.4 477.6 477.6 Mass Flow [kg/h] 5378 5378 1.301e+004 1.301e+004 Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 15.49 Molar Enthalpy [kl/kgmole] -2.375e-004 1754 -8.612e+004 -8.680e+004 Molar Enthalpy [kl/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
PF Specs Molar Flow [kgmole/h] 186.4 186.4 477.6 477.6 Mass Flow [kg/h] 5378 5378 1.301e+004 1.301e+004 Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 15.49 Molar Enthalpy [kl/kgmole] -2.375e-004 1754 -8.612e+004 -8.680e+004 Molar Entropy [kl/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Mass Flow [kg/h] 5378 5378 1.301e+004 Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 Molar Enthalpy [k//kgmole] -2.375e-004 1754 -8.612e+004 Molar Enthalpy [k//kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [k//h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Std Ideal Liq Vol Flow [m3/h] 6.217 6.217 15.49 Molar Enthalpy [kl/kgmole] -2.375e-004 1754 -8.612e+004 -8.680e+004 Molar Entropy [kl/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Molar Enthalpy [kl/kgmole] -2.375e-004 1754 -8.612e+004 -8.680e+004 Molar Entropy [kl/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kl/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Molar Entropy [kJ/kgmole-C] 198.6 204.0 238.1 237.3 Heat Flow [kJ/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007
Heat Flow [k/h] -4.428e-002 3.269e+005 -4.113e+007 -4.146e+007

Figure 39 Gas-Gas Heat Exchanger Conditions

Design Rating	worksneet	Rigorous Shell&Tube
Performance	Overall Performance	
Details	Duty	3.269e+005 kJ/h
Plots	Heat Leak	0.000e-01 kJ/h
Tables	Heat Loss	0.000e-01 kJ/h
Setup	UA	6.11e+02 kJ/C-h
Error Msg	Min. Approach	515.000 C
-		
-	Detailed Performance	534.9 C
-	Detailed Performance	534.9 C
	Detailed Performance	534.9 C
	Detailed Performance UA Curvature Error Hot Pinch Temp Cold Pinch Temp	534.9 C
	Detailed Performance UA Curvature Error Hot Pinch Temp Cold Pinch Temp Ft Factor	534.9 C

Figure 40 Gas-Gas Heat Exchanger Performance Data

8.2.9. Air Demand Analyzer

An air demand analyzer is a tool that Aspen HYSYS uses to accurately estimate and optimise the amount of air needed for the sulphur recovery process.

The air demand analyzer in Aspen HYSYS enables for the analysis and computation of the precise amount of air needed for the combustion reactions engaged in the process. The air demand analyzer finds the ideal air-to-gas ratio necessary for effective sulphur combustion by taking into account the composition of the input gas, the target sulphur recovery efficiency, and other process factors.

The air demand analyzer takes into account a number of variables, including the stoichiometry of the reactions, the amount of oxygen necessary for complete combustion, and the possibility of the formation of undesirable byproducts. We can make sure that by carrying out these computations using Aspen HYSYS, To achieve effective and dependable sulphur recovery, we can make sure that the air supply is properly managed to match the process requirements.

Additionally, the air demand analyser in Aspen HYSYS supports process optimization. We can assess the impact on the air demand and assess tradeoffs between energy consumption and sulphur recovery efficiency by simulating various scenarios and varying operating conditions, such as temperature, pressure, and feed gas composition. This makes it possible to find the ideal process conditions that balance the need for air with the intended performance goals.



Figure 41 Air Demand Analyzer

Connections	Parameters Monitor User Variables	
Connections	Name ADA-1	
Connections		
Notes		
	Sample Stream	15 -
	Target Variable	H2S/SO2 Ratio
	Target Value	7.200
	Adjusted Reaction Furnace	FUR-100-3
		OK

Figure 42 ADA Connections

INSTRUMENTATION AND PROCESS CONTROL

9.1. The Need for IPC in Chemical Processes

Real-time monitoring of process variables like temperature, pressure, flow rate, and composition is possible because of IPC. This information is critical for maintaining process stability, assuring product quality, and preventing safety issues. To maintain ideal process conditions, IPC systems enable control activities like altering setpoints, triggering safety interlocks, and executing regulatory control techniques..

9.2. Controllers and their application in Superclaus Plant

9.2.1. Temperature Control Loop

9.2.2. In a Super Claus plant, controllers play a vital role in ensuring optimal operation and achieving desired process outcomes. Temperature controllers are used to regulate and maintain temperatures in the Claus reactor, incinerator, and other equipment, optimizing reaction rates for efficient sulfur recovery. Pressure controllers maintain safe operating pressures in different plant sections, preventing overpressure and optimizing flow rates.

9.2.3. Flow Control Loop

Flow controllers manage feed gas, air, and other streams to achieve optimum stoichiometry and gas flow balance. In order to ensure effective separation processes, level controllers keep liquid levels in containers and separators constant. Analytical controllers monitor and control process parameters, facilitating compliance with quality standards and enabling real-time adjustments. In a Super Claus facility, controllers allow for precise control, optimization, and compliance, all of which contribute to safe and effective sulfur recovery procedures.

9.3. Controlling Air Flow to the Furnace

Ratio control is a type of control strategy used in process systems to maintain a specific ratio between two or more process variables. It involves adjusting one variable in response to changes in another variable to maintain the desired ratio.



Figure 43 Ratio Control Block Diagram

The ratio control system normally consists of two basic components: a primary controller and a secondary controller. While the secondary controller monitors the secondary process variable, the primary controller monitors the primary process variable. The secondary controller adjusts the manipulated variable to maintain the desired ratio based on the setpoint and feedback from the primary controller.

Ratio control is commonly used in processes were maintaining a specific proportion between two variables is critical for process performance. For example, in chemical mixing processes, it may be necessary to maintain a specific ratio of two ingredients to achieve the desired product quality or reaction rate. In fuel-air mixing applications, maintaining the correct fuel-to-air ratio is essential for efficient combustion and emissions control.



Figure 44 Ratio Controller

Ratio control has advantages such as higher process efficiency, enhanced product quality, and improved process consistency. Variations in one variable can be automatically accounted for by modifying the other variable by maintaining a constant ratio. This guarantees that the desired ratio is maintained and reduces process deviations, leading to more consistent and predictable process outcomes.

CHAPTER 10

COST ANALYSIS

Cost analysis is basically the evaluation and identification of all the expenses associated with a project. The basic purpose of cost analysis is to check the financial feasibility and profitability of a project. Cost analysis provides us with the foundation for financial planning, decision making and risk management. The prime focus of every plant is to generate revenue, so it is important to perform a detailed economic analysis before the installation of every plant. [11] [12]

We adapted the Coulson and Richardson method for our Project economic analysis.

The overall cost of the Project is the sum of fixed capital cost and overall Production cost.

Total Cost of the project = Fixed Capital Cost + Overall Production Cost

10.1. Fixed Capital Cost

The formula used for the calculation of capital cost is:

$C = 14000NQ^2$

Here,

C = capital cost in dollars

N = number of functional units = 3

Q = Plant capacity = 35040 ton/year

Using the above formula

Fixed Capital cost = $14000 \times 3 \times 35040^{0.615}$

Fixed Capital cost = \$26100000

10.2. Factorial Method of Cost Estimation

To see all the minor details of the cost we use the factorial method of cost estimation. In this method fixed capital cost is calculated on the base of physical plant cost. To find out the physical plant cost we must know the purchase cost of equipment.

Factors Increasing the Fixed capital cost:

There are the following factors which affect the fixed capital cost.

			Process type	
	Item	Fluids	Fluids- solids	Solids
1.	Major equipment, total purchase			
	cost	PCE	PCE	PCE
	f_1 Equipment erection	0.4	0.45	0.50
	f_2 Piping	0.70	0.45	0.20
	f_3 Instrumentation	0.20	0.15	0.10
	f_4 Electrical	0.10	0.10	0.10
	f_5 Buildings, process	0.15	0.10	0.05
	f_6 Utilities	0.50	0.45	0.25
	* f ₇ Storages	0.15	0.20	0.25
	f_8 Site development	0.05	0.05	0.05
	*f9 Ancillary buildings	0.15	0.20	0.30
2.	Total physical plant cost (PPC) $PPC = PCE (1 + f_1 + \dots + f_9)$			
	$= PCE \times$	3.40	3.15	2.80
	f_{10} Design and Engineering	0.30	0.25	0.20
	f_{11} Contractor's fee	0.05	0.05	0.05
	f_{12} Contingency Fixed capital = PPC (1 + f_{12} + f_{12} + f_{13})	0.10	0.10	0.10
	$= PPC \times$	1.45	1.40	1.35

Table 51 Factors affecting Fixed Cost

10.3. Purchase Cost of Equipment

Purchase cost of equipment refers to the initial investment needed to obtain the equipment and includes the actual purchase price as well as any associated expenses, such as taxes and delivery charges.

Cost of Furnace, Reactor and Separator:

Equipment	Size unit, S	Size range	Cons C,£	stant C,\$	Index n	Comment	
Agitators Propeller Turbine	driver power, kW	5-75	1200 1800	1900 3000	0.5 0.5		
Boilers Packaged up to 10 bar 10 to 60 bar	kg/h steam	$(5-50) imes 10^3$	70 60	120 100	0.8 0.8	oil or gas fired	
Centrifuges Horizontal basket Vertical basket	dia., m	0.5-1.0	35,000 35,000	58,000 58,000	1.3 1.0	carbon steel ×1.7 for ss	
Compressors Centrifugal	driver	20-500	1160	1920	0.8	electric,	
Reciprocating Conveyors	power, ku		1600	2700	0.8	50 bar	
Belt 0.5 m wide 1.0 m wide	length, m	2-40	1200 1800	1900 2900	0.75 0.75		
Crushers Cone Pulverisers	t/h kg/h	20-200	2300 2000	3800 3400	0.85 0.35		
Dryers Rotary Pan	area, m ²	5-30 2-10	21,000 4700	35,000	0.45	direct gas fired	
Evaporators Vertical tube Falling film	area, m ²	10-100	12,000 6500	20,000 10,000	0.53 0.52	carbon steel	
Filters Plate and frame Vacuum drum	area, m ²	5-50 1-10	5400 21,000	8800 34,000	0.6 0.6	cast iron carbon steel	
Furnaces Process Cylindrical Box	heat abs, kW	$10^3 - 10^4$ $10^3 - 10^5$	330 340	540 560	0.77 0.77	carbon steel ×2.0 ss	
Reactors Jacketed, agitated	capacity, m3	3-30	9300 18,500	15,000 31,000	0.40 0.45	carbon steel glass lined	
Tanks Process vertical horizontal	capacity, m ³	1-50 10-100	1450 1750	2400 2900	0.6 0.6	atmos. press. carbon steel	
floating roof cone roof		50-8000 50-8000	2500 1400	4350 2300	0.55 0.55	×2 for stainless	

Table 52 Purchase cost of miscellaneous equipment, cost factors

To calculate the values of these equipment we get the value from Table 10.2 and put into the following equation.

$$\mathbf{C}_e = \mathbf{C} \times \mathbf{S}^N$$

Here,

 $C_e = Purchased equipment cost, £, $$

C = cost constant

S = characteristic size parameter

n = index for that type of equipment

So, we get the cost.

Table 53 Purchase Cost of Equipment

Equipment	Cost (\$)
Furnace	85,145
Reactor	49,542
Separator	3,286

Condenser

 $Area = 38.82m^2$

Tube Material = Stainless Steel

Shell Material = Carbon Steel

Pressure = 1.32bar

Type Factors = Fixed tube sheet

The equation is used to calculate the cost of condenser.

Ce = bare cost from Graph $10.1 \times$ Type factor \times Pressure factor

By using Graph 10.1 we have

Bare cost = 46000

Type factor = 0.8

Pressure factor = 1

So,

 $Ce = 46000 \times 0.8 \times 1$

Ce = \$36,800



Shell	Tubes	1-10 bar	× 1.0	Floating head	× 1.0
 Carbon steel 	Carbon steel	10-20	× 1.1	Fixed tube sheet	× 0.8
② C.S.	Brass	20-30	× 1.25	U tube	× 0.85
③ C.S.	Stainless steel	30-50	× 1.3	Kettle	× 1.3
(4) S.S.	S.S.	50-70	× 1.5		

Figure 45 Heat Exchanger Cost Graph

10.4. Summary

Table 54 Summary of Purchase Cost of Equipment

Equipment	Cost (\$)
Furnace	85,145
Reactor	49,542
Separator	3,286
Condenser	36,800

10.5. Overall Production Cost

Overall production cost is related to the cost which is used in manufacturing or creating goods or delivering services. It includes all the costs associated with the production activities, such as raw materials, labour, overheads, utilities, maintenance, and any other expenses directly related to the production process.

Overall Production Cost = Fixed Cost + Variable Cost

Variable costs 1. Raw materials 2. Miscellaneous materials 3. Utilities 4. Shipping and packaging	<i>Typical values</i> from flow-sheets 10 per cent of item (5) from flow-sheet usually negligible
Sub-total A	A
 Fixed costs 5. Maintenance 6. Operating labour 7. Laboratory costs 8. Supervision 9. Plant overheads 10. Capital charges 11. Insurance 12. Local taxes 13. Royalties 	5–10 per cent of fixed capital from manning estimates 20–23 per cent of 6 20 per cent of item (6) 50 per cent of item (6) 10 per cent of the fixed capital 1 per cent of the fixed capital 2 per cent of the fixed capital 1 per cent of the fixed capital
Sub-total I	3
Direct production costs A + 1 13. Sales expense 14. General overheads 15. Research and development	B 20-30 per cent of the direct production cost
Sub-total C	2
Annual production $cost = A + B + C =$	=
Production cost $\pounds/kg = -$	Annual production cost Annual production rate

Table 55 Summary of overall production cost

10.6. Fixed Costs

Table 56 Fixed Cost

Maintenance Cost

= 5% of the capital cost = 0.0526100000 = \$1305000

Laboure Cost

= 37,917

Laboratory Cost

= 20% of the Labouré cost $= 0.2 \times 37917 = \$7583.4$

Plant overheads

= 50% of Laboure cost = \$18958

10.7. Variable Costs

Table 57 Variable Cost

Miscellaneous materials

= 10% of the maintenance cost $= 0.1 \times 1305000 = 130500

Overall Production Cost = Fixed Costs + Variable Costs

Overall Production Cost = 1305000 + 37917 + 7583.4 + 18958 + 130500

Overall Production Cost = \$1499958.4(Annually)

To find out production cost per ton

 $Production \ cost = \frac{Annual \ production \ cost}{Annual \ production \ rate}$

 $Production \ cost = \frac{1499958.4}{35040}$

Production cost = (\$)42 per ton

10.8. Pay Back Period

Cost per ton = \$239.72 per ton

Profit on Every ton = \$198

Annual Profit = 198×35040

Annual Profit = \$6937920

Pay Back Period = $\frac{\$26100000}{\$6937920}$

Pay Back Period = 3.5 Years (Approximately)

10.9. Summary of Cost Analysis

Fixed Capital Cost	\$26,100,000
Fixed Cost	\$1,369,458
Variable Cost	\$130,500
Overall Production Cost	\$1,499,958
Annual Profit	\$6,937,920
Pay Back Period	3.5 Years

Table 58 Cost Analysis Summary

The cost analysis has provided us with a valuable insight into the financial aspects and feasibility of the proposed plant. By estimating all the costs now, we can say that our project is financially viable because the capital cost is not very high and our payback period is 3.5 years, which is not much. A general rule of thumb says if the payback period is less than 5 years then the proposal should be considered financially feasible. So, we can say that we are well positioned to execute this project.

CHAPTER 11

HAZOP ANALYSIS

Hazop and Operability analysis is an essential step in the design stage of a chemical plant. It helps in identifying the potential hazards that can lead to accidents. After evaluating the list of possible hazards, it is required to take necessary precautionary actions recommended to eliminate or minimize the potential occurrence of any incident. [13]

The hazop analysis for the three major equipment of the sulphur recovery unit are as follows:

Study	Process	Guide	Deviation	Potential	Potential	Actions
Node	Parameter	Word		Causes	Consequences	Required
Coolin	Flowrate	More	More	Failure	Greater	Install
g			cooling	of inlet	decrease in	temperatu
Water			water	cooling	the outlet	re sensors
(Shell			Flowrate.	water	temperature	at the inlet
side)				valve to	of the process	and outlet
				close.	fluid than	of process
					optimum.	fluid.
						Install low
						temperatu
						re sensors
						at the
						outlet of
						tube side.
		Less	Less flow	Pipe	Outlet	Install flow
			of cooling	leakage	temperature	meters to
			water	Pipe	of the process	the inlet of
				blockage		shell side.

			than		fluid higher	Install high
			optimum		than optimum.	temperatu
						re sensors
					Less effective	at the
					heat transfer.	outlet of
						tube side.
		None	No cooling	Failure	No alteration	Install
			water flow	of inlet	in	temperatu
				cooling	temperature	re sensors
				water	of process	at the inlet
				valve.	fluid.	and outlet
						of process
						fluid.
						Install flow
						meters to
						the inlet of
						shell side.
Proce	Temperat	Hight	Hight	Lower	Less effective	High
SS	ure		outlet	cooling	heat transfer.	temperatu
Fluid			temperatu	water	Higher tube	re sensors
(Tube			re of the	flowrate.	outlet	at the
Outlet			process	Higher	temperature	outlet of
)			fluid.	tube	than required.	the tube
				inlet		side.
				fluid		Flow
				temperat		meter at
				ure.		the inlet of
						the shell
						side.

	Low	Lower	Greater	Optimum	Install flow
		outlet	cooling	temperature	meters and
		temperatu	water	of the process	temperatu
		re of the	flowrate.	fluid not	re sensors
		process	Lower	achieved.	at the inlet
		fluid.	inlet		of shell
			shell		side.
			temperat		
			ure of		
			cooling		
			water.		

Table 60 Hazop Analysis on Furnace

Study	Process	Guide	Deviation	Potential	Potential	Actions
Node	Parameter	Word		Causes	Consequences	Required
Oxygen	Flow	Low	Low	Leakage in	Incomplete	Install flow
stream			oxygen	the	combustion.	meter.
Inlet to			inlet	pipeline.		
Furnace					Flammable gas	Regular
				Valve fails	accumulation	maintenan
				to open	inside the	ce and
				completely.	furnace.	monitoring
						of the
					Can potentially	valve.
					lead to	
					explosion.	
		No	No	Malfunctio	No reaction.	Change of
			oxygen	ning of the		valve.
			supply	valve.		

					Accumulation	
					of flammable	
					gas.	
		High	High	Higher rate	No claus	Maintenan
			oxygen	of blowing	reaction.	ce of
			supply	of draft fan.		control
					Higher overall	valve and
				Failure of	outlet	draft fan.
				control	temperature.	
				valve.		
Furnace	Pressure	High	High	Blocked or	May lead to	Install high
(Combu			overall	restricted	poor	pressure
stion			pressure	aur flow.	combustion.	alarm in
Cahmbe						the
r)				Faulty	Production of	combustio
				pressure	black smoke.	n chamber.
				regulator.		Install
						systems
				Restriction	Мау	that would
				in exhaust	potentially leas	automatica
				system.	to explosion.	lly shut off
						the fuel
				Faulty		supply.
				pressure		
				relief valve.		
		Low	Low	Insufficient	Insufficient	Inspect for
			pressure	fuel supply.	heating.	leaks.
			in the	Malfunctio	Cold spots and	Check the
			combusti	ning	uneven	exhaust
			on	burner.	heating.	system.
			chamber	Leaks in		
				the system.		

		Increased	
		energy	
		consumption.	

Table 61 Hazop Analysis on Reactor

Study	Process	Guide	Deviation	Potential	Potential	Actions
Node	Parameter	Word		Causes	Consequences	required
Claus	Temperatur	High	High	Catalyst	Decreased	Improve
Reacto	e		temperatur	deactivatio	catalyst	reactor
r			e of the	n or	performance.	distributi
			reactor.	fouling.		on.
					Reduced	
				High	reactor	Install
				reaction	performance.	temperat
				rates.	Runaway	ure
					reaction.	alarms.
				Flow		
				restriction		
				or pressure		
				drop.		
		Low	Low	Poor	Slower rate of	Better
			reactor	insulation.	reaction.	insulatio
			temperatur			n.
			e	Slow	Low	
				reaction	conversion in	Install
				kinematics.	the reactor.	temperat
					ure	
--------	------	--------------	------------	----------------	------------	
					sensors.	
Volume	Less	Lesser	Catalyst	Reaction	Routinely	
		volume of	degradatio	kinetics would	check the	
		the reactor.	n	be affected.	buildup	
				Increase in	inside the	
			Loss of	reactor	reactor.	
			catalyst.	pressure.	Clean the	
					reactor.	
			Channeling		Monitor	
			of the		the	
			reactants.		pressure	
					of	
					reaction	
					using	
					pressure	
					sensors.	

CONCLUSION

The design of a Superclaus plant for sulfur recovery has been carried out mathematically. This plant has been simulated on Aspen Hysys. This process enables a 99.5% overall conversion of H₂S. Higher conversion efficiency achieved by the virtue of selective oxidation catalyst in the superclaus reactor eliminates the requirement of downstream tail gas treatment unit. The exhaust gases leaving the last unit of this process contain no more than 0.02% of SO₂. The recovered elemental sulfur finds numerous uses in chemical and manufacturing industry. Furthermore, economic analysis performed for this project shows its financial feasibility. Therefore, this project provides a sustainable and cost-effective solution to the challenge of sulfur emissions to the atmosphere, minimizing environmental impact by optimizing the process.

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