Process Design and Simulation of Claus Unit for the Conversion of H_2S to Sulfur

Name: Muhammad Arslan Zahid

Registration number: 00000275851

This work is submitted as an MS thesis in partial fulfillment of the requirement for the degree of

MS in Process Systems Engineering

Supervisor Name: Dr.Muhammad Ahsan

School of Chemical and Materials Engineering (SCME)

National University of Sciences and Technology (NUST)

H-12 Islamabad, Pakistan

Declaration

I have clarify that my research work on “Process Design and Simulation of Claus Process’’ is my own doing work. This work is not doing any one before or nothing has published a research paper. The data has been used in this research paper are referred properly.

Signature of Student

Muhammad Arslan Zahid

00000275158

Acknowledgement

I would like to express my sincere gratitude to Dr. Muhammad Ahsan Assistant Professor, and Head of Department of SCME Chemical for allowing me to undertake this work. I am grateful to my supervisors Assistant Professor Dr. Ahsan Department of SCME for his continuous guidance advice effort and invertible suggestion throughout the research. I am also grateful to my supervisor Dr Ahsan for SCME Chemical Nust for providing me the logistic support and his valuable suggestion to carry out my research successfully.

Abstract

In the many refineries there is environmental pollution due to presence of sulfur content in the different petroleum product. These sulfur content are reduce by using different methods. There is different technique to reduce the sulfur content from petroleum product. the of best are Claus process in Claus Process the hydrogen sulphide gas are reacted with oxygen at the presence of high pressure and temperature and it form water and SO_2 gas. There is a method which is used for reduction of sulfur that is incinerator procedure that is not friendly method because they are required high temperature and a high pressure. The method is released a high amount of SO_2 gas that are released to atmosphere. In the sour and Sox gases there are presence of ammonia gases and other aromatic components. These sour gases that contained some amount of sulfur and ammonia are recovery in sulfur recovery unit to get sulfur and steam energy that is used for steam generation and this steam are cost effective. The main work on this project and topic is to get simulation by using Aspen Plus software and can get a maximum recovery of sulfur. I have used Aspen Plus software for simulation of Claus process to get maximum efficiency. The result of simulation are shown the completely conversion of sour gas and H_2S gas into complete elemental sulfur. The purpose of this simulation of keep the good environment from Sox gases and H_2S gases because these gases are damaged the environmental problem. It is also effect on agriculture growth land it is reduced the growth of crops. The important work is done by a scientist who has destroy the NH_3 gases that are produced in Claus process because due to NH_3 production it caused effect on equipment it has increased the rate of corrosion in the chemical plant. In this process 90 lb/hr of oxygen are used as oxidant for removal of sulfur and Waste heat boiler are used to generation of pressure steam and production of electricity. The behavior of chemical process industry is study by Aspen Plus software. In the Aspen Plus there are optimal study of steam generation, oxygen requirement and hydrogen yield that are further study in Claus process. It is also consider that the conversion of H_2S gas is increased by increasing the concentration of oxygen in chemical plant. With increasing the concentration of oxygen has cause great effect on sulfur recovery components from 0.8 to 0.94 percent. It is also notices that with increase the concentration of oxygen concentration in air are caused decrease the effect of NH3 gas that are produced in Claus process. The decreased and reduced the concentration of NH3 is due to oxidation of different gases like SO_2, CO2 gas and N_2 gases at the temperature of 1300^{o}C.it has increase the concentration of Sulfur components and also increase the efficiency of Claus process. It has effect on increase the concentration of Carbon monoxide gases in the reaction furnace. Now we need to optimize or change the parameter of furnace that are causes effect on ammonia destruction and carbon monoxide emission.

Keywords: Sulfur Recovery Unit; Ammonia Destructive

Table of Contents

List of Figure

List of Table

CHAPTER 1

INTRODUCTION

1. Introduction

There are different amount of sour gases that are containing different quality of impurities like Hydrogen sulphide gas, Ammonia, and carbon dioxide gas and addition of other waste materials like nitrogen gas. In the petroleum product there is high quantity of sulfur content and other containments that are must be removed for the environmental pollution. The elimination of sulfur is important objective in the petroleum product like petrol, diesel and LPG ECT. The removal of sulfur is rule of EPA (Environmental protection Agency) because it causes environmental pollution. The H_2S is found in environment is cause bad effect on human skin, Eye and breathing problem. The H_2S gas is the raw of dangerous gases like SO_2, CO_2 and NH_3 gases. The methane gas is main resource of H_2S gas. When natural gases are burned in combustion engine it causes SO_2 gases and CO_2 gases. Almost all the refinery in the world is used Claus Process to removal of sulfur and many refineries are produce sulfur 10 ton per day. Sulfur is raw material of Sulfuric acid [1].

1.1 Background

In 1993 Oxygen based modification is used in Claus process there was modification on this process (1) Upgrading the existing systems and introduces a new system and (2) To reduce the equipment size [2]. Claus process is really a popular engineering for retrieving In 1993 Lurgi Company took experiment on Claus process with capacity of 10 ton per day has efficiency of 99.8 %. According to Iranian petroleum research the incinerators process environment for Sulfur recovery process. Lots of refineries tire out several thousand ppm air pollution day after day attributable to transformation for Sulfur element to SO_2.In 1994 Super Claus catalyst was introduced in which reactor operated at low temperature .temperature reduced to 255°C to 200°C and have save utility cost and also decrease a tail gas [3].In 1998 Anne Piepeu worked on Sulfur recovery Claus process it enhance level of sulphur recovery from natural refinery it worked on mechanism of reaction that occurring in sulfur recovery units the reaction between H_2S , SO_2 and CO_2 and side reaction such as a hydrolysis of COS and CS_2 and also sulfation of catalyst. In 2010 the simulation has been done on MATLAB in which all physical condition and chemical character tics have been considers. Amount of enter sulphur enter into first bed and assumed to be 159 kmol/hr and also assumed the amount of sulfur present in furnace. Therefore sour gases and fuel are converted into H_2S gas and NH_3 gas in the oil refinery. During the gasification of coal they are produced hydrogen cyanide, Hydrogen sulfide and ammonia gases are formed. The Claus process consists of two parts. The thermal section part and the Catalytic section part. The thermal reactions has contains different furnace reactions and WHB. In the reaction furnace one-third parts of hydrogen sulfide gas is reacted with sulfur dioxide and water and also Hydrogen sulphide gases are reacts with sulfur dioxide gas to formed sulfur and water at temperature of 1000°C. Exhaust gases are allowed to cool down at 315°C in waste heat boiler to extract thermal energy and sulfur components. Out of the following impurities NH_3 is one of the most thermal destructive and completely destruction ensure the hydrocarbon gases contaminations that are including benzene , toluene, ethyl benzene & xylene (required temperature above 1050°C) are completely eliminate from furnace. The incompletely destruction of ammonia gas in furnace cause ammonia gas and nitrous oxide gas carryover into catalyst bed in which NH_3 is react with SO_3 to form ammonium salt components. The ammonia salt causes deactivation of catalyst and causes pressure drops in the reactor that enhance maintenance cost. The presence of nitrous oxide in reactor. Nitrogen and water is product of Claus process. In 1998 Clark et al worked on practical experiment study on ammonia oxidation in Plug Reactor at time constant of 0.4s to 0.55s and the inlet feed concentration of oxygen gas and ammonia gas are 3% to 4% respectively. The result shown that the temperature between 700 to 1100°C the conversion of NH_3 is reduced to 10% and while enhance temperature to 1100°C the conversion of ammonia is moved toward 60% to 100% [4]. In 2001 Monnery took study and established kinetic rate expression for pyrolysis and oxidation of ammonia gas. It is noted that conversion of ammonia through oxidation process is continuously varying from between 1 to 50%. Temperature domain between of 850-950°C and its residence time of 50-750 ms and conversion of pyrolysis is never exceeding than 20%. In Claus furnace pyrolysis of ammonia reaction is predictable to control for its destruction due to limited amount of oxygen. The reactions of ammonia damage can be increase by the presence of chemical components [5]. In 1998 Clark et al took experiments to observe the effect of water and ammonia pyrolysis at different temperature in furnace and different residence time. It also observes that the presence of sulfur dioxide has increase ammonia pyrolysis. In 2009 Mendiara el al it study the effect of carbon dioxide on the oxidation of ammonia gas during the oxy-fuel combustion of methane gas in plug flow reactor at temperature range of 773°C to 1500°C. It also study that high concentration of CO_2 has cause negligible effect on methane oxidation and it also enhance the formation of nitrous oxide due to rise in H/OH ratio and it increased the conversion of ammonia gas under condition [6].In 2003 Dagaut et al it study effect of nitrous oxide and sulfur dioxide on the oxidation of hydrogen gas and carbon monoxide mixture components in CSTR reactor at normal pressure and have a fixed resistance time and at different temperature from 1127°C to up to on [7]. In the Claus furnace there are two section furnace configurations that are single section and double section and effect of time constant on feed preheating to investigate kinetic model reactions of ammonia pyrolysis is developed by Monnery scientist. The furnace double zones furnace have get achieved higher conversion levels of ammonia demolition as compared to single section zone furnace because due to pass of clean acid gas feed that around the burner into second section zones that help to raise temperature in the first section. The simulation result shown that single furnace zone could acceptable level of NH_3 destruction with using some technique such as inlet feed heating again and increase oxygen concentration enrichment that would enhance furnace temperature. In 2004 the modification of Claus process to increase a sulfur recovery by reduced a cost. This modification is combination of Oxygen enrichment and recycles streams is used. In first stage the flow rate of oxygen is not exceed than 78% [8] .In 2010 the integration and simulation has been simulated on Aspen plus. The sensitivity of different process is studies. Analysis and thermal efficiency was attained 45% and carbon dioxide and Sox gases emission. The optimum analysis of gasification cycles was according to pinch analysis [9]. In 2018 the new design of Claus Process in which H_2S absorber and desorbed , SO_2 absorption ,separation and recycling in which H_2S and flue gas is absorbed in MDEA .The absorbent of Methyl di-ethanolamine and sodium citrate absorbent are regenerated to decreased the cost of process [10]. In 2018 Solid package of Aspen Plus is used for simulation and optimization of Claus reactor. The variation of change in temperature and pressure to observed the H_2S conversion into sulfur. To observe H_2S conversion and sulphur production which are calculated through Aspen Plus and comparison with design data [11]. In 2019 objective is improving the performance of sulfur recovery by using Aspen Hysys modified three stage simulation model is used study behavior of sulfur recovery and also consider a based case. The performance of base case is 93.89%. In base case optimization took place by controlling air demand percent and also adjusting the sulfur dew point margin .these margin change the performance of Claus process to 98.60% [12]. The effectiveness of each individual Claus component would depend on this Claus reactor stages. Such as the two reactors have to remove Sulfur from sour gas has capability of 90% conversion or method three reactor places possess a capability of 97%. The clause process is unable to get conversion of 100% enter Sulfur. Aspen PLUS® takes advantage of exact fashions intended for prediction belonging to the practice performance by way of the proper group thermodynamic fashions together with Assumed a good design and style from a process. This data may provide in the iterative type to help you improve this design.

1.2 Research Goal

The aim of research is to develop a model of Claus process in Aspen Plus software to improve the design and optimization of the chemical process industry. The thesis is target on simulation, optimization and cost analysis of sulfur recovery unit.

- To develop process design and simulation in Aspen Plus software and make a numerical and mathematical model for solving the equation.(Chapter No#2)
- To study parametric study and topological study of Claus process and To check the effect by changing the different variable and parameter of chemical process.(Chapter No#3)
- To study the pinch analysis of Claus process and find the optimum value from pinch analysis study (Chapter No#4)

- To study the Cost analysis of Claus process. Frist Claus analysis is done before the optimization and second cost analysis is done after the optimization and shown the cost comparison.(Chapter No #5 & Chapter No#6)
- At last we shown the Recommendation and Conclusion of Claus Process (Chapter No# 7)

1.3 Optimization Study of Claus Process

Optimization is work on sulfur production and cost that are related to energy consumption. The literature has review on the environmental determination have abundant modification of Claus process unit. There are taking some steps for recovery of sulfur and it is effect on cost increment to separate a sulfur molecule from sour gases. The recovery of sulfur is causes good effect on the environmental surface and also takes good effect on the atmosphere. Due to recovery of sulfur it causes good on human ecosystems and human nature and Claus process are the procedure to recovery of elemental sulfur from the sour gases. There are different studies on manufacturing of sulfur from Claus process. Diwekar is worked on fuel cell power systems and ethylene procedure utility plant. Fiaschi and Lombardi have worked on impacted on the environmental influence of the sulfur recovery section part of integer gasified section. The Zarei is worked on procedure of Claus furnace reaction for optimization & modification of Claus process. The different procedure valuations of the Claus process for recovery of sulfur and there are different main objective of Claus process that are used for sulfur recovery. The performance of varies modification was evaluate by using numerical analysis. The major work to finding are Oxygen based Claus process. The types are: 1) Upgrading the existing system and launched the new systems [13].Consider an increasing the use of high amount sulfur fuel is more stringent environment limitation on sulfur emission from different source.

CHAPTER NO 2

PROCESS SIMULATION

2.1 Process Simulation

2.1.1 Process Description

The Claus process is design on base on their sour gases and exhaust gases that are released from industrial chimney without any resistance. The sulfur recovery is defining the efficiency of Claus process. The objective of Claus process are complete removal of sulfur and other main containment gases that are NH_3 gas, CO_2 gases that must be remove from Claus process. Now we are used Aspen plus Software for simulation of Claus Process. Aspen Plus is one of the best software for simulation of Claus process. The thermodynamic packaging is used for simulation of Claus process, Peng Robison method is used for simulation of Claus. Peng Robison is used for hydrocarbon components and vapor phase reaction.the objective of clauses process is to convert the H_2S gas into Sulfur and most probably from exhaust gases is come from physical and chemical and natural gas processing unit. A Claus technique is containing of waste heat boiler, thermal furnace, catalytic reactor & cooler. There is little mechanism in which Claus process is take place the oxidation reaction is exothermic in which hydrogen sulphide is reacted with oxygen and made SO_2 from response to create Sulfur. The reaction of Claus process is that H_2S is reacted with O_2 at ratio of 2/1 ratio at the presence of high temperature and high pressure and it get Hydrogen sulphide gas and water. At the ratio of 2/1 the good amount of sulfur is produced. There are two types of Claus process first is modified Claus process and second is basis Claus process. In Basic Claus process the efficiency of sulfur is 70-78% ad it is very highly exothermic reaction and it is difficult to control and it also damage the catalyst and second one is Modified Claus process in this process efficiency is 90-92%. It is very good control system for temperature control. [14].

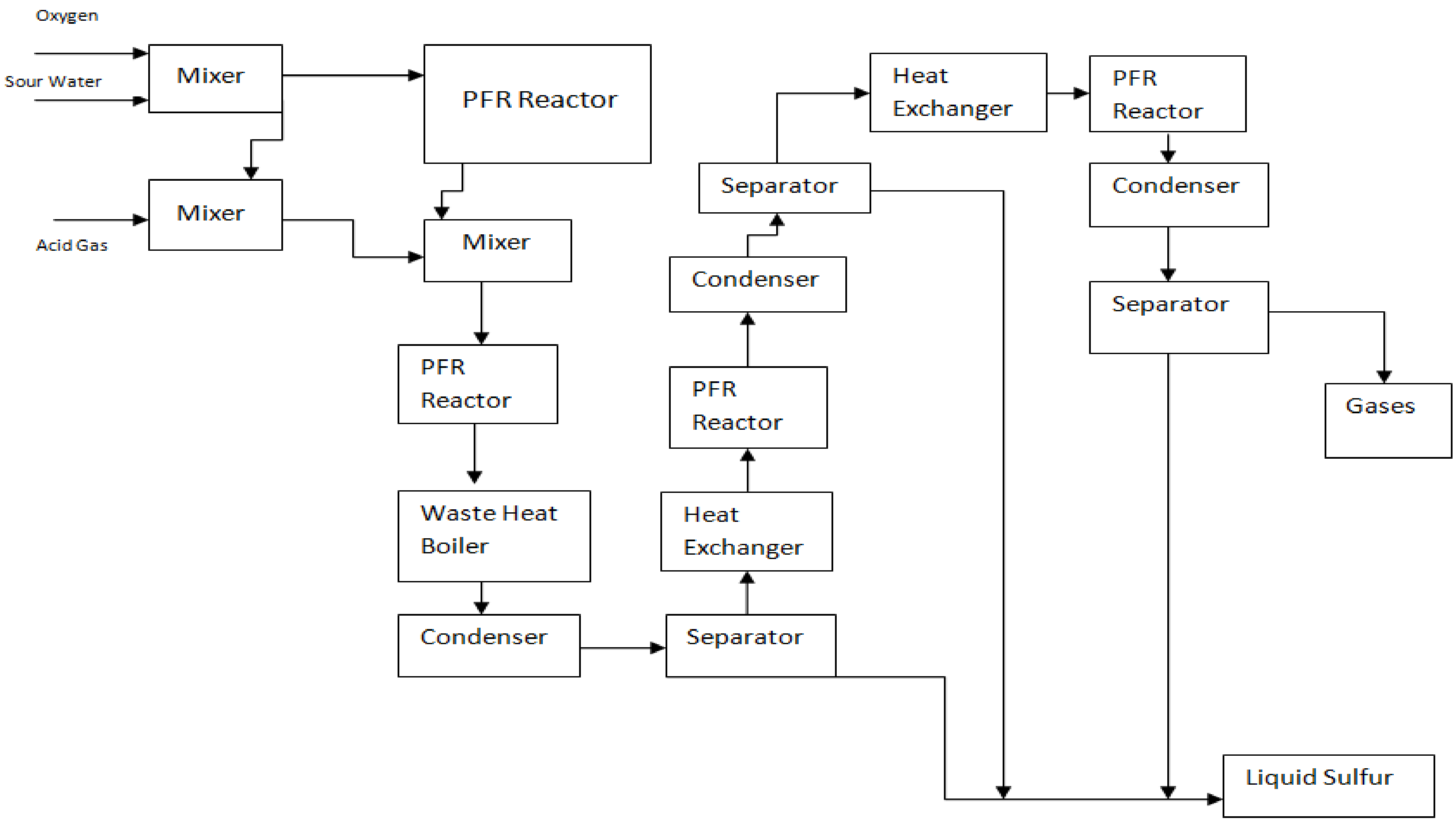


Figure 1: Block Flow diagram of Claus Process

2.2 Modeling and Optimization of Claus Process

The process is start with the chemical process reactions which are exothermic in nature, which is shown as thermal section stage. In this process the hydro sulphide gas contain acid gases is reacted with oxygen to form Sulphur dioxide and water. This gas is passed through waste heat boiler to form intermediate steam that is used for heating medium. The gases are cooled in the condenser and a high amount of sulfur is formed. The unreacted gases are moved toward the reheated in which cooling unreacted H_2S gas is further heated at reaction temperature and pressure after this amount of sulfur is produced. It again move toward condenser in which sulfur is separated at bottom of separator and unreacted gases are pass from top of the reactor. In the packed bed catalytic reactor hydrogen sulphide is reacted with oxygen at ratio of 2:1 and to form sulfur and water. [15].

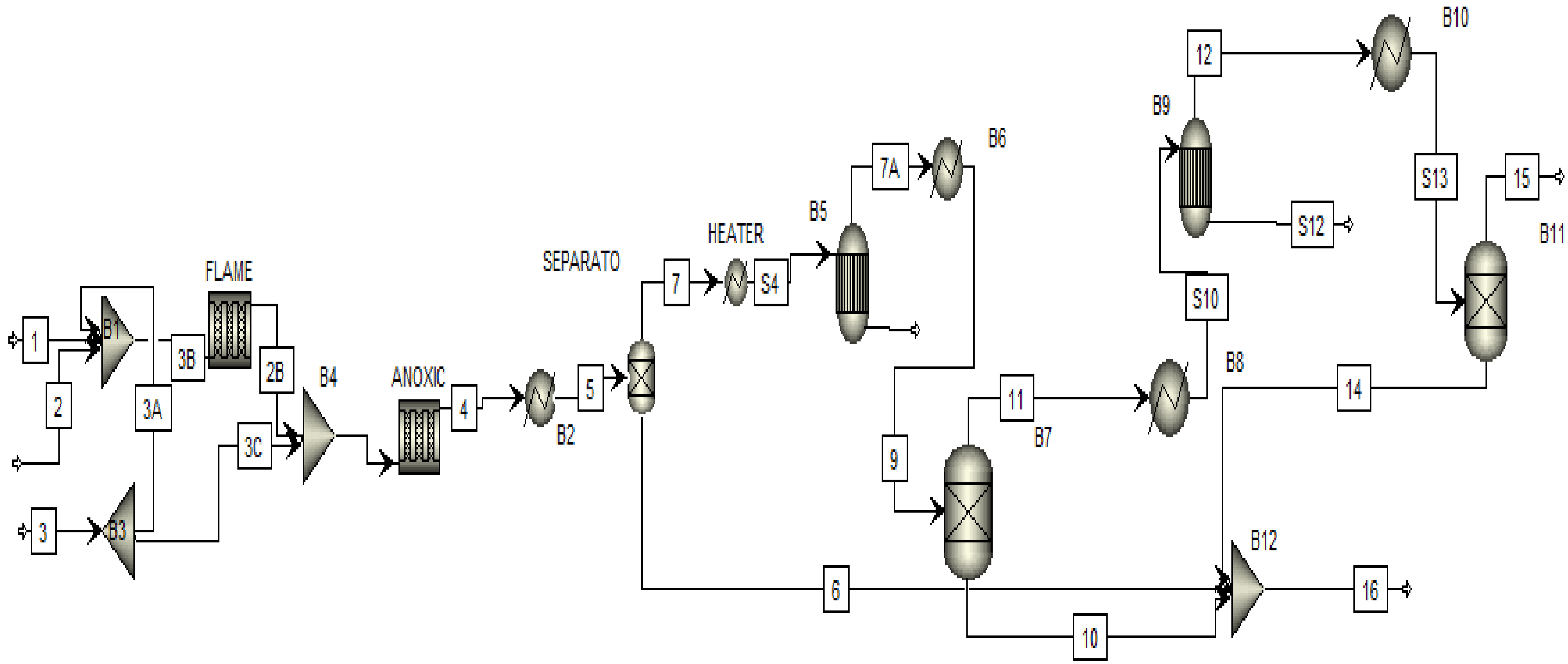


Figure 2: Process Simulation of Claus Process

2.3 First Stage Reaction

The Claus process is design on the basis of their sulfur recovery efficiency. The presence of sulfur and other containments in the gases are deciding the capacity of Claus process. The performance of Claus process is totally depend upon an amount of sulfur recovery from sour gases and a completely removal of other containment from gases.

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

$$NH_3 + 3/4\ O_2 \longrightarrow 1/2\ N_2 + 3/2\ H_2O \quad (2)$$

2.4 Second Stage Reaction

These are highly exothermic reaction and it causes increase in temperature in reaction furnace about 1350°C. There are different side reactions that are take place after this main reaction.

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

$$H_2S \longleftrightarrow 1/2\ S_2 + H_2 \quad (4)$$

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

$$NH_3 + 3/4\ SO_2 \longrightarrow 1/2\ N_2 + 3/2\ H_2O + 3/8\ S_2 \quad (6)$$

The important thing of this process efficiency is molar ratio of H_2S/SO_2 at sour gas is 2 to get highest conversion of Sulfur. There are equilibrium reaction are take place in the reaction.

2.4.1 Equilibrium Reaction

$$S_2 \longleftrightarrow S_8 \quad (7)$$

$$H_2S + 1/2\ SO_2 \longleftrightarrow 3/16\ S_8 + H_2O \quad (8)$$

In this operation acid gas which contains hydrogen sulphide that configuration is more than 50 mol% a conventional through configuration. The split flow configuration is challenges that arise when H_2S concentration in gases.

2.5 Flame Zone

The first reaction of Claus process is adiabatic reaction are take place in Plug flow reactor.

The liner reaction is oxidation reactions. Predicting the extents of reaction is occurring in flame zone and consumption of oxygen. It's make sure that no oxygen is slip toward into anoxic region it is also safety factor relate issue.

2.6 Modification of Claus Process on Basic of their Oxygen

Claus process is modified on base of their oxygen modification in which air is enriched with oxygen. This process is analyzing through process thermodynamic and kinetic. The major objective of this work is: 1) Decreasing the equipment sizing. The oxygen-base Sulfur recovery units has provide increase capacity of Claus systems at higher Sulfur recovery unit level and Dual & Double stage thermal stage system provide have a greatest capacity reverse.

2.7 Thermal Section Units

The reaction of reactions furnace and Water Heat Boiler simulation were control the process condition that lead to devastation of ammonia current in inlet streams. The furnace heating temperature and residence time constant are important parameter to promote destruction of NH_3 gas. To increase the oxygen enrichment in air, furnace temperature and feed preheating and increase the furnace length are changed. The feed used in Claus process is consists of sour water gas (SWG) air & acid gas, stream. There is complete mixing of steam before it moves toward the furnace and in this stage ammonia concentration is 125000ppm. The SO_2/H_2S ratio is 2 at the exist point of the waste heat boiler. Now we are changing the input variable of furnace to check the simulation result by taking variation of inlet air concentration and changing the fuel concentration. The temperature notices at waste heat boiler is 350^0C and temperature of waste heat boiler is maintained at 315^0C by using cooling jacket. Now at end take analysis of these exhaust gases by using analyzer. Now we find the efficiency of sulfur by calculating sulfur at outlet of furnace and sulfur at inlet of sulfur and it’s multiplied with 100. The mass of sulfur is obtained by using formula at inlet and outlet of the furnace.

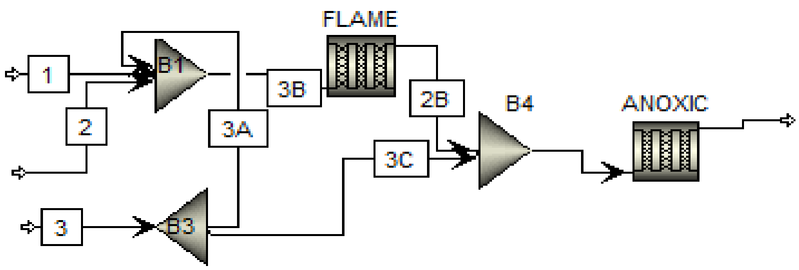


Figure 3: Simulation of Sulfur recovery unit

2.8 Reaction Kinetic of Chemical Reaction

The modeling of Claus process is divided into two sections and two zones. One section is highly rich oxygen concentration and Second section is oxygen deficient is called anoxic zone. The anoxic section is endothermic section and there is lower temperature and endothermic reaction is take place. [16].

$$-r_i = k_{o,i} \exp[\frac{-Ei}{RT}] \beta_{H2S} \beta_{NH3} \beta_{O2} \quad (a)$$

$$-r_2 = 3.58*10^7 \exp\left[\frac{-26.0}{RT}\right] (\beta_{H2S}\beta_{SO2}\beta_{H2} - \exp[-0.949 - \frac{5840}{T}] \beta_{S2}\beta_{H2O}) \quad (b)$$

$$-r_3 = 9.17*10^5 \exp\left[\frac{-45.0}{RT}\right] (\beta_{H2S}\beta_{H2} - \exp[-5.93 - \frac{10880}{T}] \beta_{S2}\beta_{H2}) \quad (c)$$

$$-r_4 = 1.52*10^{12} \exp\left[\frac{-60.0}{RT}\right] (C_{CO2}C_{H2} - \exp[-3.88 - \frac{4166}{T}] \frac{CCOCH2O}{C\,H2} \quad (d)$$

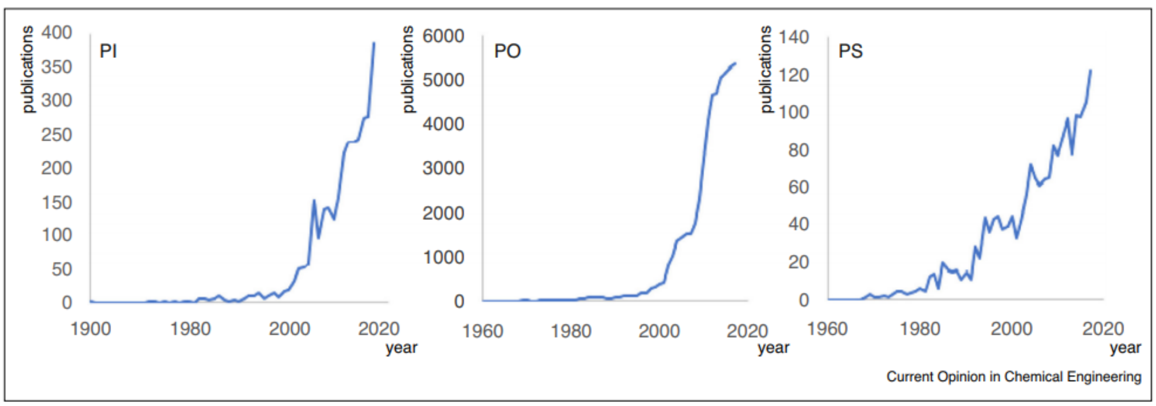
$$-r_5 = 2.29*10^4 \exp\left[\frac{-27.5}{RT}\right] C_{NH3}C_{SO2} \quad (e)$$

CHAPTER 3

OPTIMIZATION OF CLAUS PROCESS

3.1 Optimization of Chemical Process

Process Intensification and Process Optimization have cause great affect in rise the interest in research community. The process Optimization is cause significant increase or advances the speed and robustness of equipment. Process Intensification is used for process development to reduction of equipment size. In Process Intensification are included process, business & environmental aspects. Process Intensification is method of making reducing. The Process Intensification, Process Optimization and Process Systems are not a same study and field but their advance and development are correlated.



Scopus: Contributions on PI, PO and PS (from left to right) between 1960 and 2017.

Figure 4 : Contribution on PI, PO and PS

3.2 Method for Process Optimization,

The industrial motivation toward the retrofit is increasing capacity, increase productivity and safety and while decreased usage of energy, waste and operational cost. Process intensification has estimate 70-80% of project Systems Engineering and Process Intensification are decreased energy consumption and helpful to increase and improve quality, safety and conversion. There are four step heuristic methodologies that are including base case analysis, general improvement without analysis, optimization and comparison of solution.

Process Optimization is used to resolve the current challenges in chemical industry. To get benefit into engineer intensified process. Both process intensification and process intensification is powerful mathematical tool.

3.3 Technique and Process of Reaction Optimization

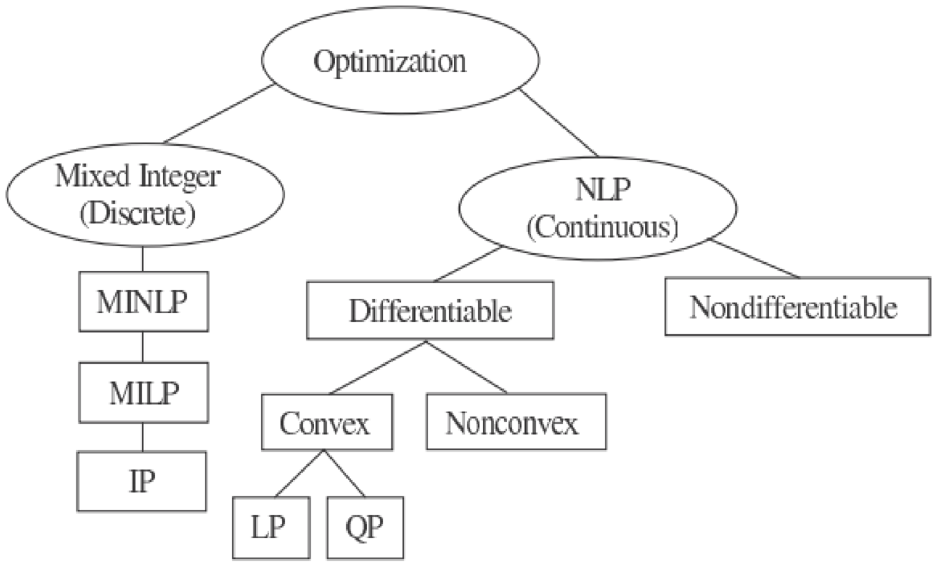
- Raw material and selection of reagent.
- The scale up technique.
- Increase quality controller aspects.
- Safety Material Data Sheet.
- Focus on environmental aspects.
- Control hazard of chemical process.

3.3.1 Scope of Optimization

The optimization is take to a system and process to find a good solution of the chemical process within constrats. The best elements are :

Objective Function

A objective function are provide a scalar quantative function performance it measure that needs of maximize and minimize. This process can be systems cost , yeild and profit.



.Figure 5 : Classification of Optimization Problem

Process Optimization is based on:

- Typical Industrial Problems
- Mathematical Programming software
- Optimization is based on mathematical equation
- The Lagrange Multiples and simple Algorithm
- On-line Optimization
- Chemical complex optimization

Optimal Design

- Uses flow sheet simulator
- Heuristics for process design and superstructure

Optimal Operations

- Plant optimal scheduling
- On-line optimization
- Supply chain optimization

Difference Optimization Language

LINDO - They are used in business application.

Optimization Capability Software

- Maple
- Matlab
- Excel-Solver
- Mathcad

Mathematical Programming

- Using GAMS
- Using Excel-Solver
- Mathematics Based optimization
- Simple method and Lagrange Method

	LP	MILP	QP	NLP	MINLP
Process Model Building				X	X
Process Design & Synthesis					
Heat Exchangers	X	X		X	X
Mass Exchangers	X	X		X	X
Separations		X		X	X
Reactors	X			X	X
Flowsheeting				X	X
Process Operations					
Scheduling	X	X			X
Supply Chain	X	X			X
Real-Time Optimization	X		X	X	
Process Control					
Model Predictive Control	X		X		
Nonlinear MPC			X	X	
Hybrid MPC		X			

Figure 6: Mathematical Programming in Systems Engineering

There is different type of sulfur.

- Formed Sulfur
- Emulsified sulfur
- Milled Sulfur

- Precipitated Sulfur

3.7 Design Variable of Optimization

3.7.1 Design Variable

The design variable is whose independent variable over which engineer are control is. These are continuous variable such as temperature, pressure or some discrete integer variable such as the number of stage in column. This decision variable is called design variables.

3.7.2 Objective Function

An objective function is a mathematics function in which we use best value of the decision variables, and reached toward the maximum and minimum value. The objective function is used to measure the value or goodness for solved the optimization problem. If it is profits in which we search toward maximum. If it is cost then moved toward minimum.

3.7.3 Constraints

There is limitation on the value of the decision variables. There are two types of value linear and non-linear and they are involved more than one decision variable. The constraints are written an equality involving more than two decision variables is called equality constraints. These reactions contain a specific concentration of oxygen and it combined with feed and it reacts with reactor. The mole balance of oxygen are reacted with reactor feed is an equality constraints. In inequality involved one or more than one decision variable is called inequality constraints.

3.7.4 Types of Optimization

There are two types of optimization that a chemical engineer needs to be considers

1) Topological Optimization

2) Parametric Optimization

3.7.4.1 Topological Optimization

In topological Optimization it compacts with the topological preparation of process equipment's. In second types is the parametric optimization it deals with operational variables such as temperature, concentration and pressure for the given piece of apparatus or process. In new chemical plant and design the new process units or upgrading the existing unit. The topological optimization is considered first because it causes large impact on overall effectiveness of plant. In another parametric optimization it is combination of both types of optimization tactics may be employed instantaneously but the topological change are causes best to optimize the process.

1) Can equipment be removed or arranged?

2) Can unwanted by-product should be eliminated?

3) An optional and alternative separation method or reactor configuration may be employed?

3.7.4.2 Parametric Optimization

In optimization of chemical process the conclusion variable should be identify in the optimization process. This is very necessary in order to decrease the computation effort as well as the time and make problem compliant. There are some variable are consider to most of the process.

1. Operating Condition for the distillation and vessel:-for example, temperature, pressure, concentration of reactant. The temperature may be control by observing catalyst properties, the sinter at high temperature or to be quiet at very low temperature.
2. Single pass transformation in the distillation and reactor, the selectivity will be determined by the condition that is mention and the single pass transformation.
3. The recovery of new reactant.
4. The purge ratios for reprocess streams that having an inerts gases.
5. Operating pressure of the separators.

3.8 Improvement of Claus Process

There is different improvement of Claus Process.

- Super Claus
- Oxygen Claus
- Better Catalyst

SuperClaus: A best catalyst is used in oxidize to sulfur and avoid the formation of sulfur dioxide. The higher conservation is obtained at good cost.

Better Catalyst: Higher conversion has been achieved with good catalyst that is provided higher surface area and also macro porosity.

CS_2 Destruction: C_2S Destruction is by product of furnace. There was laboratory worked on the special catalyst operating in the heater and furnace can destruction of C_2S before it moved toward into catalytic section.

Mathematical Process Optimization

The Mathematic process that contain 2000 different reactions and difference 142 species.A catalytic section is containing two reactors and two reactions and each reactor is containing 141 species for mass balance. The optimization problem contains three variables Furnace temperature / pressure, Air ratio / quality, Waste heat boiler temperature and pressure. These variables contain upper and lower limit boundaries.

3.9 Parametric Study of Claus Process

3.9.1 Effect of change in hydrogen concentration

To study the effect of hydrogen concentration on waste recovery heat by changing the heat transfer coefficient. The concentration of hydrogen and heat transfer coefficient both are inversely proportional to each other. If the hydrogen concentration is decrease gradually the production of steam in waste heat boiler is increased.

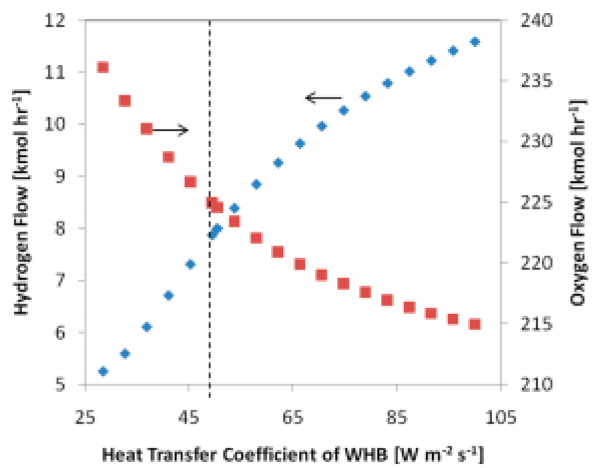


Figure 7 : Effect of change in hydrogen concentration

3.9.2 By changing the length of Reactor.

Carbon monoxide are cause big effect on the length of the reactor. They are gradually changed in length of reactor by changing the molar flow rate. In the Hydrogen sulphide gas there are causes less effect on the length of the reactor. If the molar flow rate is increase the conversion of H_2S into elemental sulfur is also increase. In SO_2 gas sulfur dioxide the are causes big effect on changing reactor length. If the length reactor increase it cause decrease in production of sulfur dioxide gas. If we increase or decrease the length of reactor is effect on conversion of hydrogen gas in increase.

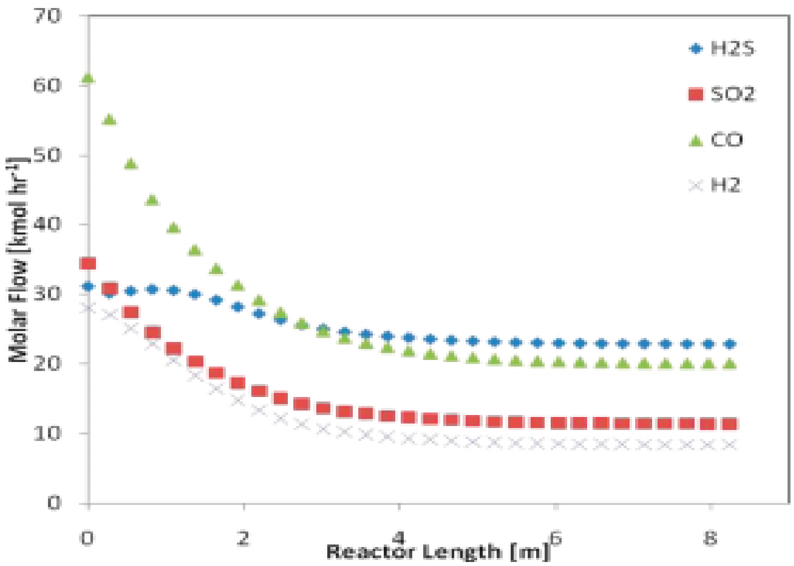


Figure 8 : Effect of Oxygen on sulfur Recovery

3.9.3 Effect of stream pressure on Claus process

It is observed that effect of steam pressure on the Claus Process when the steam pressure is high than the production of sulfur in sulfur recovery process is decreased. The steam production and Claus process.

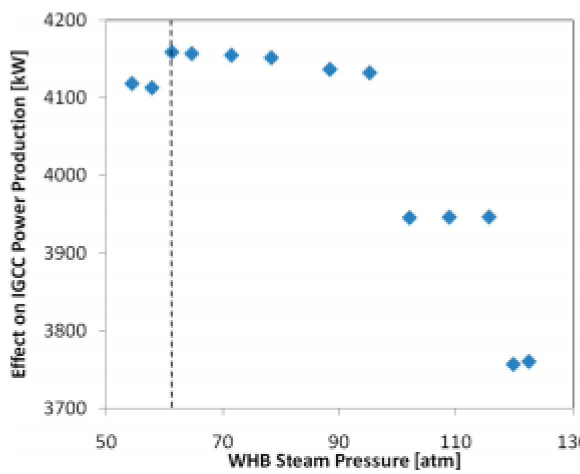


Figure 9: Effect of change in pressure on Sulfur Recovery

3.9.6 Optimization Temperature of Sulfur Recovery Unit

For the optimum operating condition, the average temperature of 2nd and 3rd reactor can be decreased. The reducing the temperature is causes increasing the sulfur recovery and low emission can be expected. The target of SRU is operates at average temperature at 214°C and 199°C respectively and temperature is gradually reduced. The variation of temperature of 2nd and 3rd temperature is causes variation in H_2S recovery. It was observed that up to 2°C temperature reduction cause no significant on total H_2S conversion. After this point for each degree centigrade reduction in temperature about 0.1 mol % increases in H_2S conversion [17].

CHAPTER 4

PINCH ANALYSIS OF CLAUS PROCESS

4.1 Pinch Analysis Technique

- There are appreciated placement principle how we study cold and hot utilities and separation system and other process systems that are related to GCC and the pinch analysis.
- There is multiple level of hot and cold value level. The mixing of cooling and heating systems the optimally with this process.
- The Network optimization and relaxation there are modified a network to reduce and eliminate a small heat exchanger which are less cost effective.
- The retrofit of presence chemical plants that are adapting a technique to dealing an existing plant layout and exchanger.
- There are systems analysis of power and heat systems and refrigeration and heat pumps systems.
- There are causes of process change where alter changing operating condition of different unit operation and other than stream to maximize the heat integration.

4.2 Key Steps of Pinch Technology

There is four steps for pinch analysis in design of heat regaining for both existing and new heat exchanger design.

- First Data extraction that are involve in collection of data for the utility and process.
- Targeting the temperature which is best for show in various respects.
- The design of heat exchanger where an initial warmth exchanger network are established.
- Last is optimization wherever initial design is basic and enhanced economically.

4.4 Data Extraction

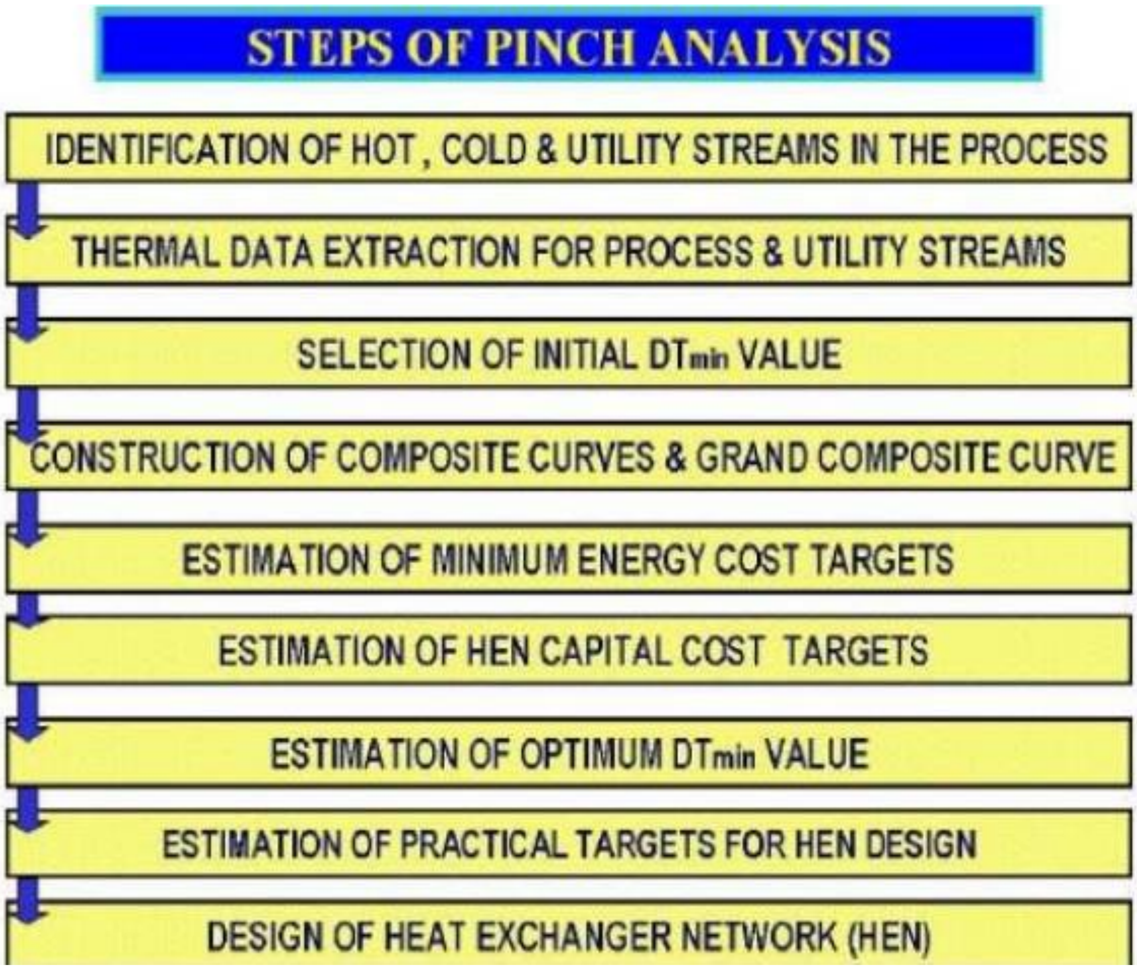


Figure 10 : Steps of Pinch Analysis

4.5 Basic Element of Pinch Technology

4.5.1 Representation of Grid

- Hot Streams that required cooling medium. It is move toward right direction.
- Cold Streams that are required heating medium. It is move toward left direction.
- A heat exchanger is represented by vertical lining that are joining the two open circles on the different streams being matched.

- Cooler and Heater are represented in open circle on the stream line being cooled and heated.
- The temperatures that can be put on the grid are easily checked on terminal difference temperature for each one unit.

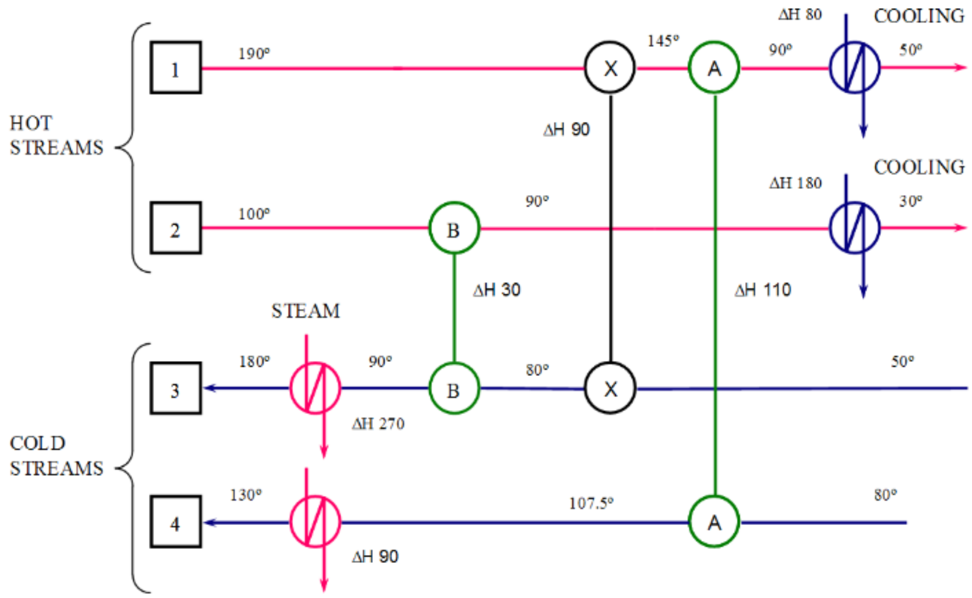


Figure 11 : Grid Diagram Heat Recovery Problem

4.5.2 Composite Curve

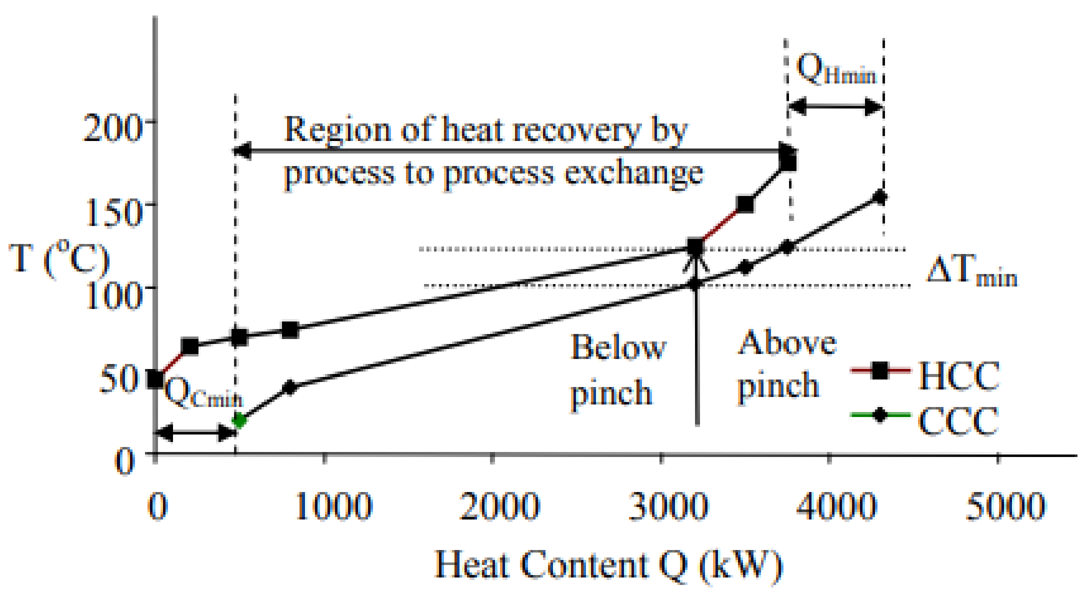


Figure 12 : Composite Curve

4.5.3 Problem Table Algorithm

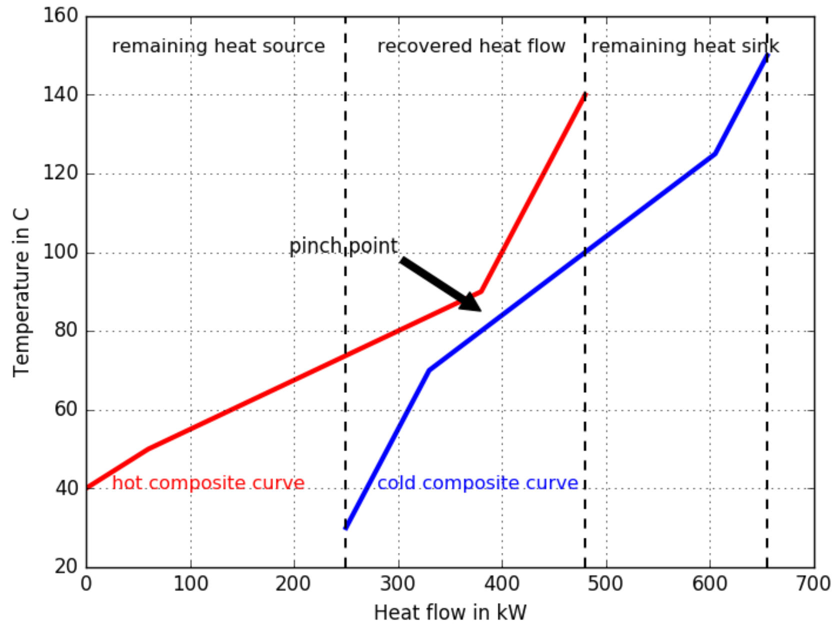


Figure 13 : Composite Curve

4.5.4 Grand Composite Curve

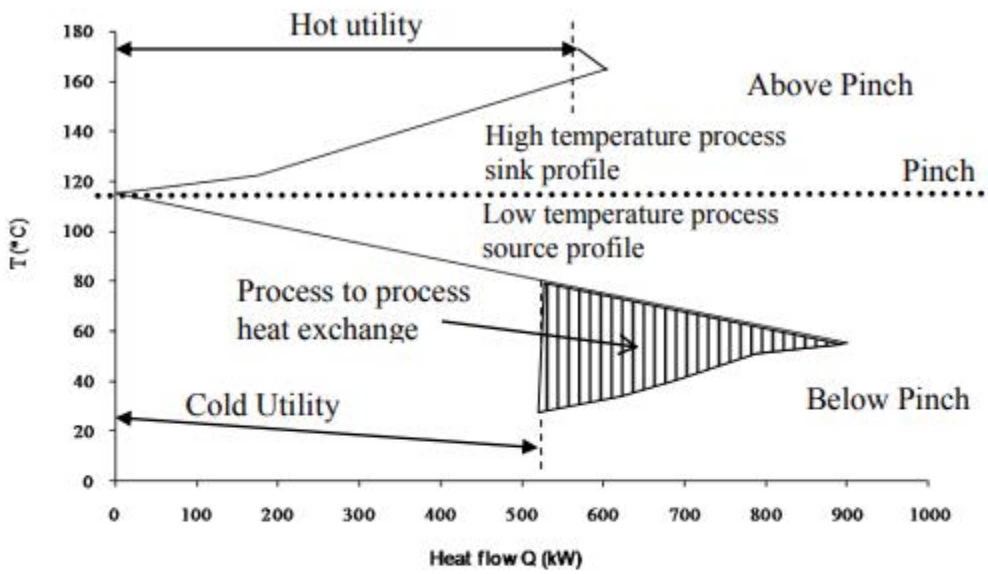


Figure 14 : Grand Composite Curve

4.5.6 The Pinch Concept

Pinch analysis is structured approached that improvement related to external. Analysis gives us opportunities such as improving efficiency, reducing operating cost and planning capital investment.

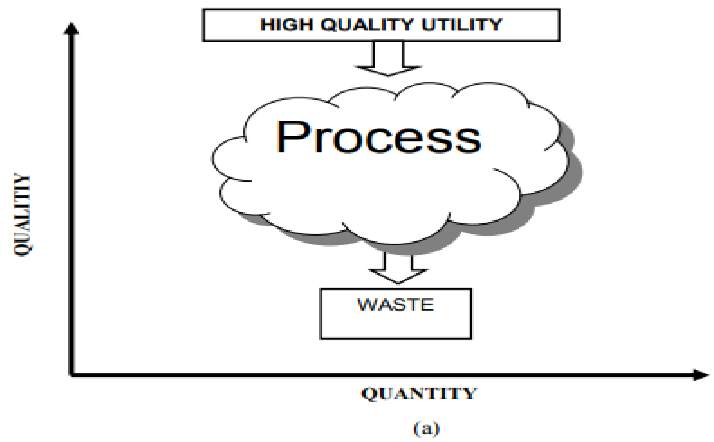


Figure 15 : The Pinch Concept

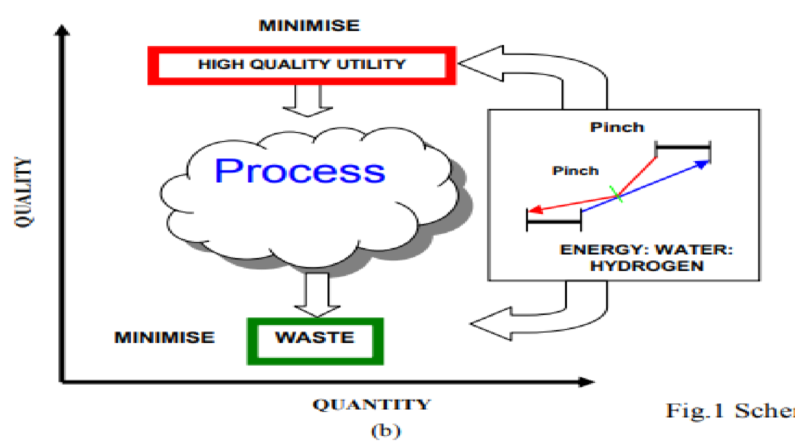


Figure 16 : The Pinch Technology

4.6 Pinch Technology vs Process Engineering

- Pinch Technology is a subdivision of process engineering.
- Our engineer are specialized information of thermodynamic and software tools. They can communicate effectively with clients and conceptual design.

- Carrying out process engineering project without the input of pinch study will led a less efficient.

How a pinch technology is different from other energy

A pinch technology is used to saving and their corresponding financial benefits.

- Maximum possibility to saving utilities.
- It study at all generally site
- It reveals the highest cogeneration potential.
- It does not include bench-mark but also account all specific factors, age, process equipment, cost product ECT.

4.6.1 Role of Thermodynamic Law in Pinch Technology

- Real Saving
- Feasible job
- significant Target

4.6.2 Important of Pinch Technology

- Pinch give best that will be achieved in systems.
- Pinch can gives the target to aim for that is less than theoretical maximum.
- The target is set the basic of heat exchanger design and also gives rules about how to design.
- Take place at wide systems. This allows seeing the interaction of two streams in process flow diagram or the utility flow sheet.
- Refine the area data where the accuracy factor is important. Pinch can show incomplete data.
- Pinch Analysis can compared result with other design tools, which can require detailed knowledge about geometry and flow sheet structure.
- Pinch is one of the best tools that can be used for conceptual design.

4.6.4 Application of Process Intensification

- Heat Integration
- Cogeneration site targeting

- Fractional Distillation Column target
- Hydrogen gas management refinery

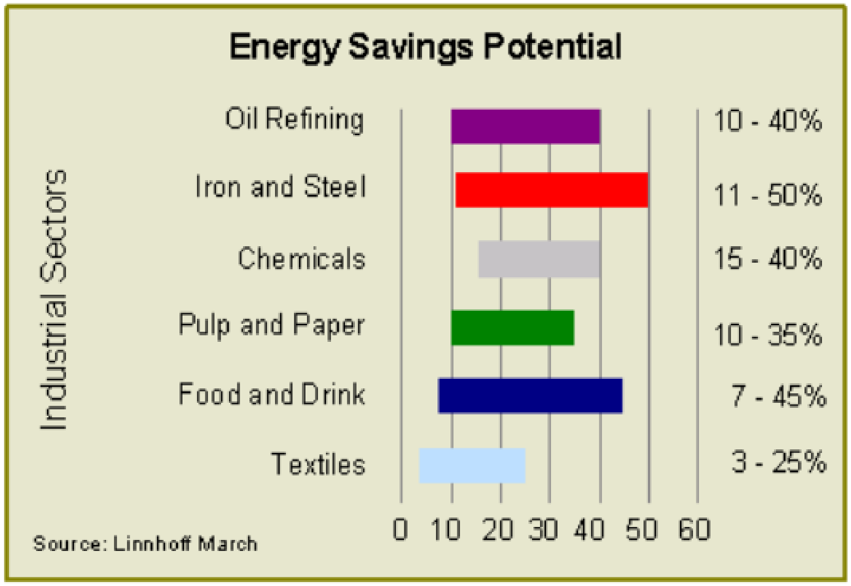


Figure 17 : Potential Energy Saving

4.7 Methodology of Pinch Analysis

Table 1: Steam Table of Pinch Analysis

Stream	Description	Type	Heat Type	T1 (K)	T2 (K)	H (kW)	m·cp(kW·K)
1	Cold	Cold	Sensible	468.15	587.15	31825.	267.437
2	Hot	Hot	Sensible	1623.65	468.15	-39209.7	33.9331
3	Hot	Hot	Sensible	587.15	448.15	-49001.4	352.528
4	Cold	Cold	Sensible	448.5	507.5	33477.1	567.408
5	Hot	Hot	Sensible	507.15	433.15	-33582.7	453.82

The temperature interval diagram was made on suitable temperature difference. The utility target is determined and stream splitting technology was employed to create a network.

4.7.1 Grid Diagram

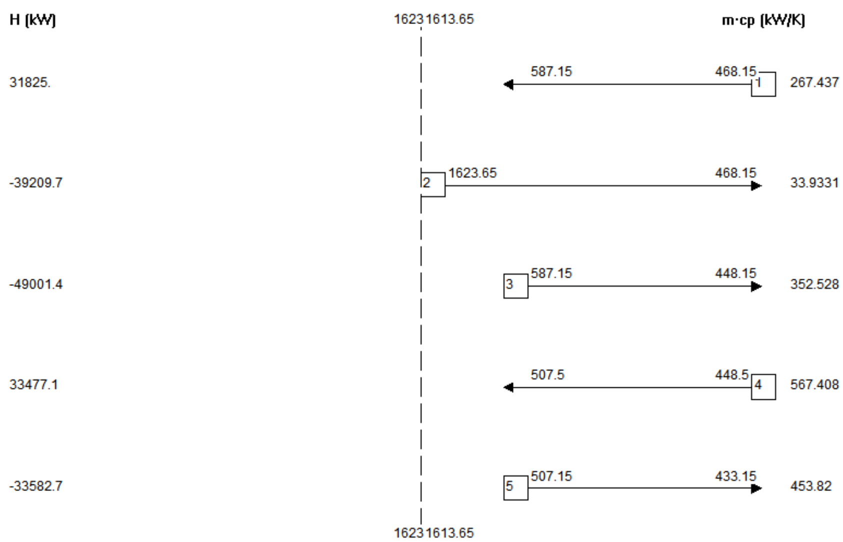


Figure 18 : Grid Diagram

4.8 Heat Exchanger Network

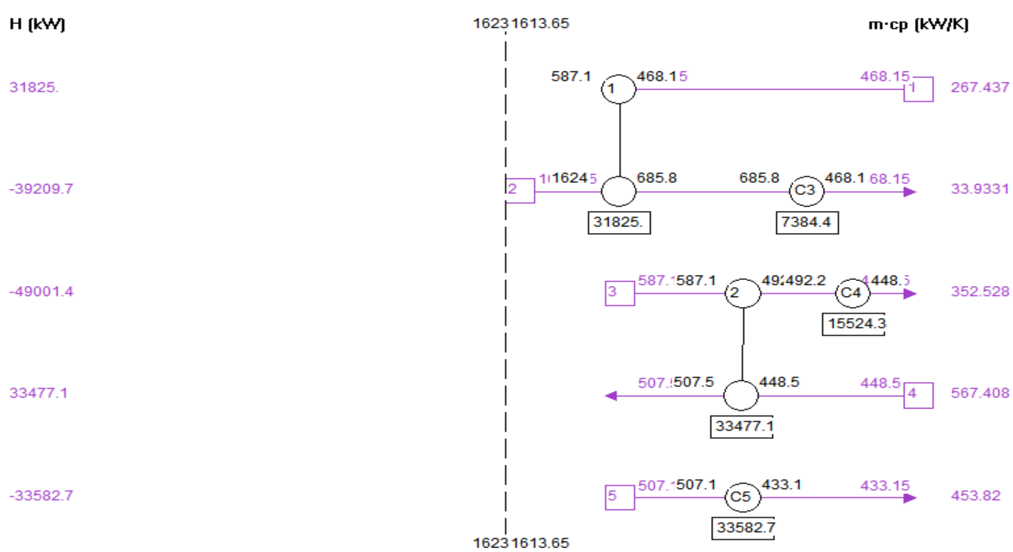


Figure 19 : Heat Exchanger Network

CHAPTER 5

COST ANALYSIS OF CLAUS PROCESS

5.1 Cost Analysis of Claus Process

A capital cost is cost that associate with existing chemical plant and modification of new chemical plant.

Order of Magnitude

These cost information is adjust by using scaling factor, capacity, and for providing the estimate cost of chemical plant. Block flow diagram is used for order of Magnitude cost estimation.

Study Estimation

In this types of cost estimation enlist a major components found in process industry. These are including equipment's like compressor, pump turbine, heat exchanger ECT. The each equipment is roughly sized and determined the cost estimation. This estimation is based on process flow diagram.

Preliminary Design Estimate

In these types of estimation accurate sizing of equipment that is used in study estimate .In the addition make layout of equipment is made up of piping, electrical equipment, and instrumentation and Utilities are also estimate. The preliminary estimate is based on Process Flow Diagram that included vessel stretches of equipment, elevation diagram.

Definitive Estimation

In this estimation that require preliminary specification of all chemical equipment, instrumentation, utilities and off site. The definitive estimate is including Process Flow Diagram, Utilities balance, and P&ID.

Detailed Estimation

In this types of estimate that require complete engineering of the process and also related all the utilities like off-site utilities. In detailed estimation it includes Process Flow Diagram, Process and Instrumentation Diagram, utilities balance and vessel sketches.

Class of Estimate	Level of Project Definition (as % of Complete Definition)	Typical Purpose of Estimate	Methodology (Estimating Method)	Expected Accuracy Range (+/- Range Relative to Best Index of 1)	Preparation Effort (Relative to Lowest Cost Index of 1)
Class 5	0% to 2%	Screening or Feasibility	Stochastic or Judgment	4 to 20	1
Class 4	1% to 15%	Concept Study or Feasibility	Primarily Stochastic	3 to 12	2 to 4
Class 3	10% to 40%	Budget, Authorization, or Control	Mixed but Primarily Stochastic	2 to 6	3 to 10
Class 2	30% to 70%	Control or Bid/Tender	Primarily Deterministic	1 to 3	5 to 20
Class 1	50% to 100%	Check Estimate or Bid/Tender	Deterministic	1	10 to 100

Figure 20 : List of Cost Estimation

The level of accuracy of estimate is depending upon:

- Effort and Time available
- Technique and Method Employed

- What is Qualification of estimator
- Study sensitivity of different parameter

5.2 Costing Technique of Module

The preliminary cost estimation is best for chemical plant. This technique is based on all cost back of purchased cost of chemical equipment evaluation. There is some technique of Module costing:

- Specify equipment types.
- There is specific equipment pressure.
- There is specific material of construction.

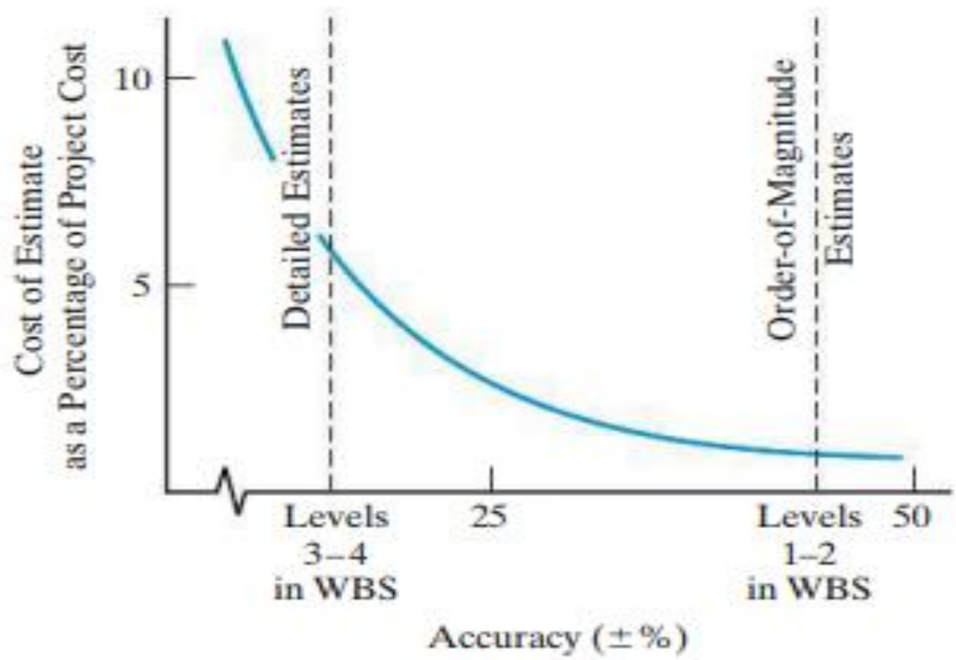


Figure 21: Accuracy of Cost Revenue Estimator Vs Cost of Making

5.3 Source of Cost Estimation

The information of cost analysis is useful for cost and revenue estimating. There are four main source of information.

- Accounting Record
- Other source take from firm
- Source from outside the firm

- Research and Development

Accounting Record

An accounting record is the primary source of information for cost analysis but they are not suitable for direct use. An accounting record is consisting of series of operating procedure for saving and keeping record detailed transaction between establishes categories of different asset. Accounting record is source of historical data but there is some limitation when they are used in making prospective estimation for economic engineering analysis.

Other Source takes from firm

There are number of people of people and record that are best source to estimating information. For Example: Firms that keep previous record that are useful to economic analysis are engineering, quality, purchased, sales, and personnel.

Source takes form outside firm

There are different source that are outside the firm that are helpful information for cost analysis. The main sources from outsider are:

- Published Information
- Current Wage

Research and Development

This information is not given or published and cannot be obtained by consulting and the only alternative may be undertake Research and Development to generate a data. First developed a pilot plant and observing the operating condition and pressure.

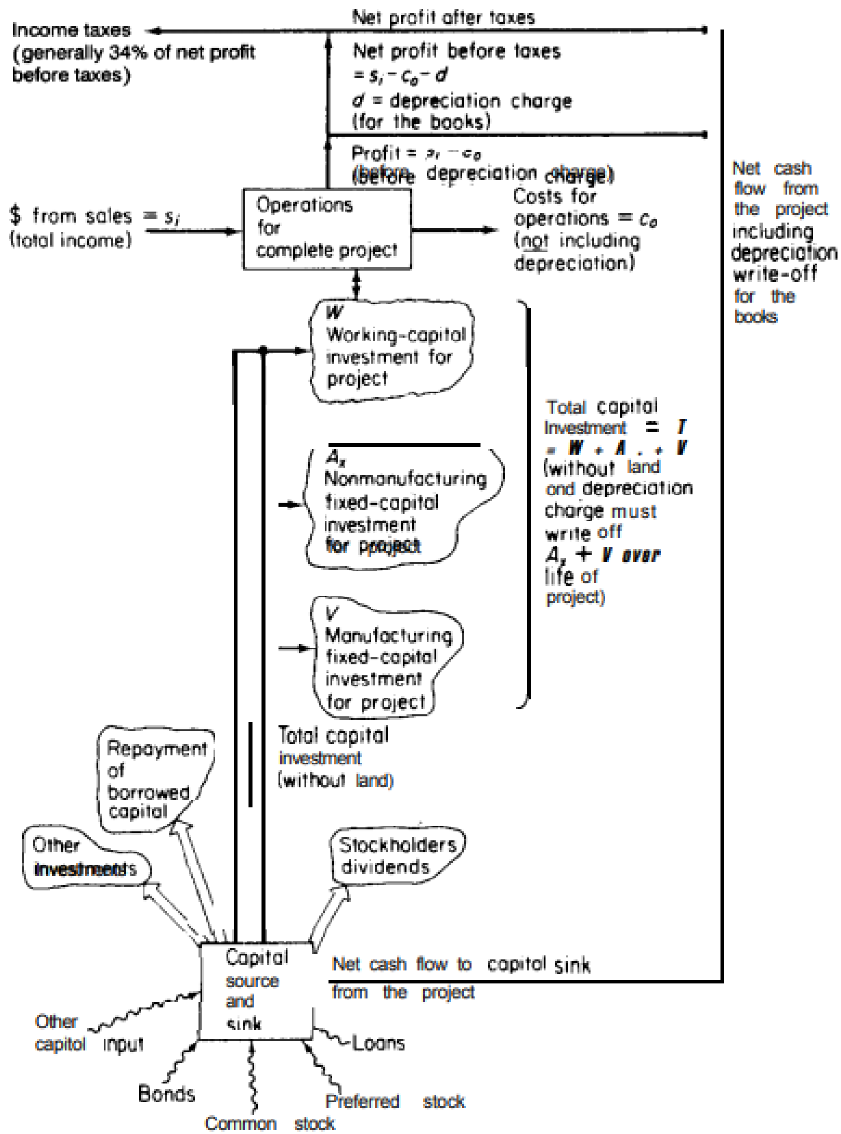


Figure 22: The cash flow diagram for industrial operation

5.5 Factor Affecting Investment and Production Cost

Whenever an Engineer of Chemical are decides cost of any product these cost must be accuracy to reliable decision the engineer must know the factor that affecting cost of product. Many companies have different arrangement with other contractor whereas raw material and equipment may be purchased lower than market value but a chemical engineer is based on raw material of reactant that is available in market place. Engineer must to be upgrade with price fluctuation, governmental regulation, company polices and other factor.

- Source of Equipment

Price Fluctuation

In the modern technology there are price fluctuation price is varies period to period. The labor cost is change by changing the price of food and goods. Therefore a chemical engineer should know the daily price and wage fluctuation.

Company Policy

The policy of company is direct effect on the cost of product. The company polices is totally depend on labor unions because there is effect of labor charge overtime work and the operator and engineer that work in company in overtime work.

Governmental Policy

The government has many regulation and rule that are cause effect on direct cost of industrial process. For example there are some tariff regulation on import and export. There are restriction on permissible depreciation rate and environmental regulation.

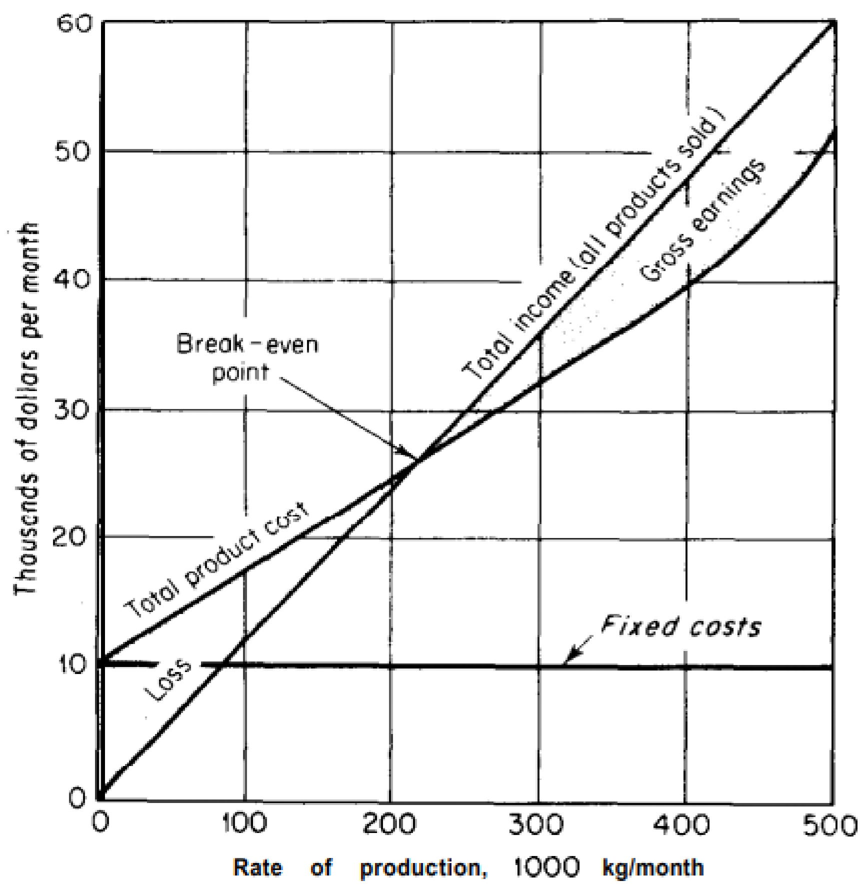


Figure 23 : Breakeven point for chemical plant

5.8 Chemical Engineering Cost Index

Year	Marshall and Swift installed-equipment indexes, 1926 = 100		Eng. News-Record construction index			Nelson-Farrar refinery construction index, 1946 = 100	Chemical engineering plant cost index 1957-1959 = loo
	All-industry	Process-industry	1913 = 100	1949 = 100	1967 = 100		
1975	444	452	2412	464	207	576	182
1976	472	479	2401	503	224	616	192
1977	505	514	2576	540	241	653	204
1978	545	552	2776	582	259	701	219
1979	599	607	3003	630	281	757	239
1980	560	675	3237	679	303	823	261
1981	721	745	3535	741	330	904	297
1982	746	774	3825	802	357	977	314
1983	761	786	4066	852	380	1026	317
1984	780	806	4146	869	387	1061	323
1985	790	813	4195	879	392	1074	325
1986	798	817	4295	900	401	1090	318
1987	814	830	4406	924	412	1122	324
1988	852	870	4519	947	422	1165	343
1989	895	914	4606	965	429	1194	355
1990 (Jan.)	904†	924	4673	979	435	1203	356

Figure 24 : Cost index of Chemical Engineering

Grass Root Plant

A grass root plant is consisting of complete plant installed on new side. This investment included all cost of land.

Battery Limit Plant

A boundary limits plant that define plant limit where it start from the production. A battery limit plant is the point where plant inlet is start from there. It include all the process equipment but exclusion of storage, Administration building, Auxiliary facilities.

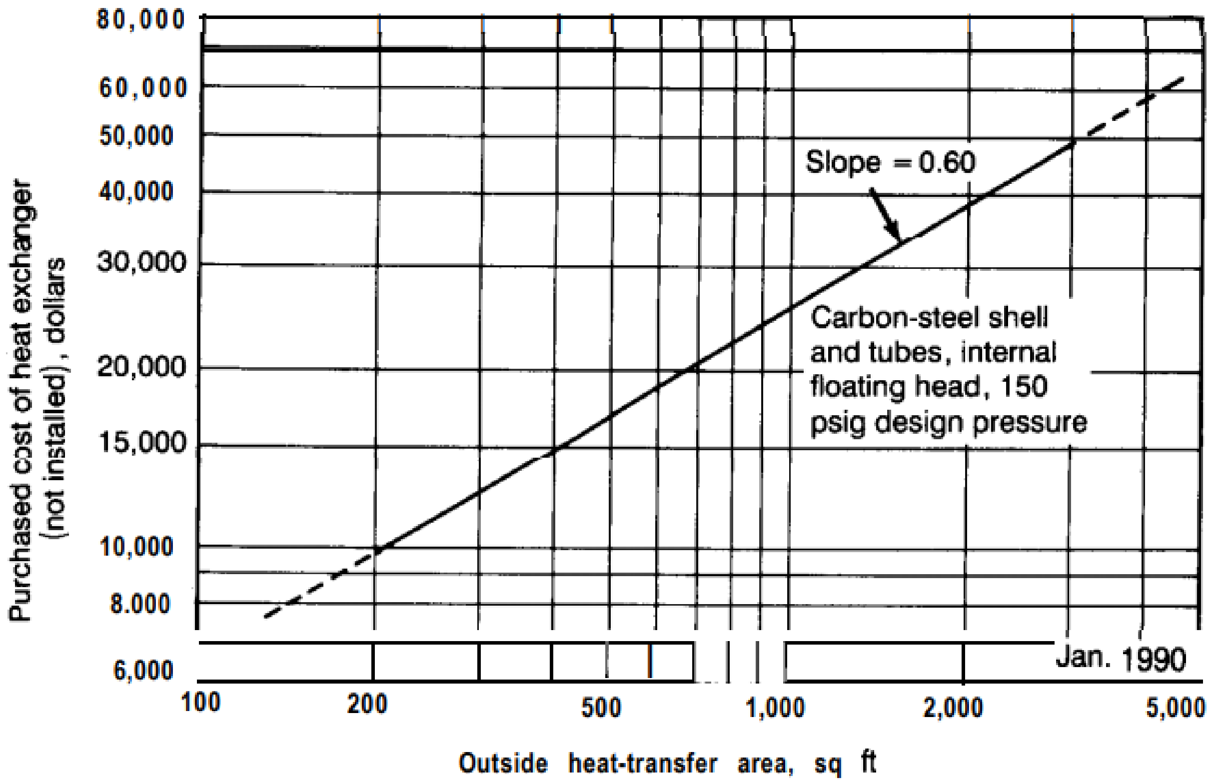


Figure 25 : Application of six-tenth-factor rule to the cost

5.11 General Overall Design of Chemical Plant

- We study the plant location.
- We study instrumentation control and chemical process.
- We study external utilities that used in chemical process.
- We study the different 3D diagram of chemical process.
- We study the structural design and building of chemical process.
- We study the handling of different material through different process.

5.12 Cost Analysis of Claus Process Sulfur Recovery Units

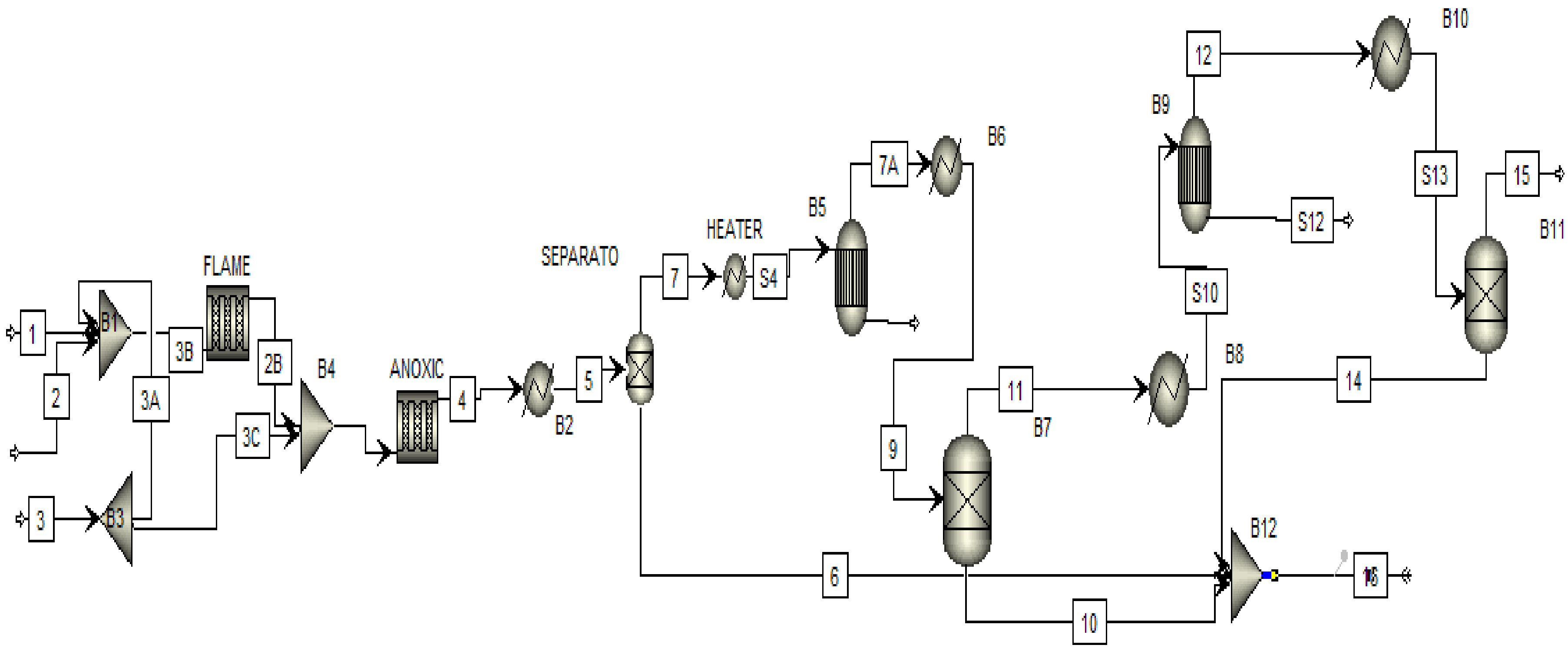


Figure 26:Process Flow Diagram of Claus Process

5.12.1 Equipment Summary of Claus Process

User Added Equipment

Exchangers	Exchanger Type	Shell Pressure	Tube Pressure	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
E-101	Floating Head	0	2	Carbon Steel / Carbon Steel	307	$ 66,100	$ 218,000	$ 66,100	$ 218,000
E-102	Floating Head	0	2	Carbon Steel / Carbon Steel	103	$ 35,100	$ 115,000	$ 35,100	$ 115,000
E-103	Floating Head	0	2	Carbon Steel / Carbon Steel	105	$ 35,300	$ 116,000	$ 35,300	$ 116,000
E-104	Fixed, Sheet, or U-Tube	0	2	Carbon Steel / Carbon Steel	48.3	$ 25,900	$ 85,200	$ 25,900	$ 85,200
E-105	Floating Head	0	2	Carbon Steel / Carbon Steel	48.3	$ 27,300	$ 89,900	$ 27,300	$ 89,900

Heater	Type	Heat Duty (MJ/h)	Steam Superheat	MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
H-101	Reformer Furnace	28600		Carbon Steel		$ 1,180,000	$ 2,510,000	$ 1,180,000	$ 2,510,000
H-102	Reformer Furnace	28700		Carbon Steel		$ 1,180,000	$ 2,510,000	$ 1,180,000	$ 2,510,000

Reactors	Type	Volume (cubic	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
R-101	Autoclave	7.08	$ 88,900	$ 356,000	$ 88,900	$ 356,000
R-102	Autoclave	7.08	$ 88,900	$ 356,000	$ 88,900	$ 356,000

Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
V-101	Horizontal	6.8	2.27	Carbon Steel		2	$ 15,900,000	$ 24,200,000	$ 26,500	$ 79,700
V-102	Horizontal	5.06	1.69	Carbon Steel		2	$ 6,940,000	$ 10,600,000	$ 15,500	$ 46,700
V-103	Horizontal	5.29	1.76	Carbon Steel		2	$ 7,770,000	$ 11,800,000	$ 16,700	$ 50,200
						Totals	**$ 33,337,500**	**$52,956,100**	**$ 2,786,200**	**$ 6,532,700**

Total Module Cost	$ 62,490,000
Total Grass Roots Cost	$ 65,760,000
Total Equipment Cost	$ 33,337,500

Figure 27 : Equipment Summary of Claus Process

5.12.2 Utilities Summary of Claus Process

Name	Total Module Cost	Grass Roots Cost	Utility Used	Efficiency	Actual Usage	Annual Utility Cost
E-101	$ 256,800	$ 366,000	Cooling Water		32300 MJ/h	$ 102,000
E-102	$ 136,000	$ 194,000	Low-Pressure Steam		897 MJ/h	$ 15,150
E-103	$ 137,000	$ 195,000	Cooling Water		2900 MJ/h	$ 9,100
E-104	$ 100,000	$ 143,000	Medium-Pressure Steam		759 MJ/h	$ 17,560
E-105	$ 106,000	$ 151,000	Cooling Water		1430 MJ/h	$ 4,500
H-101	$ 2,960,000	$ 4,220,000	Natural Gas	0.9	31800 MJ/h	$ 836,000
H-102	$ 2,970,000	$ 4,220,000	Natural Gas	0.9	31900 MJ/h	$ 839,000
R-101	$ 420,000	$ 464,000	Low-Pressure Steam		897 MJ/h	$ 15,150
R-102	$ 420,000	$ 464,000	Low-Pressure Steam		2900 MJ/h	$ 49,000
V-101	$ 28,600,000	$ 28,600,000	NA			
V-102	$ 12,500,000	$ 12,500,000	NA			
V-103	$ 14,000,000	$ 14,000,000	NA			
Totals	**$ 62,600,000**	**$ 65,500,000**				**$ 1,890,000**

Figure 28 : Utilities Summary Of Claus Process

5.12.3 Material of Construction

Add Materials

Remove all Materials

Material Name	Classification	Price ($/kg)	Flowrate (kg/h)	Annual Cost
Hydrogen Sulphide	Raw Material	$ -	5853.00	$ -
Oxygen	Raw Material	$ 1.50	2880.00	$ 35,951,040
Sulfur	Product	$ (0.19)	390.00	$ (616,660)
Hydrogen	Product	$ (12.00)	718.00	$ (71,702,352)
Nitrogen	Product	$ (10.00)	4009.76	$ (333,692,227)
Nitrogen	Raw Material	$ 10.00	1193.60	$ 99,331,392
Ammonia	Raw Material	$ 9.00	1264.00	$ 94,671,072

Economic Options

Cost of Land	$ 10,000,000
Taxation Rate	45%
Annual Interest Rate	10%
Salvage Value	$ 15,000,000
Working Capital	$ 38,100,000
FCI_L	$ 150,000,000
Total Module Factor	1.18
Grass Roots Factor	0.50

Figure 29 : Material of Construction

5.12.4 ECONOMIC INFORMATION AND CALCULATION

Economic Information Calculated From Given Information

Revenue From Sales	$ 406,011,239
C_{RM} (Raw Materials Costs)	$ 229,953,504
C_{UT} (Cost of Utilities)	$ 1,890,000
C_{WT} (Waste Treatment Costs)	$ -
C_{OL} (Cost of Operating Labor)	$ 936,740

Factors Used in Calculation of Cost of Manufacturing (COM_d)

Comd = 0.18*FCIL + 2.76*COL + 1.23*(CUT + CWT + CRM)

Multiplying factor for FCIL	0.18
Multiplying factor for C_{OL}	2.76
Facotrs for C_{UT}, C_{WT}, and C_{RM}	1.23
COM_d	$ 314,752,912

Factors Used in Calculation of Working Capital

Working Capital = $A*C_{RM} + B*FCI_L + C*C_{OL}$

A	0.10
B	0.10
C	0.10

Project Life (Years after Startup)	10
Construction period	2

Distribution of Fixed Capital Investment (must sum to one)

End of year One	60%
End of year Two	40%
End of year Three	
End of year Four	
End of year Five	

Figure 30 : Economic Information and Calculation

5.12.5 Cash Flow Diagram

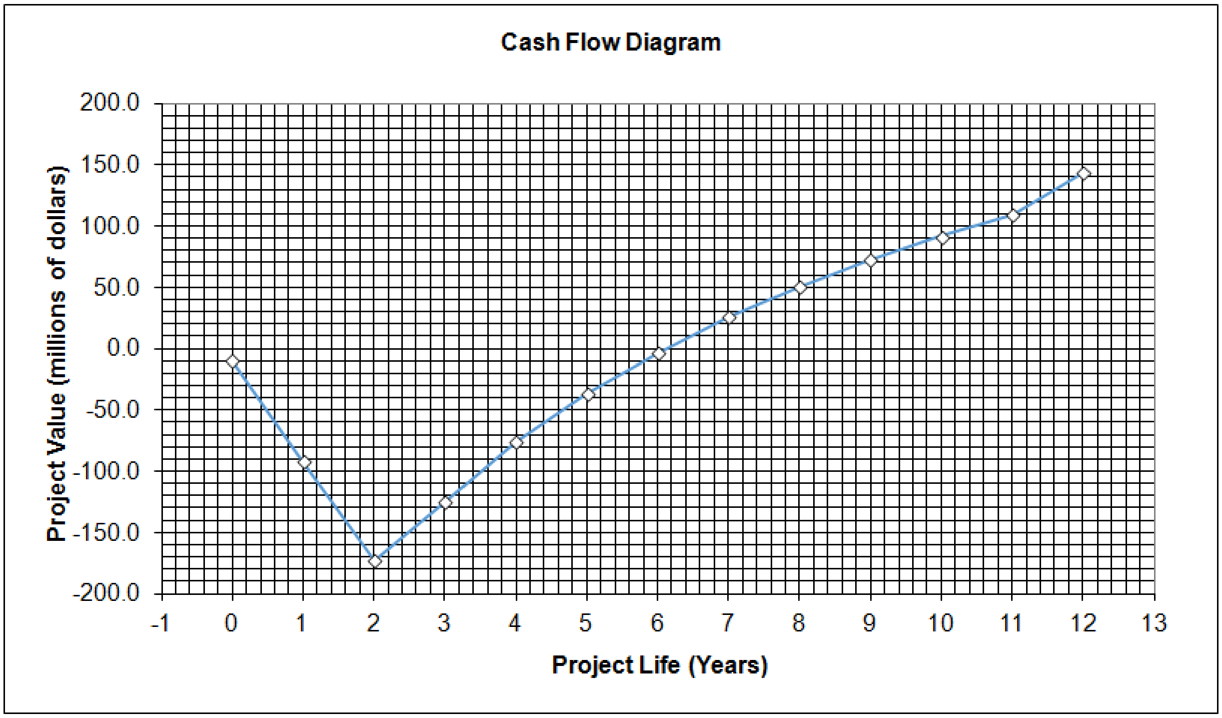


Figure 31 : Cash Flow Diagram

5.12.6 Discount and Non-Discount Profitability Criteria

Discounted Profitibility Criterion

Net Present Value (millions)	143.08
Discounted Cash Flow Rate of Return	24.62%
Discounted Payback Period (years)	2.9

Non-Discounted Profitibility Criteria

Cumulative Cash Position (millions)	427.67
Rate of Return on Investment	28.51%
Payback Period (years)	2.2

Year	Investment	d_k	$FCI_L - Sd_k$	R	COM_d	$(R - COM_d - d_k)*(1-t)+d_k$	Cash Flow (Non-discounted)	Cash Flow (discounted)	Cumulative Cash Flow (discounted)	Cumulative Cash Flow (Non-discounted)
0	10.00		150.00				(10.00)	(10.00)	(10.00)	(10.00)
1	90.00		150.00				(90.00)	(81.82)	(91.82)	(100.00)
2	98.10		150.00				(98.10)	(81.07)	(172.89)	(198.10)
3		30.00	120.00	406.01	314.75	63.69	63.69	47.85	(125.04)	(134.41)
4		48.00	72.00	406.01	314.75	71.79	71.79	49.03	(76.00)	(62.62)
5		28.80	43.20	406.01	314.75	63.15	63.15	39.21	(36.79)	0.54
6		17.25	25.95	406.01	314.75	57.95	57.95	32.71	(4.08)	58.49
7		17.25	8.70	406.01	314.75	57.95	57.95	29.74	25.66	116.45
8		8.70	-	406.01	314.75	54.11	54.11	25.24	50.90	170.55
9			-	406.01	314.75	50.19	50.19	21.29	72.19	220.74
10			-	406.01	314.75	50.19	50.19	19.35	91.54	270.94
11			-	406.01	314.75	50.19	50.19	17.59	109.13	321.13
12			-	406.01	314.75	58.44	106.54	33.95	143.08	427.67

Figure 32 : Discount and Non-Discount Profitabity Criteria

5.12.7 Variable Key Parameter over Plant Life

	Lower Limit	Upper Limit	Base Value
FCIL	-20%	30%	$ 150,000,000
Price of Product	-20%	5%	$ 406,011,239
Working Capital	0%	0%	$ 38,100,000
Income Tax Rate*	0%	0%	45%
Interest Rate*	0%	0%	10%
Raw Material Price	-10%	10%	$ 229,953,504
Salvage Value	0%	0%	$ 15,000,000

Figure 33 : Variable Parameter Over Plant Life

CHAPTER 6

Analysis of Cost Improvement in Chemical Technology

In the R&D and design of chemical plant the capital cost are universal estimation. In the chemical plant performance is overestimated. The product cost is trending to increasing significant between realized cost and estimate. There are number of factor that depends upon decrease cost of chemical plant.

- Improving the technology
- Learning by designer and plant operator
- Economic analysis of large equipment
- Using the cheap raw material cost

6.1 Cost Improvement

This is relationship between better worker performance and decreased cost and improved management and production and technical improvement. This phenomenon is types of manufacturing process are called learning curve. The learning phenomena are not factor that promote the relationship between declined cost unit and cumulative production. There are generic factor of learning improvement are learning by plant improvement, improvement the technical ability, improved the economic scale and decrease raw material cost.

6.1.1 Rate of Cost Improvement

The rate of Cost Improvement is defined as there are same manner of as the learning curve. There are slope of regression between fitted logarithm cost on Y-axis and logarithm of industry production on X-axis.

$$C_n = C_1 n^b$$

The curve of improvement is 100% is minus with rate of improvement. If the rate of improvement is 20% then rate of curve is 80%.

6.1.2 Factor Affect Rate of Improvement

- The characterize the technology
- The characterize the marketplace
- The characterize the management

The first factor is important for rate of improvement because of the state of product and market product and other factor cause less variant in product technology.

The Factor that characterize the Technology

We are considering 4 hypotheses that are regarding relationship between cost improvement and technical characterizes.

- **The higher level of complexity are cause high improvement**

The hypothesis are implies that higher the number of complexity cause the higher number of interlink step process and it offer greater the number of opportunities to improve the process. The more step are implied to improvement through process simplification and it causes higher proficiency.

- **If product has price it causes less cost improvement**

Higher the capital investment is causes rapid improvement in chemical process because process will provide less value of performance and it also cause less cost improvement.

Solid processing is may related to rapid cost improvement

Solid process is involved more physical unit operation other than gas and liquid and physical operation involve in less technological improvement. The solid processes are weak as compared to gas processing. There are some elementary factor in which heat and material balance are more difficult to take extrapolate from one plant to next changes. There is less show of improvement in solid processing.

In Technological display greater economical scale show more rapid improvement in cost

There is relationship between learning curve and technological innovation and other economical scale are discussed in context of CPI. A learning improvement are implies in the state of art of product, labor, improved management and organization and an advance product technology. Economic scale is shown range of cost unit decline as well as level of production increments.

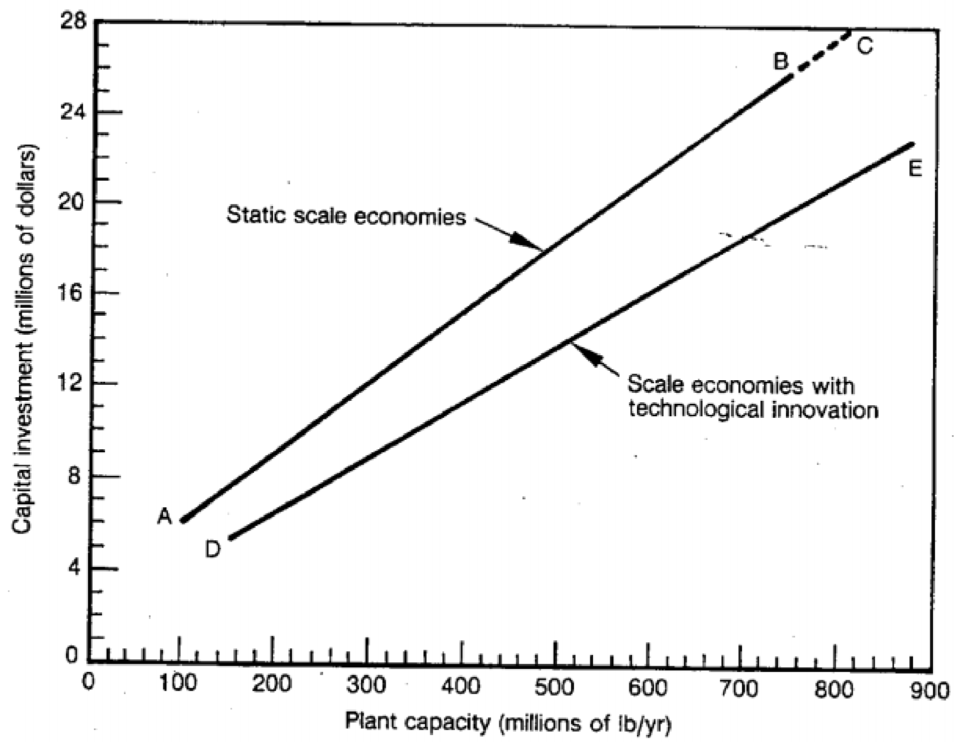


Figure 34 : Scale Economic with and without technical change

6.1.2 Factor that Affect Characterize the Market Place

There are three hypotheses that are relationship between market factor and cost improvement.

- **The actual change feedstock prices will effect of improvement cost**

The hypothesis is show that cost improvement in raw material will be reelected the more rapid in production improvement. The cost improvement is most rapid for intermediate rather than primary chemical used. The predecessor chemical are causes more rapid cost improvement.

- **The higher demand of growth are causes more rapid learning because of higher demand will create powerful incentive to power reduced cost to capture market value.**
- **The concentration Level and competition in industry may affect cost improvement.**

Some of the economic told that concentration has reduced the incentive investment in the Research and Development Department.

Factor that are characterize the Management

The management has cause more affect in cost improvement but they are cause effect in management. This relation is hard to prove. However there are two hypotheses.

- **The higher level of R&D is causes more rapid cost improvement.**
- **We can do careful management to maximizing collect information from earlier chemical plant and provided continuity for follow up plant and that effect rate of cost improvement after commercialization of new process or market product.**

6.2 Understanding Cost Improvement in Chemical Processing

There are 37 chemical process and products that are factor associated with cost improvement. First examine hypotheses that related to technology, Marketplace, management and analysis cost improvement that is form of database. Whenever data is not found then we can used case studies and literature value to discuss factors qualitatively and finally present statistical model for cost improvement.

Capital Intensity

The capital makes big contribution on product cost have caused more rapid economic improvement is not sure by the cost analysis. There are two relationships way between cost improvement and cost analysis that could support the factors that actually cause cost improvement , better management , technological innovation ect that can have limit effect on the feedstock costs but they have potentially have great effect on the capital cost.

Process Factor

There are no relationship between "scaling factor" and cost improvement for technological analysis. The scaling factor is measure economics scale analysis of capital cost. The most important factor is cost of chemical. There is relationship between cost improvement slope and cost economies after other factor are controlled variable.

Table 1 : Capital Intensity of Different Chemical Groups

Chemical Type	Average Capital Cost per Pound, as a Percent of 1969 Product Price
Organics	18.7
Inorganics	26.9
Fibers	29.3
Metals	28.0
All	21.3

Process Complexity

The process Complexity has offered more opportunity for improvement of technical processes by using complexity methods.

6.4 Cost Improvement and Marketplace

The price change in feedstock are causes big effect on prices cost on product. There is most implication that is applied on cost analysis.

- We are expecting that there is less cost improvement in primary chemicals as compare to secondary chemical. The refined chemical raw material will be less variable therefore that improving the reliability the chemical process. In the addition there are causes opportunity for introducing feedstock and that are greater than secondary chemical involved.
- There is prediction that the rate of cost improvement in primary chemical cost is faster than improvement in secondary chemicals.

- There are expecting that less cost improvement in feedstock where rising cost are associates with mineral depletion.

- **Table 2 : Correlation between Improvement Slopes and Feed Stock Factor**

Factor[a]	Pearson Correlation	Statistical Significance
Cost improvement slope of precursor chemical (19)	+0.60	0.006
Product is a "secondary" chemical (37)	−0.43	0.009
Process uses "raw" solid feedstock (41)	+0.55	0.0005

[a]Numbers of observations are shown in parentheses.

6.5 Cost Improvement and Management

In the first hypotheses there are relationship between cost improvement and industrial management for the chemical process. They are cause higher level of development and research expenditure of product cost and it causes rapid improvement. The second hypotheses are on management information transfer and organization of rapid improvement cost.

Cost Improvement and R&D Expenditure

There is magnitude of relationship between R&D expenditure and cost improvement has very important implication of industrial competitiveness. We have hoped to test relationship between different R&D expenditure on refinement of different processes and cost improvement slopes by using different multiple regression model.

- Lieberman Equation cannot contain four factors that are use to drove the cost improvement in the chemical processes. This relationship would affect the factors are taken to unknowns.
- R&D are cause significant contribution to examine and explain cost improvement variation which are combined cumulative industry output and strongly related with cost analysis. The relationship between cost improvement

and cumulative output are much stronger than R&D expenditure and also cost analysis.

- Lieberman has measure of R&D expenditure that admittedly the crude. It is ratio of sale of R&D expenditure and company sale. There are causal linked between cost improvement and R&D expenditure.

6.6 Cost Analysis of Claus Process after Improvement

6.6.1 Equipment Cost

Table 3: Cost Analysis of Claus Process after Improvement

User Added Equipment

Exchangers	Exchanger Type	Shell Pressure	Tube Pressure	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
E-101	Floating Head	0	2	Carbon Steel / Carbon Steel	60	$ 28,900	$ 95,000	$ 28,900	$ 95,000
E-102	Floating Head	0	2	Carbon Steel / Carbon Steel	12.8	$ 26,000	$ 85,400	$ 26,000	$ 85,400
E-103	Floating Head	0	2	Carbon Steel / Carbon Steel	559	$ 108,000	$ 356,000	$ 108,000	$ 356,000
E-104	Fixed, Sheet, or U-Tube	0	2	Carbon Steel / Carbon Steel	32.7	$ 23,800	$ 78,200	$ 23,800	$ 78,200
E-105	Floating Head	0	2	Carbon Steel / Carbon Steel	70.8	$ 30,400	$ 99,900	$ 30,400	$ 99,900

Heater	Type	Heat Duty (MJ/h)	Steam Superheat	MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
H-101	Reformer Furnace	28600		Carbon Steel		$ 1,180,000	$ 2,510,000	$ 1,180,000	$ 2,510,000
H-102	Reformer Furnace	28700		Carbon Steel		$ 1,180,000	$ 2,510,000	$ 1,180,000	$ 2,510,000

Reactors	Type	Volume (cubic	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
R-101	Autoclave	7.08	$ 88,900	$ 356,000	$ 88,900	$ 356,000
R-102	Autoclave	7.08	$ 88,900	$ 356,000	$ 88,900	$ 356,000

Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
V-101	Horizontal	6.8	2.27	Carbon Steel		2	$ 15,900,000	$ 24,200,000	$ 26,500	$ 79,700
V-102	Horizontal	5.06	1.69	Carbon Steel		2	$ 6,940,000	$ 10,600,000	$ 15,500	$ 46,700
V-103	Horizontal	5.29	1.76	Carbon Steel		2	$ 7,770,000	$ 11,800,000	$ 16,700	$ 50,200
						Totals	**$ 33,364,900**	**$ 53,046,500**	**$ 2,813,600**	**$ 6,623,100**

Total Module Cost	**$ 62,590,000**
Total Grass Roots Cos	**$ 65,900,000**
Total Equipment Cost	**$ 33,364,900**
Lang Factor	**4.74**
Lang Factor Cost	**$ 158,100,000**

Utilities Summary

Name	Total Module Cost		Grass Roots Cost		Utility Used	Efficiency	Actual Usage	Annual Utility Cost	
E-101	$	112,079	$	160,000	Cooling Water		115000 MJ/h	$	-
E-102	$	101,000	$	143,000	Low-Pressure Steam		897 MJ/h	$	15,150
E-103	$	420,000	$	597,000	Cooling Water		2900 MJ/h	$	9,100
E-104	$	92,000	$	131,000	Low-Pressure Steam		759 MJ/h	$	12,820
E-105	$	118,000	$	168,000	Cooling Water		1430 MJ/h	$	4,500
H-101	$	2,960,000	$	4,220,000	Natural Gas	0.9	31800 MJ/h	$	836,000
H-102	$	2,970,000	$	4,220,000	Natural Gas	0.9	31900 MJ/h	$	839,000
R-101	$	420,000	$	464,000	Low-Pressure Steam		897 MJ/h	$	15,150
R-102	$	420,000	$	464,000	Low-Pressure Steam		2900 MJ/h	$	49,000
V-101	$	28,600,000	$	28,600,000	NA				
V-102	$	12,500,000	$	12,500,000	NA				
V-103	$	14,000,000	$	14,000,000	NA				
Totals	**$**	**62,700,000**	**$**	**65,700,000**				**$**	**1,780,000**

Figure 35 : Utilities Summary

Material of Construction

Economic Options

Cost of Land	$	10,000,000
Taxation Rate		45%
Annual Interest Rate		10%
Salvage Value	$	15,000,000
Working Capital	$	38,900,000
FCI_L	$	150,000,000
Total Module Factor		1.18
Grass Roots Factor		0.50

Economic Information Calculated From Given Information

Revenue From Sales	$	406,533,029
C_{RM} (Raw Materials Costs)	$	237,942,624
C_{UT} (Cost of Utilities)	$	1,780,000
C_{WT} (Waste Treatment Costs)	$	-
C_{OL} (Cost of Operating Labor)	$	936,740

Factors Used in Calculation of Cost of Manufacturing (COM_d)

Comd = 0.18*FCIL + 2.76*COL + 1.23*(CUT + CWT + CRM)

Multiplying factor for FCIL		0.18
Multiplying factor for C_{OL}		2.76
Facotrs for C_{UT}, C_{WT}, and C_{RM}		1.23
COM_d	$	324,444,230

Figure 36 : Material of Construction

Cash Flow Diagram

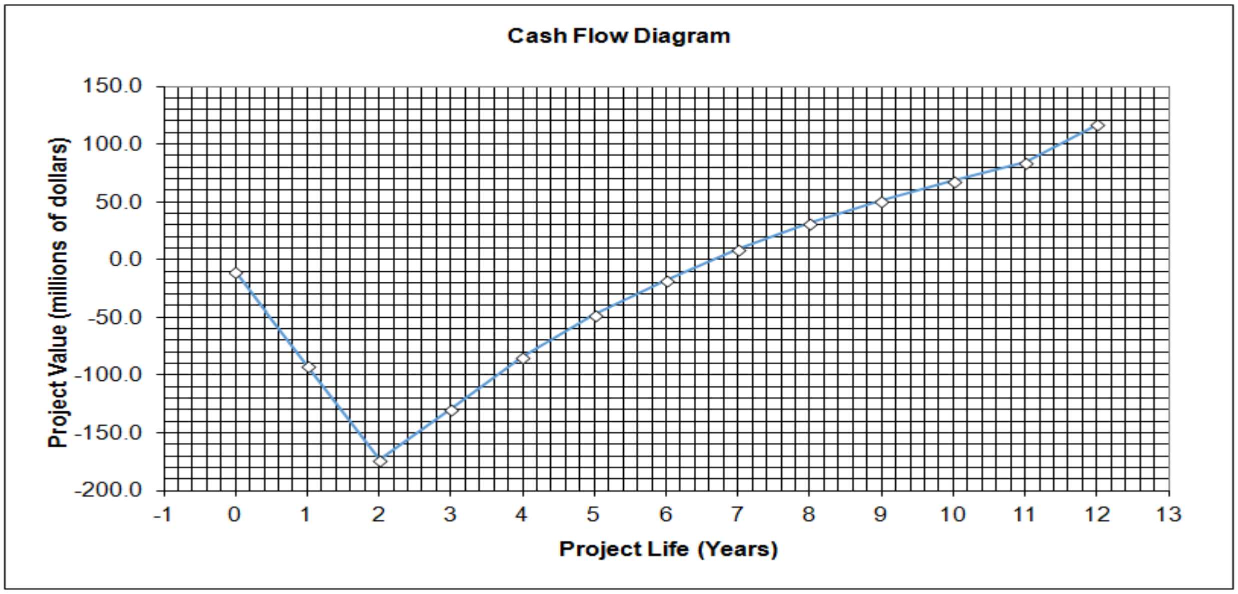


Figure 37 :Cash Flow Diagram

Discounted Profitibility Criterion

Net Present Value (millions)	117.06
Discounted Cash Flow Rate of Return	22.20%
Discounted Payback Period (years)	3.2

Non-Discounted Profitibility Criteria

Cumulative Cash Position (millions)	377.24
Rate of Return on Investment	25.15%
Payback Period (years)	2.4

Parameter over Plant Life

	Lower Limit	Upper Limit	Base Value
FCIL	-20%	30%	$ 150,000,000
Price of Product	-20%	5%	$ 406,533,029
Working Capital	0%	0%	$ 38,900,000
Income Tax Rate*	0%	0%	45%
Interest Rate*	0%	0%	10%
Raw Material Price	-10%	10%	$ 237,942,624
Salvage Value	0%	0%	$ 15,000,000

* Please note that variations for percentages are a percent of a percent.
For example, a 10% variance on a 12% interst rate would imply a 1.2% uncertainty

Figure 38 : Parameter over Plant Life

CHAPTER 7

RESULT AND DISCUION

7.1 Result and Discussion

The Claus process is design on the basis of their property method. A Peng-Robinson method is used to simulation of Claus process. The efficiency of Claus process is depending upon sulfur production. The main objective of Claus process is to removal sulfur from petroleum product because it is environmental friendly. It is good for atmosphere and human ecosystem. At the same temperature and pressure and flowrate for oxygen we get 25.57 lb mol/hr of sulfur.

Table 4: Heat and Material Balance Table

Heat and Material Balance Table		
Stream ID		16
Temperature	F	352.6
Pressure	psia	13.05
Vapor Frac		1.000
Mole Flow	lbmol/hr	61.124
Mass Flow	lb/hr	8666.386
Volume Flow	cuft/hr	40815.796
Enthalpy	MMBtu/hr	2.671
Mole Flow	lbmol/hr	
H2S		
SO2		
WATER		4.738
CO2		
CO		
O2		
H2		
N2		
NH3		
S2		30.581
S8		25.805

7.2 Effect Of Change in Length and Diameter of Furnace

Table 5 : Effect of Change in Length and Diameter of Furnace

Heat and Material Balance Table		
Stream ID		16
Temperature	F	344.1
Pressure	psia	13.05
Vapor Frac		1.000
Mole Flow	lbmol/hr	52.949
Mass Flow	lb/hr	12462.250
Volume Flow	cuft/hr	34989.165
Enthalpy	MMBtu/hr	2.112
Mole Flow	lbmol/hr	
H2S		
SO2		
WATER		4.692
CO2		
CO		
O2		
H2		
N2		
NH3		
S2		0.009
S8		48.249

7.2.1 Effect of Increasing Oxygen flow rate on Sulfur Recovery

If we increase the quantity of oxygen in air it causes increase the sulfur recovery from hydrogen sulphide gas and it's also caused decreased the formation of SO_2 gas which is not good for chemical industry and high quantity of oxygen uses in Claus process are also affect in decreased the formation of NH_3 in Claus process. Ammonia gas causes corrosion in chemical industry.

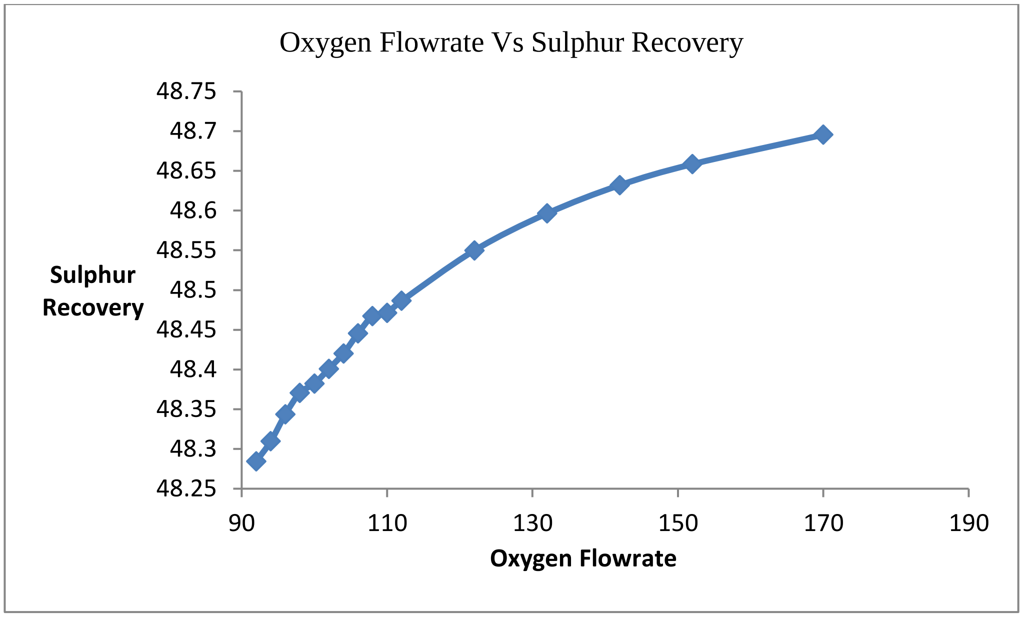


Figure 39 : Effect of Oxygen on sulfur Recovery

7.3 Effect of Change in Temperature on Sulfur Recovery

It is observed that increase the temperature of reactor it causes decreased in sulfur recovery from Sulfur recovery unit. In Claus process there are exothermic reaction take place in reactor. In exothermic reaction we used cooling medium to control the temperature otherwise it formed by product in the reactor like formation of SO_2 and NH_3 in the reaction which is not good for process.

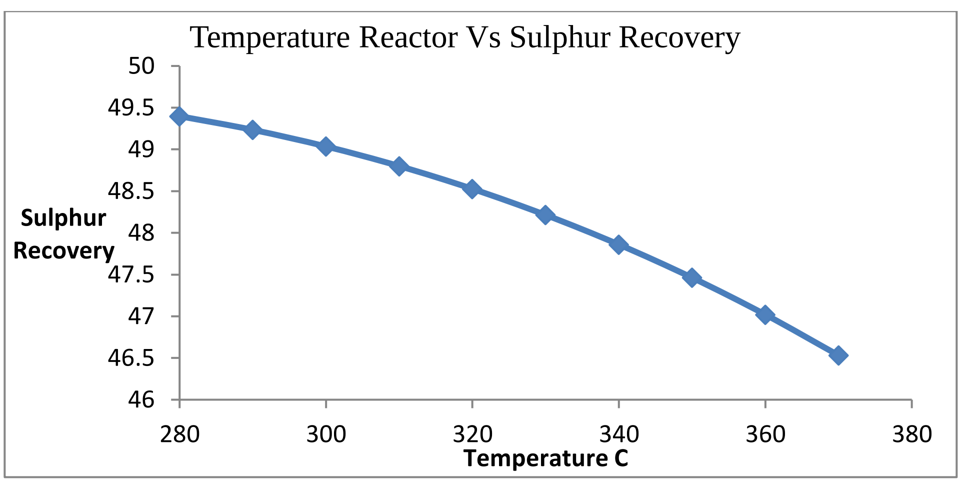


Figure 40 :Effect of change in Temperature on Sulfur Recovery

7.4 Effect of Pressure Reactor on Sulfur Recovery

It is observed that effect of pressure on the sulfur recovery unit. If we increase the operating condition like pressure of reactor it causes to increase the sulfur. The increase pressure is directly proportional to sulfur recovery but increasing pressure did not cause big effect on sulfur recovery unit. There are little bit effect of sulfur recovery on Claus process.

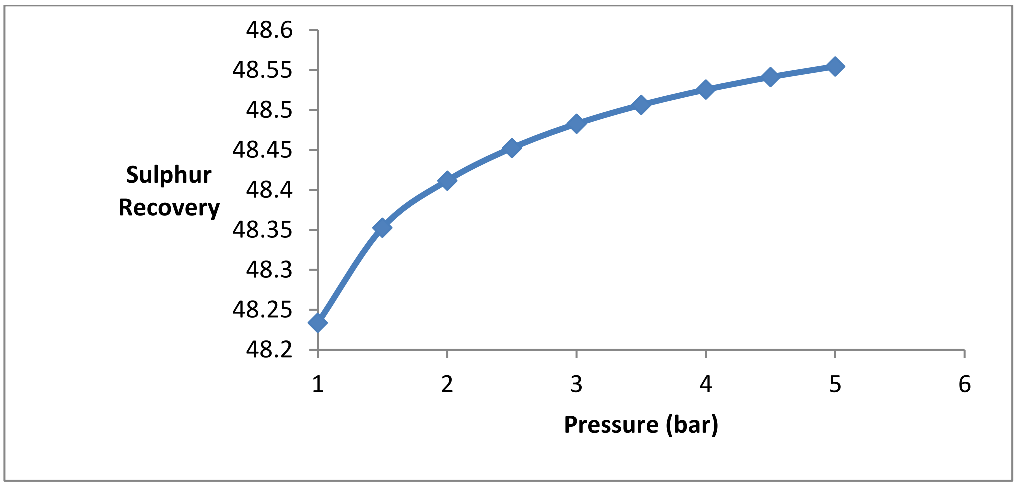


Figure 41: Effect of change in pressure on Sulfur Recovery

7.5 Sulfur Recovery vs Reactor Length

Reactor length on sulfur recovery unit. This graph shows that the length of reactor is increased from 28.3 m to 40 m. From 28.3 m to 35m the sulfur recovery increasing and after 35 m the recovery of sulfur is decreased. Its notices that there are little affect to increase length of reactor.

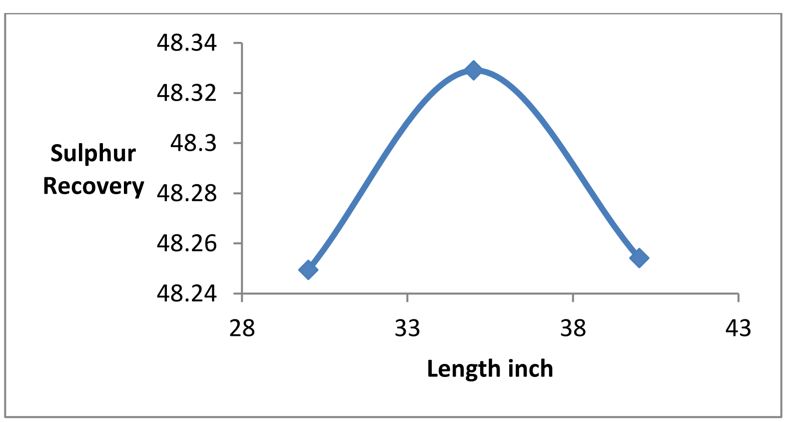


Figure 42: Effect of Length of Reactor on Sulfur Recovery

7.6 Cost Analysis Result

Discounted Profitibility Criterion

Net Present Value (millions)	143.08
Discounted Cash Flow Rate of Return	24.62%
Discounted Payback Period (years)	2.9

Non-Discounted Profitibility Criteria

Cumulative Cash Position (millions)	427.67
Rate of Return on Investment	28.51%
Payback Period (years)	2.2

Year	Investment	d_k	FCI_L-Sd_k	R	COM_d	$(R-COM_d-d_k)*(1-t)+d_k$	Cash Flow (Non-discounted)	Cash Flow (discounted)	Cumulative Cash Flow (discounted)	Cumulative Cash Flow (Non-discounted)
0	10.00		150.00				(10.00)	(10.00)	(10.00)	(10.00)
1	90.00		150.00				(90.00)	(81.82)	(91.82)	(100.00)
2	98.10		150.00				(98.10)	(81.07)	(172.89)	(198.10)
3		30.00	120.00	406.01	314.75	63.69	63.69	47.85	(125.04)	(134.41)
4		48.00	72.00	406.01	314.75	71.79	71.79	49.03	(76.00)	(62.62)
5		28.80	43.20	406.01	314.75	63.15	63.15	39.21	(36.79)	0.54
6		17.25	25.95	406.01	314.75	57.95	57.95	32.71	(4.08)	58.49
7		17.25	8.70	406.01	314.75	57.95	57.95	29.74	25.66	116.45
8		8.70	-	406.01	314.75	54.11	54.11	25.24	50.90	170.55
9			-	406.01	314.75	50.19	50.19	21.29	72.19	220.74
10			-	406.01	314.75	50.19	50.19	19.35	91.54	270.94
11			-	406.01	314.75	50.19	50.19	17.59	109.13	321.13
12			-	406.01	314.75	58.44	106.54	33.95	143.08	427.67

Figure 43 : Cost Analysis before Analysis

Discounted Profitibility Criterion

Net Present Value (millions)	117.06
Discounted Cash Flow Rate of Return	22.20%
Discounted Payback Period (years)	3.2

Non-Discounted Profitibility Criteria

Cumulative Cash Position (millions)	377.24
Rate of Return on Investment	25.15%
Payback Period (years)	2.4

Figure 44 : Cost Analysis after Analysis

CHAPTER 8

CONCLUSION & RECOMMENDATION

8.1 Conclusion

The simulation is based on Claus process .it is a sulfur recovery process in which sulfur is extracted from sour gases and exhaust gases. If sulfur is not removed from sour gases it causes SO_2, CO_2 gases. When petroleum products that contain sulfur components are burned and combusted in engine it is produce SO_2, CO_2 gases which is causes bad for environment. Now in the Claus process the sulfur components are extracted from petroleum product before it burned in engine. The presence of SO_2 in air is causes acid rain and also effect in breathing problem like asthma. We are used Aspen plus software for simulation of Claus process and the property method which is helps for simulation is Peng-Robison. The Peng-Robison method is used for hydrocarbon and vapor gases components. After the simulation of Claus process we have worked on Optimization of Claus process. There are two types of optimization first topological optimization and parametric optimization. In topological optimization there are reduction of size of equipment and reduce external utilities. The objective of topological optimization is to maximum consumption of internal utilities. Due to theses objective of topological optimization I have decided to done pinch analysis because in pinch analysis the size of equipment is less. There is maximum utilization of internal hot and cold utilities. The size of equipment is optimized. After the pinch analysis and topological optimization I have work on parametric optimization in the parametric optimization. We can change the parameter of Claus process to check the result and we can change the operating condition of Claus process to get maximum efficiency. Frist we have change the concentration and flowrate of oxygen due to change of flowrate the unreacted H_2S gas is converted into sulfur. The unreacted H_2S gas is converted into elemental sulfur and it increase the performance of Claus process. Secondly change the temperature of reactor when the temperature of reactor is changed the conversion of H_2S gas into sulfur is decreased. Due to increase in temperature the deactivation of catalyst is increased the production of by-product is increased. When the temperature of catalyst is increasing the some problems is causes with catalyst like fouling, coking and sintering. The Claus process is an exothermic reaction. The temperature of reaction is increased due to proceeds to reaction. Now we have installed cooling jacket to control the temperature of reactor. The cooling water is moving toward the jacket and temperature of reactor is maintained. The third optimization length of reactor is changing from 35.5 inch to 50 inch and the diameter of reactor is increased from 30 inch to 50 inch in this parametric optimization when the length of reactor is increasing the NH_3 production is decreasing along the length and formation of sulfur is increasing along the length. There are many research papers are worked on the NH_3 formation because due to NH_3 formation it causes corrosion and it damage the chemical equipment. To avoid from ammonia formation we increase the size of equipment and increase the length and diameter of the reactor. The fourth optimization is take place on the effect of pressure on sulfur recovery units. We are notices that there are minimum effect of sulfur recovery due to increase in pressure. These steps are not followed because increase in pressure causes great cost investment. After the simulation and optimization of Claus process the final steps is cost analysis. I have done two time of cost analysis my first cost analysis is done before optimization and second optimization is done after the cost analysis. I have used Capcost software for cost analysis of Claus process. After the two time cost analysis we have notices that profit of this process is increased and optimization of Claus process is more effective for the Claus process.

8.2 Recommendation

The Claus process is design for removal of sulfur from sour gases because these gases are causes environmental pollution and it is damage the human ecosystems. The second reason of design this process is increase the performance of engine due to sulfur components present in engine it causes knocking and produces big noise in the engine. The decomposition of NH_3 gas by increasing and decreasing the length of each equipment .NH_3 gas is causes corrosion in chemical plant. There are few modification are carried out for optimization of Claus process by increasing the capacity of Claus process. Process Intensification will be applied on Claus process to reduce the size of equipment. Increasing the effectiveness of heat exchanger network is required by using process intensification. Now in Claus process there are three reactors are used. There is so much research paper in reactor because there will be one reactor is used as compared to three reactor. The efficiency of separator is increasing by using process intensification method.

CHAPTER 9

REFERENCE

9.1 References

[1] Nopmongcol, U.; Beardsley, R.; Kumar, N.; Knipping, E.; Yarwood, G. Changes in United States deposition of nitrogen and sulfur compounds over five decades from 1970 to 2020. Atmos. Environ. 2019, 209, 144−151.

[2] Duissenov, D. Production and Processing of Sour Crude and Natural Gas-Challenges Due to Increasing Stringent Regulations; Institutt for petroleumsteknologi og anvendt geofysikk, 2013.

[3] Gupta, A. K.; Ibrahim, S.; Al Shoaibi, A. Advances in sulfur chemistry for treatment of acid gases. Prog. Energy Combust. Sci. 2016, 54, 65−92.

[4] Ibrahim, S.; Al Shoaibi, A.; Gupta, A. K. Role of toluene to acid gas (H2S and CO2) combustion in H2/O2−N2 flame under Claus condition. Appl. Energy 2015, 149, 62−68.

(5) Rahman, R. K.; Raj, A.; Ibrahim, S.; Khan M, I. I.; Al Muhairi, N. O. Reduction in natural gas consumption in sulfur recovery units through kinetic simulation using a detailed reaction mechanism. Ind. Eng. Chem. Res. 2018, 57, 1417−1428.

[6] Weiland, S.; Hatcher, N.; Jones, C.; Weiland, R., Ammonia destruction in the reaction furnace; Optimized Gas Treating Inc. www.digitalrefining.com/article/1001297, 2016.

[7] Al Hamadi, M.; Ibrahim, S.; Raj, A. Effects of Oxygen Enrichment on Natural Gas Consumption and Emissions of Toxic Gases (CO, Aromatics, and SO2) in the Claus Process. Ind. Eng. Chem. Res. 2019, 58, 16489−16501.

[8] Li, D.; Dowling, N.; Marriott, R.; Clark, P. Kinetics and Mechanisms for Destruction of Ammonia in the Claus Furnace; Alberta Sulphur Research Ltd. Chalk Talk: Calgary AB, Canada, 2016.

[9] Ibrahim, S.; Rahman, R. K.; Raj, A. Effects of H2O in the Feed of Sulfur Recovery Unit on Sulfur Production and Aromatics Emission from Claus Furnace. Ind. Eng. Chem. Res. 2017, 56, 11713−11725.

[10] Clark, P.; Dowling, N.; Huang, M. Ammonia Destruction in the Claus Furnace. Proceedings of the Brimstone 1998 Sulphur Recovery Symposium, 1998; Vol. 1998, pp 15−18.

[11] Monnery, W. D.; Hawboldt, K. A.; Pollock, A. E.; Svrcek, W. Y. Ammonia pyrolysis and oxidation in the Claus furnace. Ind. Eng. Chem. Res. 2001, 40, 144−151.

[12] Otomo, J.; Koshi, M.; Mitsumori, T.; Iwasaki, H.; Yamada, K. Chemical kinetic modeling of ammonia oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion. Int. J. Hydrogen Energy 2018, 43, 3004−3014.

[13] He, X.; Shu, B.; Nascimento, D.; Moshammer, K.; Costa, M.; Fernandes, R. X. Auto-ignition kinetics of ammonia and ammonia/ hydrogen mixtures at intermediate temperatures and high pressures. Combust. Flame 2019, 206, 189−200.

[14] Okafor, E. C.; Naito, Y.; Colson, S.; Ichikawa, A.; Kudo, T.; Hayakawa, A.; Kobayashi, H. Measurement and modelling of the laminar burning velocity of methane-ammonia-air flames at high pressures using a reduced reaction mechanism. Combust. Flame 2019, 204, 162−175.

[15] MacLean, D.; Wagner, H. G. The structure of the reaction zones of ammonia-oxygen and hydrazine-decomposition flames. Symposium (International) on Combustion; Elsevier, 1967; Vol. 1967, pp 871−878.

[16] Manna, M. V.; Sabia, P.; Ragucci, R.; de Joannon, M. Oxidation and pyrolysis of ammonia mixtures in model reactors. Fuel 2020, 264, 116768.

[17] Vandooren, J. Comparison of the experimental structure of an ammonia seeded rich-hydrogen-oxygen-argon flame with the calculated ones along several reaction mechanisms. Combust. Sci. Technol. 1992, 84, 335−344.

[18] Mendiara, T.; Glarborg, P. Ammonia chemistry in oxy-fuel combustion of methane. Combust. Flame 2009, 156, 1937−1949.

[19] Dagaut, P.; Lecomte, F.; Mieritz, J.; Glarborg, P. Experimental and kinetic modeling study of the effect of NO and SO2 on the oxidation of CO· H2 mixtures. Int. J. Chem. Kinet. 2003, 35, 564−575.

[20] Glarborg, P.; Kubel, D.; Dam-Johansen, K.; Chiang, H.-M.; Bozzelli, J. W. Impact of SO2 and NO on CO oxidation under postflame conditions. Int. J. Chem. Kinet. 1996, 28, 773−790.

[21] Nabikandi, N. J.; Fatemi, S. Kinetic modelling of a commercial sulfur recovery unit based on Claus straight through process: Comparison with equilibrium model. J. Ind. Eng. Chem. 2015, 30, 50−63.

[22] ZareNezhad, B.; Hosseinpour, N. Evaluation of different alternatives for increasing the reaction furnace temperature of Claus SRU by chemical equilibrium calculations. Appl. Therm. Eng. 2008, 28, 738−744.

[23] Zarei, S.; Ganji, H.; Sadi, M.; Rashidzadeh, M. Kinetic modeling and optimization of Claus reaction furnace. J. Nat. Gas Sci. Eng. 2016, 31, 747−757.

[24] Rahman, R. K.; Ibrahim, S.; Raj, A. Oxidative destruction of monocyclic and polycyclic aromatic hydrocarbon (PAH) contaminants in sulfur recovery units. Chem. Eng. Sci. 2016, 155, 348−365.

[25] Ibrahim, S.; Rahman, R. K.; Raj, A. Roles of hydrogen sulfide concentration and fuel gas injection on aromatics emission from Claus furnace. Chem. Eng. Sci. 2017, 172, 513−527.

[26] Abdoli, P.; Hosseini, S. A.; Mujeebu, M. A. Effect of Preheating Inlet Air and Acid Gas on the Performance of Sulfur Recovery Unit□ CFD Simulation and Validation. Forsch. Im. Ingenieurwes. 2019, 83, 81− 89.

[27] Kazempour, H.; Pourfayaz, F.; Mehrpooya, M. Modeling and multi-optimization of thermal section of Claus process based on kinetic model. J. Nat. Gas Sci. Eng. 2017, 38, 235−244.

[28] Abdoli, P.; Hosseini, S. A.; Mujeebu, M. A. Influence of O2 enrichment in dry air on combustion temperature, contaminant production and sulfur recovery, in SRU reaction furnace. Forsch. Im. Ingenieurwes. 2018, 82, 99−106.

[29] Selim, H.; Gupta, A. K.; Sassi, M. Novel error propagation approach for reducing H2S/O2 reaction mechanism. Appl. Energy 2012, 93, 116−124.

[30] Zhou, C.; Sendt, K.; Haynes, B. S. Experimental and kinetic modelling study of H2S oxidation. Proc. Combust. Inst. 2013, 34, 625− 632.

[31] Mohammed, S.; Raj, A.; Shoaibi, A. A. Effects of fuel gas addition to Claus furnace on the formation of soot precursors. Combust. Flame 2016, 168, 240−254.

[32] Rahman, R. K.; Raj, A. A reaction kinetics study and model development to predict the formation and destruction of organosulfur species (carbonyl sulfide and mercaptans) in Claus furnace. Int. J. Chem. Kinet. 2018, 50, 880−896.

[33] Bassani, A.; Pirola, C.; Maggio, E.; Pettinau, A.; Frau, C.; Bozzano, G.; Pierucci, S.; Ranzi, E.; Manenti, F. Acid Gas to Syngas (AG2STM) technology applied to solid fuel gasification: Cutting H2S and CO2 emissions by improving syngas production. Appl. Energy 2016, 184, 1284−1291.

[34] Ibrahim, S.; Raj, A. Kinetic Simulation of Acid Gas (H2S and CO2) Destruction for Simultaneous Syngas and Sulfur Recovery. Ind. Eng. Chem. Res. 2016, 55, 6743−6752.

[35] Bongartz, D.; Ghoniem, A. F. Chemical kinetics mechanism for oxy-fuel combustion of mixtures of hydrogen sulfide and methane. Combust. Flame 2015, 162, 544−553.

[36] Starik, A. M.; Savelieva, V. A.; Sharipov, A. S.; Titova, N. S. Enhancement of hydrogen sulfide oxidation via excitation of oxygen molecules to the singlet delta state. Combust. Flame 2016, 170, 124− 134.

[37] Savelieva, V. A.; Starik, A. M.; Titova, N. S.; Favorskii, O. N. Numerical Analysis of Hydrogen Sulphide Conversion to Hydrogen during Its Pyrolysis and Partial Oxidation. Combust. Explos. Shock Waves 2018, 54, 136−146.