DESIGN AND DEVELOPMENT OF A PROCESS FOR DESULFURIZATION OF COAL



By

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School of Chemical and Materials Engineering National University of Sciences and Technology June 2023

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CERTIFICATE

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DEDICATION

This Work is dedicated to our Parents and Teachers, who always had our back when we needed them the most.

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We would like to express our deepest gratitude to Allah, the Generous and Almighty, for His countless blessings and rewards, which granted us the strength and ability to complete this thesis. We are grateful to our parents for their unconditional love and support, which has always been our guiding light. They have always been there for us, through thick and thin, and we know that we can always count on them. We are also grateful to our supervisor, Dr. Tayyaba Noor, for her guidance and mentorship, and for always believing in us. She has been a constant source of support and encouragement, and we are so grateful for her guidance.

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Authors

ABSTRACT

Having so many large reserves of coal, Pakistan is facing an energy crisis because coal is not being utilized. The primary purpose is that in coal incineration in electricity plant life, high sulfur content material of coal poses serious environmental problems due to sulfur dioxide emission. It causes acid rain which has dangerous outcomes on lakes and flora and causes corrosion. Basically, we've three coals, one is regional, 2nd is Baluchistan and third is Choa Saidan shah coal.

Bestway uses Baluchistan coal as a fuel for electricity source. This coal contains total moisture (M) is 9.52%, volatile moisture (VM) is 34.21%, ash is 22.21%, and Sulphur is four%. To conquer this, we will appoint extraordinary techniques for coal desulfurization. So, Baluchistan coal (Lignite) earlier than usage may be subjected to 3 physical, chemical, and organic desulfurization strategies. But physical and organic strategies are useless, time eating, and they can be applied pleasantly at the bench scale. Maximum of the effective lignite desulfurization strategies is based on chemical strategies. possible techniques for sulfur dioxide removal from coals may be divided into critical classes: elimination of sulfur dioxide during combustion and removal of sulfur dioxide from flue gases after combustion. One question arises at that moment, why can we need to take away sulfur before combustion as opposed to during and after combustion. The need for sulfur elimination is to promote coal to clients whether they've hooked up pollutants or no longer, to lessen transportation and combustion cost, and to lessen load on flue fuel scrubber. So, leaching is one of the most commonplace techniques employed for coal desulfurization.

Alkali leaching is an effective technique for demineralization of coal with the aid of reducing most of the mineral-rich constituents. It can be due to the synergistic impact of alkali reagents, which have excessive affinity towards coal minerals and the capability to penetrate the interior of the coal matrix. At some stage in alkali leaching, alkali reacts with the silica, alumina, and clay-bearing minerals within the coal and response product transformed into hydrated alkali-bearing silicate, aluminate, and aluminosilicate complexes (sodalite). It was discovered that the consequences of the leaching temperature, agitation time and particle length on the removal of different varieties of sulfur are very extensive. Sulfur restoration will increase with agitation time and temperature. With the help of the chemical leaching procedure, we can cast off 50–60% Sulphur and 80% ash, respectively.

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LIST OF SYMBOLS

 Δ H: Change in enthalpy A: Area C: Cost ^oC: Degree centigrade C: constant in USD Ce: purchased equipment cost in USD D: Diameter F: Flow Rate g: Acceleration due to gravity H: Height J: Joule L: *h* Mol: Mole n: index P: Pressure Q: Energy Flow rate t: time S: size unit V: Volume W: *h* Cp: Specific Heat Capacity at Constant Pressure T: Temperature V: e

K: Thermal Conductivity h: Thermal Conductivity

CHAPTER 1

INTRODUCTION

1.1 Overview

Our beloved country Pakistan is blessed with numerous coal reserves. Pakistan's largest coal reserves are found in Sindh, measuring approximately 175 billion tons. Tharparkar division of Sindh is said to host huge deposits. Pakistan holds 3,377 million tons (MMst) of proven coal reserves as of 2016, ranking 20th in the world and accounting for about 0% of the world's total coal reserves of 1,139,471 million tons (MMst).

Despite all these numerous reserves, we have continued to face some serious energy crisis over the past few decades. This is happening due to underutilization of this coal because of environmental concerns. Environmental concerns are raised due to the presence of toxic Sulphur compounds in coal. Sulphur on combustion produces SO2 gas, which is highly toxic for the environment. So far, the post-treatment of effluent SO2 gas has been made possible to counter these environmental concerns. But even this idea is just like "Putting dust under the carpet" because toxic fumes of burnt Sulphur still contaminate the process and the equipment. So, it's necessary to do pre-treatment. i.e., Desulphurization of coal, to make it useful for combustion as well as harmless to the process, industrial equipment, and the environment.

The desulfurization of coal is a crucial aspect of sustainable energy production, aiming to mitigate the environmental impact of sulfur emissions during coal combustion. In collaboration with Bestway Cement Industry, our group project focuses on the design and development of an innovative process for coal desulfurization using the chemical leaching method. This project seeks to address the pressing need for cleaner and more efficient coal utilization, contributing to environmental protection and regulatory compliance in the energy sector.

1.2 Discussion Background

Coal, as a vital energy resource, plays a significant role in global power generation, industrial processes, and heating applications. However, the high sulfur content in coal presents a major challenge due to the formation of sulfur dioxide (SO2) during combustion. The release of SO2 into the atmosphere contributes to air pollution, acid rain formation, and detrimental effects on ecosystems and human health. To combat these issues, it is crucial to develop effective desulfurization processes to reduce sulfur emissions from coal combustion.

The "Chemical Leaching" process offers a promising solution for coal desulfurization. This method involves the use of leaching agents that selectively react with sulfur compounds in coal, resulting in their removal.

Chemical leaching offers several advantages, including high desulfurization efficiency, flexibility in process design, and adaptability to various coal types and sulfur concentrations. By implementing an efficient and environmentally friendly desulfurization process, we can enhance the sustainability of coal utilization and meet stringent emission regulations.

1.3 Methodology

Our project will employ a comprehensive approach, encompassing literature review, laboratory-scale experiments, and process optimization. Through an in-depth review of existing research and case studies, we will identify suitable leaching agents, their concentrations, and optimal process conditions for efficient sulfur removal. The laboratory experiments will utilize coal samples provided by Bestway Cement Industry, enabling us to determine the ideal leaching agent, concentration, temperature, and contact time to achieve maximum desulfurization while minimizing any adverse effects on coal quality.

The obtained experimental data will be meticulously analyzed to establish the optimal process conditions and guide the design of a pilot-scale chemical leaching unit. The pilot-scale implementation will further validate the effectiveness and feasibility of the developed desulfurization process, paving the way for potential industrial-scale application in coal-based energy production.

1.4 Conclusion

In conclusion, our group project on the design and development of a chemical leaching process for coal desulfurization represents a significant step towards sustainable and environmentally conscious coal utilization. Through collaboration with Bestway Cement Industry, we aim to contribute to cleaner energy production, reduced sulfur emissions, and regulatory compliance. The successful implementation of this project holds the potential to revolutionize coal desulfurization technologies, not only benefiting the cement industry but also having broader implications for various coal-dependent sectors.

CHAPTER 2

LITERATURE REVIEW

Coal is one of the most utilized fossil fuels for energy production across the globe leading to higher amount of emission of sulfur dioxide (SO2) in the atmosphere. Combustion of coal containing higher contents of sulfur is a major factor responsible for acid rain and associated environmental degradation. The currently used physicochemical approaches for removal of sulfur from coal are expensive, toxic in nature, and inappropriate for different types of coal.

Almost all coal utilization systems depend heavily on sulfur, which is present in significant amounts in inorganic elements of coal. To separate coal's inorganic components from its organic components, various techniques have been used. Prior to use, coal is desulfurized using various physical, chemical, and biological processes. Physical and biological techniques, on the other hand, are inefficient, time-consuming, and limited to bench-scale use. Most efficient coal desulfurization systems rely on chemical processes. Chemical desulfurization, leaching, extraction, flotation, Ox desulfurization, and Bio desulfurization are the primary desulfurization techniques. Pyritic sulfur, which is less prevalent than organic sulfur in coal, is easier to remove with alkaline desulfurization. Some of the sulfur removal techniques are mentioned below along with their pros and cons:

2.1 Hydrodesulfurization

An important procedure in petroleum refining operations today is called hydrodesulfurization (HDS), which adds hydrogen to eliminate undesirable sulfur compounds. In terms of the environment, HDS is an extremely significant process. To do this successfully, we looked at a Y-type zeolite catalyst that was Ni-Pd co-loaded and had outstanding hydrocracking activity for aromatic compounds. The sulfur level of diesel fuels should go below 0.005 weight percent in the near future. It is, however, quite challenging to achieve while still meeting the needs of its economy.

The HDS process involves catalytic treatment with hydrogen to convert the various sulfur compounds present to hydrogen sulfide. The hydrogen sulfide is then separated and converted to elemental sulfur by the Claus process. From this point some of the hydrogen sulfide is oxidized to sulfur dioxide by air and sulfur is formed by the overall reaction:

 $2H_2S + SO_2 \rightarrow 3S(s) + 2H_2O$

The HDS represents a crucial component of current petroleum refining operations in terms of both environmental and economic considerations. We can guess the success of this method from the fact that soon, the content of sulfur in diesel fuels should be lower than 0.005 wt%, but of course at the cost of some economical expenses now. Moreover, hydrodesulfurization is applicable on an industrial scale only for fluid fuels, preferably gases. This is because it becomes difficult to develop an economical continuous process of solid phase at commercial scale. That's why this method, despite its extreme efficiency, cannot be applied for the desulphurization of coal.

2.2 Bio desulfurization

A well-known laboratory process called "Biological Desulfurization," or "Bio desulfurization," uses bacterial cultures (thermophilic or mesophilic bacteria) to oxidize pyrite and so remove sulfur from coals.

The application of microbial resources for removal of sulfur from coal is an ecofriendly technique and could be successfully employed at industrial scale after laboratory scale process optimization. The process of sulfur removal by microbes is carried out by enzymes and is considerably influenced by different factors, including pH, temperature, nutrient composition, shaking or standing condition, coal types, and most importantly type of microorganisms used. Different bacteria and fungi isolated from coal contaminated sites as well as noncontaminated sites exhibiting sulfur removal potential can be used as next generation tool for the development of clean coal technology. Furthermore, through the application of modern genetic manipulation techniques, enhanced expression of genes responsible for desulfurization can be performed to accelerate the process of sulfur removal from coal.

2.3 Froath Flotation Method

Froath flotation is the separation of minerals that vary little in density but differ greatly in wettability by surface active agents i.e., surfactants that stabilize the foam that forms on the surface of a stirred suspension of minerals in water. Mineral processing uses the ore flotation method to separate and concentrate ore by rendering the surface of the ore hydrophobic or hydrophilic. The surface either repels or attracts water. Most minerals need to be coated with a water repellent to keep them floating. When minerals are coated with a small amount of chemicals or oils, finely ground mineral particles remain dry and stick to air bubbles. Agitation coats the mineral particles to create a paste of ore, water, and appropriate chemicals. The latter binds to the surface of mineral particles, making them hydrophobic. Non-wet particles adhere to the air bubbles and are carried to the upper surface of the pulp where they enter the foam and the foam containing these particles is removed. Foam flotation is the separation of minerals that vary little in density but differ greatly in wettability by surfactants that stabilize the foam that forms on the surface of a stirred suspension of minerals in water.

The froath flotation method is a mineral processing method that separates valuable minerals from gangue minerals by utilizing the difference in surface physicochemical properties of valuable minerals and vein minerals. Ore flotation is characterized by the contact of three phases: suspended mineral particles, aqueous electrolyte solution, and gas. In foam flotation, crushed ore is stirred in water and various chemical reagents are added to attach selected minerals to the air bubbles. The foam or floating fraction is commonly referred to as the concentrate.

Most of the sulfur in lignite is commonly present as pyritic sulfur and varies in size and form. Conventional coal refining mineral processing techniques such as gravity separation can be applied to coarse particles. To release the finely distributed pyritic sulfur in coal, it must be finely ground. Conventional foam flotation is applied to lignite for three purposes:

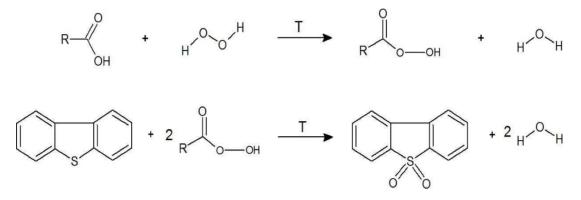
- 1. Recovery of coal in sludge to obtain a low sulfur and ash product.
- 2. Mitigation of pollution by purifying process water, called black water, removed from coal industries.
- 3. Manufactures coal for cooking by separating the macerals from the coal.

The natural floatability of coal depends on the mineral content or ash content of the coal. That is the rank of coal. All coal oxidizes when exposed to air. This effect is likely due to surface oxidation that readily occurs under normal atmospheric conditions. This is characterized by the formation of acid groups on the coal surface, leading to a decrease in the hydrophobicity of the coal. With less carbide, it oxidizes easily and loses most of its floatability. Gangue flotation was preferred over coal flotation in such cases.

2.4 Chemical Desulphurization Methods

Oxidation by Performic Acid

Performic acid is a very strong oxidizing reagent that oxidizes sulfur-containing amino acids. It is a colorless liquid, soluble in organic solvents such as water, alcohol, ether, benzene, and chloroform. Its strong oxidizing properties are used to break disulfide bonds in oxidation reactions.



Performic Acid, an organic acid, has the potential of oxidation of the organic matrix of coal at low temperatures. Research on performic acid oxidation, using both mineral matter of coal and some commercial minerals, showed that clay minerals and silicates are almost inert to performic acid oxidation. However, carbonates and sulfur minerals are not resistant to performic acid, even at low temperatures. So, desulphurization of coal can be achieved by performic acid oxidation.

2.5 Chemical Leaching Process

Alkaline Desulfurization is more effective in removing the pyritic sulfur from the coal, which is the less abundant form than organic sulfur. Total sulfur contents are considerably reduced by aqueous NaOH treatment. This process involves the reaction of crushed coal slurry with aqueous NaOH and nitric acid (HNO₃) at elevated temperatures of 200°C to 300°C and atmospheric pressure conditions.

 $30NaOH + 8FeS_2 \rightarrow 4Fe_2O_3 + 14Na_2S_2O_3 + 15H_2O$ $NaOH + CH_3 - SH \rightarrow CH_3 - SNa + H_2O$ $FeS_2 + 2HNO_3 \rightarrow Fe NO_{3 2} + H_2S + S$

Both NaOH and HNO₃ are used in equivalent proportions alternatively for chemical leaching, to keep neutral pH of the overall product.

Although Physical sulfur removal techniques are the most practical ones so far, these methods are ineffective, time consuming and they can be applied only on the bench scale. Their effectiveness isn't enough to remove sulfur from coal up to an environmentally friendly level. Chemical methods of Sulphur removal are very effective, efficient and can remove enough sulfur. That's why we have considered "Chemical Leaching Process", which is a chemical technique.

We want to separate inorganic and pyritic sulphuric parts of coal from organic part. To obtain as much as possible, the pure combustible organic portion (without Sulphur compounds) with max carbon chains.

Most of the research work on coal desulfurization has been focused on pyritic sulfur removal, which represents in most cases at least half of the total sulfur content in coal, since organic sulfur is more difficult to remove by conventional processes.

CHAPTER 3

PROCESS DESCRIPTION

3.1 Description

Alkali leaching is an effective method for demineralization of coal by reducing most of the mineral-rich constituents. It may be due to the synergistic effect of alkali reagents, which have high affinity towards coal minerals and the ability to penetrate the interior of the coal matrix. During alkali leaching, alkali reacts with the silica, alumina, and clay-bearing minerals in the coal and reaction product converted into hydrated alkali-bearing silicate, aluminate, and aluminosilicate complexes (sodalite). It was found that the effects of the leaching temperature, agitation time and particle size on the removal of different forms of sulfur are very significant. Sulfur recovery increases with agitation time and temperature.

3.2 Chemical Equation

 $\begin{array}{l} 30NNNN + 8NNN_2 \rightarrow 4NN_2 N_3 + 14NN_2 N_2 N_3 + 15N_2 O \\ NNNN + NN_3 - NN \rightarrow NN_3 - SNa + N_2 O \\ 2NaOH + NNN_2 \rightarrow NN_2NNN_3 + N_2N \\ 2NNNN + NN_2 N_3 \rightarrow 2NaAlN_3 + N_2 O \\ NNN_2 + 2NNN_3 \rightarrow NN (NN_3) _2 + N_2N + N \end{array}$

3.3 Process Flow Diagram

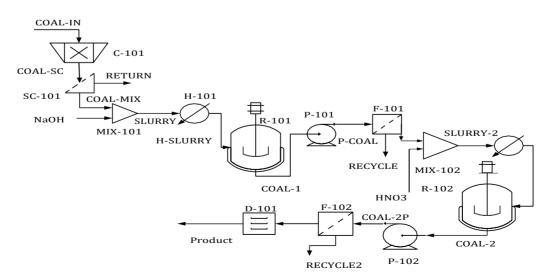


Figure 3-1 Design and Development of a process for Desulphurization of coal

CHAPTER 4

MATERIAL BALANCE

The material balance was carried out by applying the law of conservation of mass to each of the important components present within the proposed design.

Material balance is a quantitative description of the mass conservation of a system. The principle of mass balance states that the mass at the input to the system must equal the mass at the output plus the mass of accumulation in the system since mass cannot be created or destroyed.

4.1 Significance of Material Balance

Material balance is important because it provides a way to track the flow of materials in your system. This information can be used for:

- Identify waste sources
- Optimize process efficiency
- Ensuring product safety

For example, chemical plants can use material balances to track the flow of raw materials, intermediate products, and finished products. This information can be used to identify sources of waste such as leaks and spills. It can also be used to optimize plant efficiency by ensuring that the right amount of each raw material is used to produce the required amount of product. Finally, it can be used to ensure product safety by ensuring that all relevant safety standards are met. Material balance is a powerful tool that can be used to improve the efficiency, safety, and environmental impact of any system.

4.2 Sieve Shaker

To use the sieve shaker to separate coal, the following steps are typically taken:

• The coal sample is placed on the top sieve.

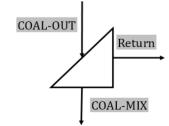


Figure 4-1 Sieve Shaker

- The platform is then shaken or vibrated.
- The sieve shaker is run for a predetermined amount of time.
- The sieves are then removed and the particles that are retained on each sieve are weighed.

The weights of the particles on each sieve can then be used to calculate the percentage of the coal sample that is in each size fraction.

Table 4-1 Sieve Shaker Material Balance

		IN	OUT	
	Units	COAL-OUT	Return	COAL-MIX
Mass-flow	kg/h	6653	1330.8	5322.2

4.3 Mixer

The mixture undergoes full processing and agitation within the mixer. Agitation facilitates the dissolution, dispersion, or suspension of coal particles in the solvent. The breakdown of coal particles occurs due to intense agitation. The result is a

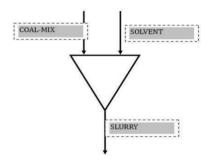


Figure 4-2 Mixer

homogeneous slurry, with coal particles finely dispersed or dissolved in the solvent.

		IN		OUT
Mass-flow	Units	COAL-MIX	SOLVENT	SLURRY
COAL	kg/h	5322.2	0	5322.2
NaOH	kg/h	0	958	958
Water	kg/h	0	15008.6	15008.6
Total	kg/h	5322.2	15967	21289.2

4.4 Alkali Leaching Reactor

The dissolution of metal oxides into an alkaline solution is a common reaction to be encountered during the alkylating process. We consider the reaction between a metal oxide, such as Fe2O3 (iron(III) oxide), and an alkaline leaching agent, typically sodium hydroxide (NaOH), in the presence of water (H2O).

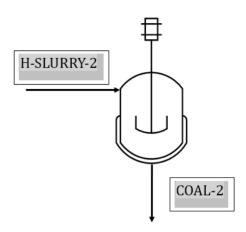


Figure 4-3 Alkali Leaching Reactor

Reactions:

 $\begin{aligned} 30NaOH + 8FeS2 &\rightarrow 4Fe2O3 + 14Na_2 S_2O_3 + 15H_2O \\ 2NaOH + CH3 - SH &\rightarrow CH_3 - SNa + H_2O \\ 2NaOH + SiO2 &\rightarrow Na2SiO3 + H2O \\ 2NaOH + Al2O3 &\rightarrow 2NaAlO_3 + H_2O \end{aligned}$

	Units	IN	OUT
COAL	Kg/h	5322.2	4284.38
NaOH	Kg/h	958	95.8
Water	Kg/h	15009	15242.5
Na2SiO3	Kg/h	0	1095.08
NaAlO2	Kg/h	0	349.71

Table 4-3 Alkali Leaching Reactor Material

NaOH	Kg/h	958	95.8
Water	Kg/h	15009	15242.5
Na2SiO3	Kg/h	0	1095.08
NaAlO2	Kg/h	0	349.71
Fe2O3	Kg/h	0	34.423
Na2S2O3	Kg/h	0	119.291
CH3-SNa	Kg/h	0	75.7223
Sulfur-Removed	%	40	
Ash-Removed	%	80	

4.5 Acidic Leaching Reactor

Table 4-4 Acidic Leaching Reactor Material Balance
--

	Units	IN	OUT
COAL	kg/h	4472.35	4407.15
Water	kg/h	75.33	75.33
HNO3	kg/h	75.33	7.533
Fe(NO3)2	kg/h	0	94.43
H2S	kg/h	0	17.85
S	kg/h	0	16.8
Sulfur-Removed	%	60	
Ash-Removed	%	80	

4.6 Overall Material Balance

Components	Mass Flow	In		(Dut	
Crusher Block	kg/h	429581		42	9581	
Sieve Shaker	kg/h	6653		5322.2	1330.8	
Mixer-1	kg/h	5322.2 15966.6		21288.8		
Alkali Reactor	kg/h	21288.8		21297		
Pump-1	kg/h	21297		21	1297	
Filter Press-1	kg/h	21297		4472.45	16824.55	
Pump-2	kg/h	4472.45		4472.45 4472.45		72.45
Mixer-2	kg/h	4472.45 150.66		4623.01		
Pump-3	kg/h	4623.01		4623.01		
Acidic Reactor	kg/h	4623.01		4619.093		
Pump-4	kg/h	4619.093		461	19.093	
Filter Press-2	kg/h	4619.093		4423.95	195.143	

Table 4-5 Overall Material Balance

CHAPTER 5

ENERGY BALANCE

An energy balance is an instrument that tracks the progression of energy into, though, and out of a framework. With regards to industry, an energy equilibrium can be utilized to follow the progression of energy from the mark of energy creation to the place of energy utilization. This data can be utilized to distinguish regions where energy is being squandered, and to foster techniques for further developing energy proficiency.

5.1 Significance of energy balance in industry

There are a few justifications for why energy balance is significant in industry. To start with, energy is an important asset that ought to be utilized effectively. Second, energy productivity can prompt expense reserve funds for organizations. Third, energy proficiency can assist with diminishing ozone harming substance outflows and further develop air quality.

There are many advantages to further developing energy productivity in industry. Probably the most well-known benefits include:

- Cost investment funds
- Expanded efficiency
- Worked on natural execution

5.2 Crusher

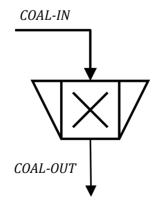


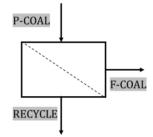
Figure 5-1 Crusher

	Units	Values
Wi	kwh/t	13
D _{pb}	mm	0.149
D _{pa}	mm	5
М	ton/h	6.653
Duty	KW	58.62

Table 5-1 Crusher Energy Balance

5.3 Filter Press

The basic relationship used for particle size reduction and grinding operations is the equation = 0.3162 * Wi * Dpb * Dpa * m. It will calculate the special energy needed to process comminution. The equation can be explained in a simplified way



$$\frac{P}{m} = 0.3162 * Wi * \left(\frac{1}{\sqrt{Dpb}} - \frac{1}{\sqrt{Dpa}}\right)$$

Figure 5-2 Filter Press

 W_i = Work index D_{pb} = Product particle size D_{pa} = Reactant particle size

m = mass flowrate

		IN	OUT	
	Units	P-COAL	F-COAL	RECYCLE
Coal	kg/h	4472.37	4472.37	0
Solvent	kg/h	16824.63	0	16824.63
Total		21297	21297	I

Table 5-2 Filter Press Energy Balance

5.4 Heater

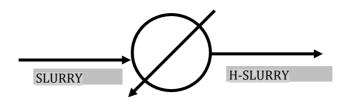


Figure 5-3 Heater

Table 5-3 Heater Energy Balance

	Units	IN	OUT
Temperature	С	25	250
Mass-Enthalpy	kJ/kg	-1216.54	-1003.59
Mass-flowrate	kg/h	21289.2	21289.2
Duty	kW	1259.35	

5.5 Alkali Leaching Reactor

The needed quantity for the substance or solution is defined as the volume to be used. It's the same as 16657 liters. This is the amount that you're aiming for at the end of this process. 2% allowance: This is a percentage increase, or an amount added to the overall volume required. It is a 2% increase on the volume of this case. In the case of any losses, errors, or compensations in each process, they will typically be included.

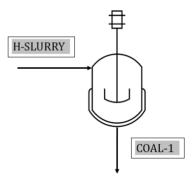


Figure 5-4 Alkali Leaching

Equations

By using these equations and available data, we find out the parameter of energy for leaching reactor:

Energy Flow =
$$-F_{A0} \cdot C_{PA} (T - T_0) + (H_B(T) - H_A(T)) \cdot r_A V + Q$$

 $H_A (T) = H_A (T_0) + C_{PA} (T - T_0)$
 $H_B (T) = H_B (T_0) + C_{PB} (T - T_0)$
 $\Delta H_r(T) = (H_B(T) - H_A(T)) \cdot r_A \cdot V$
(Where, $A = FeS_2 \otimes B = H_2S$)

Available Data

By using; $V = T \ge V_0 \& T = 60 \min \text{ or } 1 \text{ hr}$

Total Volume Needed = 16657 lit

By Providing 2% Allowance

Volume of Reactor = V = 17000 lit

	Units	FeS ₂	$Na_2S_2O_3$	
Molar Flow (F _{A0})	mol/h	0.431	0.7545	
%Conv (X _A)	%	60%	-	
Rate of Rxn (-r _A)	mol/lit.h	-1.52x10 ⁻⁵	+1.52x10 ⁻⁵	
Std. Enthalpy of form (H(T ₀))	kJ/mol	-95.06	-1117	
Specific Heat (C _P)	kJ/kg.K	0.61	0.59	
Enthalpy of form (H(T))	kJ/mol	42.19	-984.45	
Heat of Rxn (ΔH_{rxn} (T))	kJ/mol	-100604.93	-130178.6645	
-F _{A0} . C _{PA} (T – T ₀)	kJ.mol/kg.h	-59.15		
Heat Flow (Q)	kJ/h	-1168813.48		
Total Energy Flow	MJ or mega-watt-days	-1269.5 or -8.472		

Table 5-4 Alkali Leaching	Reactor Energy Balance
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5.6 Pump

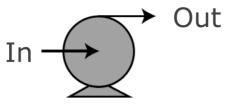


Figure 5-5 Pump Material Balance

		IN	OUT
Temperature	С	250	250
Pressure	kPa	100	1500
Density	kg/m ³	1000	1000
Mass Flow Rate	kg/h	21297	21297
Duty	kW	1.94	

5.7 Acidic Leaching Reactor

	Units	FeS ₂	H ₂ S	
Molar Flow (F _{A0})	mol/h	0.431	0.5235	
%Conv (X _A)	%	60%	-	
Rate of Reaction (-r _A)	mol/lit.h	-1.52x10 ⁻⁵	+1.52x10 ⁻⁵	
Std. Enthalpy of form (H(T ₀))	kJ/mol	-95.06	-20.15	
Specific Heat (C _P)	kJ/kg.K	0.61	1.012	
Enthalpy of form (H _T)	kJ/mol	42.19	207.55	
Heat of Reaction ($\Delta H_{Reaction}$)	kJ/mol	-100604.93	196.64	
-F _{A0} . C _{PA} (T - T ₀)	kJ.mol/kg.h	-59.15		
Heat Flow (Q)	kJ/h	-1168813.48		
Total Energy Flow	MJ	-1168.68 or -7.8		

Table 5-6 Acidic Leaching Reactor Energy Balance

5.8 Overall Energy Balance

	Units	FeS ₂	$Na_2S_2O_3$	H ₂ S	CH₃-SH	CH ₃ -SNA
Molar Flow (F _{A0})	mol/h	0.431	0.7545	0.5235	1.080	1.081
%Conv (X _A)	%	60%	-	-	45%	-
Rate of Rxn (-r _A)	mol/lit.h	-1.52x10 ⁻⁵	+1.52x10 ⁻⁵	+1.52x10 ⁻⁵	-2.85x10 ⁻⁵	+2.85x10 ⁻ ⁵
Std. Enthalpy of form (H(T ₀))	kJ/mol	-95.06	-1117	-20.15	-28.6	309.2
Specific Heat (C _P)	kJ/kg.K	0.61	0.59	1.012	2.598	1.912
Enthalpy of form (H(T))	kJ/mol	42.19	-984.45	207.55	555.95	739.4
Heat of Rxn (ΔH_{rxn})	kJ/mol	-100604.9	-130178.6	196.64	88.88	88.88
-F _{A0} . C _{PA} (T – T ₀)	kJ.mol/kg.h	-59.15		-	-631.31	1
Heat Flow (Q)	kJ/h	-1168813.48			-1168813.48	
Total Energy Flow	MJ	-1269.5 or -8.472			-1169.4 or -7.79	

Table 5-7 Overall Energy Balance

CHAPTER 6

EQUIPMENT DESIGN

6.1 Reactor

Designing a reactor involves several considerations depending on the precise application and sort of reactor. But here are some trendy aspects to remember in gadget design for a reactor:

Reactor kind: Determine the precise sort of reactor you're designing, including a chemical reactor, nuclear reactor, or biological reactor. Every type has precise necessities and considerations.

Reactor Vessel: The reactor vessel is the main factor that houses the response. It needs to be designed to face up to the running situations, consisting of temperature, stress, and corrosive nature of the reactants. The fabric choice and thickness should be appropriate for the situations.

Agitation and mixing: If the reaction calls for agitation or mixing, don't forget the design of agitators, impellers, or mixers. The layout should make sure green blending and save you lifeless zones or stagnant areas in the reactor.

Heat transfer: If warmth switch is concerned, don't forget the design of warmth exchangers, jackets, or coils inside the reactor vessel. Those elements facilitate warmth switch for exothermic or endothermic reactions, maintaining the preferred temperature variety.

Inlet and Outlet structures: Design suitable systems for introducing reactants, controlling float charges, and disposing of products or through-merchandise. recall elements which include strain drop, distribution uniformity, and minimizing any potential for leaks.

Instrumentation and Manipulation: Decide the instrumentation required for monitoring and controlling the reactor parameters, along with temperature, stress, pH, or awareness. consider the position and integration of sensors, control valves, and automation systems.

Fabric selection: Pick materials compatible with the reactants, operating situations, and corrosion resistance necessities. don't forget factors which includes fabric electricity, thermal enlargement, and the want for specialized coatings or linings.

Scaling-up considerations: If the layout entails scaling up from laboratory to industrial scale, account for factors like reaction kinetics, mass switch boundaries, and system dynamics. make certain that the design can cope with the increased scale at the same time as preserving efficiency and protection.

It's far crucial to be aware that reactor design is a complicated engineering mission and often calls for the knowledge of chemical, mechanical, or nuclear engineers, relying on specific applications. Consulting with experts in the field is noticeably encouraged to make certain a safe and green layout.

Calculations for Reactor Design:

Energy Flow = $-F_{A0}$. $C_{PA}(T - T_0) + (H_B(T) - H_A(T))$. r_A . V + Q $H_A(T) = H_A(T_0) + C_{PA}(T - T_0)$ $H_B(T) = H_B(T_0) + C_{PB}(T - T_0)$ (Where, $A = NaOH + H_2O \& B = Na_2S_2O_3$) Specific Heat (C_P) Values at 250 °C & 1 bar: Specific Heat of Ash ($C_{P Ash}$) = 0.9284 kJ/kg.K Specific Heat of Carbon ($C_{P Carbon}$) = 0.71 kJ/kg.K Specific Heat of H_2 ($C_{P H2}$) = 14.3 kJ/kg.K Specific Heat of N_2 ($C_{P N2}$) = 1.04 kJ/kg.K Specific Heat of Cl (C_P Cl) = 0.96 kJ/kg.K Specific Heat of Sulphur (C_P s) = 0.75 kJ/kg.K Specific Heat of O_2 (C_{P 02}) = 0.92 kJ/kg.K Average Specific Heat of Coal (C_{P.avg Coal}) = 1.3253 kJ/kg.K Specific Heat of NaOH (CP_NaOH) = 3.6 kJ/kg.K Specific Heat of $H_2O(C_{P_H2O}) = 1.855 \text{ kJ/kg.K}$ Average Specific Heat of Solvent ($C_{P.avg_Solvent}$) = 0.9399 x 1.855 + 0.06001 x 3.6 Average Specific Heat of Solvent (C_{P.avg_Solvent}) = 1.96 kJ/kg.K Volume of reactor = 17000 Lit

By using Enthalpy Tables:

 $\begin{aligned} H_A (T_0) &= -241.9 \text{ kJ/kg.K} & H_B (T_0) &= -1117 \text{ kJ/kg.K} \\ H_A (T) &= H_A (T_0) + C_{PA} (T - T_0) &= 199.1 \text{ kJ} \\ H_B (T) &= H_B (T_0) + C_{PB} (T - T_0) &= -984.45 \text{ kJ} \end{aligned}$

Now using; V/F_{A0} = T/C_{A0} to find C_{A0}, C_{A0} = 9.95 x 10⁻⁵ moles/Lit And using; V/F_{B0} = T/C_{B0} to find C_{B0}, C_{B0} = 0.01 moles/Lit

Total Percent Sulphur removed = % Conversion = 40% Using this Conversion, we can find rate of reaction (r_A); $r_A = 9.95 \ge 10^{-5}$ moles/hr Now, Specific Heat of Na₂S₂O₃ (C_{P_Na2S2O3}) = 0.92 kJ/kg.K

6.2 Jaw Crusher

Designing a jaw crusher includes worn-out numerous elements to make sure it's efficiency, sturdiness, and protection. right here are a few key aspects to consider within the equipment worn-out of a jaw crusher:

Feed material traits: Recognize the characteristics of the fabric that will be fed into the crusher, inclusive of its hardness, abrasiveness, and moisture content material. These statistics will affect the choice of materials for the jaw plates and the worn-out of the crushing chamber.

Crushing Chamber Geometry: decide the gold standard shape and size of the crushing chamber based totally on the preferred product size, throughput potential, and particle distribution. do not forget elements together with the nip perspective, stroke, and kinematics to ensure green crushing.

Jaw Plates: Pick appropriate substances for the jaw plates primarily based on the feed material characteristics. don't forget substances with excessive put on resistance and durability to face up to the crushing forces and abrasive put on. The worn-out must facilitate easy alternative of a jaw plates.

Eccentric Shaft and Bearings: Worn-out a robust eccentric shaft that transfers the crushing motion to the jaw plates. worn-out bearings capable of withstanding heavy loads and provide proper lubrication to decrease friction and heat technology.

Toggle gadget: Lay worn tired a dependable toggle system that enables worn- outlet tired and ultimate of the jaw crusher. Don't forget the toggle plate, toggle seats, and anxiety rods to offer the essential mechanical advantage and make certain right alignment of the jaw plates.

Force machine: Decide the suitable driving system, along with a motor or hydraulic power, based totally on the desired electricity, velocity, and control abilities. make certain sufficient strength and torque to conquer the crushing forces and provide clean operation.

Safety capabilities: Incorporate protection features into the worn- out to guard operators and limit risks. Remember features inclusive of protection guards, emergency stops, and isolation mechanisms to save you injuries and offer easy get admission to for upkeep and upkeep.

Discharge machine: Lay worn tired an efficient discharge system to eliminate overwhelmed cloth from the crusher. recall elements inclusive of the discharge beginning length, shape, and configuration to ensure proper waft and save you blockages.

Structural Integrity: Worn-out a robust and sturdy shape to aid the jaw crusher, resist the crushing forces, and decrease vibrations. do not forget factors which include fabric choice, reinforcement, and proper bracing to ensure structural integrity.

Accessibility and renovation: Worn-out the crusher for easy get right of entry to critical components and renovation tasks. do not forget capabilities which include removable jaw plates, inspection doorways, and platforms to facilitate recurring protection and repairs.

It's far crucial to notice that designing a jaw crusher requires the know-how of mechanical engineers and may involve specialized software programs and simulation tools. Consulting with professionals within the subject is especially endorsed to make sure a safe and green worn-out.

Designing of Crusher:

Design Parameter	Formula	Value	
Feed Size Range		(125+1020)/2	0.572 m
		= 572.5 mm	
Feed opening width	Assumed to be 1.5 times the	1145 mm	1.145 m
	maximum feed size		
Product size	Assumed to be 1/4 of the	143.125 mm	0.143 m
	feed size		
Theoretical		19969.6 m ³ /h	27957.44
maximum capacity			kg/h
Capacity (Design)	Assumed to be 75% of the		20968.08
	theoretical maximum		kg/h
	capacity		
Required motor	$P = Q \ge E$	21.46 kW	
power			
Crusher speed		122 RPM	

Table 6-1 Designing of Crusher

Crusher length	Assumed to be 4 times the feed opening width	4580 mm	4.58 m
Crusher width	Assumed to be 1.5 times the feed opening width	1717.5 mm	1.717 m
Reduction ratio	Given	4:1	
Operating temperature	Given	25°C	

The theoretical feed capacity of a jaw crusher can be calculated using the following formula:

Q = (60 * L * W * S) / (H * K)

Where: Q = Theoretical feed capacity (in m^3/h)

L = Length of the jaw crusher's receiving opening (in meters)

W = Width of the jaw crusher's receiving opening (in meters)

S = Stroke of the jaw crusher (in meters)

H = Speed of rotation of the jaw crusher eccentric shaft (in revolutions per minute)

K = Constant related to machine characteristics

Assuming the following values:

Length of receiving opening = 1.527 meters (1.145/ 0.75)

Width of receiving opening = 1.145 meters

Stroke of the jaw crusher = 0.172 meters (1.145 x 15%)

Now calculate the theoretical feed velocity:

V = 0.5 x (g x L) / (W x 1000)

where g is the acceleration due to gravity (9.81 m/s^2)

V = 0.5 x (9.81 x 1.527) / (1.145 x 1000)

V = 0.0517 m/s

Finally, we can calculate the speed (RPM) using:

 $RPM = (60 \times V) / (L \times W)$

RPM = (60 x 0.0517) / (1.527 x 1.145)

RPM = 122

Speed of rotation of the jaw crusher eccentric shaft = 122 rpm = 2.033 rps

Constant related to machine characteristics = 1.6

Substituting the values, we get:

Q = (60 * 1.527 * 1.145 * 0.172) / (2.033 * 1.6) Q = 5.55 m³/s = 19969.6 m³/h Capacity = 19969.6 * 1.4 = 27957.44 kg/h

Work indexes for dry crushing[†] or wet grinding[‡]

Material	Specific gravity	Work index, W_i
Bauxite	2.20	8.78
Cement clinker	3.15	13.45
Cement raw material	2.67	10.51
Clay	2.51	6.30
Coal	1.4	13.00
Coke	1.31	15.13
Granite	2.66	15.13
Gravel	2.66	16.06
Gypsum rock	2.69	6.73
Iron ore (hematite)	3.53	12.84
Limestone	2.66	12.74
Phosphate rock	2.74	9.92
Quartz	2.65	13.57
Shale	2.63	15.87
Slate	2.57	14.30
Trap rock	2.87	19.32

† For dry grinding, multiply by 4.

$$\frac{P}{m} = 0.3162 W_i \left(\frac{1}{\sqrt{D_{Pa}}} - \frac{1}{\sqrt{D_{Pa}}}\right)$$

To convert the theoretical feed capacity from m^3/h to kg/h for coal, we need to know the density of the coal. Assuming a density of 1.4 kg/m³ for coal,

The feed capacity in kg/h can be calculated as:

5322.208 kg/h = 5.87 ton/h = $0.047 \text{ m}^3/\text{h} \times 1.4 \text{ kg/m}^3 \times 3600$ (conversion factor from hours to seconds.

6.3 Fluidized Bed dryer

The design of fluidized mattress dryer involves numerous key considerations to make sure green and effective drying of the cloth being processed. here are a few essential factors to do not forget when designing a fluidized bed dryer.

Length and shape: the dimensions and shape of the fluidized mattress must be optimized to achieve the favored drying potential and uniformity. The bed peak needs to be enough to accommodate the preferred residence time of the cloth.

Distributor plate: A distributor plate is commonly used at the lowest part of the mattress to evenly distribute the drying medium (air or gas) throughout the mattress. It needs to be designed to prevent channeling and ensure uniform fluidization.

Drying Medium

Airflow charge: The airflow price should be cautiously decided to offer ok fluidization of the material at the same time as minimizing the chance of entrainment or carryover.

Temperature: The temperature of the drying medium must be selected based on the traits of the fabric being dried and the favored drying fee. Care ought to be taken to avoid overheating or thermal degradation of the product.

Humidity manipulates depending at the utility, the moisture content material of the drying medium may additionally want to be controlled to attain the desired drying results.

Material Handling

Feed mechanism: The method of introducing the cloth into the fluidized bed should be designed to make sure uniform distribution and save you agglomeration or excessive particle breakage.

Discharge mechanism: The layout should facilitate clean and efficient discharge of the dried cloth from the fluidized mattress.

Heat transfer

Heat transfer surface: The design should maximize the heat switch location between the drying medium and the cloth to make certain efficient drying. this can be accomplished using Heat transfer surfaces including tubes, plates, or fluidized mattress internals.

Controls and safety

Instrumentation and controls: The dryer must be prepared with appropriate sensors and controls to screen and adjust parameters such as temperature, airflow price, and humidity. This allows for specific management of the drying system and ensures safe operation.

Material and Construction

Material selection: choice of production materials should consider factors including the corrosiveness or abrasiveness of the cloth being dried, in addition to the running temperature and stress.

It's important to say that the specific layout considerations can also range depending on the meant utility and the properties of the material being dried. Consulting with specialists in drying technology and equipment design is recommended to make sure and superior fluidized bed dryer design to your requirements.

Calculations

Cross-sectional area of the bed = Abed = $(mf / (Umf * \rho p * \epsilon)) * (1 - \epsilon)$ where: mf = mass flow rate of coal feed (5322.208 kg/hr) Umf = minimum fluidization velocity (0.7 m/s) ρp = density of coal particles (1400 kg/m³) ϵ = bed porosity (assumed to be 0.4) Plugging in the values, we get $A_{bed} = (5322.208 / (0.7 * 1400 * 0.4)) * (1 - 0.4) = 8.15 m^2$ Cross-sectional area of the dryer: $A_{dryer} = A_{bed} / (1 - \epsilon)$ Plugging in the values, we get: $A_{dryer} = 8.15 / (1 - 0.4) = 13.6 m^2$

6.4 Filter Press

The layout of a filter out press entails diverse components and issues to obtain green stableliquid separation. right here are the important thing device layout aspects to consider for a clear out press

Material: The body is commonly made of sturdy materials such as metallic or stainlesssteel to offer structural integrity and withstand the mechanical forces throughout operation. **Layout:** The body layout has to permit for clean meeting and disassembly of clear out plates, in addition to facilitate the application of hydraulic stress for cake compression.

Filter Plates

Cloth: Clear out plates are generally fabricated from polypropylene, forged iron, or stainless-steel. The cloth choice relies upon elements consisting of the chemical compatibility with the manner fluid and the specified electricity.

Configuration: Clear out plates have a recessed design with numerous channels and ports for liquid and gasoline waft. The variety and association of plates rely on the preferred filtration place and capability.

Filter Cloth

Cloth: Clear out cloths are typically made from substances like polypropylene, polyester, or nylon, selected primarily based on chemical compatibility and favored filtration residences.

Attachment: The filter out cloth is securely attached to the filter plates for the usage of gaskets, clamps, or other sealing mechanisms to save you leakage and ensure right filtration.

Filtrate Collection

Channeling: The clear out press design must comprise proper go with the flow channels and series structures to make certain efficient removal of the filtrate (liquid) from the filter out plates.

Filtrate Outlet: Filtrate retailers and piping ought to be designed to save you leakage or bypassing of the process fluid.

it is crucial to note that the unique design features may range relying on the scale, ability, and supposed software of the filter press. Consulting with manufacturers or experts in filter press era is recommended to make certain the design meets your filtration requirements.

Calculations:

Given feed rate of Coal + NaOH Solution = 21296.91 kg/h Total concentration of coal particles = 21% First, calculate the total solids (TS) in the feed: TS = (21/100) x 21296.91 = 4472.93 kg/h Lets take general Filter press efficiency of 98%:

Next, we need to calculate the filtrate (Liquid NaOH) flowrate (Qf):

Qf = 0.98 x (21296.91 - 4472.93) = 15703.15 kg/h

Finally, we can calculate the filtration rate (FR):

FR = Qf / A

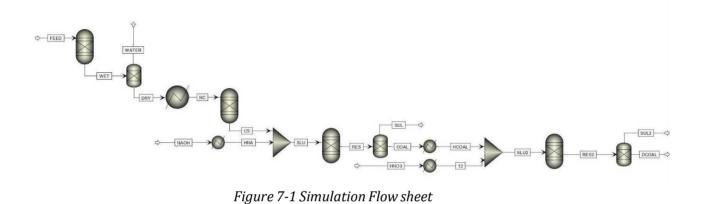
where A is the filtration area. Assuming a typical filtration rate of 100-1000 kg/m²/h for a filter press, we can take a value of 400 kg/m²/h as a proximate value. Therefore:

 $A = Qf / FR = 15703.15 / 400 = 39.26 m^2$

CHAPTER 7

SIMULATION

7.1 Simulation Main Flow Sheet



7.2 Coal Component Input

To input coal as a component, the following steps were performed on Aspen Plus:

- 1. Open Aspen Plus V10.
- 2. Click on the Properties tab at the left corner.
- 3. Click on Components and type "COAL" under Component ID.
- 4. Change the type from Conventional to Non-Conventional.

	_			
۲	COAL	Nonconventional		
	ASI	Nonconventional		
Þ	С	Solid	CARBON-GRAPHITE	С
₽	H2	Conventional	HYDROGEN	H2
Þ	N2	Conventional	NITROGEN	N2
Þ	CL2	Conventional	CHLORINE	CL2
Þ	S	Solid	SULFUR	S
▶	02	Conventional	OXYGEN	02
▶	H2O	Conventional	WATER	H2O
₽	NAOH	Conventional	SODIUM-HYDROXIDE	NAOH
₽	NA2SO3	Conventional	SODIUM-SULFITE	NA2503
Þ	NA2S	Conventional	SODIUM-SULFIDE	NA2S
₽	ниоз	Conventional	NITRIC-ACID	HNO3
►	H2SO4	Conventional	SULFURIC-ACID	H2SO4
	NO2	Conventional	NITROGEN-DIOXIDE	NO2

Figure 7-2 Components List

7.3 Fluid Packages

To input fluid packages, the following steps were performed:

- 1. Click on the Properties tab at the left corner.
- 2. Click on methods and select specifications.
- 3. Click on Method name and select Peng-Rob.
- 4. Go to NC Props and select COAL.
- 5. Click on the enthalpy tab and select HCOALGEN.
- 6. Click on the density tab and select DCOALIGT.

🥝 Global	Flowsheet	Sections	Referenced	C	omments		
Property m	ethods & d	ptions —		_	Method name		
Method fil	ter	COMMON	/ 👻		PENG-ROB	Method	ls Assistant
Base meth	od	PENG-RO	в –				
Henry com	ponents		-		Modify —		
Petroleur	n calculatio	on options -			EOS	ESPRSTD	-
		STEAM-TA	-		Data set		1 🚔
Water so	ubility	3	-		Liquid gamma		-
	,				Data set		
-	e calculatio	on options			Liquid molar enthalpy	HLMX106	-
Chemistr	y ID		-		Liquid molar volume	VLMX20	-
🔽 Use tr	ue compor	nents			Heat of mixing		
					Poynting correction	1	
					Use liquid reference	state enthalpy	,
					Use liquid reference	e state enthalpy	·

Figure 7-3 Fluid Packages for CS

Property Methods	Comments									
	COAL •									
roperty models for Model name	nonconventional com		on codes							
Enthalpy	HCOALGEN	•	I 1	1	1					
Density	DCOALIGT	•								
PROXANAL	ULTANAL	501	ANAL							

Figure 7-4 Setup for Simulation

The fluid package is the set of equations that helps the program come up with relevant fluid properties at given states. Since a process is nothing but a change of states, the simulation needs underlying relationships to come up with values of properties pertaining to the system. The selection of the fluid package depends on the type of components involved.

7.4 Simulation Setup

Before simulating the process, we must make it ready for our simulation. To tell the aspen plus to provide us with certain tools. We setup our simulation using the following steps:

- 1. Go to the simulation environment.
- 2. Go to the setup tab and click on the specifications, dropdown the sub stream menu and select the "MCINCPSD".

Global □	escription	Accounting	Diagnostics	Comments	
Title					
litie			Clabel anti-		
Global unit set	METCBA	R -	Global settings — Input mode	Steady-State	-
			Stream class	MCINCPSD	-
			Flow basis	Mole	•
			Ambient pressure	e 1.01325	bar 🔹
			Ambient temp.	10	C ~
		,	Valid phases		-
		1	Free water	No	-

Figure 7-5 Setup for Simulation

By selecting the "MCINPSD" you are telling the aspen plus that we have conventional and non-conventional solids with their PSD. So, he should simulate the environment accordingly.

7.5 Simulating Meshes

You need to create a mesh so aspen plus can calculate the weight fraction on each mesh. You need to follow the following steps:

- Go to the components in the simulation environment and click on the solids tab, then click on PSD.
- Select the option Equidistant on Mesh type and specify the size range. In our project, we assumed that we got the coal in gravel aggregate (4.75 mm to 75 mm).
- Now click on calculate and aspen plus will find the weight fraction on each mesh.
- Now we are ready to simulate the equipment.

PSD mesh ID	PSD	
- PSD Mesh		
PSD mesh type	Equidistan	t 🔹
No. of intervals		20 🗘
Lower limit	Upper limit	Size units
75		Number of intervals for particle Enter a number between 0 and
		Create PSD Mesh ber of intervals, data will be herever this PSD is used.

Figure 7-6 Simulating Meshes

7.6 COAL STREAM

So far, we have only made the aspen plus ready for our simulation, Now, it's to simulate the process, so first is to simulate the material stream. Follow the steps to simulate the making of the coal stream.

- 1. Make a material stream in simulation environment.
- 2. Enter the feed specifications and enter the proximal, ultimate and sulfur analysis in the dialogue box.
- 3. Now the feed stream is ready to be used.

 Specifications 							
State variables				 Co	mposition		
Substream name	ONC		•	Μ	ass-Frac 🔹		Ŧ
Temperature	25	С	•		Component	Value	
Pressure	1	bar	•	>	COAL		1
Total flow basis	Mass •			×	ASH		
Total flow rate	70000	kg/hr	•		Total		1

Figure 7-7 Feed specifications

٢	🕜 Componer	nt Attrik	oute	
Component ID		⊘C0	AL	•
Att	ribute ID	⊘ SU	LFANAL	•
	Element	:	Value	
	PYRITIC		1.6198	5
	SULFATE		0.53995	1
\geq	ORGANIC		2.170	2

Figure 7-9 Sulfur Analysis

•) 🥝 Componen	nt Attribute	
Component ID Attribute ID		⊘COAL	•
		PROXANAL	•
	Element	Value	
	MOISTURE	7.0	51
	FC	35.	97
	VM	34.2	21
	ASH	22.	21

Figure 7-8 Proximate Analysis

📀 🥝 Component Attribute					
Component ID					
Att	ribute ID	ØULTANAL -			
	Element	t Value			
	ASH	22.21			
	CARBON	60.06			
	HYDROGEN	4			
	NITROGEN	1.4			
	CHLORINE	0			
	SULFUR	4.33			
	OXYGEN	8			

Figure 7-10 Specifications of Jaw Crusher

7.7 Jaw Crusher

Now according to plant design mentioned in the above section we need to reduce the size of the coal from 5 mm to 149 microns for that purpose, we are designing a jaw crusher in simulation. The reason for this size reduction is explained in the plant design section. We followed the following steps for the design of jaw crusher:

- 1. Go to the solids section on model pallet.
- 2. Now select the crusher and paste it onto the simulation environment.
- Now go to the parameters tab and enter the downstream size reduction and select US. Bureau of Mines and then select Jaw Crusher.
- 4. Specify the bond's work index (for coal it is 13) and run your simulation.

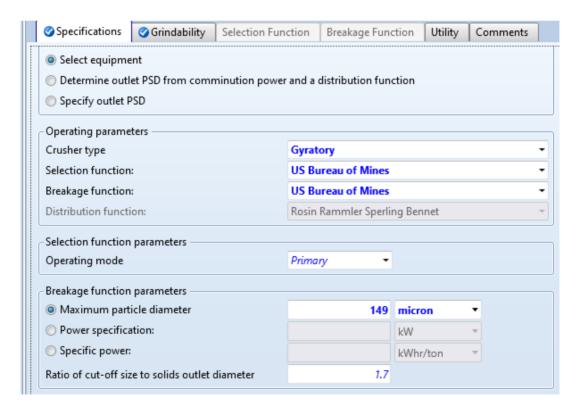


Figure 35: Jaw Crusher

7.8 Yield Reactor

Yield is technically not a reactor; it is more of a convector used to non-conventional solids into conventional solids so that it can react with our solvent as non-conventional components are theoretical type compounds so for the sulfur present in the coal to react with our solvent, we need to make it conventional. This reactor is found in the reactor ribbon on model pallet. You can simply paste it on the simulation environment and input the data shown in the following figures:

Flash Type	Temperature	Pressure	-		Component	Basis	Basis Yield
femperature	250	С	•	•	ASH	Mass	0.222
emperature chan	ige	С	*		C (CISOLID)	Mass	0.6000
Pressure	1.01325	bar	•		H2	Mass	0.04
Duty		cal/sec	*		N2	Mass	0.014
Vapor fraction					CL2	Mass	
					S (CISOLID)	Mass	0.0433
Culutarian ID	(2) MC	•		Con	nponent yields		
					1 2		
Substream ID	WNC	•			Component	Basis	Basis Yield
Component attr	ributes		nent Value			Basis Mass	
Component attr Component ID	ributes OASH	▼ Eler	ment Value		Component		Yield
Component attr	ributes	Elen MOISTU	JRE O	~ ~ ~	Component H2	Mass	Yield 0.04 0.014
Component attr Component ID	ributes OASH	Eler MOISTU FC		~ ~ ~	Component H2 N2	Mass -	Yield 0.04 0.014
Component attr Component ID	ributes OASH	Elen MOISTU	JRE O		Component H2 N2 CL2	Mass Mass - Mass Yield per u	Vield 0.04 0.014 unit mass of tota

Figure 7-11 Yield Reactor Specifications

7.9 Alkali & Acidic Reactor

The working and benefits of using alkali and acidic reactors are mentioned in the design section and steps involving both reactors are pretty much the same. Both the reactors are Stoic reactors, and we added the data shown in the following figure and calculated the results.

Operating conditions Flash Type	Temperature 🝷	Pressure
Temperature	250	c .
Pressure	1.01325	bar 🔹
Duty		cal/sec "
Vapor fraction		

Figure 7-12 Alkali Reactor Specifications

eactants			Pro	ducts	
Component	Coefficient			Component	Coefficient
S (CISOLID)	-3		•	NA2SO3	1
NAOH	-6		•	NA2S	2
				H2O	3
•			► ►	H2O	3
>				H2O	3
•				H2O	3
>				H2O	3
Products generation				H2O	3
	kmol/hr	Ŧ		H2O	3

Figure 7-13 Alkali Reactor Specifications

Operating conditions —			
Flash Type	Temperature -	Pressure	-
Temperature	95	С	•
Pressure	1.01325	bar	•
Duty		cal/sec	*
Vapor fraction			
Vapor fraction			

Figure 7-14 Acidic Reactor Specifications

CHAPTER 8

ECONOMICS ANALYSIS

8.1 Cost Analysis

The cost of a project decides whether the project is feasible or not. Economic analysis is very important for the financially evaluate the project and all or its components. Since the prime goal of a project is to do business and produce revenue, that's why cost is a major factor for the decision of equipment installation.

Cost is one of the most important parameters in efficient management of a project.

Time and quality usually trade off with price of a project for desired results. We adapted the Coulson and Richardson method for our Project economic analysis.

8.2 Fluidized Bed Dryer

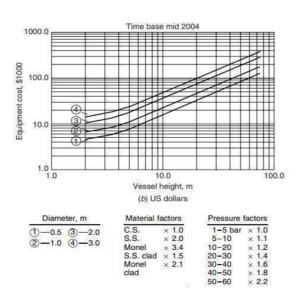
Diameter (d) = 2.0 m

Length (l) = 4.21 m

Since we used carbon steel material because of the cost factor, therefore **material factor** is 1.

Pressure factor is also 1 for 1-5 bar pressure.

Total cost of desalter = (bare vessel cost) * (material factor) * (pressure factor)



= USD 6472.96

8.3 Jaw Crusher

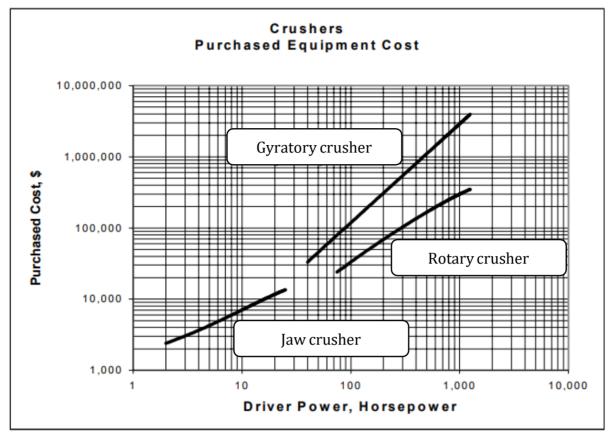


Figure: Jaw Crusher Cost Graph

Table 8-1 Cost of Jaw Crusher

Duty	28.76	hp
Cost in 2004	14000	USD

8.4 Heater

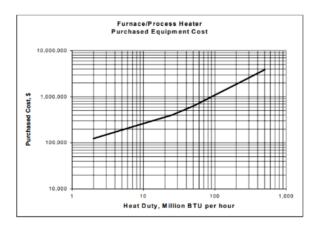
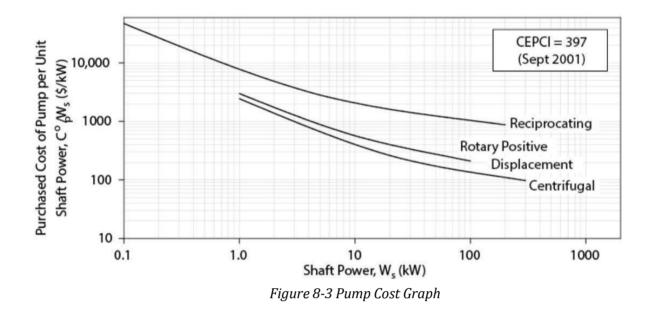


Figure 8-2 Heater Cost Graph

8.5 Pumps



Shaft Power (kW) = 1.9 kW Purchased Cost in 2004 (USD) = 1346.49 USD

8.6 Reactor

Volume of reactor = 17 m3 Vessel material = glass lined NNNNh NNNN NNNNNNNNN = NN = NNN Where Ce is the purchased equipment cost in USD, C is a constant in USD, S is size unit, and n is the index

Equipment	Size unit, S	Size range	Con: 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	$(5-50)\times 10^3$	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 power, kW	20-500	1160	1920	0.8	electric, max. press.
Reciprocating	power, kn		1600	2700	0.8	50 bar
Conveyors 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 7700	0.45 0.35	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, m ³	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
Storage floating roof cone roof		50-8000 50-8000	2500 1400	4350 2300	0.55 0.55	×2 for stainless

Table 6.2. H	Purchase cost of mi	scellaneous equipment	, cost factors I	for use in equa	tion 6.7.	Cost basis mid 2004
--------------	---------------------	-----------------------	------------------	-----------------	-----------	---------------------

N = USD31000

N = 0.45

N = reactor *NNNNNNN NN N*3= 17*N*3

 $Ce = USD31000 \times 17^{0.45}$

Ce = USD110933.8

8.7 Plate and frame filter press

Area = 39.26 m2 Vessel material = cast iron NNNNh NNNN NNNNNNNN = NN = NNN Where Ce is the purchased equipment cost in USD, C is a constant in USD, S is size unit, and n is the index.

From table 6.2 in Coulson Richardson's Chemical Engineering Series Volume 6

Equipment	Size	Size	Cons		Index	Comment
	unit, S	range	C,£	C,\$	n	
Agitators		5 75	1000	1000	0.5	
Propeller	driver	5-75	1200 1800	1900 3000	0.5	
Turbine	power, kW		1800	3000	0.5	
Boilers						
Packaged		·5 501 103	20	100	0.0	oil or gas fire
up to 10 bar	kg/h steam	$(5-50) \times 10^3$	70	120	0.8	
10 to 60 bar			60	100	0.8	
Centrifuges		05.40	25.000	50.000		
Horizontal basket	dia., m	0.5-1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	$\times 1.7$ for ss
Compressors						
Centrifugal	driver	20-500	1160	1920	0.8	electric,
	power, kW		1.000	0700	0.0	max. press.
Reciprocating			1600	2700	0.8	50 bar
Conveyors						
Belt	length, m	2-40				
0.5 m wide			1200	1900	0.75	
1.0 m wide			1800	2900	0.75	
Crushers						
Cone	t/h	20-200	2300	3800	0.85	
Pulverisers	kg/h		2000	3400	0.35	
Dryers						
Rotary	area, m ²	5-30	21,000	35,000	0.45	direct
Pan		2-10	4700	7700	0.35	gas fired
Evaporators						0
Vertical tube	area, m ²	10-100	12,000	20.000	0.53	carbon steel
Falling film	area, m	10-100	6500	10,000	0.52	carbon steer
			0.00	10,000	0.04	
Filters	2	5 50	5 400	0000	0.0	
Plate and frame	area, m ²	5-50	5400	8800	0.6	cast iron
Vacuum drum		1-10	21,000	34,000	0.6	carbon steel
Furnaces						
Process						
Cylindrical	heat abs, kW	$10^{3} - 10^{4}$	330	540	0.77	carbon steel
Box		$10^{3} - 10^{5}$	340	560	0.77	×2.0 ss
Reactors						
Jacketed,	capacity, m ³	3-30	9300	15,000	0.40	carbon steel
agitated			18,500	31,000	0.45	glass lined
Tanks						-
Process	capacity, m ³					
vertical	capacity, in	1-50	1450	2400	0.6	atmos. press.
horizontal		10-100	1750	2900	0.6	carbon steel
Storage						
floating roof		50-8000	2500	4350	0.55	×2 for
cone roof		50-8000	1400	2300	0.55	stainless

8.8 Purchased Equipment cost

Equipment	Cost (USD)
Jaw Crusher	14,000
Mixer (1&2)	20,000
Heater 1	170000
Reactor 1	110933.8
Reactor 2	110933.8
Pump 1	1346.49
Pump 2	1346.49
Plate and frame filter press 1	9133.55
Plate and frame filter press 2	9133.55
Fluidized Bed dryer	6472.96
Total	USD 1.3 million

Table 8-2 Purchased Equipment cost

8.9 Indexing

Index in 2004 = 111

Index in 2023 = 320

Cost in 2023 = (<u>Cost in 2004)*(Index in 2023)</u>

Index in 2004

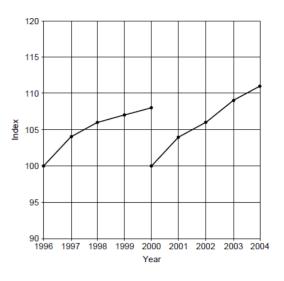


Figure 8-4 Index Graph

8.10 Total cost

Table 6.1. Typical factors for estimation of project fixed
--

		Process type	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	
*f7 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	

8.11 Physical Plant Cost

Equipment Erection	0.45
Piping	0.45
Instrumentation	0.15
Electrical	0.1
Process	0.1
Storages	0.20
Utilities	0.45
Total Physical Plant Cost	USD 3.79 million

Table 8-3 Physical plant Cost

8.12 Fixed Capital Cost

f_{10} Design and Engineering f_{11} Contractor's fee	0.30 0.05	0.25 0.05	0.20 0.05
f ₁₂ Contingency	0.10	0.10	0.10
Fixed capital = PPC $(1 + f_{10} + f_{11} + f_{12})$ = PPC ×	1.45	1.40	1.35

Design and Engineering	0.25
Contingencies	0.05
Contractor's fees	0.10
Fixed Capital cost	USD 5.306 million

	•
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	
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 B	
Direct production costs A + B 13. Sales expense 14. General overheads 15. Research and development	20–30 per cent of the direct production cost
Sub-total C	
Annual production $cost = A + B + C =$	
Production cost $\pounds/kg = \frac{Ann}{Ann}$	nual production cost nual production rate

Table 6.6. Summary of production costs

Table 8-5 Fixed & Variable Cost

Local Taxes	USD 0.11 M
Insurance	USD 0.053 M
Capital Charges	USD 0.53 M
plant overheads	USD 0.05 M
laboratory	USD 0.02 M
Supervision	USD 0.02 M
Operating labor	USD 0.10 M
Maintenance	USD 0.53 M

8.14 Variable Operating Cost

	Т	'able	8-6	Variable	e Oper	atina	Cost
--	---	-------	-----	----------	--------	-------	------

Raw material	10 M
Miscellaneous	1.4 M
Utilities	0.6 M
Total	USD 12 million

8.15 Whole Plant Summary

Purchased Equipment Cost (PCE)	USD 1.31 million
Physical Plant Cost (PPC)	USD 3.79 million
Fix Capital	USD 5.306 million
Fix Operating Cost	USD 1.47 million
Variable Operating Cost	USD 12 million
Direct Production Cost	USD 13.47 million
Annual Production Cost	USD 17.51 million
Annual profit	USD 29.18 million
Payback Time	1 year 5 months

Table 8-7 Whole Plant Summary

CHAPTER 9

HAZOP ANALYSIS

A Hazard and Operability study of the proposed is fundamental to its technical feasibility from a safety point of view. Conventionally, such analyses usually involve using specific guidewords to assess the cause, effects, and preventative measures for the process. Examples of said guidewords may be "high temperature", "low pressure" or something else of the sorts. These guidewords vary with the equipment under study within a system. Each component within a system must be considered for a thorough risk assessment. The guidewords are essentially deviations that may potentially be encountered within the equipment and help to imagine several possible scenarios. HAZOP involves.

9.1 Key Words

Nodes Pipe sections or vessels containing where process chemicals may be present.

Super nodes Several nodes considered together as one node for quicker studies.

Hazard Potential source of harm.

Harm Actual injury or damage to equipment, personnel, or environment.

Risk Probability of harm occurring and its associated level of damage.

9.2 Methodology

- Identify all major nodes and super nodes.
- Identify why the node was chosen for the HAZOP study.
- Choose a key process parameter for said node.
- Apply all relevant guidewords for chosen parameter. These would result in unwanted deviations within the process. List down the deviations.
- Determine the potential causes of the deviations identified and add them to the table.

Study Node	Process	Guide	Causes	Consequences	Action Required
	Parameters	Words			
Valve (V-1)	Flow	No	Valve actuator stuck	Crusher consumes	Try to manually force open the
			due to rusting or	energy when empty.	valve if possible.
			sedimentation.		A bypass valve line must be
			Controller fails to open		Do cleansing action of stuck
			valve		valve actuator
		Low	Valve actuator partially	Mechanical energy	A bypass valve line must be
			stuck due to rusting or	loss due to partial	installed to save productivity
			sedimentation.	empty operating	loss during maintenance.
			Controller fails to	crusher	Do cleansing action of partially
			properly open valve		stuck valve actuator
Screening Mesh	Flow	Low	Mesh holes are partially	Inefficient Screening	Cleansing action applied to
(SC-101)			blocked due to stuck	of coal particles	mesh screen by water spray
			particles		and pressurized air ejector

Table 9-1 HAZOP Analysis Crusher (C-101)

Table 9-2 HAZOP MIXER (M-101)

Study	Process	Guide	Causes	Consequences	Action Required
Node	Parameters	Words			
Valve	Flow	No	Valve actuator stuck due to	Composition of mixture	Try to manually force open the
(V-2)			rusting or sedimentation.	will be altered due to	valve if possible.
			Controller fails to open	unavailability of one	A bypass valve line must be
			valve	component	installed to avoid composition
					change.
		Low	Valve actuator partially	Composition of mixture	Try to manually force open the
			stuck due to rusting or	will be altered due to	valve properly if possible.
			sedimentation.	partial availability of one	A bypass valve line must be
			Controller fails to properly	component	installed to avoid composition
			open valve		change.
Valve	Flow	No	Valve actuator stuck due to	Composition of mixture	Try to manually force open the
(V-3)			rusting or sedimentation.	will be altered due to	valve if possible.
			Controller fails to open	unavailability of one	A bypass valve line must be
			valve	component	installed to avoid composition
					change.
		Low	Valve actuator partially	Composition of mixture	Try to manually force open the
			stuck due to rusting or	will be altered due to	valve properly if possible.
			sedimentation.	partial availability of one	A bypass valve line must be
			Controller fails to properly	component	installed to avoid composition
			open valve		change.

		High	The valve actuator becomes	Composition of mixture	Try to manually force close the
			loose and open more than	will be altered due to	valve to required opening if
			required.	excess inflow of NaOH	possible.
			Controller opens valve more	solution	A bypass valve line must be
			than required		installed to avoid composition
					change.
	Flow	No	Valve actuator stuck due to	The temperature of	A bypass valve line must be
(V-4)			rusting or sedimentation.	Energy loss due to	installed to avoid heat loss
				empty heating	during maintenance.
		Low	Valve actuator partially	The temperature of the	Try to manually force open the
			stuck due to rusting or	heating compartment	valve properly if possible.
			sedimentation.	will increase more	Do cleansing action of partially
				than the requirement.	stuck valve actuator
		High	Controller opens valve more than required	Required temperature of material won't be achieved.	Do maintenance action of loosened valve actuator
	Flow	No	Valve actuator stuck due	The temperature of the	Try to manually force open the
(V-5)			to rusting or	heating compartment	valve if possible.
			sedimentation.	will increase	Do cleansing action of stuck valve
				drastically.	actuator
		Low	Valve actuator partially	Energy loss due to	A bypass valve line must be
			stuck due to rusting or	heating of lesser	installed to avoid heat loss.
			sedimentation.	material than requirement	Do cleansing action of partially stuck valve actuator
	1				

Table 9-3 HAZOP Analysis Pump (P-101)

Study Node	Process Parameters	Guide Words	Causes	Consequences	Action Required
Valve (V-6)	Flow	No	rusting or codimontation	Cavitation and Seal damage can occur due to dry running of pump	Try to manually force open the valve if possible. Do cleansing action of stuck valve actuator
		Low	Variable Flow Drive (VFD),	Cavitation caused by insufficient liquid at suction Impeller	A bypass valve line must be installed to avoid heat loss.
			causing deviation of flowrate from required value		Do maintenance of VFD on pump
		High	Variable Flow Drive (VFD), not working on pump, causing deviation of flowrate from required value.	Mechanical energy losses are due to pressure drop caused by overloading of liquid at suction.	Try to manually force close the valve to required opening if possible. Do maintenance of VFD on pump
Pump (P-101)	State	As well as	Vapor or bubbles can be formed due to lower suction pressure than NPSH.	These vapors cause cavitation, that leads to damage of pump components.	Stand-by pump needs to be installed and turned on during priming and maintenance of original pump.

Study	Process	Guide	Causes	Consequences	Action Required
Node	Parameters	Words			
Line	Pressure	Low	It can also occur due to	It can also cause early	Try to manually force
			friction present	clogging which eventually	open the valve
(L-7)			because of scaling in	leads to inefficient filtration	properlyif possible.
			pipeline. Variable Flow	and reduction of life of filter	Scale inhibitors or scale
			Drive (VFD), not	membrane.	remover (dissolver) are
			working on pump	It can also lead to lowering	applied to either
				of overall process flowrate.	prevent or remove
					scaling from
					pipeline.
		High	Feed mixture coming at	It can also cause filter	Try to manually force
			high pressure due to	housing to deform or crack,	close the valve to
			more valve opening	that eventually leads to	required opening if
			than required.	lower product quality and	possible. Do
				inefficient filtration	maintenance action of
					loosened valve actuator.

Table 9-4 HAZOP Analysis Filter (F-101)

Fluidized Bed Dryer (D-101)

Study Node		Guide Words	Causes	Consequences	Action Required
Dryer (D-101)	Temperature	Low	It can also decrease below required drying temperature due to failure of fuel valve opening to minimum required limit.	reduced efficiency of the	Opening of incoming air mustbe kept constant between thedesigned range to keep air flowrate of process within required range.
		High	It can also increase above required drying temperature due to failure of fuel valve opening to maximum required limit	Higher temperature can also cause internal structure of dryer compartment to distort or even explosion if it increases too much	Opening of incoming air must be kept constant between the designed rangeto keep air flowrate of process within required range.



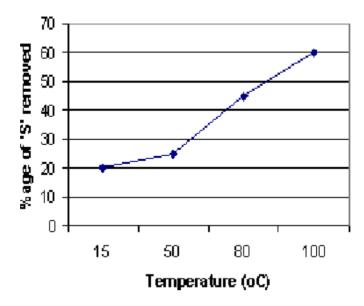


Figure 0-1 % Removal of Sulfur Vs Temperature

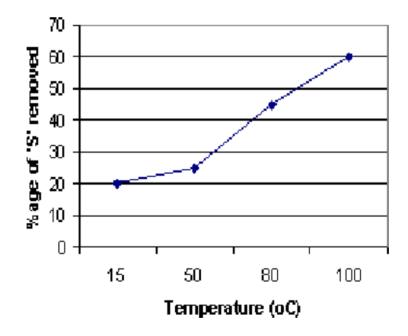


Figure 0-2 % Removal of Sulfur Vs Temperature

Finally, we reached he outcome that percentages of sulphur removed is directly proportional with rise in temperature as well as reduction in particle size, until we attain optimization.

CONCLUSION

We approached the conclusion that with the help of the chemical leaching process, we can remove 50–60% Sulphur and 80% ash, respectively. Based on the mass and energy balance and economic analysis, we conclude that the chemical leaching process is the most efficient process in terms of economics and sustainability.

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