PRODUCTION OF ETHANOL USING CELLULOSIC MATERIAL

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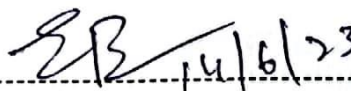
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CERTIFICATE

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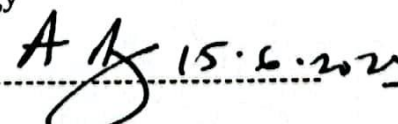

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DEDICATION

This FYP Thesis is dedicated to individuals who believed in the potential of this group, especially, our beloved families, friends, and teachers who played a significant role in bringing us this far.

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ABSTRACT

Due to rising demand worldwide, it is predicted that within ten years, the amount of energy consumed will increase by almost 50%. The primary source of energy, petroleum oil, is rapidly running out both in Pakistan and globally. This predicament will highlight the necessity for alternative and renewable resources to meet the steadily growing demand for vitality.

Ethanol can be mixed with diesel to form up to 20-80 Ethanol-Diesel mixtures. It's common to think of the production of ethanol from maize feedstock and sugar as posing a threat to food production, food consumption, and rising food and biofuel costs. This is why the manufacture of ethanol from cellulose-based biomass is so attractive, as it reduces competition with the food industry by employing non-edible biomass as a feedstock. Furthermore, compared to bioethanol and gasoline, cellulosic ethanol ensures lower carbon emissions. Our project's primary goal is to demonstrate the manufacture of cellulosic ethanol on Aspen plus using agricultural wastes as raw materials (namely, rice husk) that are conveniently and affordably available in Pakistan. The primary goal is to manufacture affordable, environmentally friendly ethanol. The process starts with the pretreatment of biomass, then moves on to the gasification of biomass, fermentation of syngas to ethanol, and finally, the distillation of ethanol-water mixture to produce 95% pure weight/weight ethanol while using less energy and under optimal temperature and pressure (TP) conditions. The project's findings show that cellulosic ethanol is in fact the most dependable energy source that will help us achieve sustainable development.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

INTRODUCTION

1.1 What is Ethanol?

The family of chemical molecules known as alcohols includes the clear, colorless, and flammable liquid known as ethanol. It has two carbon atoms, six hydrogen atoms, and one oxygen atom in its chemical formula, C_2H_5OH. Grain alcohol and alcohol are two frequent names for ethanol.

Ethanol serves as a valuable chemical feedstock and bio-based fuel in the context of chemical engineering and biofuels. It is generally made by fermenting sugars and starches found in renewable sources like corn, sugarcane, cellulosic biomass, and different agricultural waste products.

Several crucial characteristics of ethanol make it a useful substance:

- Fuel Use: Ethanol is utilized in the transportation industry as a biofuel additive or as a stand-alone fuel. It is either blended with gasoline (E10, E15, or higher blends) or used in flex-fuel cars that can run on high ethanol blends (E85). Burning ethanol releases energy and emits fewer greenhouse gases than burning fossil fuels, which helps to lower carbon dioxide emissions.

- Ethanol has excellent solvent properties and is frequently used in cleaning solutions, cosmetics, personal care items, and medications. It is appropriate for a variety of industrial applications because it can dissolve both polar and non-polar compounds.

- Chemical Intermediate: In the chemical sector, ethanol is a key building block. It serves as a precursor for the creation of many other chemicals and derivatives, including ethylene, acetic acid, ethyl acetate, and other solvents that are used to make adhesives, coatings, and resins for use in plastics.

- Alcoholic beverages like beer, wine, and spirits all contain ethanol as a fundamental ingredient. It contributes significantly to the sensory qualities and flavor preservation of these drinks, as well as the euphoric effects that make them intoxicate.

- Applications in Medicine and Sanitation: Due to its antiseptic qualities, ethanol is frequently used as a component of hand sanitizers, disinfectants, and medical sterilizing treatments.

In order to minimize greenhouse gas emissions, rely less on non-renewable resources, and promote a more sustainable and energy-diverse future, the production and usage of ethanol has gained popularity as a viable substitute for fossil fuels.

In conclusion, ethanol is a versatile substance with a wide range of uses in the chemical, medicinal, energy, and beverage industries. It is a crucial element in the effort to create a more sustainable and low-carbon economy due to its renewable nature, cleaner combustion capabilities, and wide range of applications.

1.2 History of Bio Ethanol from Cellulosic Materials

Over the course of several decades, there have been numerous notable advances and advancements in the field of producing cellulosic ethanol. To lessen dependency on fossil fuels and address environmental concerns, researchers started investigating the possibilities of cellulosic ethanol as an alternative fuel source in the 1970s. Early research centered on deciphering the intricate structure of cellulosic biomass, creating pretreatment techniques to dissolve cellulose and hemicellulose, and finding enzymes effective at hydrolyzing materials. The suitability of several feedstocks, including agricultural wastes, forestry waste, and specialized energy crops, was assessed to produce cellulosic ethanol.

Pilot-scale cellulosic ethanol production plants were set up all over the world in the 2000s. These facilities were created to demonstrate the technical viability and scalability of the manufacture of cellulosic ethanol. To effectively break down cellulose and hemicellulose into fermentable sugars, a number of pretreatment procedures, including acid hydrolysis, steam explosion, and enzymatic hydrolysis, were created and tested. Higher sugar yields from lignocellulosic feedstocks were made possible by improvements in enzymatic hydrolysis' efficiency and cost-effectiveness brought about by advancements in enzyme engineering and biotechnology. In order to increase the variety of available feedstocks, fermentation procedures using specialized microbes that can

ferment a wider range of sugars, such as glucose and xylose, were also created.

With the creation of massive production facilities, the commercialization of cellulosic ethanol experienced a key turning point in the 2010s. Cellulosic ethanol is now more economically viable and competitive with regular ethanol and fossil fuels thanks to technological developments and process optimization. To increase ethanol yields and reduce production costs, businesses invested in cutting-edge pretreatment technology, enhanced enzyme cocktails, and optimized fermentation techniques. Government subsidies and other forms of policy assistance and encouragement, such as renewable fuel mandates, were crucial in advancing the production of cellulosic ethanol on a commercial scale. As a result, numerous commercial-scale cellulosic ethanol facilities with expanded production capacities and improved operational efficiency were put into service all over the world.

The goals of cellulosic ethanol research and development still center on improving sustainability, cost-effectiveness, and efficiency. Continuous improvements in pretreatment techniques, fermentation technologies, enzymatic hydrolysis, and feedstock selection are made to boost process economics and lessen environmental effects. To optimize the value derived from lignocellulosic biomass, integration of cellulosic ethanol production with other biorefinery processes, such as the manufacture of high-value chemicals or bio-based products, is also being investigated. Further advancements in the manufacture of cellulosic ethanol are anticipated to be fueled by ongoing innovation in the fields of enzyme engineering, microorganism genetic engineering, and bioprocess optimization.

The progress of research, technology advancement, and commercialization initiatives over time are highlighted by the history of cellulosic ethanol. Despite persisting difficulties, cellulosic ethanol is seen as a possible replacement for fossil fuels in the quest for a greener and more sustainable future due to ongoing developments and the global focus on renewable and sustainable energy sources.

1.3 Scope and Limitations

Scope of Biomass for Production of Syngas and Ethanol

An important topic for research and development is the manufacture of ethanol and syngas from biomass, which offers a sustainable and renewable energy source. This procedure uses biomass feedstocks like organic waste, agricultural waste, energy crops, and other feedstocks to lessen its dependency on finite fossil fuels and help reduce greenhouse gas emissions. This technology encourages the use of renewable resources and aids in the transition to a future with cleaner energy by turning biomass into syngas and ethanol.

The quantity and widespread accessibility of biomass feedstocks is a significant benefit of biomass to the production of syngas and ethanol. It is possible to set up production facilities in a variety of locations because these feedstocks can be found in different geographical areas. Due to this accessibility, the conversion process is guaranteed a steady and continuous supply of raw materials.

Additionally, ethanol and syngas produced from biomass have the potential to be carbon neutral or even carbon negative. The carbon absorbed during the growth of the biomass feedstock balances the carbon released during the burning of these fuels. The entire carbon footprint is decreased as a result of this closed carbon cycle, which also helps to slow down global warming.

Another important advantage of biomass to the generation of syngas and ethanol is the diversity of the energy mix. We can lessen reliance on a single energy source and increase energy security and resilience by implementing this technology in the energy industry. Additionally, this diversification supports an energy portfolio that is more sustainable and balanced.

The biomass conversion process creates useful byproducts such lignin, organic acids, and charcoal in addition to syngas and ethanol. These byproducts are used in a variety of industrial processes, such as the creation of bio-based materials, chemicals, and soil amendments. Utilizing these byproducts advances a circular economy and adds value to the whole biomass conversion process.

Limitations of Biomass for Production of Syngas and Ethanol

Despite its potential, biomass to syngas and ethanol production has a number of drawbacks that need to be resolved in order for it to be widely used and economically viable.

In the beginning, geographical location, seasonal variations, and logistical difficulties can all have a substantial impact on the availability and logistics of biomass feedstocks. Given that reliable and affordable access to biomass feedstocks is necessary, these factors may have an impact on the cost and viability of biomass conversion processes.

Production of ethanol and syngas from biomass continues to face difficulties with cost competitiveness. The cost of producing syngas and ethanol from biomass can be higher than it is for conventional fossil fuel-based methods. Costlier feedstock conversion, transportation, and collection technologies are mostly to blame. Continuous technological breakthroughs and cost-cutting initiatives are necessary to achieve cost parity with fossil fuels.

The process of turning biomass into syngas and ethanol is also fraught with technical difficulties. Complex procedures like pretreatment, enzymatic hydrolysis, fermentation, and gasification are a part of the procedure. To enhance efficiency and obtain high conversion rates, these processes need to be carefully optimized. Low conversion rates, enzyme effectiveness, and reactor scaling up for industrial-scale production are difficulties.

Concerns about resources and the environment are raised by the large-scale production of biomass for energy. It could have an effect on how much land is used, how much water is used, how good the soil is, and how much food is produced. The long-term profitability of biomass to syngas and ethanol production depends on ensuring sustainable biomass sourcing and limiting environmental consequences.

Frameworks for supportive market infrastructure and regulation are also necessary for the growth of biomass to syngas and ethanol production. This entails setting up processing facilities, distribution systems, and market demand for the ethanol and syngas generated. To encourage investment, market development, and the expansion of the biomass conversion sector, the government must provide adequate policy support through mandates, mandated actions, and regulations.

Furthermore, to solve the current limits of biomass conversion technology, constant technological developments are required. Enhancing pretreatment's effectiveness,

scalability, and cost-effectiveness should be the main goals of research and development.

1.4 Why Choose Bagasse as Feed

Bagasse is the fibrous byproduct left over after the juice from sugarcane stalks is extracted. Due to its availability and renewable nature, it is frequently utilized as a biomass feedstock for energy generation and a variety of other applications. It is a byproduct of the sugar industry.

Depending on variables including sugarcane type, processing techniques, and ambient circumstances, bagasse content may vary slightly. However, cellulose, hemicellulose, and lignin make up the majority of bagasse's three basic ingredients. Here is a table outlining bagasse's general composition:

Table 1 – Bagasse Composition

Component	Approximate Composition (%)
Cellulose	40-50
Hemicellulose	20-25
Lignin	20-25
Other components	5-10

The primary polysaccharide in bagasse is cellulose, which provides structural.
integrity to the plant cell walls. Hemicellulose is a polysaccharide group that surrounds cellulose fibers and contributes to the overall structure of biomass. Lignin is a complex polymer that functions as a binding agent and gives cell walls their rigidity. These three components constitute the preponderance of bagasse's biomass content.

Bagasse is abundant in Pakistan due to numerous factors. First, Pakistan is one of the largest sugarcane-producing nations, and the country is home to a significant number of sugar facilities. As a byproduct of the sugarcane industry, bagasse is readily available in significant quantities.

In addition, bagasse is a desirable biomass feedstock due to its renewable nature and the economic benefits associated with its use. Pakistan's sugar industry recognizes bagasse's value as a potential energy source and has increased its investment in technologies to extricate maximum value from this abundant biomass residue. Sugar mills use bagasse for cogeneration of electricity and heat, which reduces their reliance on fossil fuels and contributes to energy security and sustainability.

In addition, bagasse has the potential to be used in the production of biofuels, such as cellulosic ethanol, via processes such as biomass gasification and fermentation. This is consistent with the global trend toward renewable and sustainable energy sources, making bagasse an attractive resource for bioenergy production in Pakistan.

The combination of a flourishing sugarcane industry, an abundance of bagasse as a byproduct, and an increasing recognition of its value as a renewable resource has made bagasse readily available in Pakistan for various applications, especially in the energy sector.

PROCESS DESCRIPTION

2.1   Process Flow Diagram

Figure 1 Process Flow Diagram

2.2 Process Description

The production of ethanol through the pyrolysis and fermentation of biomass is a promising route for the sustainable production of biofuels. The procedure begins with the preparation of biomass feedstock, such as wood particles or agricultural residues, by means of size reduction, drying, and impurity elimination. The biomass is then fed into a gasification apparatus for thermochemical conversion. In this facility, biomass is exposed to high temperatures and an oxygen-depleted environment under controlled conditions, resulting in the production of syngas. Carbon monoxide (CO), hydrogen (H_2), carbon dioxide (CO_2), and trace quantities of methane (CH_4) and nitrogen (N_2) make up the majority of the syngas.

The unprocessed syngas produced by biomass gasification must be purified to eliminate impurities and contaminants. Through processes such as filtration, scouring, and catalytic conversion, tars, particulates, sulfur compounds, and trace metals are removed. Syngas purification is essential for enhancing the purity and stability of syngas for use in downstream processes. After the cleansing phase, the conditioned syngas is subjected to additional conditioning to optimize its composition for ethanol fermentation. This involves modifying the ratio of carbon monoxide to hydrogen (CO/H_2) to promote ethanol production. Utilizing the water-gas shift reaction to convert excess CO to CO_2 and H_2 improves the efficiency of ethanol synthesis.

After conditioning the syngas, it is available for ethanol fermentation. In the fermentation device, specialized microorganisms such as acetogenic bacteria such as Clostridium ljungdahlii or Clostridium autoethanogenum or specific yeast strains such as Saccharomyces cerevisiae are introduced. Through biochemical reactions, these microorganisms metabolize the components of syngas (CO and H_2) into ethanol. To ensure optimal microbial activity and ethanol production, the fermentation process is meticulously regulated, with temperature, pH, and nutrient availability optimized.

The mélange that results from fermentation contains ethanol, residual syngas components, water, and byproducts. To isolate ethanol from the fermentation liquid, the mixture is subjected to separation processes, mainly distillation or fractional distillation. Additional purification processes, such as molecular sieve dehydration or azeotropic distillation, can be used to remove water and further concentrate ethanol. These purification steps assist in achieving the desired ethanol concentration, such as

anhydrous ethanol, which is appropriate for a variety of applications, such as fuel blending and chemical synthesis.

In addition to producing ethanol, the gasification procedure may also produce valuable byproducts. As co-products, for instance, syngas-derived compounds or biochar can be recovered alongside ethanol. These byproducts have multiple applications, including chemical synthesis, energy generation, and soil amendment. The recovery and use of co-products contribute to the overall effectiveness and viability of the biomass gasification and fermentation process.

To preserve its quality, the produced ethanol is stored in suitable containers, such as tanks or barrels. Through an established network, ethanol is distributed to end-users such as fuel distributors, compounding facilities, and chemical manufacturers. Compared to fossil fuels, the production of ethanol through biomass gasification and fermentation offers significant environmental benefits. It reduces greenhouse gas emissions and reliance on nonrenewable resources, making the energy sector more sustainable.

This comprehensive overview of the various stages involved in converting biomass into a valuable biofuel is provided by the detailed process description of ethanol production via biomass gasification and fermentation.

2.2 Main Reactions Involved

If the biomass feedstock is bagasse, which is a fibrous residue obtained from sugarcane processing, the reactions involved in the conversion of bagasse to syngas and further to ethanol are as follows:

Biomass Gasification:
- $C_6H_{10}O_5$ (Cellulose) + $H_2O \rightarrow C_6H_{12}O_6$ (Glucose)
- $C_6H_{10}O_5$ (Cellulose) + $O_2 \rightarrow 6CO + 5H_2$
- $C_5H_8O_4$ (Hemicellulose) + $H_2O \rightarrow C_5H_{10}O_5$ (Xylose)
- $C_5H_8O_4$ (Hemicellulose) + $O_2 \rightarrow 5CO + 4H_2$
- $C_{10}H_{16}O_8$ (Lignin) + $H_2O \rightarrow C_{10}H_{18}O_9$ (Monosaccharides)
- $C_{10}H_{16}O_8$ (Lignin) + $O_2 \rightarrow 10CO + 8H_2$

Syngas Production:
- $C_6H_{12}O_6$ (Glucose) $\rightarrow 2C_2H_5OH$ (Ethanol) + $2CO_2$
- $C_5H_{10}O_5$ (Xylose) $\rightarrow 2C_2H_5OH$ (Ethanol) + $2CO_2$
- $C_{10}H_{18}O_9$ (Monosaccharides) $\rightarrow 2C_2H_5OH$ (Ethanol) + $2CO_2$
- $C_6H_{12}O_6$ (Glucose) $\rightarrow 2CH_3OH$ (Methanol) + $2CO$
- $C_5H_{10}O_5$ (Xylose) $\rightarrow 2CH_3OH$ (Methanol) + $2CO$
- $C_{10}H_{18}O_9$ (Monosaccharides) $\rightarrow 2CH_3OH$ (Methanol) + $2CO$

Ethanol Fermentation:
- C_2H_5OH (Ethanol) $\rightarrow C_2H_4$ (Ethylene) + H_2O

- C2H5OH (Ethanol) + CO2 → C2H4O (Acetaldehyde) + H2O
- C2H5OH (Ethanol) + H2O → C2H5O2 (Ethyl Acetate)
- C2H5OH (Ethanol) → CH3CHO (Acetaldehyde) + H2
- C2H5OH (Ethanol) + C6H8O7 (Citric Acid) → C2H4O2 (Acetic Acid) + H2O

MASS BALANCE

The foundation of the material balance is the law of conservation of mass, which asserts that mass can never be generated or destroyed and is always conserved in all processes. The concept of mass conservation is used to analyze physical systems utilizing the concept of material balance, also referred to as mass balance. By taking into consideration the material entering and leaving a system, mass fluxes that would have been undiscovered or challenging to measure without this methodology can be found. Chemical engineering calculations typically make use of material balances, particularly when designing equipment and calculating flows into and out of a gas absorption column as well as reflux ratios and boil-up ratios. This is how the general mass balance equation is expressed:

Accumulation within the system = (Mass into the system) – (Mass out of the system) + (Generation within the system) – (Consumption within the system)

(Eq. 4.1)

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

3.1 Separator 1

Input = Output + Accumulation $\pm$ Generation/Consumption

From law of conservation of mass, we get:

mass flow rate of component in = mass flow rate

of component out. Results are tabulated as follows:

Table 2 - Separator Mass Balance

Stream Name	Units	S2	CELLULOSE	H2O	HEMICEL	LIGNIN	S6
Mass Flows	kg/hr	1945.14	857.812	173.118	499.904	394.866	19.4515
H2O	kg/hr	173.118	0.0	173.118	0.0	0.0	0.0
SO2	kg/hr	19.45	0.0	0.0	0.0	0.0	19.4515
CELULOSE	kg/hr	857.812	857.812	0.0	0.0	0.0	0.0
HEMICEL	kg/hr	499.9	0.0	0.0	499.904	0.0	0.0
LIGNIN	kg/hr	394.866	0.0	0.0	0.0	394.866	0.0

3.2 Reactor P1A

From law of conservation of mass, we get:

$$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$$

Reaction involved is:

$$HEMICEL \rightarrow 0.4\ HEMA1 + 0.6\ HEMA2$$

Table 3 - Reactor P1A Mass Balance

Stream Name	Units	CELLULOSE	HEMICEL	LIGNIN	S8
Mass Flows	kg/hr	857.812	499.904	394.866	1752.58
CELULOSE	kg/hr	857.812	0.0	0.0	857.812
HEMICEL	kg/hr	0.0	499.904	0.0	0.0
LIGNIN	kg/hr	0.0	0.0	394.866	394.866
HEMA-2	kg/hr	0.0	0.0	0.0	299.942
HEMA-1	kg/hr	0.0	0.0	0.0	199.962

3.3   Reactor P1B

From law of conservation of mass, we get:

$$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$$

Reactions involved are:

$$LIGNIN \rightarrow LIGA$$
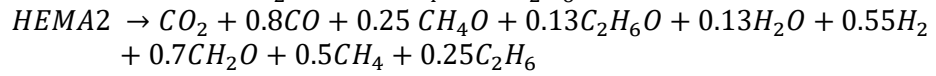
$$CELLULOSE \rightarrow ACTCELLT$$

$$CELLULOSE \rightarrow 6C + 5H_2O$$

$$HEMA1 \rightarrow 0.6\ XYLOSE + 0.17\ C_2H_4O_2 + 0.33\ F_2$$
$$HEMA1 \rightarrow 0.2\ H_2 + CO_2 + CO + 0.5\ CH_2O + 0.25\ CH_4O + 0.13\ C_2H_6O$$
$$+ 0.13H_2O + 0.7\ CH_4 + 0.3C_2H_6 + 0.7C$$
$$HEMA2 \rightarrow CO_2 + 0.8CO + 0.25\ CH_4O + 0.13C_2H_6O + 0.13H_2O + 0.55H_2$$
$$+ 0.7CH_2O + 0.5CH_4 + 0.25C_2H_6$$
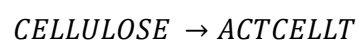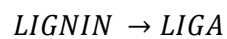
Table 4 – Reactor P1B Mass Balance

Stream Name	Units	S6	S8	S9
Mass Flows	kg/hr	19.4515	1752.58	1772.03
CH4O	kg/hr	0.0	0.0	24.49
H2O	kg/hr	0.0	0.0	45
SO2	kg/hr	19.4515	0.0	19.45
CELULOSE	kg/hr	0.0	857.812	0.0
LIGNIN	kg/hr	0.0	394.866	0.0
H2	kg/hr	0.0	0.0	2.83
CO	kg/hr	0.0	0.0	72.92
CO2	kg/hr	0.0	0.0	134.55
C2H6O	kg/hr	0.0	0.0	17.61
F-F	kg/hr	0.0	0.0	23.3
C	kg/hr	0.0	0.0	64.4
C2H4O2	kg/hr	0.0	0.0	7.27
LIGA	kg/hr	0.0	0.0	394.866
XYLOSE	kg/hr	0.0	0.0	65.4417
ACTCELLT	kg/hr	0.0	0.0	789.187
CH2O	kg/hr	0.0	0.0	59.5
C2H6	kg/hr	0.0	0.0	24.16
CH4	kg/hr	0.0	0.0	27.04
HEMA-2	kg/hr	0.0	299.94	0.0
HEMA-1	kg/hr	0.0	199.96	0.0

3.4   Reactor P1C

From law of conservation of mass, we get:

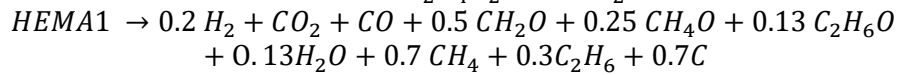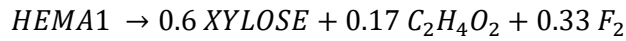*mass flow rate of component in = mass flow rate of component out*
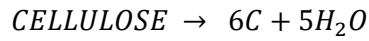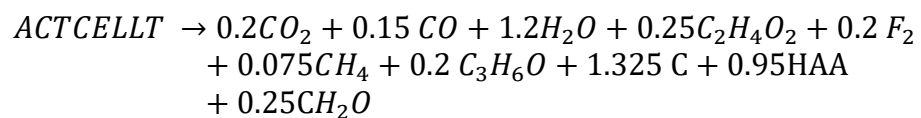
Reactions involved are:

$$ACTCELLT \rightarrow LVG$$

$$ACTCELLT \rightarrow 0.2CO_2 + 0.15\ CO + 1.2H_2O + 0.25C_2H_4O_2 + 0.2\ F_2$$
$$+ 0.075CH_4 + 0.2\ C_3H_6O + 1.325\ C + 0.95HAA$$
$$+ 0.25CH_2O$$

14

Table 5 – Reactor P1C Mass Balance

Stream Name	Units	S9	S10
Mass Flows	kg/hr	1772.03	1772.03
CH_4O	kg/hr	24.49	24.49
H_2O	kg/hr	45.0	55.53
SO_2	kg/hr	19.45	19.45
H_2	kg/hr	2.83	2.83
CO	kg/hr	72.92	74.96
CO_2	kg/hr	134.55	138.84
C_2H_6O	kg/hr	17.6	17.6
F-F	kg/hr	23.26	32.62
C	kg/hr	64.38	72.13
LVG	kg/hr	0.0	710.26
$C_2H_4O_2$	kg/hr	7.27	14.57
HAA	kg/hr	0.0	27.76
LIGA	kg/hr	394.86	394.86
XYLOSE	kg/hr	65.44	65.44
ACTCELLT	kg/hr	789.2	0.0
CH_2O	kg/hr	59.53	63.18
C_2H_6	kg/hr	24.16	24.16
CH_4	kg/hr	27.0	27.63
C_3H_6O	kg/hr	0.0	5.65

3.5   Reactor P1D

From law of conservation of mass, we get:

mass flow rate of component in = mass flow rate of component out

Reactions involved are:

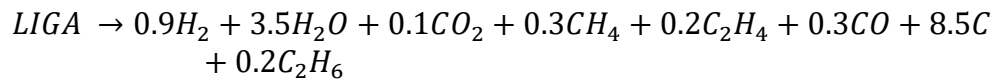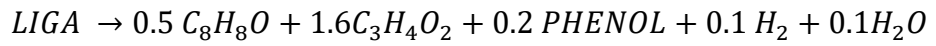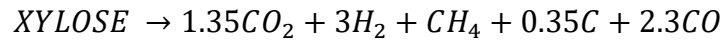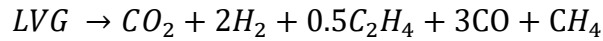$$LIGA \rightarrow 0.5\ C_8H_8O + 1.6C_3H_4O_2 + 0.2\ PHENOL + 0.1\ H_2 + 0.1H_2O$$

$$LIGA \rightarrow 0.9H_2 + 3.5H_2O + 0.1CO_2 + 0.3CH_4 + 0.2C_2H_4 + 0.3CO + 8.5C + 0.2C_2H_6$$

Table 6 – Reactor P1D Mass Balance

Stream Name	Units	S10	S11
Mass Flows	kg/hr	1772.0	1772.0
CH4O	kg/hr	24.49	24.49
H2O	kg/hr	55.53	151.6
SO2	kg/hr	19.45	19.45
PHENOL	kg/hr	0.0	9.47
H2	kg/hr	2.83	5.67
CO	kg/hr	74.96	87.64
CO2	kg/hr	138.84	145.48
C2H6O	kg/hr	17.6	17.6
F-F	kg/hr	32.62	32.62
C	kg/hr	72.13	226.23
LVG	kg/hr	710.26	710.26
C2H4O2	kg/hr	14.57	14.57
HAA	kg/hr	27.76	27.76
C8H8O	kg/hr	0.0	30.23
LIGA	kg/hr	394.86	0.0
XYLOSE	kg/hr	65.44	65.44
CH2O	kg/hr	63.18	63.18
C2H6	kg/hr	24.16	33.24
CH4	kg/hr	27.63	34.89
C2H4	kg/hr	0.0	8.46
C3H4O2	kg/hr	0.0	58.0
C3H6O	kg/hr	5.65	5.65

3.6 Reactor CSTR1

From law of conservation of mass, we get:
mass flow rate of component in = mass flow rate of component out
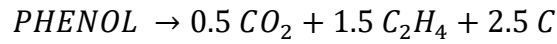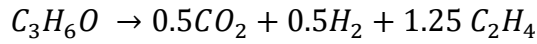Reactions involved are:

$$HAA \rightarrow 2CO + 2H_2$$

$$C_2H_4O_2 \rightarrow 2CO + 2H_2$$

$$C_3H_4O_2 \rightarrow CO_2 + C_2H_4$$

$$F_2 \rightarrow CH_4 + 2CO + 2C$$

$$C_8H_8O \rightarrow CO + CH_4 + 4C + C_2H_4$$

$$C_3H_6O \rightarrow 0.5CO_2 + 0.5H_2 + 1.25\,C_2H_4$$

$$PHENOL \rightarrow 0.5\,CO_2 + 1.5\,C_2H_4 + 2.5\,C$$

$$LVG \rightarrow CO_2 + 2H_2 + 0.5C_2H_4 + 3CO + CH_4$$

$$XYLOSE \rightarrow 1.35CO_2 + 3H_2 + CH_4 + 0.35C + 2.3CO$$
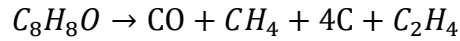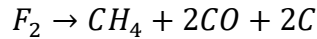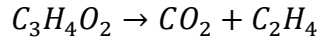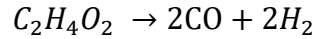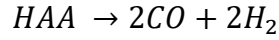
Table 7 – CSTR 1 Mass Balance

Stream Name	Units	H20	S11	S12
Mass Flows	kg/hr	173.12	1772.03	1945.15
CH4O	kg/hr	0.0	24.49	24.49
H2O	kg/hr	173.12	151.61	324.73
SO2	kg/hr	0.0	19.45	19.45
PHENOL	kg/hr	0.0	9.47	9.47
H2	kg/hr	0.0	5.67	20.0
CO	kg/hr	0.0	87.64	386.25
CO2	kg/hr	0.0	145.47	301.86
C2H6O	kg/hr	0.0	17.6	17.6
F-F	kg/hr	0.0	32.62	32.62
C	kg/hr	0.0	226.23	226.23
LVG	kg/hr	0.0	710.26	134.10
C2H4O2	kg/hr	0.0	14.57	14.57
HAA	kg/hr	0.0	27.76	27.76
C8H8O	kg/hr	0.0	30.22	30.22
XYLOSE	kg/hr	0.0	65.44	65.44
CH2O	kg/hr	0.0	63.18	63.18
C2H6	kg/hr	0.0	33.24	33.24
CH4	kg/hr	0.0	34.89	91.9
C2H4	kg/hr	0.0	8.46	58.31
C3H4O2	kg/hr	0.0	58.01	58.01
C3H6O	kg/hr	0.0	5.65	5.65

3.7   Reactor CSTR2

From law of conservation of mass, we get:

$$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$$

Table 8 - CSTR 2 Mass Balance

Stream Name	Units	AIR	S7	S12	S4
Mass Flows	kg/hr	1100	20	1945.15	3065.15
CH4O	kg/hr	0	0	24.49	24.49
H2O	kg/hr	0	20	324.73	344.73
N2	kg/hr	843.79	0	0	843.79
O2	kg/hr	256.2	0	0	256.2
S02	kg/hr	0	0	19.45	19.45
PHENOL	kg/hr	0	0	9.47	9.47
H2	kg/hr	0	0	20.0	20.0
CO	kg/hr	0	0	386.24	386.24
CO2	kg/hr	0	0	301.86	301.86
C2H60	kg/hr	0	0	17.60	17.60
F-F	kg/hr	0	0	32.62	32.62
C	kg/hr	0	0	226.23	226.23
LVG	kg/hr	0	0	134.10	134.10
C2H4O2	kg/hr	0	0	14.57	14.57
HAA	kg/hr	0	0	27.76	27.76
C8H8O	kg/hr	0	0	30.23	30.23
XYLOSE	kg/hr	0	0	65.44	65.44
CH2O	kg/hr	0	0	63.18	63.18
C2H6	kg/hr	0	0	33.24	33.24
CH4	kg/hr	0	0	91.90	91.90
C2H4	kg/hr	0	0	58.31	58.31
C3H4O2	kg/hr	0	0	58.01	58.01
C3H6O	kg/hr	0	0	5.65	5.65

3.8 Gasifier

From law of conservation of mass, we get:

mass flow rate of component in = mass flow rate of component out

Table 9 - Gasifier Mass Balance

Stream Name	Units	S4	S1
Mass Flows	kg/hr	3065.15	3065.15
CH4O	kg/hr	24.49	0
H2O	kg/hr	344.73	53.74
N2	kg/hr	843.79	843.79
NH3	kg/hr	0	0.098
O2	kg/hr	256.2	0
S02	kg/hr	19.45	19.45
PHENOL	kg/hr	9.47	0
H2	kg/hr	20.0	119.53
CO	kg/hr	386.24	1851.53
CO2	kg/hr	301.86	160.34
C2H60	kg/hr	17.60	0
F-F	kg/hr	32.62	0
C	kg/hr	226.23	0
LVG	kg/hr	134.10	0
C2H4O2	kg/hr	14.57	0
HAA	kg/hr	27.76	0
C8H8O	kg/hr	30.23	0
XYLOSE	kg/hr	65.44	0
CH2O	kg/hr	63.18	0
C2H6	kg/hr	33.24	0
CH4	kg/hr	91.90	16.73

C2H4	kg/hr	58.31	0
C3H4O2	kg/hr	58.01	0
C3H6O	kg/hr	5.65	0

3.9 Separator

From law of conservation of mass, we get:

mass flow rate of component in = mass flow rate of component out

Table 10 - Separator Mass Balance

Stream Name	Units	S3	S13	S14
Mass Flows	kg/hr	3065.15	2185.16	879.98
H2O	kg/hr	53.74	53.74	0
N2	kg/hr	843.71	0	843.71
NH3	kg/hr	0.098	0	0.098
S02	kg/hr	19.45	0	19.45
H2	kg/hr	119.55	119.55	0
CO	kg/hr	1851.53	1851.53	0
CO2	kg/hr	160.34	160.34	0
CH4	kg/hr	16.73	0	16.73

3.10 Mixer

From law of conservation of mass, we get:

mass flow rate of component in = mass flow rate of component out

Table 11 - Mixer Mass Balance

Stream Name	Units	S13	S15	S16
Mass Flows	kg/hr	2185.16	567.5	2752.66
H2O	kg/hr	53.74	567.5	621.24
H2	kg/hr	119.55	0	119.55
CO	kg/hr	1851.53	0	1851.53
CO2	kg/hr	160.34	0	160.34
CAE	kg/hr	0	500.0	500.0

3.11 Fermenter

From law of conservation of mass, we get:

$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$
Reactions involved are:
$$CO + H_2O \rightarrow C_6H_2O + CO_2$$
$$CO_2 + H_2 \rightarrow C_6H_2O + H_2O$$
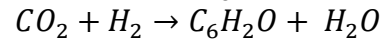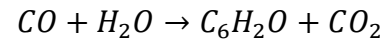
Table 12 – Fermenter Mass Balance

Stream Name	Units	S16	S17
Mass Flows	kg/hr	2752.66	3042.66
H2O	kg/hr	621.24	1223.8
H2	kg/hr	119.55	148.1
CO	kg/hr	1851.53	92.57
CO2	kg/hr	160.34	100.14
C2H60	kg/hr	0	1478
CAE	kg/hr	500.0	500.0

3.12 Flash Drum Separator

From law of conservation of mass, we get:

$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$

Table 13 - Flash Drum Separator Mass Balance

Stream Name	Units	S17	S18	S28
Mass Flows	kg/hr	3042.66	340.82	2701.85
H2O	kg/hr	1223.85	0	1223.85
H2	kg/hr	148.1	148.1	0
CO	kg/hr	92.57	92.57	0
CO2	kg/hr	100.14	100.14	0
C2H60	kg/hr	1478	0	1478
CAE	kg/hr	500.0	500.0	0

3.13 Distillation Column1

From law of conservation of mass, we get:

$$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$$

Table 14 - Distillation column 1 Mass Balance

Stream Name	Units	S28	S20	S21
Mass Flows	kg/hr	2701.85	2071.21	630.64
H2O	kg/hr	1223.85	213.5	630.64
C2H60	kg/hr	1478	1478	1.06e^-5

3.14 Distillation Column2

From law of conservation of mass, we get:

$$mass\ flow\ rate\ of\ component\ in = mass\ flow\ rate\ of\ component\ out$$

Table 15 - Distillation column 2 Mass Balance

Stream Name	Units	S20	S25	S26
Mass Flows	kg/hr	2071.21	1544.17	527.043
H2O	kg/hr	213.5	66.18	527.03
C2H60	kg/hr	1478	1477.98	0.01265

ENERGY BALANCE

Energy is the term used to describe a body's capacity to accomplish work. Among the several types of energy are kinetic energy, potential energy, chemical energy, and internal energy. In a moving or dynamic system, these energies are interconvertible, making it challenging to separate them all out. However, in other situations, a particular type predominates.

We may evaluate a system and determine whether energy has been conserved using the energy balance. This balance in a chemical system is typically calculated using heat flow or enthalpy, where enthalpy is the total amount of heat present in a system. Internal energy and work are additional foundation for energy balance in chemical engineering. Energy balances are typically used to estimate the heat transfer between various surfaces or layers so that the equipment can be designed appropriately. They can also be used to estimate the number of utilities needed to run a plant.

4.1 General Energy Balance Equation

The law of conservation of energy states that although energy cannot be generated or destroyed, it can be changed from one form to another. This assumption is expressed in thermodynamics by the general energy balance equation, which is as follows:

$$\Delta U + \Delta E_k + \Delta E_p = \boldsymbol{Q} - W_{shaft} + W_f$$

(Eq 5.1)

$$here, \; W_{shaft} = P\Delta V \; \& \; H = U + P\Delta V$$

The symbols used in the above equation are explained below:

Table 16 - Symbols used in equations.

Symbol	Meaning
U	Internal Energy
H	Enthalpy
E_k	Kinetic Energy
E_p	Potential Energy
Q	Heat
W_{shaft}	Shaft Work
W_{flow}	Flow Work
P	Pressure
V	Volume

Assumptions & Simplifications

1. The Enthalpy of each stream was calculated using the following formula:

$$H_T = m \int_{To}^{T} CpdT$$

(Eq 5.2)

2. Kinetic energy & potential energy changes are negligible. Open system, so flow work is included and H is used instead of U. Applying the simplifications above, we arrive at the simplified energy balance equation:

$$\Delta H = \boldsymbol{Q} + W$$

(Eq 5.3)

3. To calculate C_p of a mixed stream, containing more than one chemical species, the summability relation was used:

C_p(mixture) = x_A $C_{p,A}$ + x_B $C_{p,B}$ + x_C $C_{p,C}$ + …

24

(Eq 5.4)

4. To calculate energy losses by convection and radiation, the following relations were used:

$$Qcon = \alpha con \times (Ts - Ta) \times As + \varepsilon \times \sigma \times ((Ts + 273.15)^4 - (Ta + 273.15)^4) \times As$$

$$Qrad = \varepsilon \times \sigma \times ((Ts + 273.15)^4 - (Ta + 273.15)^4) \times As$$

Once the required material balances were carried out, we were able to conduct energy balances on appropriate equipment.

4.2 Reactor P1A

Table 17 – Energy Balance on Reactor P1A

Extent (kmol/hr)	Heat of reaction (kJ/hr)	Reference Component
3.78	-1.19e^-10	HEMICEL

Reaction involved is:

$$HEMICEL \rightarrow 0.4\ HEMA1 + 0.6\ HEMA2$$

4.3 Reactor P1B

Table 18 – Energy Balance on Reactor P1B

Extent (kmol/hr)	Heat of reaction (kJ/kmol)	Reference Component
0.42	4.13e^6	CELLULOSE
4.86	0.0	CELLULOSE
0.73	183236	HEMA-1
2.0	0.0	LIGNIN
0.78	596442	HEMA-1
2.27	832710	HEMA-2

Reactions involved are:

$$LIGNIN \rightarrow LIGA$$

$$CELLULOSE \rightarrow ACTCELLT$$

$$CELLULOSE \rightarrow 6C + 5H_2O$$

$$HEMA1 \rightarrow 0.6\ XYLOSE + 0.17\ C_2H_4O_2 + 0.33\ F_2$$
$$HEMA1 \rightarrow 0.2\ H_2 + CO_2 + CO + 0.5\ CH_2O + 0.25\ CH_4O + 0.13\ C_2H_6O$$
$$+ 0.13H_2O + 0.7\ CH_4 + 0.3C_2H_6 + 0.7C$$
$$HEMA2 \rightarrow CO_2 + 0.8CO + 0.25\ CH_4O + 0.13C_2H_6O + 0.13H_2O + 0.55H_2$$
$$+ 0.7CH_2O + 0.5CH_4 + 0.25C_2H_6$$
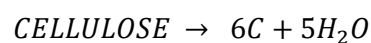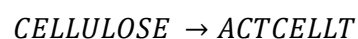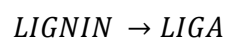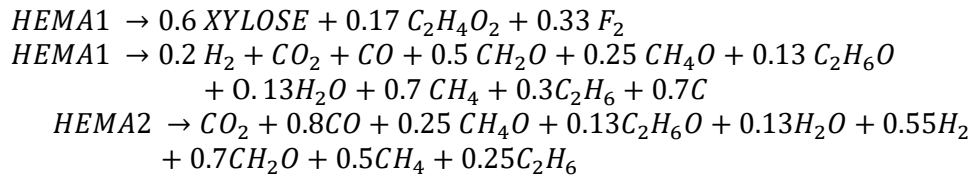
4.4 Reactor P1C

Table 19 – Energy Balance on Reactor P1C

Fractional Conversion	Extent (kmol/hr)	Heat of reaction(kJ/kmol)	Reference Component
0.1	0.48	1.10e^6	ACTCELLT
0.9	4.38	0.0	ACTCELLT

Reactions involved are:

$$ACTCELLT \rightarrow LVG$$

$$ACTCELLT \rightarrow 0.2CO_2 + 0.15\ CO + 1.2H_2O + 0.25C_2H_4O_2 + 0.2\ F_2$$
$$+ 0.075CH_4 + 0.2\ C_3H_6O + 1.325\ C + 0.95HAA$$
$$+ 0.25CH_2O$$
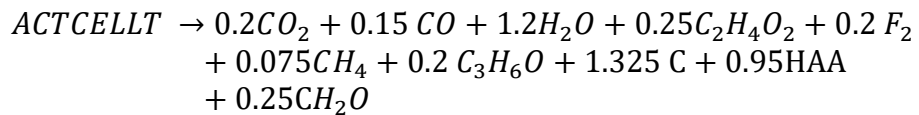
4.5 Reactor P1D

Table 20 – Energy Balance on Reactor P1D

Fractional Conversion	Extent(kmol/hr)	Heat of reaction (kJ/kmol)	Reference Component
0.3	0.50	-24187.7	LIGA
0.8	1.51	5.67e^6	LIGA

Reactions involved are:

$$LIGA \rightarrow 0.5\ C_8H_8O + 1.6C_3H_4O_2 + 0.2\ PHENOL + 0.1\ H_2 + 0.1H_2O$$

$$LIGA \rightarrow 0.9H_2 + 3.5H_2O + 0.1CO_2 + 0.3CH_4 + 0.2C_2H_4 + 0.3CO + 8.5C$$
$$+ 0.2C_2H_6$$
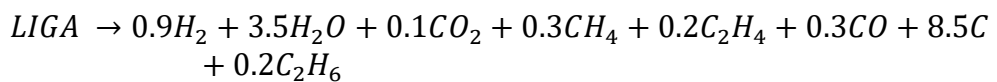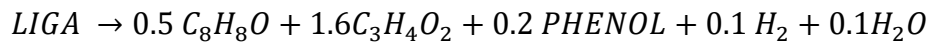
4.6 CSTR 1

Table 21 – Energy Balance on Reactor CSTR 1

	IN	OUT
Enthalpy (kW)	209.21	917.7
Total Duty (kW) =	708.5	

Reactions involved are:

$$HAA \rightarrow 2CO + 2H_2$$

$$C_2H_4O_2 \rightarrow 2CO + 2H_2$$

$$C_3H_4O_2 \rightarrow CO_2 + C_2H_4$$

$$F_2 \rightarrow CH_4 + 2CO + 2C$$

$$C_8H_8O \rightarrow CO + CH_4 + 4C + C_2H_4$$

$$C_3H_6O \rightarrow 0.5CO_2 + 0.5H_2 + 1.25\,C_2H_4$$

$$PHENOL \rightarrow 0.5\,CO_2 + 1.5\,C_2H_4 + 2.5\,C$$

$$LVG \rightarrow CO_2 + 2H_2 + 0.5C_2H_4 + 3CO + CH_4$$

$$XYLOSE \rightarrow 1.35CO_2 + 3H_2 + CH_4 + 0.35C + 2.3CO$$
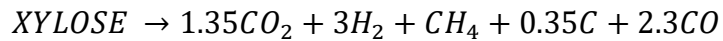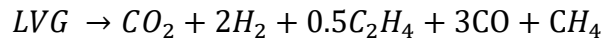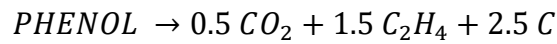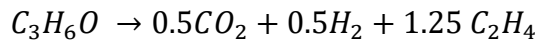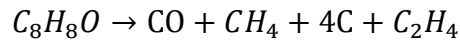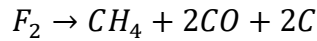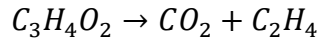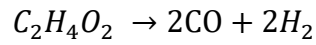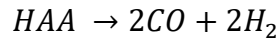
4.7   CSTR2

Table 22– Energy Balance on Reactor CSTR 2

	IN	OUT
Enthalpy (kW)	959.23	1124.7
Total Duty (kW) =	165.48	

4.8   Gasifier

Table 23 – Energy Balance on Gasifier

Streams	IN	OUT
Enthalpy (kW)	1124.71	-1577.05
Duty (kW)	-2701.76	
Temperature	800 degree C	

4.9 Fermenter
Reactions involved are:

$$CO + H_2O \rightarrow C_6H_2O + CO_2$$
$$CO_2 + H_2 \rightarrow C_6H_2O + H_2O$$
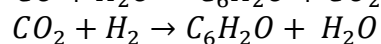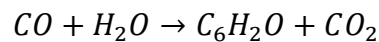
Table 24 – Energy Balance on Fermenter

Extent (kmol/hr)	Heat of reaction (kJ/kmol)	Fractional conversion	Reactant
10.46	-70059.3	0.95	CO
21.61	-86692	0.95	CO2

	IN	OUT
Enthalpy kW	-4437.39	-7588.28
Duty (kW)	-3150.89	
Temperature	60 degree C	

EQUIPMENT DESIGN

5.1 Distillation Column

To calculate the column top temperature, the system was simplified into a pseudo-binary form by selecting the high-key and low-key components. Once these components were chosen and their compositions were fixed, the next step was to determine the temperature at the column ends.

The column top temperature was obtained by performing dew point calculations at various temperatures and selecting the temperature that satisfied the given equation.

Equation 7.2 =

$$\sum x_i = \sum \frac{y_i}{K_i} = 1$$

The composition and K values for each component were readily obtained literature for the process streams. By evaluating various temperatures through bubble point calculations, it was determined that a temperature of 79 °C satisfied the relation for the column top temperature.

Similarly, for the column bottom temperature, bubble point calculations were performed at different temperatures. It was found that a temperature of 100°C satisfied the given relation.

Equation 7.1 =

$$\sum y_i = \sum K_i x_i = 1$$

After obtaining the temperatures for the column top and bottom, the next step was to determine the minimum number of stages required. This calculation was accomplished using Fenske's Equation, which provides the minimum number of plates needed for the desired distillate and bottoms compositions.

Fenske's Equation takes into account factors such as the relative volatility of the components and the desired separation efficiency. By applying this equation, the minimum number of stages required for the given distillate and bottoms compositions was calculated.

Equation 7.3=

$$N_m = \frac{\log\left[\frac{x_{LK}}{x_{HK}}\right]_d \log\left[\frac{x_{HK}}{x_{LK}}\right]_b}{\log \alpha_{LK}}$$

Nm= 16

5.1.1 Minimum Reflux Ratio

To calculate the parameter theta (θ) in the Underwood equation, the following steps can be followed. First, obtain the equilibrium data for the components and determine their relative volatility (α). Then, calculate the Murphree vapor efficiency (η) using the equation (η = (α - 1) / (α - θ)). Assume an initial value for θ and calculate η. Iterate the calculation by adjusting θ until η converges to a desired accuracy. Finally, use the determined value of θ in the Underwood equation for further distillation design.

Equation 7.4=
$$\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q$$

Use q=0 as feed used is liquid to find Theta.

Calculated Theta = 1.71 and then using equation 7.5 find minimum reflux ratio.

Equation 7.5=
$$\sum \frac{\alpha_i x_{i,d}}{\alpha_i - \theta} = R_m + 1$$

5.1.2 Number of Ideal stages

Using the formula:
Rm + 1 = 3.35
Rm = 2.35
R = 1.4*Rm
R = 3.29

$$\frac{Rm}{Rm + 1} = 0.59$$
$$\frac{R}{R + 1} = 0.74$$

Now from graph,

$$\frac{Nm}{N} = 0.69$$

Minimum Number of plates = Nm =16
Actual number of plates = N = 23
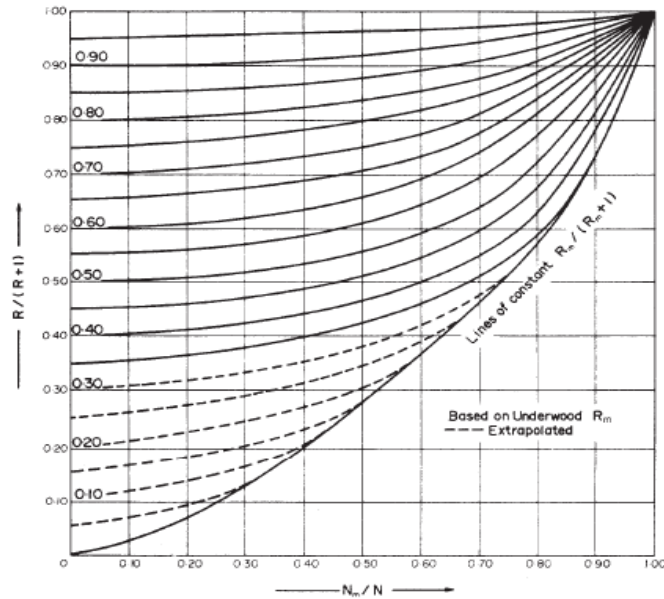
Figure 1 - Underwood equation graph

5.1.3 Feed Point Calculations

$$\log\left[\frac{N_r}{N_s}\right] = 0.206 \log\left[\left(\frac{B}{D}\right)\left(\frac{x_{f,\text{HK}}}{x_{f,\text{LK}}}\right)\left(\frac{x_{b,\text{LK}}}{x_{d,\text{HK}}}\right)^2\right]$$

where N_r = number of stages above the feed, including any partial condenser,

N_s = number of stages below the feed, including the reboiler,

B = molar flow bottom product,

D = molar flow top product,

$x_{f,\text{HK}}$ = concentration of the heavy key in the feed,

$x_{f,\text{LK}}$ = concentration of the light key in the feed,

$x_{d,\text{HK}}$ = concentration of the heavy key in the top product,

$x_{b,\text{LK}}$ = concentration of the light key if in the bottom product.

Using Given data:
Xf Hk= 0.51
Xf Lk= 0.49
Xb Lk= 0.05
Xd Hk=0.90
B= 29.25 kmol/hr
D= 35.7 kmol/hr

Hence Feed entry stage =2

5.1.4 Efficiency

Use O'Connel relation to calculate efficiency
Equation 7.6=

$$E_o = 51 - 32.5 \log(\mu_a \alpha_a)$$

Using given data
μ = 0.533 cp ;
α = 1.71
 μα = 0.911
Efficiency = 0.74
Hence actual number of stages =42

5.1.5 Diameter and Height of column

$$\hat{u}_v = (-0.171 l_t^2 + 0.27 l_t - 0.047) \left[\frac{(\rho_L - \rho_v)}{\rho_v} \right]^{1/2} \qquad (11.79)$$

where $\hat{u}_v$ = maximum allowable vapour velocity, based on the gross (total) column
    cross-sectional area, m/s,

l_t = plate spacing, m, (range 0.5–1.5).

The column diameter, D_c, can then be calculated:

$$D_c = \sqrt{\frac{4 \hat{V}_w}{\pi \rho_v \hat{u}_v}} \qquad (11.80)$$

where $\hat{V}_w$ is the maximum vapour rate, kg/s.

   This approximate estimate of the diameter would be revised when the detailed plate design is undertaken.

Diameter = 0.82m
Height = 8.4m
Plate Spacing = 0.2m

5.1.6 Distillation Column Specifics

Table 25 - Distillation Column specifications

Specification of distillation Column	
Minimum No. of plates	16
Ideal Stages	23
No. of Actual plates	42
Type of Plates	sieve tray
Minimum trays	16
Reflux Ratio	2.8
Column Diameter (m)	0.82
Column Height (m)	8.4

5.2 Liquid Vapor Flash Drum

The design of a vapor flash drum involves determining the required separation efficiency and operating conditions. Factors such as flow rates, drum size, internals, and inlet/outlet arrangements are considered. By carefully considering these parameters, an efficient vapor-liquid separation can be achieved, meeting process requirements and ensuring effective operation.

5.2.1 Fraction of liquid in vapor phase

$$F_L V = W_l/W_v \sqrt{(\rho_v/\rho_l)} \qquad \textit{Equation 7.7}$$

Using Given data:

$F = 6746.32 \; kmol/hr \qquad \rho_F = 0.000786 \; g/cc \qquad W_F = 15345 \; kg/hr$

$L = 4537.58 \; kmol/hr \qquad \rho_l = 0.85407 \; g/cc \qquad W_L = 55931.8 \; kg/hr$

$V = 2208.74 \; kmol/hr \qquad \rho_v = 0.000786 \; g/cc \qquad W_V = 97522.3 \; kg/hr$

Flv= 0.0173

5.2.2 K$_{drum}$ Value

$(w_l/w_v)\sqrt{\rho_v/\rho_l}$
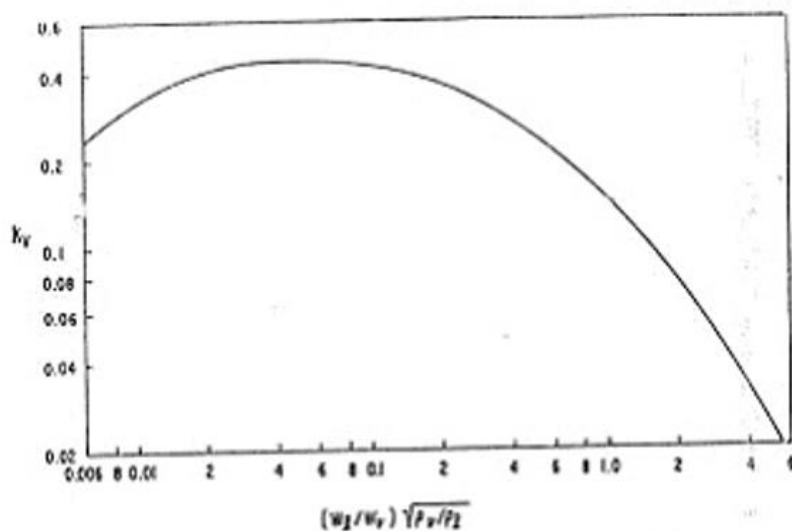
Figure 2 - Value for Kdrum

Using Flv = 0.0173
From graph:
K = 0.35

5.2.3 Permissible vapor velocity

$$u_perm = K_drum\sqrt{((\rho_L - \rho_V)/\rho_V)} \qquad \text{Equation 7.8}$$

Density of ethanol = 789 kg/m^3
Density of water = 1000 kg/m^3

u_perm = 11.53 ft/s

5.2.4 Area

$$A_e = (VM_WV)/(u_perm(3600)\rho_V) \qquad \text{Equation 7.9}$$

Using above equation
Area = 9.814 m^2

7.2.5 Diameter

$$D = \sqrt{((4A_e)/\pi)} \qquad \text{Equation 7.10}$$

Using
Area = 9.814 m^2
We calculate:
Diameter = 3.53m

5.2.6 Volume and Length

$Volume=Volumetric\ flow\ rate \times Residence\ Time$ 　　　Equation 7.11
Residence time =0.4 hrs
Volumetric Flow rate =65.5 m^3/hr
Hence
Volume = 26.2 m^2

Length = Volume/Area
Hence Length = 3m

5.2.7 Flash Drum specifications

Table 26 - Flash Drum Specifications

Specification	Value
Volume	26.1955m3
Area	9.81m^2
Diameter	3.53m
Length	3m

Temperature	77°C
Pressure	1atm

5.3 Reactor Design

$$W = F_{Ao} \int_0^x -\frac{1}{r_A} dx \qquad\qquad \text{Equation:7.12}$$

Rate of disappearance of syngas is given Langmuir-Hinshelwood mechanism,

Table 27 - Data for reactor

Data	Values
K	4.28e+06 kgmole/m^3
a	189 kgmole/m3.s
Temperature	212°C
Pressure	1atm
Feed Flow rate	163.5 kmol/hr

5.3.1 Conversion and Partial Pressure Calculations

Table 28 – Conversion in Reactor

Conversion	CO	CO_2	H2	C2H6O	H_2O
0.95	0.018	0.012	0.41	0.18	0.38

$$P_A = \frac{x_A}{x_T} \times P \qquad\qquad \text{Equation 7.13}$$

Table 29 – Partial Pressure in Reactor

pCO	pCO2	pH2	pC2H6O	pH20
1.82	1.22	41.5	18.2	38.5

5.3.2 Volume

By using
V=w/p
W= weight of catalyst
P= bulk density of catalyst

Volume= 29 m3

Table 30 – Volume of Reactor

Length(m)	2
Diameter(m)	2.52
Volume (m3)	29
Material	Carbon Steel

5.3.3 Pressure Drop Calculations

Table 31 – Pressure drop in Reactor

Particle Diameter (m)	0.00335
Porosity	0.403
Particle Density (Kg/m3)	2320
ΔP	13.2kPa

Pressure Drop is calculated by:

$$\frac{\Delta P}{L} = \left(\frac{150\mu v_o}{D_p^2} \times \frac{1-\varepsilon^2}{\varepsilon^3}\right) + \left(\frac{1.75\rho_g v_o^2}{D_p} \times \frac{1-\varepsilon}{\varepsilon^2}\right)$$

PROCESS SIMULATION & PARAMETRIC ANALYSIS

6.1 Introduction

In order to model and simulate Ethanol Production Plant, Aspen Plus V10 was used. Chemical Reaction, Separation, Distillation and Drying were considered main processing units. For a large number of components, ASPEN PLUS stores physical property parameters in several databases. A property method is a collection of methods, models and the physical properties of all streams used by ASPEN PLUS to calculate the chemical and thermodynamic equilibrium. In this work, ASPEN PLUS was used to calculate all the physical properties required with the NRTL property package, as this best suited the non-ideal behavior of Ethanol Production.

6.2 Procedure

We simulated the process through the following procedure:

1. Every Component was added in the list.
2. Selected property package was NRTL for non-ideal behavior of Ethanol Production
3. After adding the components and selecting the package, the property table is automatically generated.
4. Simulation window is entered, and all the unit operations are added and specifications are done. (Reactor-1 is added and given the stoichiometry and similarly all the other unit operations are added and specified)
5. Simulation was run and the results were noted and matched with the manual results.

6.3 Equipment Specifications

Simulatin Main Flow Sheet
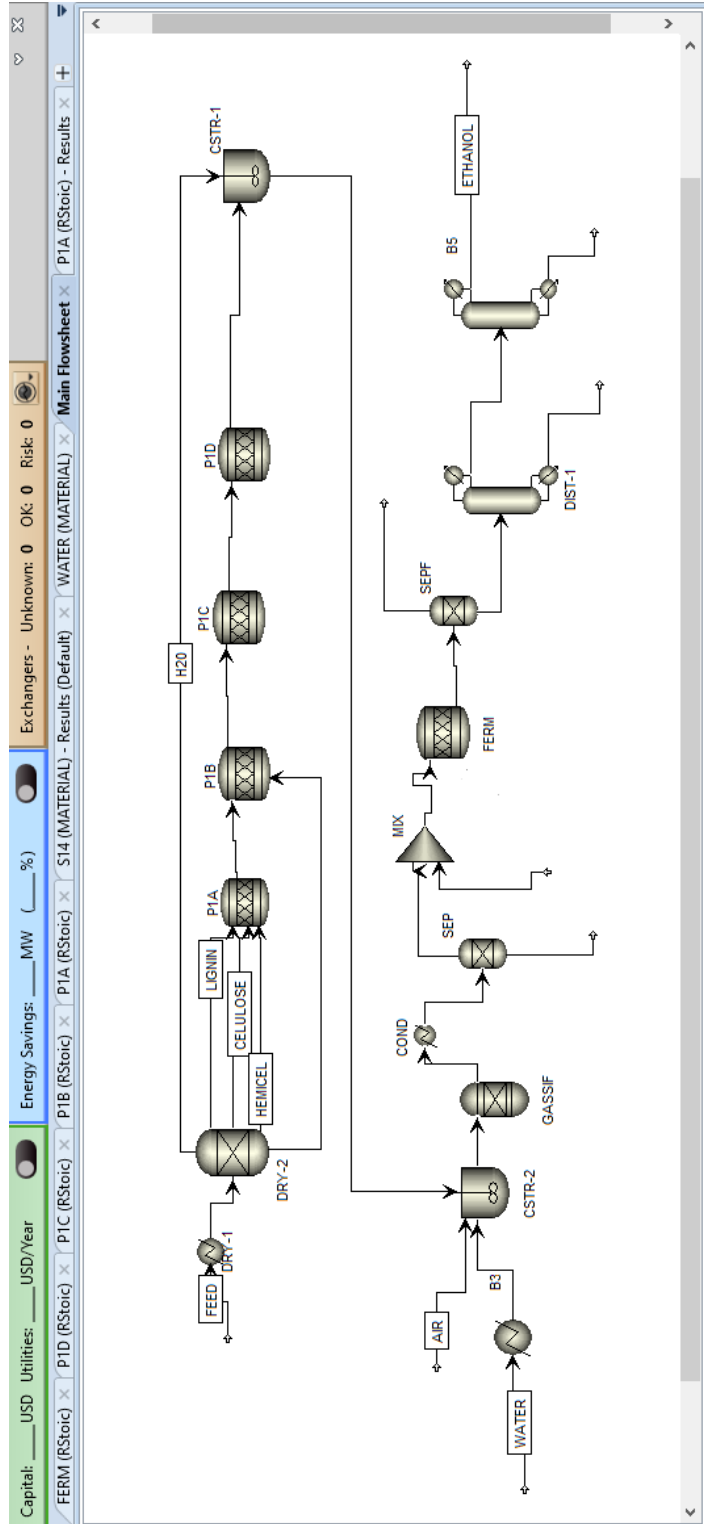
Figure 3 - Main flowsheet on Aspen Plus

Component List

Figure 4 - Component List 1

Figure 5 - Component List 2

Property Package

Figure 6 - Property Package

Heater 1

Figure 7 - Heater 1 Specs

P1A Reactor

Figure 8 - P1A Reactor specs
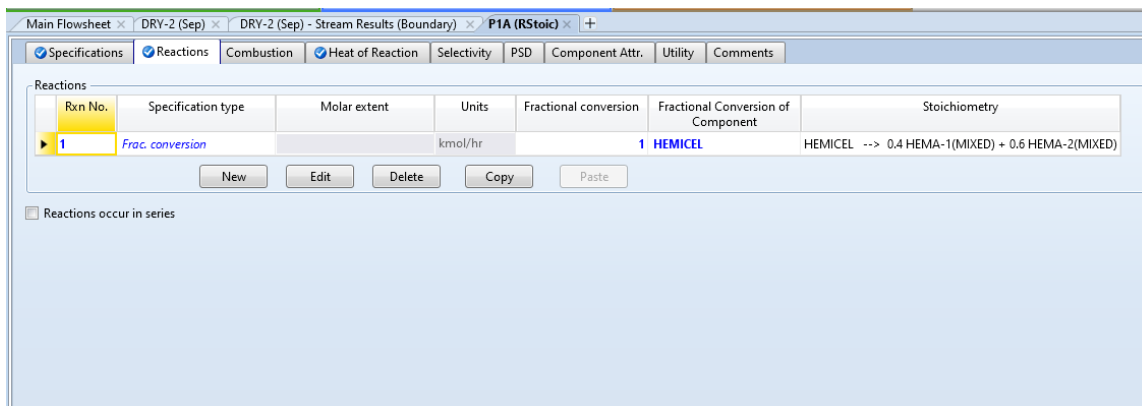
Figure 9 - P1A Reactions

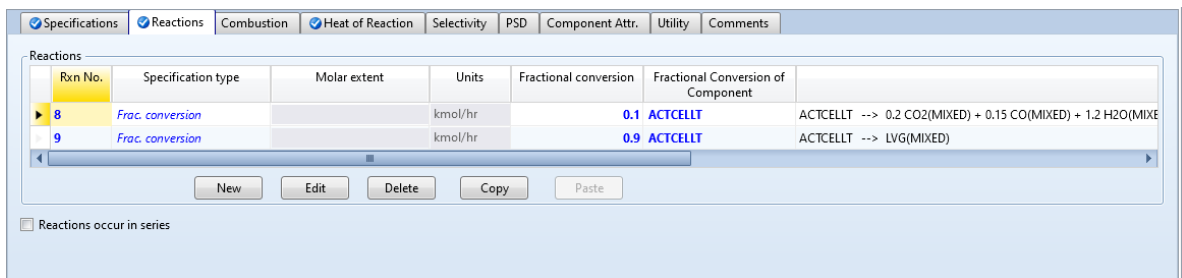## P1B Reactor
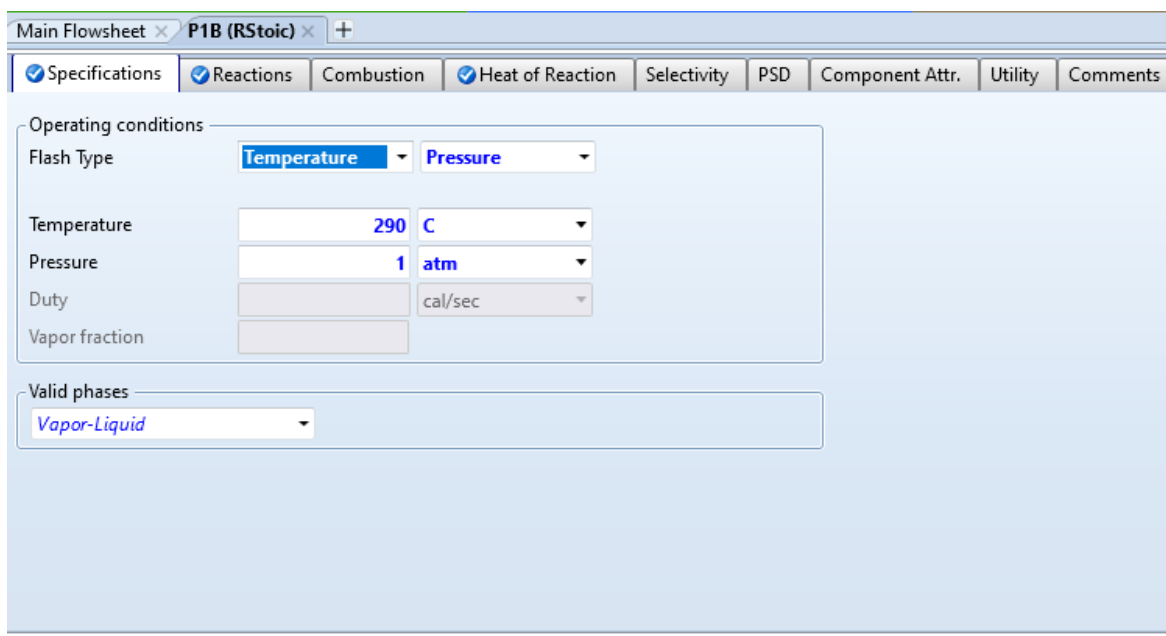
Figure 10 - P1B Reactor specs

Figure 11 - P1B Reactions 1

Figure 12 - P1B Reactions 2

P1C Reactor

Figure 13 - P1C Reactor specs

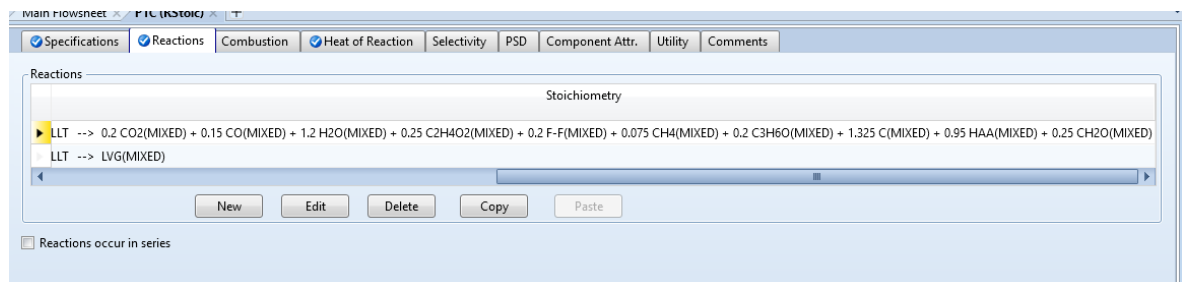*Figure 14 - P1C Reactions 1*
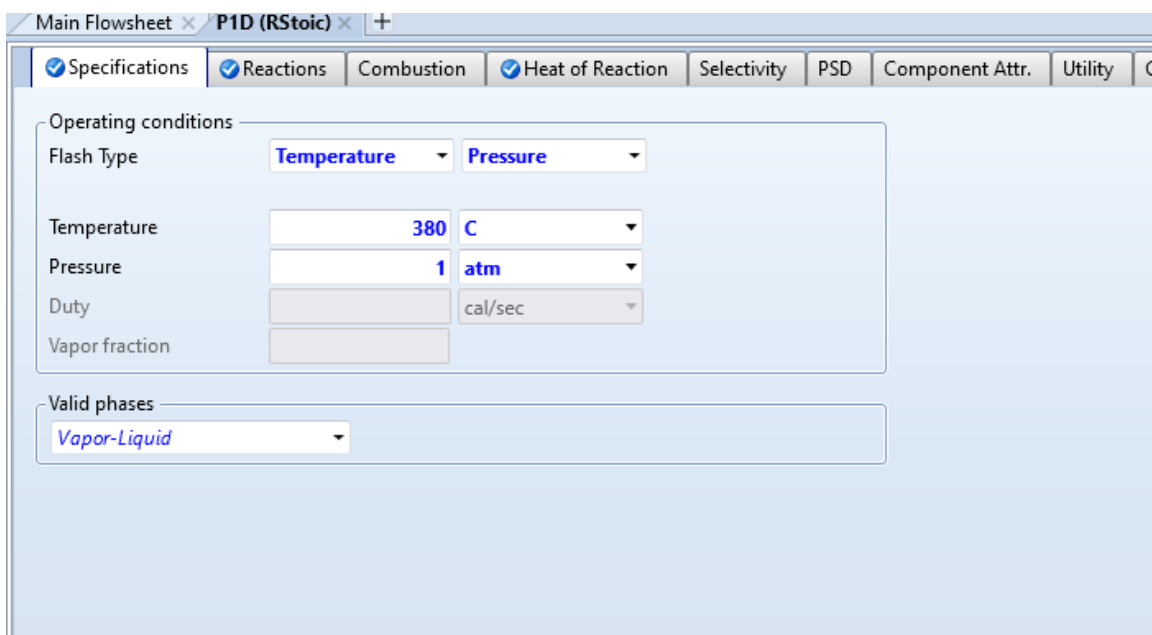

Figure 15 - P1C Reactions 2

P1D Reactor

Figure 16 - P1D Reactor specs
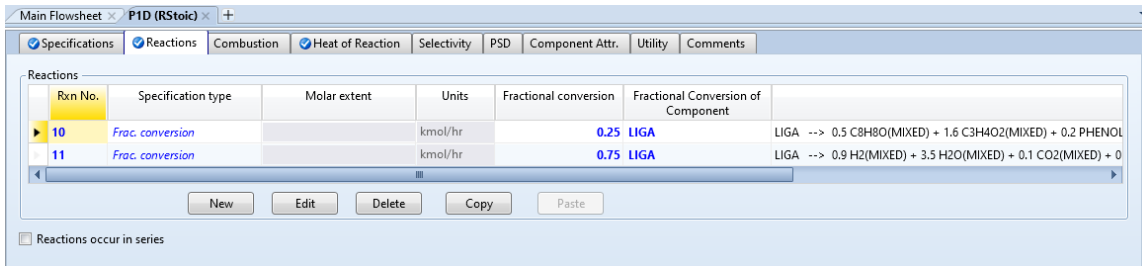
Figure 17 - P1D Reactions 1
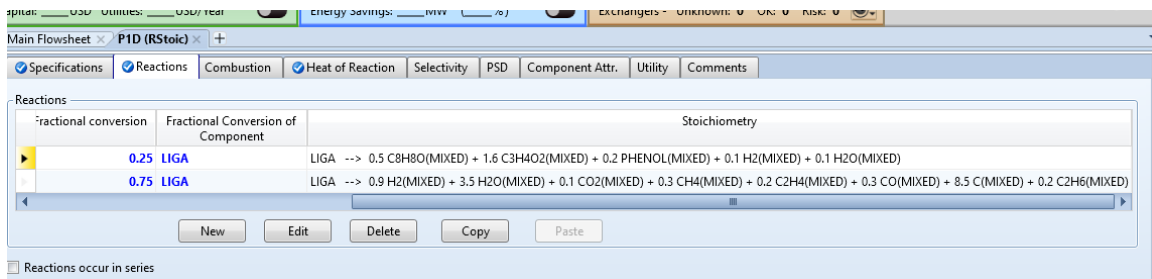
Figure 18 - P1D Reactions 2

CSTR-1

Figure 19 - CSTR 1 Specs

Figure 20 - CSTR 1 Reactions

Heater 2

Figure 21 - Heater 2 specs

CSTR-2

Figure 22 - CSTR 2 Specs

Figure 23 - CSTR 2 Reactions

Fermentation

Figure 24 - Fermentation Reactions

Distillation – 1

Figure 25 - Distillation 1 specs

Distillation – 2

Figure 26 - Distillation 2 specs

6.4 Stream Compositions

Feed

Figure 27 - Feed

Air IN

Figure 28 - Air IN

Water IN – 1

Figure 29 - Water IN 1

Water IN – 2

Figure 30 - Water IN 2

Waste Stream

	Units	S14	
Enthalpy Flow	cal/sec	26154	
Average MW		27.9627	
+ Mole Flows	**kmol/hr**	**31.4699**	
+ Mole Fractions			
+ Mass Flows	**kg/hr**	**879.985**	
– Mass Fractions			
CH4O		0	
H2O		0	
N2		0.958778	
NH3		0.000111876	
O2		0	
SO2		0.0221044	

Figure 31 - Waste Stream

Wasted SYN-GAS

Figure 32 – Wasted SYN-GAS

Product (Ethanol)

Figure 33 - Product results

6.5 Worksheet

Figure 34 - Worksheet

6.6 Simulation Conclusion

Through this Simulation in Aspen Plus V10.0, we are achieving 1.5 ton of 95% pure fuel grade ethanol. The results were similar to our manual calculation

INSTRUMENTATION & PROCESS CONTROL

7.1 Introduction

A control system is a means of regulating the desired output. In the image below, a control system is depicted in block diagram form.
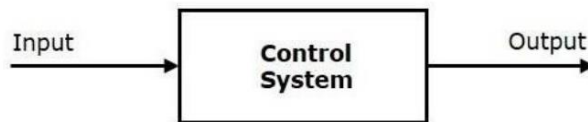
The control system is represented here by a single block. This moniker for the control system refers to the way in which several inputs are used to control the output. We will modify this input using some technique. The open loop and shutdown control systems that the blocks employ within the control system, as well as how to modify these inputs to obtain the desired result, will be thoroughly covered in the following section.

Examples include a washing machine and a traffic signal management system.

The traffic light control system is one illustration. Here, the controller's input signal sequence is used, and one of the three lights is lit for a while as the output. During this period, the other two lights are off. Based on the transportation analysis at a certain intersection, the light times can be determined for both on and off. Therefore, the input signal determines the output. As a result, the system for controlling traffic lights operates according to a schedule.

7.2 Control Systems' Classification

We can classify the control systems in the following ways, based on certain parameters.

7.2.1 Continuous time and Discrete-time Control Systems

Based on the type of signal used, continuous time control systems and discrete time control systems can be divided into different categories.

In continuous time control systems, all signals are time-continuous. Discrete time control systems, however, use one or more discrete time signals.

7.2.2 SISO and MIMO Control Systems

Based on the quantity of available inputs and outputs, the control systems can be divided into SISO and MIMO controllers.

One input and one output are present in SISO (Single Input and Single Output) control systems.

MIMO (Multiple Inputs and Multiple Outputs) control systems, on the other hand, have multiple inputs and multiple outputs.

7.2.3 Open Loop and Closed Loop Control Systems

Based on the feedback path, open loop and closed loop control systems can be distinguished.

In open loop control systems, the output is not fed back to the input. As a result, the control is independent of the desired output.

The block diagram of the open loop control system is displayed in the accompanying figure.
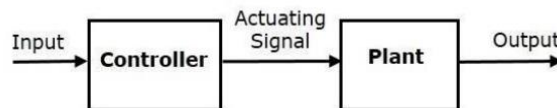
Figure 35 - Open Loop Feedback system

7.2.3.1 Open Loop

In this case, the controller produces an actuation signal in response to an input. This signal is an input to a controlled plant or process. The plant generates a controlled output. An example of an open loop control system is the traffic light control system that was previously explained.

The output of closed loop control systems is sent back into the input. As a result, the control measurement is determined by the planned output.

The accompanying figure displays the block diagram of a closed loop negative feedback control system.
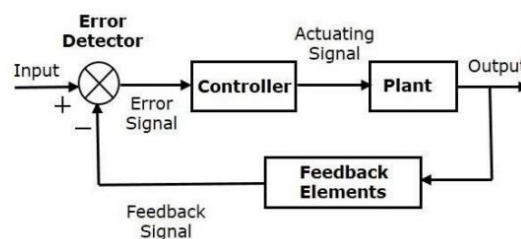
Figure 36 - Closed Loop Feedback system

7.2.3.2 Closed Loop

The error detector emits an error signal that distinguishes between the input and the feedback signal. By treating the output of the entire system as an input to this block from the block (feedback elements), the feedback signal is obtained. Instead of a direct input, the controller receives information from the error signal.

In order to control the plant, the controller produces an actuating signal.

This combination automatically modifies the control system's output until the requested response is received. Thus, closed loop control systems are another name for automatic control systems. An example of a traffic light control system using an input sensor is a closed-loop control system. (Cooper D. J. et al., 2006)

In the following table, some differences are shown between the open and the closed loop systems.

Table 32 - Difference between open and closed control systems

Open Loop Control Systems	Closed Loop Control Systems
Control action is independent of the desired output.	Control action is dependent of the desired output
Feedback path is not present.	Feedback path is present
These are also called as non-feedback control	These are also called as feedback control systems.

If any output, in whole or in part, is sent back to the input side and employed as a component of the input system, that is referred to as feedback. The effectiveness of control systems can be increased in large part through feedback. In this chapter, let's talk about feedback and its various forms.

7.3 Types of Feedback

There are two types of feedback

- Positive feedback
- Negative feedback

7.3.1 Positive Feedback

The positive feedback includes the input reference, R(s) and the output feedback. The diagram below shows the positive feedback control system block diagram.
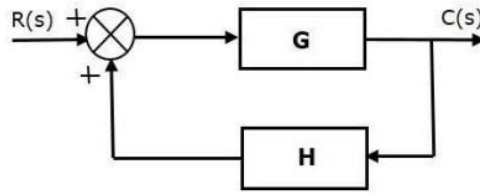
Figure 37 - Positive feedback

Later chapters discuss the concept of transfer function. Consider the transfer function of the positive feedback control system for the time being,

$T = G1 - GH$ *(Equation1)*

Where,

- T is the overall transfer function or positive feedback system gain.
- G is the open loop gain, the frequency function.
- H is a feedback path gain that is a frequency function.

7.3.2 Negative Feedback

Negative feedback reduces input, R(s) and system output error. The following figure shows a block diagram of the negative feedback system.
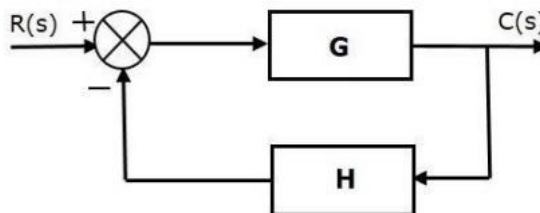
Figure 38 - Negative Feedback

Transfer function of negative feedback control system is,

$T = G1 + GH$

(Equation 2)

Where,

- T shall be the transfer function or the overall negative feedback management system gain.
- G, which is the frequency function, is an open loop gain.
- H is the feedback path gain that is the frequency function.

7.4 Control loop on CSTR
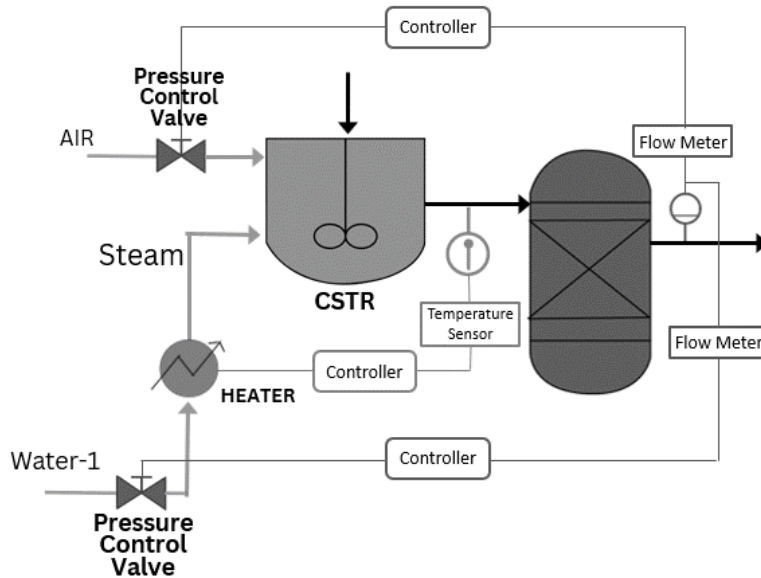
Figure 39 - Control Loop on CSTR

For representation, Control loop on CSTR-II and Gassifier in our floe sheet has been shown above. Three Feed Backward Control loops have been installed

1. Flow Meter measure the outlet of GASSIF to adjust the flow of O2 inlet in AIR stream

2. Flow Meter measure the outlet of GASSIF to adjust the flow of H20 inlet in Water stream

3. Temperature measure the outlet of CSTR to adjust the Temperature of Steam entered into CSTR

7.5 Control Loops in Plant

The following are the necessary control loops for the entire plant:

Table 33 - Necessary Control Loops

Equipment	Controller	Manipulated Variables	Controlled Variables
Heater 1 and Separator	Temperature Controller	Temperature of Separator Outlet	Heat output of Heater
P1A	Temperature Controller	Temperature of Reactor Outlet	Heat output of Reactor's Heater
P1B	Temperature Controller	Temperature of Reactor Outlet	Heat output of Reactor's Heater
P1C	Temperature Controller	Temperature of Reactor Outlet	Heat output of Reactor's Heater
P1D	Temperature Controller	Temperature of Reactor Outlet	Heat output of Reactor's Heater
CSTR-2 and Gasifier	Flow Controller	Outlet flow of Gasifier	Air IN flow rate
	Flow Controller	Outlet flow of Gasifier	Water IN flow rate
	Temperature Controller	Outlet Temperature of CSTR	Heat output of Water-1 IN Heater
Fermenter	Flow Controller	Flow of ethanol Produced from Fermenter	Water-2 IN Flow Rate

ECONOMIC ANALYSIS

Economic analysis plays an important role in determining the profitability and sustainability of chemical plant construction. It provides a comprehensive assessment of the financial impact and potential risks associated with such undertakings. A thorough economic analysis enables decision makers to assess the costs and benefits associated with building and operating a facility, including factors such as capital expenditures, operating costs, raw material procurement, labor costs and market demand. . This analysis helps estimate potential return on investment, profitability, and cash flow projections, enabling informed decision making. In addition, economic analysis can help identify potential bottlenecks and inefficiencies, optimize resource allocation, reduce risk, and proactively take action to ensure the long-term economic viability of chemical plants. We adapted Coulson and Richardson method for our Project economic analysis

8.1: Distillation Columns
8.1.1 Distillation Column-1
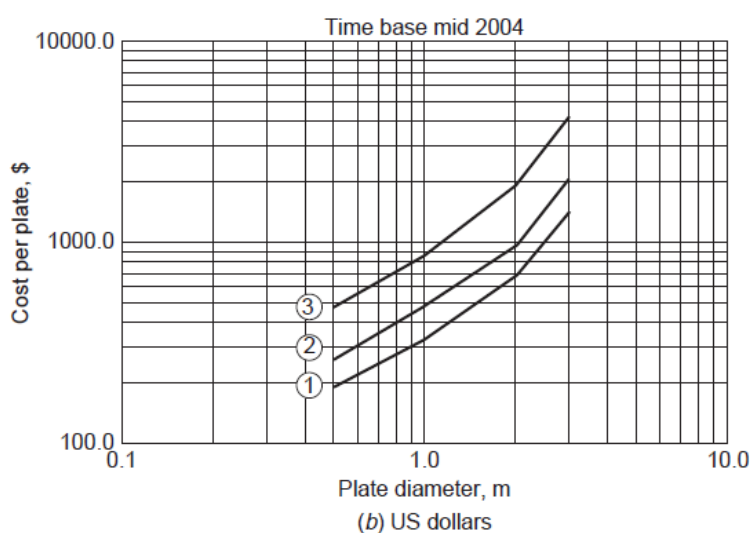
Figure 40 - Distillation column pricing

	Cost	£/m^3 ($/m^3)		
Size, mm	25	38		50
Saddles, stoneware	840 (1400)	620 (1020)		580 (960)
Pall rings, polypropylene	650 (1080)	400 (650)		250 (400)
Pall rings, stainless steel	1500 (2500)	1500 (2500)		830 (1360)

Table 35 - Distillation Cost calculations

Table 34 - Distillation Column Packing Pricing

Cost Calculation	
plate type	sieve
material factor (Stainless Steel)	1.7
plate diameter(m)	0.9
Volume of Packing m3	5.80
from graph:	
cost per plate $	320
no of plates	44
total cost $	228,111
Total cost $	
total cost of DC $	228,111
index in 2004	1252
index in 2023	1921
Cost in 2023/ $	(Cost2004)*(index2023)/(Index2023)
Cost in 2023/ $	350,000

8.1.2 Distillation Column-2

Table 36 - Distillation 2 cost calculations

plate type	sieve
material factor (Stainless Steel)	1.7
plate diameter(m)	1.5
Volume of Packing m3	9.9
from graph:	
cost per plate $	490
no of plates	50
total cost $	280249
Total cost $	
total cost of DC $	280249
index in 2004	1252
index in 2023	1952
Cost in 2022/ $	(Cost2004)*(index2022)/(Index2022)

Cost in 2022/ $	430,000

Table 6.2. Purchase cost of miscellaneous equipment, cost factors for use in equation 6.7. Cost basis mid 2004

Equipment	Size unit, S	Size range	Constant C,£	C,$	Index n	Comment
Agitators						
Propeller	driver	5–75	1200	1900	0.5	
Turbine	power, kW		1800	3000	0.5	
Boilers						
Packaged						oil or gas fired
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						
Horizontal basket	dia., m	0.5–1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	×1.7 for ss
Compressors						
Centrifugal	driver	20–500	1160	1920	0.8	electric, max. press.
	power, kW					
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						
Vertical tube	area, m^2	10–100	12,000	20,000	0.53	carbon steel
Falling film			6500	10,000	0.52	
Filters						
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		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

Figure 41 - Miscellaneous Equipment Cost

8.2 Reactors

8.2.1 Reactor-1

Volume (m3) = 6
C = 15000
N = 0.4
Using Equation: Ce = CSn
Price of reactor = $ 30,827
Index in 2004 = 1252 ; Index in 2022 = 1921
Cost in 2023 = $cost 2001 * (Index 2023/Index 2001)$ = $ 47,300

8.2.2 Reactor-2

Volume (m3) = 12.5
C = 15000
N = 0.4
Price of reactor = $ 41,059
Cost in 2023 = $cost 2001 * (Index 2023/Index 2001)$ = $ 63,000

8.2.3 Reactor-3

Volume (m3) = 4
C = 15000
N = 0.4
Using Equation: Ce = CS^n
Price of reactor = $ 25,365
Cost in 2023 = $cost 2001 * (Index 2023/Index 2001)$ = $ 39,000

8.2.4 Reactor-4

Volume (m3) = 10
C = 15000
N = 0.4
Using Equation: Ce = CS^n
Price of reactor = $ 50,730
Cost in 2023 = $cost 2001 * (Index 2023/Index 2001)$ = $ 78,000

8.2.5 CSTR-1

Volume (m3) = 11
C = 15000
N = 0.4
Using Equation: Ce = CSn
Price of reactor = $ 52,594.30
Cost in 2023 = $cost 2001 * (Index 2023/Index 2001)$ = $ 82,000

8.2.6 CSTR-2

Volume (m3) = 39
C = 15000
N = 0.4
Using Equation: Ce = CSn
Price of reactor = $ 70,553
Cost in 2023 = $cost2001 * (Index2023/Index2001)$ = $ 110,000

8.2.7 Gasifier

Volume (m3) = 44
C = 15000
N = 0.4
Using Equation: Ce = CSn
Price of reactor = $ 91,719
Cost in 2023 = $cost2001 * (Index2023/Index2001)$ = $ 143,000

8.2.1 Fermentor

Volume (m3) = 10
C = 15000
N = 0.4
Using Equation: Ce = CSn
Price of reactor = $ 57,683
Cost in 2023 = $cost2001 * (Index2023/Index2001)$ = $ 92,000

8.3 Separator

8.3.1 Separator-2

Diameter: 1.5m
Pressure (bar) = 1
Material of Construction = Carbon Steel
Price of Separator = $ 43,000

8.3.2 Separator-2

Diameter: 3.5m
Pressure (bar) = 1
Material of Construction = Carbon Steel
Price of Separator = $ 78,000

8.4 Heaters

8.4.1 Heater-1

Heat Duty = 416 KWH
Material of Construction = Carbon Steel
Type = Box
Using Equation: $Ce = CS^n$
C = 560, n = 0.77
By solving
Cost of Furnace = $ 59,000

8.4.1 Heater-2

Heat Duty = 3520 KWH
Material of Construction = Carbon Steel
Type = Box
Using Equation: $Ce = CS^n$
C = 560, n = 0.77
By solving
Cost of Furnace = $ 300,000

Total Purchase Cost = $ 1,914,300

8.5 Total Cost

Item	Process type		
	Fluids	Fluids–solids	Solids
1. Major equipment, total purchase cost	PCE	PCE	PCE
f_1 Equipment erection	0.4	0.45	0.50
f_2 Piping	0.70	0.45	0.20
f_3 Instrumentation	0.20	0.15	0.10
f_4 Electrical	0.10	0.10	0.10
f_5 Buildings, process	0.15	0.10	0.05
*f_6 Utilities	0.50	0.45	0.25
*f_7 Storages	0.15	0.20	0.25
*f_8 Site development	0.05	0.05	0.05
*f_9 Ancillary buildings	0.15	0.20	0.30
2. Total physical plant cost (PPC) $PPC = PCE (1 + f_1 + \cdots + f_9)$ $= PCE \times$	3.40	3.15	2.80
f_{10} Design and Engineering	0.30	0.25	0.20
f_{11} Contractor's fee	0.05	0.05	0.05
f_{12} Contingency	0.10	0.10	0.10
Fixed capital $= PPC (1 + f_{10} + f_{11} + f_{12})$ $= PPC \times$	1.45	1.40	1.35

*Omitted for minor extensions or additions to existing sites.

8.5.1 Physical Plant Cost

Figure 42 - Costing f factors table

Physical Plant Cost Table	
f1 (Equipment erection)	0.4
f2 (Piping)	0.7
f3 (Instrumentation)	0.2
f4 (Electrical)	0.1
f5 (Buildings, process)	0
*f6 (Utilities)	0.5
*f7 (Storages)	0.15
*f8 (Site development)	0
*f9 (Ancillary buildings)	0.15
f10 (Design and Engg.)	0.3
f11 (Contractor's fee)	0.05
f12 (Contingengency)	0.1
Total Physical plant Cost	**$2,590,800.00**

Table 37 - Physical plant cost table

8.5.2 Fixed operating cost

Fixed Operating Cost	
Maintenance (3% of FC)	112,699.80
Operating Labor	12,100.00
Plant Overheads (40% of OL)	4,840.00
Laboratory (20% of OL)	2,420.00
Capital Charges (2% of FC)	75,133.20
Insurance (1% of FC)	37,566.60
Local Taxes (1% of FC)	37,566.60
TOTAL	282,326.20

Table 38 - Fixed operating cost

8.5.3 Variable Operating Cost

Table 39 – Variable Operating Cost

Materia	Requirement	Units
Bagasse Feed Rate	13.6	tonnes/day
Bagasse Feed Price	22	/tonne
Bagasse Feed Price	299	/day
Bagasse Feed Price	103,822	/yr
Catalyst Quantity Required	22.2	tonnes/yr
Catalyst Price/tonne	8,300	/tonnes
Catalyst Price	184,260.00	/yr
Miscellaneous Cost	$52,840	
Cooling Water Required	6.4	tonnes/day
Cooling water price	0.50	/tonne
Cooling water price	3.20	/day
Cooling Water Price/ year	1,110.40	/yr
Electric Power Required	119	MJ/day
Electric Power Required	30345	MJ/yr
Cost of electricity	455.18	/yr
TVC	341,377.58	

8.5.4 Revenue

Product	Production (tonnes/yr)	Price ($/tonne)	Revenue Generated
Ethanol	3226	870.00	2,806,620.00
Syngas	612	540.00	330,480.00
		Total Revenue /yr	3,137,100.00
		Total Profit/ yr	2,513,396.23

Table 40 - Revenue

8.6 Total Summary

Table 41 - Plant Cost Summary Table

Initial Investment	4,320,159.00
Plant Running Cost	623,703.78
Revenue	3,137,100.00
Profit	2,513,396.23
Payback Period	3 years

CHAPTER 9

HAZOP ANALYSIS

HAZOP, or Hazard and Operability Study, serves as a vital research tool for identifying potential hazards that could lead to catastrophic incidents. It finds extensive application across various industries, particularly in the chemical sector, to assess the likelihood of operational problems or hazards occurring within a specific unit or process stream. A multidisciplinary team comprising typically 6 to 12 members, including operations engineers, mechanical engineers, process engineers, electrical engineers, chemical engineers, HSE consultants, and project managers, conducts the HAZOP study. This team employs a critical and analytical approach, dedicating weeks of collaborative effort to comprehensively analyze the unit or stream under investigation.

During the study, the team engages in frequent meetings to discuss and assess all relevant records and parameters that may affect the process's trajectory. The HAZOP study necessitates the examination of multiple Process Flow Diagrams (PFDs) and Piping and Instrumentation Diagrams (P&IDs), which are intricate documents requiring collective effort to decipher. Each unit is individually scrutinized, making the overall process laborious and time-consuming, often extending beyond a month for completion.

Despite the demanding nature of this technique, HAZOP analysis is widely regarded as the most comprehensive and effective approach to proactively address potential issues in a process. Its primary objective is to explore the root causes of failures and implement preventive measures. The study involves meticulously breaking down each unit or process into its smallest components, subjecting them to systematic examination using predefined guide words.

Deviations in terms of temperature, pressure, flow, and composition are rigorously evaluated against relevant guide words to uncover potential hazards.

In summary, conducting a HAZOP analysis in a chemical plant is an essential step towards ensuring safety by comprehensively understanding and mitigating potential process risks.

9.1 Methodology

The HAZOP study encompasses the following procedural steps:

- Develop a comprehensive flow sheet, highlighting the interconnections and units within the process.
- Select a specific unit, such as a kiln or mill, for in-depth analysis.
- Provide a rationale for choosing the selected unit, outlining the factors that make it critical for examination.
- Identify a specific process parameter to focus on during the study.
- Apply the predefined guide words to the chosen process parameter, systematically exploring potential deviations from these guide words as documented in the provided tables.
- Identify potential causes that may lead to deviations and assess the necessity of implementing preventive systems to avert disasters.
- Evaluate the possible outcomes resulting from identified deviations.
- Recommend appropriate preventive measures based on the findings, aiming to mitigate or eliminate potential risks.
- Thoroughly document all relevant data and present comprehensive records of the HAZOP study.

These steps form the basis of conducting a systematic and thorough HAZOP study, facilitating the identification and mitigation of potential hazards in the analyzed process.

9.2   Distillation Column

Table 42 - HAZOP Distillation Column

Parameter/Node	Guide Word	Deviation	Causes	Consequences	Safeguards/Actions
Temperature	Less	Lower than expected operating temperature	Faulty temperature control system	Incomplete separation, impurities in ethanol product	Regular maintenance and calibration of temperature control system
Temperature	More	Higher than expected operating temperature	Failure of cooling system	Potential degradation of heat-sensitive compounds, reduced ethanol purity	Installation of redundant cooling systems, automatic temperature monitoring and shut-off mechanisms
Pressure	Less	Lower than expected operating pressure	Faulty pressure control valve	Reduced separation efficiency, impurities in ethanol product	Regular maintenance and calibration of pressure control valve
Pressure	More	Higher than expected operating pressure	Blockage in condenser or column trays	Potential damage to column internals, safety risks	Installation of pressure relief valves, regular inspection of condenser and trays
Flow Rate	Less	Lower than expected feed flow rate	Pump failure or blockage in feed lines	Reduced production rate, decreased ethanol yield	Installation of redundant pumps, routine inspection of feed lines
Level	More	Excessive liquid in reboiler	High feed flow rate or incorrect level control	Potential flooding of reboiler, reduced separation efficiency	Installation of level sensors, automated shutdown system in case of high level
Sealing	Other	Leakage from column trays or condenser	Faulty gaskets or seals	Environmental contamination, safety risks	Regular inspection and replacement of gaskets and seals

9.3   Plug Flow Reactor

Table 43 - HAZOP Plug Flow Reactor

Parameter/Node	Guide Word	Deviation	Causes	Consequences	Safeguards/Actions
Temperature	Less	Lower than expected operating temperature	Faulty temperature control system	Incomplete reaction, reduced ethanol production	Regular maintenance and calibration of temperature control system
Temperature	More	Higher than expected operating temperature	Failure of cooling system	Thermal degradation of catalyst, reduced reaction efficiency	Installation of redundant cooling systems, automatic temperature monitoring and shut-off mechanisms
Pressure	Less	Lower than expected operating pressure	Faulty pressure control valve	Reduced contact time between reactants, decreased ethanol yield	Regular maintenance and calibration of pressure control valve
Pressure	More	Higher than expected operating pressure	Blockage in the reactor bed	Potential damage to reactor vessel, safety risks	Installation of pressure relief valves, regular inspection of reactor bed

Flow Rate	Less	Lower than expected reactant flow rate	Pump failure or blockage in feed lines	Insufficient reactant contact, decreased ethanol production	Installation of redundant pumps, routine inspection of feed lines
Flow Rate	More	Higher than expected reactant flow rate	Malfunctioning control valve	Poor reactor bed distribution, reduced reaction efficiency	Installation of flow rate control valves, routine inspection of control valve performance
Catalyst	Other	Use of incorrect catalyst type	Incorrect catalyst selection	Inefficient reaction, low ethanol yield	Strict adherence to recommended catalyst specifications, periodic analysis of catalyst performance
Level	Less	Insufficient reactant in the reactor	Pump failure or inadequate feed supply	Incomplete reaction, reduced ethanol production	Installation of level sensors, automated shutdown system in case of low level
Level	More	Excessive reactant in the reactor	Pump failure or overfeed	Potential overflow, safety risks	Installation of level sensors, automated shutdown system in case of high level
Sealing	Other	Leakage from reactor vessel	Faulty gaskets or seals	Environmental contamination, safety risks	Regular inspection and replacement of gaskets and seals

9.4   Condenser

Table 44 - HAZOP Condenser

Parameter/ Node	Guide Word	Deviation	Causes	Consequences	Safeguards/Actions
Temperature	Less	Lower than expected operating temperature	Faulty temperature control system	Inefficient condensation, reduced ethanol recovery	Regular maintenance and calibration of temperature control system
Temperature	More	Higher than expected operating temperature	Failure of cooling system	Potential degradation of heat-sensitive compounds, reduced ethanol quality	Installation of redundant cooling systems, automatic temperature monitoring and shut-off mechanisms
Pressure	Less	Lower than expected operating pressure	Faulty pressure control valve	Reduced condensation efficiency, lower ethanol recovery	Regular maintenance and calibration of pressure control valve
Pressure	More	Higher than expected operating pressure	Blockage in condenser or discharge line	Potential damage to condenser, safety risks	Installation of pressure relief valves, regular inspection of condenser and discharge line
Flow Rate	Less	Lower than expected cooling water flow rate	Pump failure or blockage in water lines	Reduced heat transfer, increased ethanol losses	Installation of redundant pumps, routine inspection of water lines
Flow Rate	More	Higher than expected cooling water flow rate	Malfunctioning control valve	Potential flooding of condenser, reduced condensation efficiency	Installation of flow rate control valves, routine inspection of control valve performance

Table 45 - HAZOP Condenser 2

Cooling Water Temperature	Less	Lower than expected cooling water temperature	Insufficient heat exchange, poor condensation	Decreased ethanol recovery, lower efficiency	Regular maintenance of heat exchangers, adjustment of cooling water flow rates
Cooling Water Temperature	More	Higher than expected cooling water temperature	Failure of cooling water chilling system	Reduced condensation efficiency, decreased ethanol recovery	Installation of redundant chilling systems, automatic temperature monitoring and shut-off mechanisms
Cooling Water Quality	Other	Use of improper cooling water quality	Contaminated or corrosive cooling water	Impurities in ethanol product, equipment damage	Strict control of cooling water quality, regular water analysis
Sealing	Other	Leakage from condenser	Faulty gaskets or seals	Environmental contamination, safety risks	Regular inspection and replacement of gaskets and seals

9.5 CSTR

Table 46 - HAZOP CSTR

Parameter/ Node	Guide Word	Deviation	Causes	Consequences	Safeguards/Actions
Temperature	Less	Lower than expected operating temperature	Faulty temperature control system	Reduced fermentation rate, decreased ethanol yield	Regular maintenance and calibration of temperature control system
Temperature	More	Higher than expected operating temperature	Failure of cooling system	Potential denaturation of enzymes, reduced fermentation efficiency	Installation of redundant cooling systems, automatic temperature monitoring and shut-off mechanisms
Pressure	Less	Lower than expected operating pressure	Faulty pressure control valve	Reduced mixing and mass transfer, decreased ethanol production	Regular maintenance and calibration of pressure control valve
Pressure	More	Higher than expected operating pressure	Blockage in the reactor or discharge line	Potential damage to reactor, safety risks	Installation of pressure relief valves, regular inspection of reactor and discharge line
pH Level	Less	Lower than expected pH level	Insufficient nutrient supply or pH control system failure	Reduced microbial activity, decreased fermentation efficiency	Regular monitoring and adjustment of nutrient supply and pH control

Table 47 - HAZOP CSTR 2

Substrate Concentration	Less	Lower than expected substrate concentration	Insufficient feed supply or pump failure	Reduced fermentation rate, decreased ethanol production	Installation of redundant pumps, routine inspection of feed lines
Substrate Concentration	More	Higher than expected substrate concentration	Malfunctioning control valve	Inadequate mixing, reduced fermentation efficiency	Installation of control valves, routine inspection of valve performance
Agitation Speed	Less	Lower than expected agitation speed	Motor failure or equipment malfunction	Poor mixing, decreased fermentation efficiency	Regular maintenance and inspection of agitation system
Agitation Speed	More	Higher than expected agitation speed	Malfunctioning control system	Excessive foaming, increased energy consumption	Installation of control systems, routine inspection of system performance
Foaming	Other	Excessive foaming in the reactor	High levels of proteins or fermentation by-products	Potential overflow, safety risks	Installation of foam control systems, routine monitoring of fermentation parameters
Sealing	Other	Leakage from reactor vessel	Faulty gaskets or seals	Environmental contamination, safety risks	Regular inspection and replacement of gaskets and seals

9.6 Gasifier

Table 48 - HAZOP Gasifier

Parameter/ Node	Guide Word	Deviation	Causes	Consequences	Safeguards/Actions
Temperature	Less	Lower than expected operating temperature	Faulty temperature control system	Incomplete gasification, reduced syngas production	Regular maintenance and calibration of temperature control system
Temperature	More	Higher than expected operating temperature	Failure of cooling system	Potential damage to gasifier internals, safety risks	Installation of redundant cooling systems, automatic temperature monitoring and shut-off mechanisms
Pressure	Less	Lower than expected operating pressure	Faulty pressure control valve	Reduced gasification efficiency, decreased syngas production	Regular maintenance and calibration of pressure control valve
Pressure	More	Higher than expected operating pressure	Blockage in gasifier or discharge line	Potential damage to gasifier, safety risks	Installation of pressure relief valves, regular inspection of gasifier and discharge line
Feedstock Composition	Other	Use of improper feedstock composition	Contaminated or incompatible feedstock	Impurities in syngas, reduced ethanol quality	Strict control and testing of feedstock quality
Feedstock Flow Rate	Less	Lower than expected feedstock flow rate	Feed pump failure or blockage in feed lines	Reduced gasification rate, decreased syngas production	Installation of redundant feed pumps, routine inspection of feed lines

Table 49 - HAZOP Gasifier 2

Feedstock Flow Rate	More	Higher than expected feedstock flow rate	Malfunctioning control valve	Potential flooding of gasifier, reduced gasification efficiency	Installation of flow rate control valves, routine inspection of control valve performance
Oxygen Supply	Less	Insufficient oxygen supply	Failure of oxygen delivery system or low oxygen concentration	Reduced gasification rate, decreased syngas production	Installation of redundant oxygen supply systems, routine inspection of oxygen delivery
Oxygen Supply	More	Excessive oxygen supply	Malfunctioning control system or high oxygen concentration	Increased risk of combustion, safety risks	Installation of control systems, routine inspection of system performance
Tar Removal	Other	Inadequate tar removal	Faulty tar removal system or inadequate cleaning	Clogging of syngas lines, reduced ethanol production	Regular maintenance and cleaning of tar removal system
Gasifier Bed Level	Less	Insufficient bed material	Inadequate feed or system failure	Incomplete gasification, reduced syngas production	Installation of level sensors, automated shutdown system in case of low level
Gasifier Bed Level	More	Excessive bed material	Excessive feed or improper level control	Potential bed flooding, reduced gasification efficiency	Installation of level sensors, automated shutdown system in case of high level
Sealing	Other	Leakage from gasifier vessel	Faulty gaskets or seals	Environmental contamination, safety risks	Regular inspection and replacement of gaskets and seals

CONCLUSIONS

In conclusion, the construction of a bioethanol factory in Pakistan offers great promise and potential for the long-term growth of the nation. Pakistan can gain a number of advantages by utilizing the plentiful biomass resources that are accessible, including wheat straw, rice straw, and sugarcane bagasse. First, by lowering reliance on imported fossil fuels, indigenous bioethanol production would improve energy security. The objective of a more resilient and self-sufficient energy sector is aligned with this diversification of the energy mix.

Production of bioethanol also has major environmental benefits. Pakistan may aid in worldwide efforts to mitigate climate change by substituting gasoline with bioethanol. Bioethanol is a cleaner and more environmentally friendly fuel choice due to the lower net greenhouse gas emissions connected to its manufacturing. In addition, the synthesis of bioethanol offers a workable method for handling and making use of agricultural waste, solving environmental issues related to the disposal of biomass wastes.

In Pakistan, constructing a bioethanol factory would also promote rural development and job growth. The biomass supply chain offers opportunities for farmers, agricultural laborers, and small business owners to actively participate, generating income and promoting economic empowerment in rural areas. This all-inclusive strategy fosters grassroots sustainable development and encourages fair growth.

The development of allied industries is also made possible by the introduction of the bioethanol industry. Lignin and other byproducts from the manufacturing of bioethanol can be used to make bio-based chemicals, materials, and energy. This promotes the development of a bioeconomy, fosters innovation, and aids in the advancement of sustainable industrial growth.

Additionally, by lowering the nation's reliance on unstable international oil markets, the construction of a bioethanol factory would help to stabilize prices. The national economy and consumers both benefit from this fuel price stability, which shields them from the effects of fluctuations in the price of crude oil on a worldwide scale.

Additionally, the construction of a bioethanol facility would promote information exchange, technological uptake, and capacity building in the field of renewable energy and biofuels. By fostering local innovation, research, and skills, this will assist the growth of a knowledge-based economy that is also sustainable.

It is clear that constructing a bioethanol plant in Pakistan is a strategic move towards achieving energy security, cutting greenhouse gas emissions, advancing rural development, and stimulating economic growth in light of these compelling benefits. It offers an environmentally beneficial and sustainable energy option, which is in line with the nation's aims for sustainable development. Pakistan can set sail for a greener, more resilient, and richer future by embracing bioethanol production.

BIBLIOGRAPHY

1. Almeida Benalcázar, E., Noorman, H., Maciel Filho, R., & Posada, J. A. (2020, March 27). Modeling ethanol production through gas fermentation: A biothermodynamics and mass transfer-based hybrid model for microbial growth in a large-scale bubble column bioreactor - biotechnology for biofuels and Bioproducts. BioMed Central. Retrieved January 21, 2023, from https://biotechnologyforbiofuels.biomedcentral.com/articles/10.1186/s13068-020-01695-y

2. Syngas fermentation for production of ethanol - iopscience. (n.d.). Retrieved January 1, 2023, from https://iopscience.iop.org/article/10.1088/1757-899X/1143/1/012014/meta

3. Lanzatech. (n.d.). Retrieved February 17, 2023, from https://lanzatech.com/

4. Zaman, S., Yuan, Z., Vohra, M., Heijden, H. van der, Surisetty, V. R., Subramanian, N. D., Srirangan, K., Roddy, D. J., Munasinghe, P. C., Mohanty, P., Mei, D., Liew, W. H., Liu, Y., … Centi, G. (2020, May 22). Process design and evaluation of syngas-to-ethanol conversion plants. Journal of Cleaner Production. Retrieved December 21, 2023, from
https://www.sciencedirect.com/science/article/pii/S0959652620321259

5. Zuo, Z.-J., Peng, F., & Huang, W. (2016, October 3). Efficient synthesis of ethanol from CH4 and syngas on a Cu-Co/Tio2 catalyst using a stepwise reactor. Nature News. Retrieved January 5, 2023, from
https://www.nature.com/articles/srep34670

6. Top ethanol companies. VentureRadar. (n.d.). Retrieved December 27, 2023, from https://www.ventureradar.com/keyword/Ethanol

7. David M. Kennes-Veiga, Carla Fernández-Blanco, María C. Veiga, Christian Kennes (2011, January 8). Ethanol production from syngas
https://www.sciencedirect.com/science/article/abs/pii/B9780323918787000137

8. David Kennes, Haris Nalakath Abubackar, Marío Diaz, María C Veiga, Christian Kennes (2015, October 22) Bioethanol production from biomass: carbohydrate vs syngas fermentation
https://onlinelibrary.wiley.com/doi/full/10.1002/jctb.4842