Process Design for Production of Linear Low Density Polyethylene from Ethanol “Green plastic”

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Certificate

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Dedication

We dedicate our work to our family and SCME

Acknowledgement

First of all we bow before **ALLAH, The Almighty**, for HIS countless blessing and help.

We are thankful to **Dr. Arshad Hussain,** our project supervisor, who guided us throughout the project and encouraged us to give our best.

We are grateful to our **parents**, without their support and backing, the project was not possible. They supported us through out and kept our hopes high at hard times.

We are thankful to our friends for their support and assistance.

We are obliged to have supportive **SCME faculty** and we did like to thank **Sir Muhammad Ahsan**, **Dr. Erum Pervaiz** and **Miss Monaza Sarwar** for their support and help.

Nomenclature

Streams:

S1	Feed	S11	Co-monomer Feed
S1a	Feed + Recycle	S12	Nitrogen + Catalyst Feed
S1b	Feed at high pressure	S13	Reactor Top Stream
S1c	Preheated Feed	S14	Reactor Bottom Stream
S2	Heated Reactor Feed	S15	Cyclone Top Stream
S3	Reactor Top Outlet	S16	Cyclone Bottom Stream
S4	Reactor Bottom Outlet	S16a	Screen Filtrate (Catalyst Recycle)
S3a	Reactor Top + Ethylene Recycle	S16b	Polymer Residue on Screen
S5	Cooled Distillation 1 Feed	S17	Mixed Gases Recycle
S4a	Pre-cooled Distillation 1 Feed	S17a	Cooled Mixed Gases
S4b	Cooled Separator Feed	S17b	Membrane Feed
S6	Distillation 1 Top Stream(Ethylene)	S18	Membrane Permeate
S7	Distillation 1 Bottom Stream	S19	Purge
S7a	Separator + Distillation Mix	S20	Heated Recycle
S8	Cooled Distillation 2 Feed	S21	Membrane Reject
S9	Distillation 2 Top (Ethanol Recycle)	S21a	Compressed Recycle Gasess
S10	Waste Water	S21b	Heated Recycle Gases
S6a	Pre-heated Monomer Feed	S14a	Gases to Mixer for Recycle
S6b	Heated Monomer Feed	S14b	Polymer Product

cp	Heat Capacity
ΔTm	Log Mean Temperature Difference
m	Meter
mm	Millimeter
cm	Centimeter
m2	Meter square
m3	Meter cube
cm2	Centimeter square
cm3	Centimeter cube
KJ	Kilo Joule
kg	Kilogram
h	Hour
cv	Heat Capacity of Vapor
cl	Heat Capacity of Liquid
cs	heat capacity of Solid
mmol	Millimole
gmol	gram mole
L	Length
D	Diameter
H	Height
ð	Thickness
ε	Void Ratio
α	Selectivity
µ	Viscosity
ƛ	Latent Enthalpy of steam
θ	Stage Cut
Am	Area of Membrane
y1	Mole Fraction
y2	Mole Fraction
Tsb	Temperature of Solids Leaving
Tsa	Temperature of Air Entering
Tsv	Temperature of Vaporization
Nt	Number of transfer Units
qT	Energy
°C	Centigrade
°K	Kelvin
°F	Fahrenheit
P	Inlet Pressure
I.D	Internal Diameter
j	Joint Factor
e	Wall Thickness
ρ	Density
Eu	Euler
P	Permeance
ROR	Rate of Return
MJ/kg	Mega Joule per kilogram
U	Overall Heat Transfer Coefficient
Pt	Tube Pitch
Ds	Shell Diameter
IB	Baffle Spacing

GS	Mean Velocity
Ft	Friction Factor
W	Watt
H2	Hydrogen
N2	Nitroge
Re	Reynolds Number
ΔP	Pressure Difference
PCE	Purchase Cost of Equipment
Hi	Internal Pipe Heat Transfer Coefficient
O.D	Outer diameter
As	Cross Sectional Area
Pr	Prandtl Number
Nu	Nusselt Number
de	Equivalent diameter
Np	Number of Tube Passes
ut	Tube Side Velocity
jh	Heat Transfer Factor
s	Second
do	Tube Outside Diameter
BWG	Birmingham Wire Gauge
Q	Volumetric Flow Rate
a	Packing surface area per unit volume
aw	Effective interfacial area of packing per unit volume
CT	Total molar concentration
DL	Liquid diffusivity
Dv	Diffusivity of vapor
Dp	Size of packing
Fp	Packing factor
Gm	Molar flow-rate of gas per unit area
G	Gravitational acceleration
HG	Height of gas film transfer unit
HL	Height of liquid film transfer unit
HOG	Height of overall gas phase transfer unit
HOL	Height of overall liquid phase transfer unit
H	Henry’s constant
KG	gas phase mass transfer coefficient
KL	liquid phase mass transfer coefficient
Lw	Liquid mass flow-rate
L*w	Liquid mass flow-rate per unit area
N	Number of stages
NG	Number of gas-film transfer units
NL	Number of liquid-film transfer units
NOG	Number of overall gas-phase transfer units
Si	Stripping factor
P	Partial pressure
x1	Concentration of solute in solution at column base
x2	Concentration of solute in solution at column top
Z	Height of packing

Abstract

With growing demand of plastic day by day, oil is depleting and prices are increasing, there is a need for an alternative to oil for plastic production. Pollution is a major concern in today's world and plastic is prime cause. A simple solution to this issue is green plastic, plastic produced from plants that is environment friendly. Project is aimed at producing liner low density polyethylene (lldpe) from ethanol. Ethanol will be taken from market, extracted from molasses (green source). Production of green plastic will reduce the consumption of oil and produced plastic will be environment friendly. Gas phase polymerization will be used as the temperature requirements are low and the process is feasible.

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Chapter – 1 **Introduction**

1.1 History

Polyethylene was first synthesized by the German chemist Hans von Pechmann who prepared it by accident in 1898 while investigating diazomethane. When his colleagues Eugen Bamberger and Friedrich Tschirner characterized the white, waxy substance that he had created, they recognized that it contained long -CH_2- chains and termed it polymethylene.

The first industrially practical polyethylene synthesis (diazomethane is a notoriously unstable substance that is generally avoided in industrial application) was discovered in 1933 by Eric Fawcett and Reginald Gibson, again by accident, at the Imperial Chemical Industries (ICI) works in Northwich, England. Upon applying extremely high pressure (several hundred atmospheres) to a mixture of ethylene and benzaldehyde they again produced a white, waxy, material. Because the reaction had been initiated by trace oxygen contamination in their apparatus, the experiment was, at first, difficult to reproduce. It was not until 1935 that another ICI chemist, Michael Perrin, developed this accident into a reproducible high-pressure synthesis for polyethylene that became the basis for industrial LDPE production beginning in 1939. Because polyethylene was found to have very low-loss properties at very high frequency radio waves, commercial distribution in Britain was suspended on the outbreak of World War II, secrecy imposed and the new process was used to produce insulation for UHF and SHF coaxial cables of radar sets. During World War II, further research was done on the ICI process and in 1944 Bakelite Corporation at Sabine, Texas and Du Pont at Charleston, West Virginia, began large scale commercial production under license from ICI.

The breakthrough landmark in the commercial production of polyethylene began with the development of catalyst that promote the polymerization at mild temperatures and pressures. The first of these was a chromium trioxide–based catalyst discovered in 1951 by Robert Banks and J. Paul Hogan at Phillips Petroleum. In 1953 the German chemist Karl Ziegler developed a catalytic system based on titanium halides and organo-aluminium compounds that worked at even milder conditions than the Phillips catalyst. The Phillips catalyst is less expensive and easier to work with, however, and both methods are heavily used industrially. By the end of the 1950s both the Phillips- and Ziegler-type catalysts were being used for HDPE production. In the 1970s, the Ziegler system was improved by the incorporation of magnesium chloride. Catalytic systems based on soluble catalysts, the metallocenes, were reported in 1976 by Walter Kaminsky and Hansjörg Sinn. The Ziegler- and metallocene-based catalysts families have proven to be very flexible at copolymerizing ethylene with other olefins and have become the basis for the wide range of polyethylene resins available today, including very low density polyethylene and linear low-density polyethylene. Such resins, in the form of UHMWPE fibers, have (as of 2005) begun to replace aramids in many high-strength applications.

1.2 Polyethylene

Polyethylene is available with a wide array of engineering properties to provide toughness, chemical abrasion and impact resistance, low coefficient of friction, durability in the elements and near-zero moisture absorption. These properties make polyethylene an ideal material for many applications. On the other hand, polyethylene is not degradable polymer under normal environmental conditions. It takes a long time for complete degradation. It is this reason that it ends up in landfills and oceans, which is a great environmental issue.

1.2.1 Classifications

Previously polyethylene was classified on the basis of the type of manufacturing processes that is either high pressure or low pressure polyethylene. American standard of testing material (ASTM) has classified polyethylene into grades based on density as shown in Table 1.1

Table 1.1 ASTM grades of polyethylene

Grade	**Density (g/cm^3)**
Low Density	0.910-0.925
Linear Low Density	0.926-0.940
High Density	0.941-0.959

The very low density polyethylene (VLDPE) was introduced by Kurtz, which has a density less than 0.91 g/cm^3. Recently, classification based on structure has been used. Figure 1.2 shows the structural differences between various grades of polyethylene.

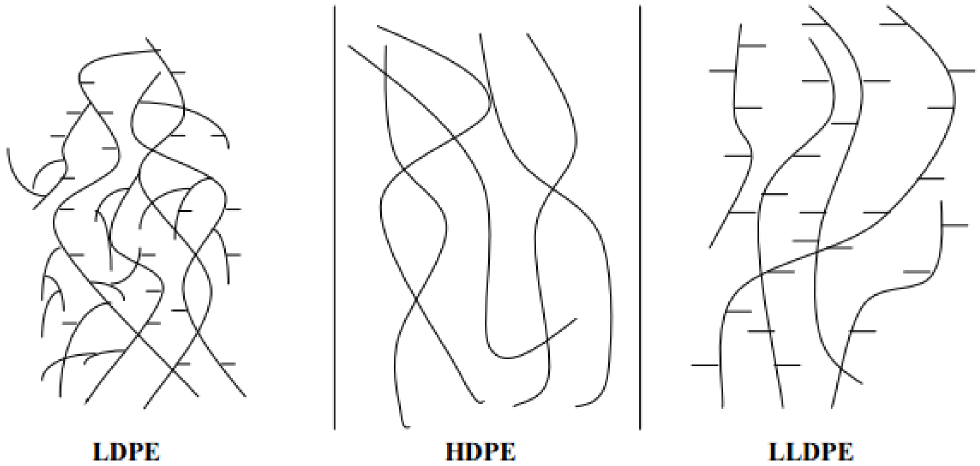


Figure 1.1 Schematic structures of different grades of polyethylene.

1.2.2 Linear Low Density Polyethylene (LLDPE)

Union Carbide and Dow chemical first commercialized LLDPE in the late 1970s. The annual global production of LLDPE is approximately 13.6 million tons. In the early 1990s, the LLDPE industry was revitalized with the introduction of several new product families, including novel single-site-catalyzed very low density polyethylene (VLDPE) called plastomers, super-hexene LLDPE, and metallocene-catalyzed (mLLDPE) for commodity applications. Work continues by resin companies around the world on new classes of LLDPE for a variety of applications. The difference between LLDPE and LDPE is that the former has narrow molecular weight distribution and does not contain long chain branching. LLDPE is a linear polymer having short branches made by copolymerization of ethylene with alpha olefins (e.g. 1-butene, 1-hexene and 1-octene). It is generally represented by formula [−CH2−CH2−CH2−CH−(Cn-2H2(n-2) +1)], where n represents the number of carbon atoms. Generally, LLDPE resins do not contain long chain branches; however, some of its resins may contain some long chain branches such as VLDPE.

1.2.2.1 Manufacturing processes of linear low density polyethylene

LLDPE is produced by the addition of alpha-olefins - butene, hexene or octene - during the polymerisation of ethylene to give a resin with a similar density to LDPE but the linearity of HDPE. Solution, slurry or gas phase processes are used to make LLDPE but the licensing of low-cost gas phase technology by Union Carbide (now Univation) and later BP Chemicals (INEOS) has contributed to the popularity of this resin. Many processes can swing between LLDPE and HDPE production although many plants tend to be dedicated to one of the two resins.

In the gas phase process, ethylene with the co-monomer and hydrogen are fed to the base of a fluid bed reactor into which the catalyst is injected. Polymerization takes place at 60-100oC and 22 bar pressure. The polymer particles formed are kept in a fluidized state by the gas stream. The polymer leaves the reactor as a white powder and is sent to a degasser where unreacted olefins are removed. Advantages claimed for the gas phase route include low temperature operation and lower operating costs.

The recent introduction of metallocene catalysts enables the production of resins with narrow molecular weight distribution giving much improved physical properties. The latest generation metallocenes are said to overcome the poor processability problems and can produce resins with properties similar to high pressure LDPE. Some companies are developing non-metallocene single site catalysts for LLDPE. New catalyst systems are also allowing more effective use of comonomers to improve performance such that claims have been made of butene copolymers with the performance of traditional hexene copolymers, and similarly for hexene copolymers with octene copolymer performance.

1.2.2.2 Properties of linear low density polyethylene

Conventional LLDPE covers the density range of 0.926–0.940. It has higher impact, tensile strength and puncture resistance than LDPE. LLDPE is a saturated hydrocarbon and is generally unreactive. The most reactive parts of the polymer molecule are tertiary carbons at short-chain branch points and double bonds at chain ends. LLDPE is stable in alcohols, alkaline solutions, and saline solutions. It is not attacked by weak organic or inorganic acids. It has heterogeneous composition and higher density fraction with minimal branching and form spherulitic structure. The amount of crystallinity in LLDPE increases by decreasing α-olefins co-monomer contents and it becomes stiffer by increasing its crystallinity.

1.2.2.3 Applications of linear low density polyethylene

LLDPE is used in packaging especially for film, bags and sheets. Injection molding is the second largest product area for LLDPE. Its applications include food containers, trash cans and lids, etc. Pipe and tubing are extruded from LLDPE at limited seal with higher burst strength. LLDPE is also used in the insulation of wires and cable for low and medium voltage applications. The ESCR and improved flexibility make it ideal for blow molded bottle applications. Its rotational molded articles are used for storage tank and outdoor furniture.

1.3 BioPlastic

Bioplastics are plastics derived from renewable biomass sources, such as vegetable fats and oils, corn starch, pea starch or microbiota. Bioplastic can be made from agricultural by-products and also from used plastic bottles and other containers using microorganisms. Common plastics, such as fossil-fuel plastics (also called petrobased polymers), are derived from petroleum or natural gas. Production of such plastics tends to require more fossil fuels and to produce more greenhouse gases than the production of biobased polymers (bioplastics). Some, but not all, bioplastics are designed to biodegrade. Biodegradable bioplastics can break down in either anaerobic or aerobic environments, depending on how they are manufactured. Bioplastics can be composed of starches, cellulose, biopolymers, and a variety of other materials.

1.3.1 Bio-derived polyethylene "Green Plastic"

The basic building block (monomer) of polyethylene is ethylene. Ethylene is chemically similar to, and can be derived from ethanol, which can be produced by fermentation of agricultural feedstock such as sugar cane or corn. Bio-derived polyethylene is chemically and physically identical to traditional polyethylene – it does not biodegrade but can be recycled. Bio derivation of polyethylene can also reduce greenhouse gas emissions considerably. Brazilian chemicals group Braskem claims that using its method of producing polyethylene from sugar cane ethanol captures (removes from the environment) 2.5 tons of carbon dioxide per ton of polyethylene produced, while the traditional petrochemical production method results in emissions of close to 3.5 tons.

Braskem plans to introduce commercial quantities of its first bio-derived high density polyethylene, to be used in a packaging such as bottles and tubs, in 2010, and has developed a technology to produce bio-derived butene, which is required to make the linear low density polyethylene types used in film production.

1.3.2 Bioplastics and biodegradation

The terminology used in the bioplastics sector is sometimes misleading. Most in the industry use the term bioplastic to mean a plastic produced from a biological source.

All (bio- and petroleum-based) plastics are technically biodegradable, meaning they can be degraded by microbes under suitable conditions. However, many degrade so slowly that they are considered non-biodegradable. Some petrochemical-based plastics are considered biodegradable, and may be used as an additive to improve the performance of commercial bioplastics. Non-biodegradable bioplastics are referred to as durable. The biodegradability of bioplastics depends on temperature, polymer stability, and available oxygen content. The European standard EN13432, published by the International Organization for Standardization, defines how quickly and to what extent a plastic must be degraded under the tightly controlled and aggressive conditions (at or above 140 °F) of an industrial composting unit for it to be considered biodegradable. This standard is recognized in many countries, including all of Europe, Japan and the US. However, it applies only to industrial composting units and does not set out a standard for home composting. Most bioplastics (e.g. PH) only biodegrade quickly in industrial composting units. These materials do not biodegrade quickly in ordinary compost piles or in the soil/water. Starch-based bioplastics are an exception, and will biodegrade in normal composting conditions.

The term "biodegradable plastic" has also been used by producers of specially modified petrochemical-based plastics that appear to biodegrade. Biodegradable plastic bag manufacturers that have misrepresented their product's biodegradability may now face legal action in the US state of California for the misleading use of the terms biodegradable or compostable. Traditional plastics such as polyethylene are degraded by ultra-violet (UV) light and oxygen. To prevent this, process manufacturers add stabilising chemicals. However with the addition of a degradation initiator to the plastic, it is possible to achieve a controlled UV/oxidation disintegration process. This type of plastic may be referred to as degradable plastic or oxy-degradable plastic or photodegradable plastic because the process is not initiated by microbial action. While some degradable plastics manufacturers argue that degraded plastic residue will be attacked by microbes, these degradable materials do not meet the requirements of the EN13432 commercial composting standard. The bioplastics industry has widely criticized oxo-biodegradable plastics, which the industry association says do not meet its requirements. Oxo-biodegradable plastics – known as "oxos" – are conventional petroleum-based products with some additives that initiate degradation. The ASTM standard for oxo-biodegradables is called the Standard Guide for Exposing and Testing Plastics that Degrade in the Environment by a Combination of Oxidation and Biodegradation (ASTM 6954). Both EN 13432 and ASTM 6400 are specifically designed for PLA and Starch based products and should not be used as a guide for oxos.

Chapter – 2 **Process Description**

The whole plant has been divided into 2 sections.

- Monomer Preparation Section
- Polymerization Section

2.1 Process Flow Diagram

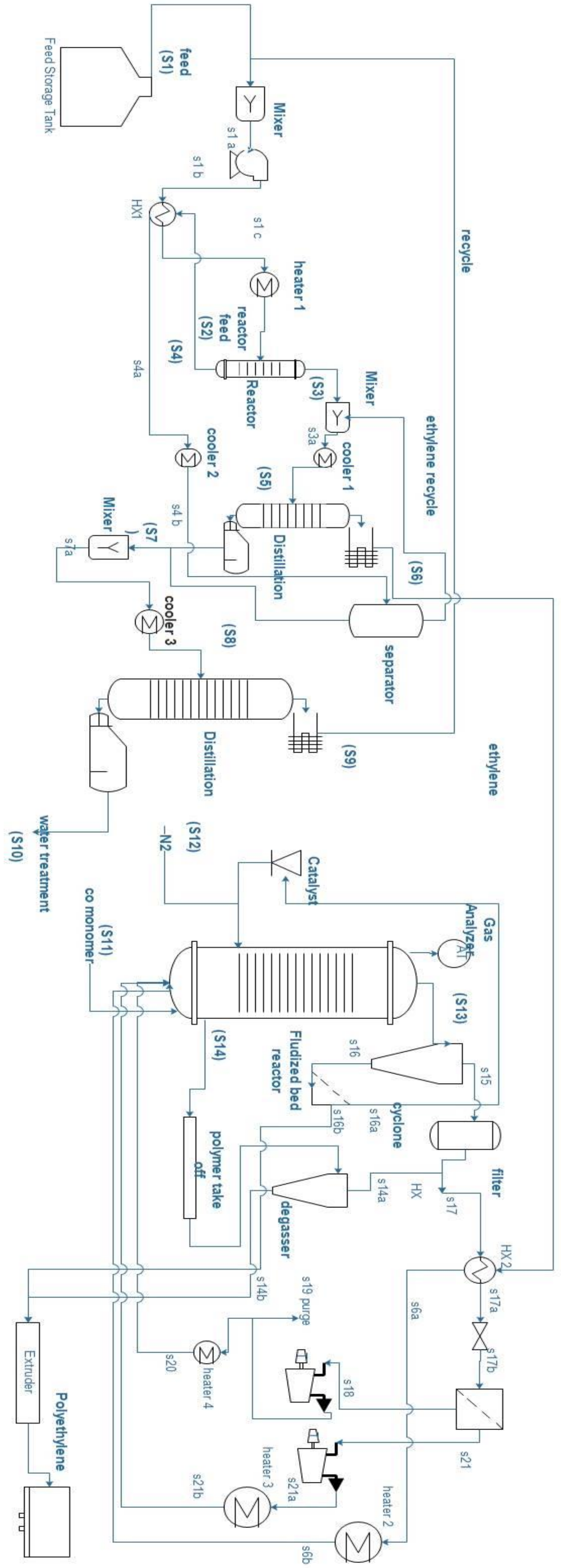


Figure 2.1 Process Flow Diagram

2.2 Monomer Preparation Section

As discussed earlier, the plant was divided into 2 sections. This section gives a brief view of processes in monomer preparation.

Ethanol is being converted to Ethylene (monomer for polyethylene) by catalytic dehydration.

2.2.1 Feed Preparation

Basic raw material for this process is 97% Ethanol that is readily available in market. Since Pakistan has many sugar mills and every sugar mill has molasses as by-product, the combined distilleries of these sugar mills convert this molasses to ethanol which is readily available at reasonable cost and various grades.

The feed is first stored in a floating roof tank and then supplied to the plant. Before being pumped to reactor, a recycle stream is mixed with it and then the main stream (S1a) is pumped to fixed bed reactor via a shell and tube heat exchanger and a heater to preheat (S1c) and then heat (S2) it to desired temperature.

2.2.2 Dehydration of Ethanol

The feed that enters the reactor is 95% ethanol at 424ºC and 42 bar. The reactor being used for dehydration is a fixed bed reactor and catalytic dehydration is being carried out. The reactions that take place inside reactor along with their conversions are as follows:

Reactions	**Conversion**
$C_2H_5OH \leftrightarrow H_2O + C_2H_4$	70 %
$2\ C_2H_5OH \rightarrow H_2O + (C_2H_5)O$	0.5 %
$C_2H_5OH \rightarrow H_2 + CH_3COH$	0.08 %
$C_2H_5OH + 2H_2 \rightarrow H_2O + 2CH_4$	0.01 %
$C_2H_5OH + H_2O \rightarrow 2H_2 + CH_3COOH$	0.025 %
$C_2H_5OH + H_2 \rightarrow H_2O + C_2H_6$	0.01 %

So the overall conversion for ethanol to ethylene is 70%

The catalyst employed for the process is γ-alumina. The reactions are highly exothermic and the outlet streams of the rector have low temperature (206ºC) as compared to inlet stream (424ºC). No external heat is required for the reaction as the feed streams provide sufficient heat for the reaction. There are some by-products of this reaction too but the conversion rates are very less and they can be ignored.

The top product stream of the reactor contains ethylene with small fractions of water and ethanol which are separated from it via distillation. The bottom outlet stream contains water ethanol and fractions of ethylene. Ethylene is separated from it and sent to distillation column.

2.2.3 Ethylene Separation

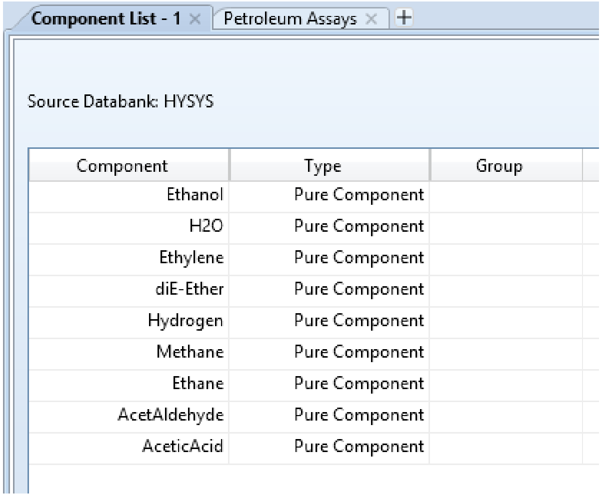
The top product stream of fixed bed reactor contains ethylene with ethanol and water. Ethylene has to be separated from these components before it is sent to polymerization section. To do so, a distillation column is used. Feed is cooled to room temperature and sent to “distillation column 1”. This column completely separates ethylene from rest of components. Separated ethylene is sent to polymerization section as monomer. The bottom stream of reactor is sent to a separator for ethylene recovery. The recovered ethylene is sent back to “distillation column 1”. The bottom stream of distillation column is sent to another distillation column for ethanol recovery.

2.2.4 Ethanol Recovery

The residue streams now contains ethanol and water. Ethanol has to be separated from water to avoid the wastage. This is done using another distillation column. The feed is cooled to room temperature and sent to “distillation column 2”. Here ethanol is sent back to main stream as top product of distillation column while bottom product contains water that is sent for treatment.

2.3 Aspen HYSYS Simulation of Monomer Preparation

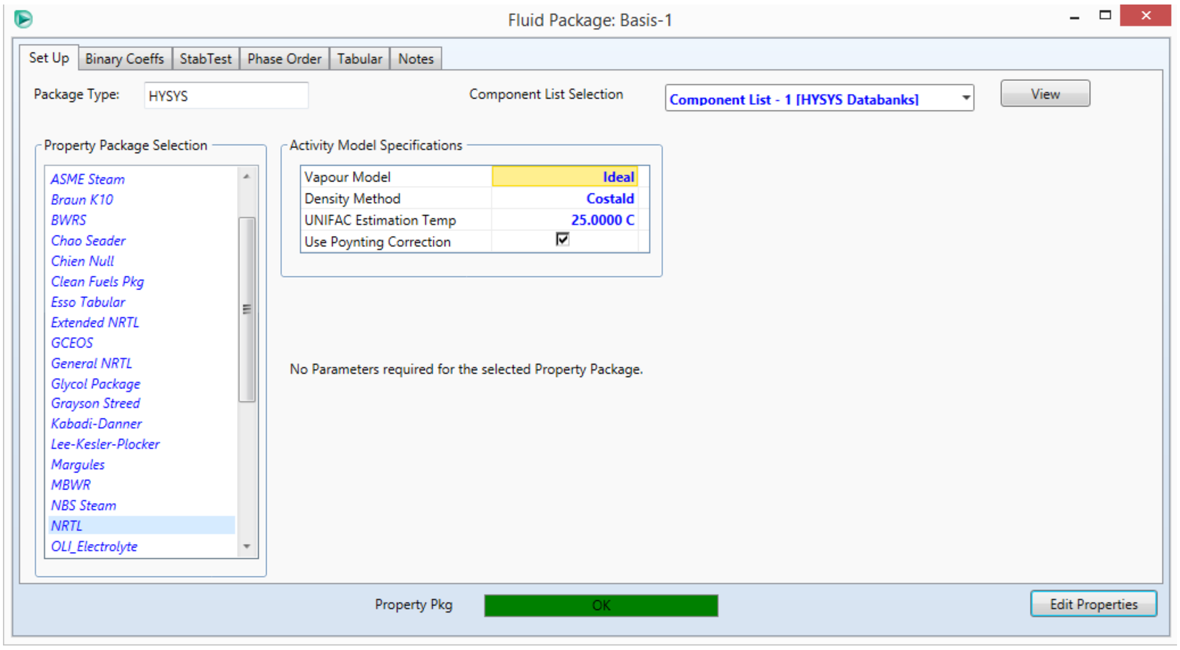
The monomer preparation section of plant was simulated on Aspen HYSYS to check the validity of the results. Following are the screenshots of Aspen HYSYS modeling:



Source Databank: HYSYS

Component	Type	Group
Ethanol	Pure Component	
H2O	Pure Component	
Ethylene	Pure Component	
diE-Ether	Pure Component	
Hydrogen	Pure Component	
Methane	Pure Component	
Ethane	Pure Component	
AcetAldehyde	Pure Component	
AceticAcid	Pure Component	

Figure 2.2 Components List



Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

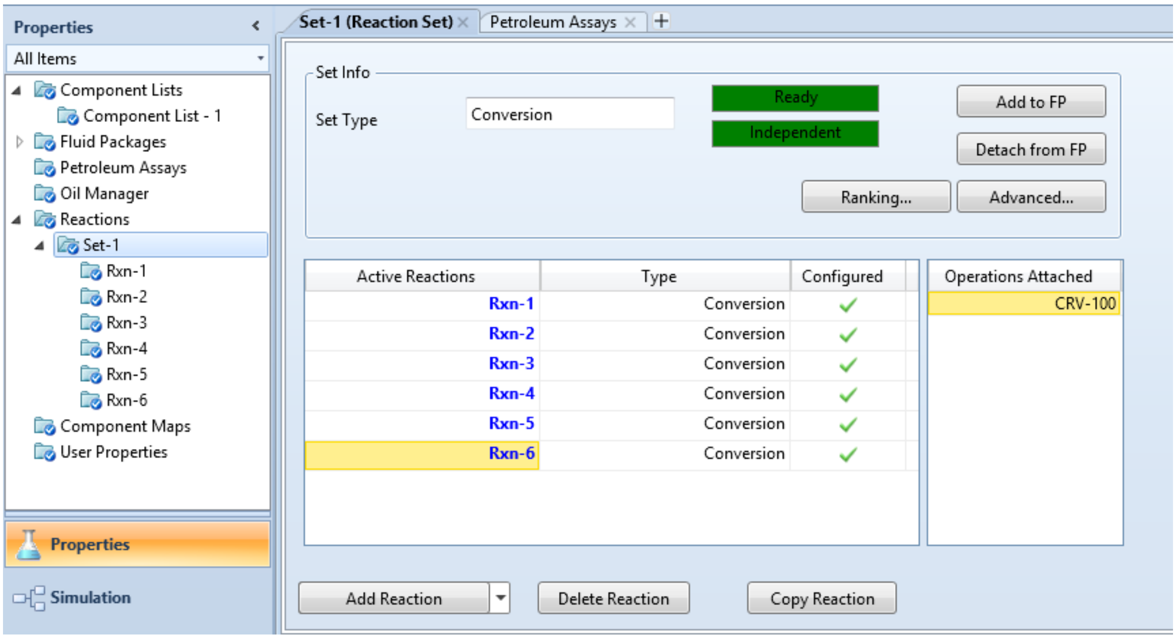
Activity Model Specifications

Vapour Model	Ideal
Density Method	Costald
UNIFAC Estimation Temp	25.0000 C
Use Poynting Correction	☑

No Parameters required for the selected Property Package.

Property Pkg: OK

Figure 2.3 Fluid Package



Set Type: Conversion

Ready

Independent

Active Reactions	Type	Configured
Rxn-1	Conversion	✓
Rxn-2	Conversion	✓
Rxn-3	Conversion	✓
Rxn-4	Conversion	✓
Rxn-5	Conversion	✓
Rxn-6	Conversion	✓

Operations Attached
CRV-100

Figure 2.4 Reactions Set

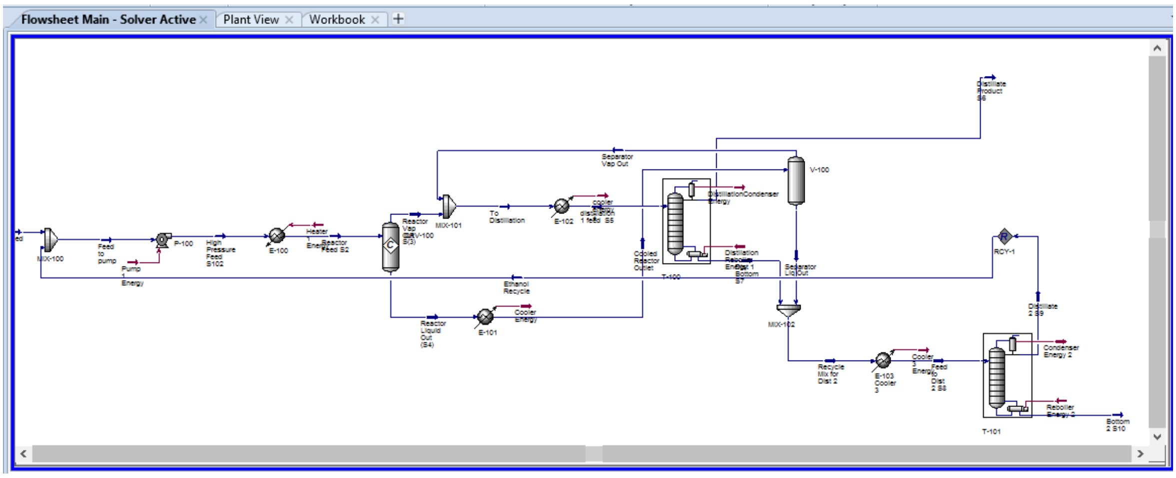
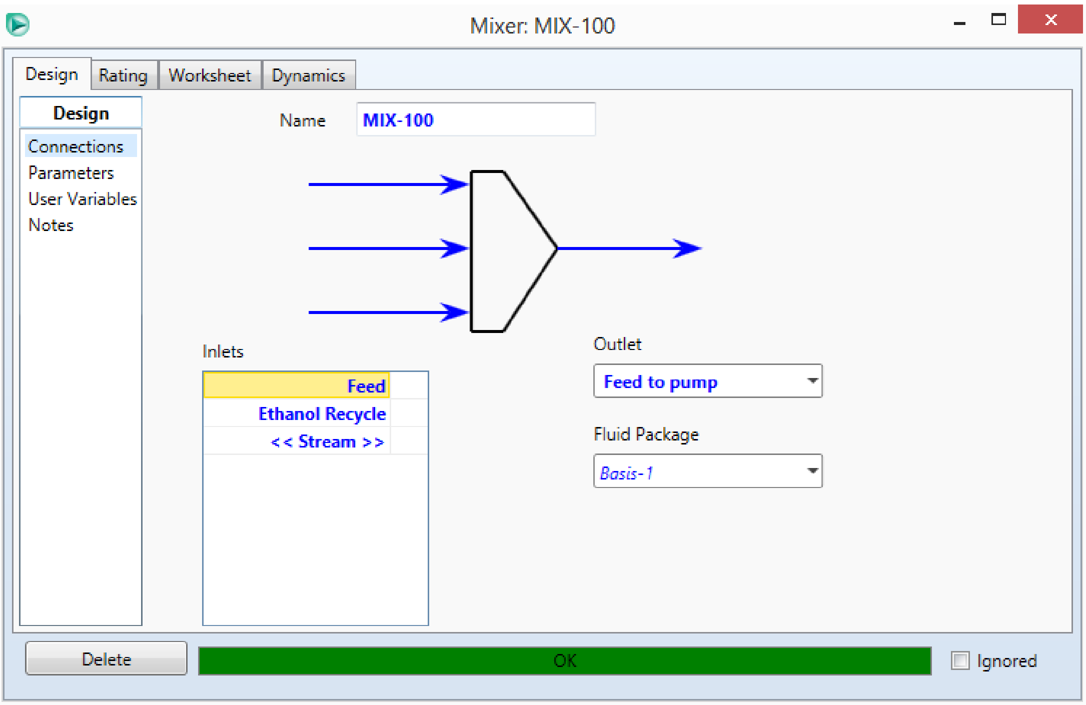


Figure 2.5 Simulation Flowsheet



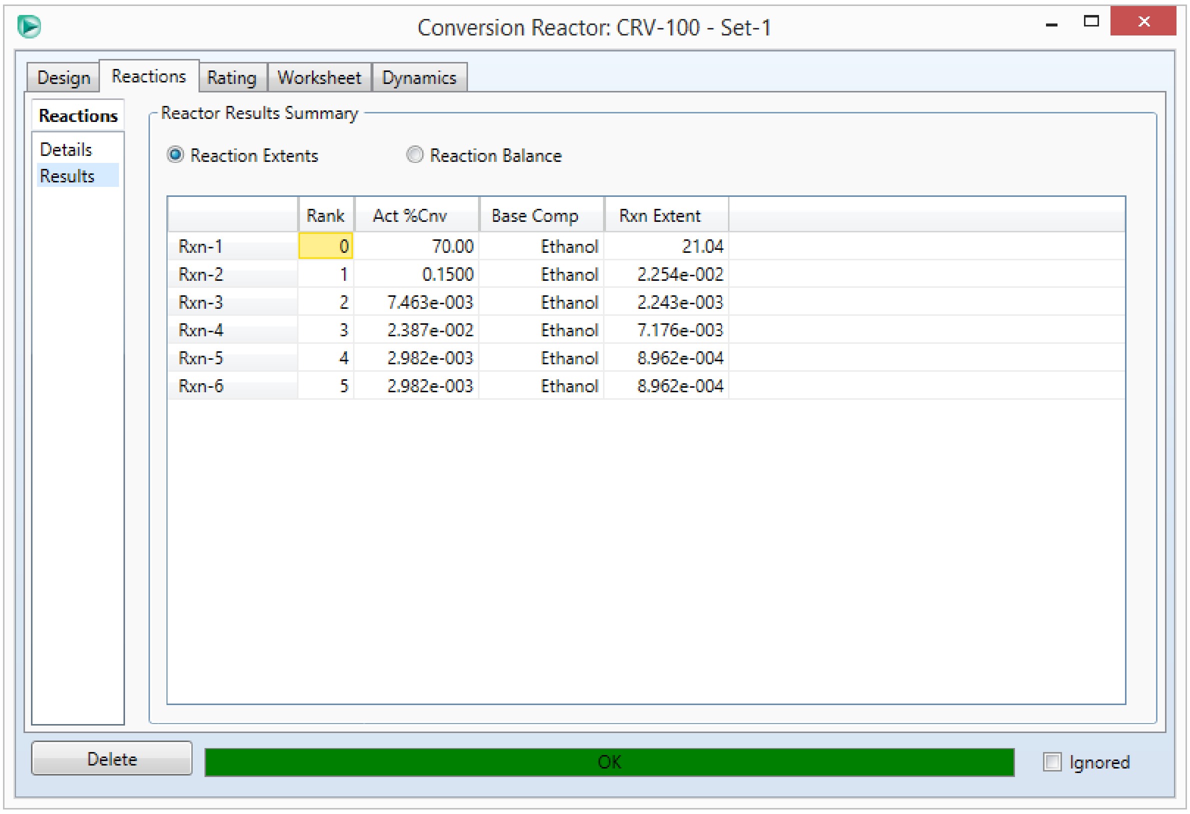
Name: MIX-100

Inlets: Feed, Ethanol Recycle, << Stream >>

Outlet: Feed to pump

Fluid Package: Basis-1

Figure 2.6 Mixer



Conversion Reactor: CRV-100 - Set-1

Reactions

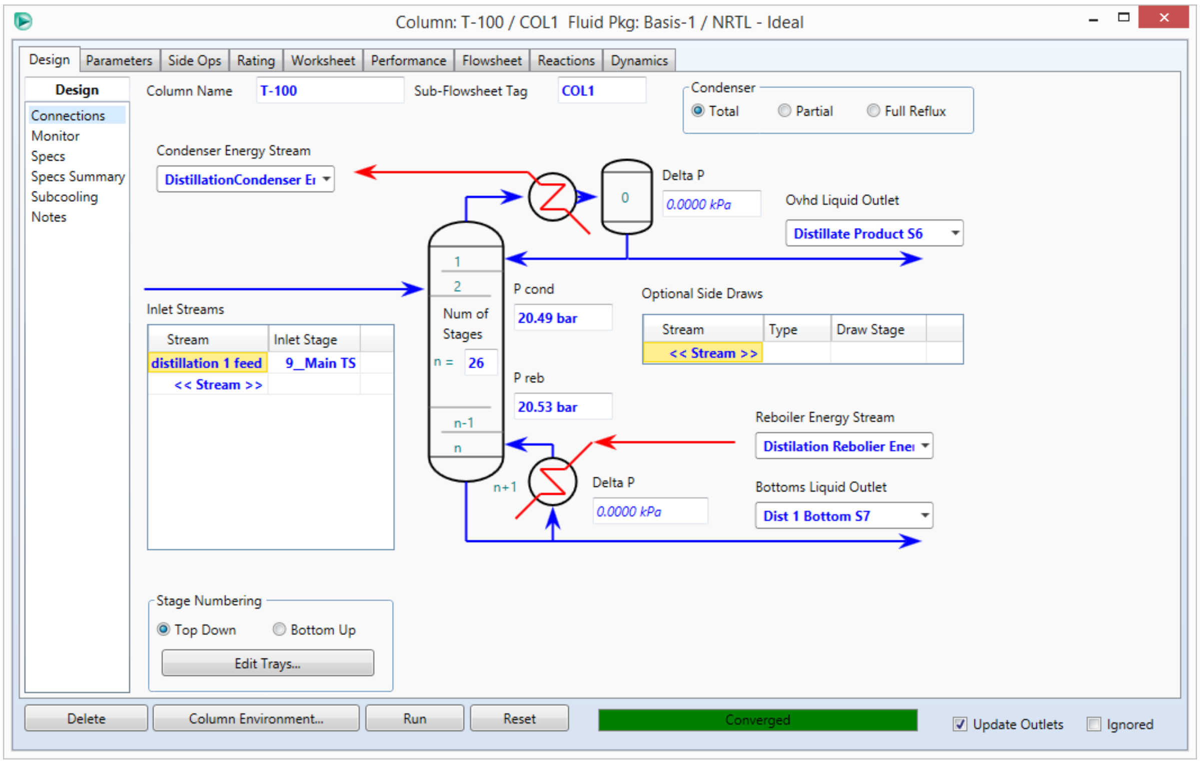
Reactor Results Summary

● Reaction Extents ○ Reaction Balance

	Rank	Act %Cnv	Base Comp	Rxn Extent
Rxn-1	0	70.00	Ethanol	21.04
Rxn-2	1	0.1500	Ethanol	2.254e-002
Rxn-3	2	7.463e-003	Ethanol	2.243e-003
Rxn-4	3	2.387e-002	Ethanol	7.176e-003
Rxn-5	4	2.982e-003	Ethanol	8.962e-004
Rxn-6	5	2.982e-003	Ethanol	8.962e-004

☐ Ignored

Figure 2.7 Reactor Conversions



Column: T-100 / COL1 Fluid Pkg: Basis-1 / NRTL - Ideal

Column Name: T-100

Sub-Flowsheet Tag: COL1

Condenser: ● Total ○ Partial ○ Full Reflux

Condenser Energy Stream: DistillationCondenser Er

Delta P: 0.0000 kPa

Ovhd Liquid Outlet: Distillate Product S6

P cond: 20.49 bar

Num of Stages: n = 26

P reb: 20.53 bar

Inlet Streams

Stream	Inlet Stage
distillation 1 feed	9__Main TS
<< Stream >>	

Optional Side Draws

Stream	Type	Draw Stage
<< Stream >>		

Reboiler Energy Stream: Distilation Rebolier Ener

Delta P: 0.0000 kPa

Bottoms Liquid Outlet: Dist 1 Bottom S7

Stage Numbering: ● Top Down ○ Bottom Up

☑ Update Outlets ☐ Ignored

Figure 2.8 Distillation Column 1 Design

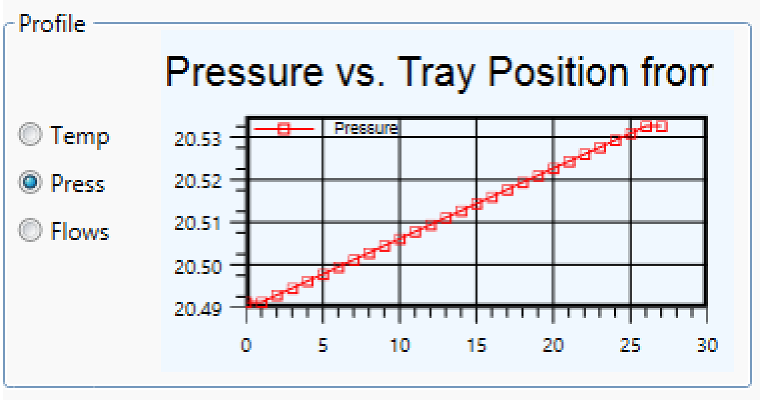
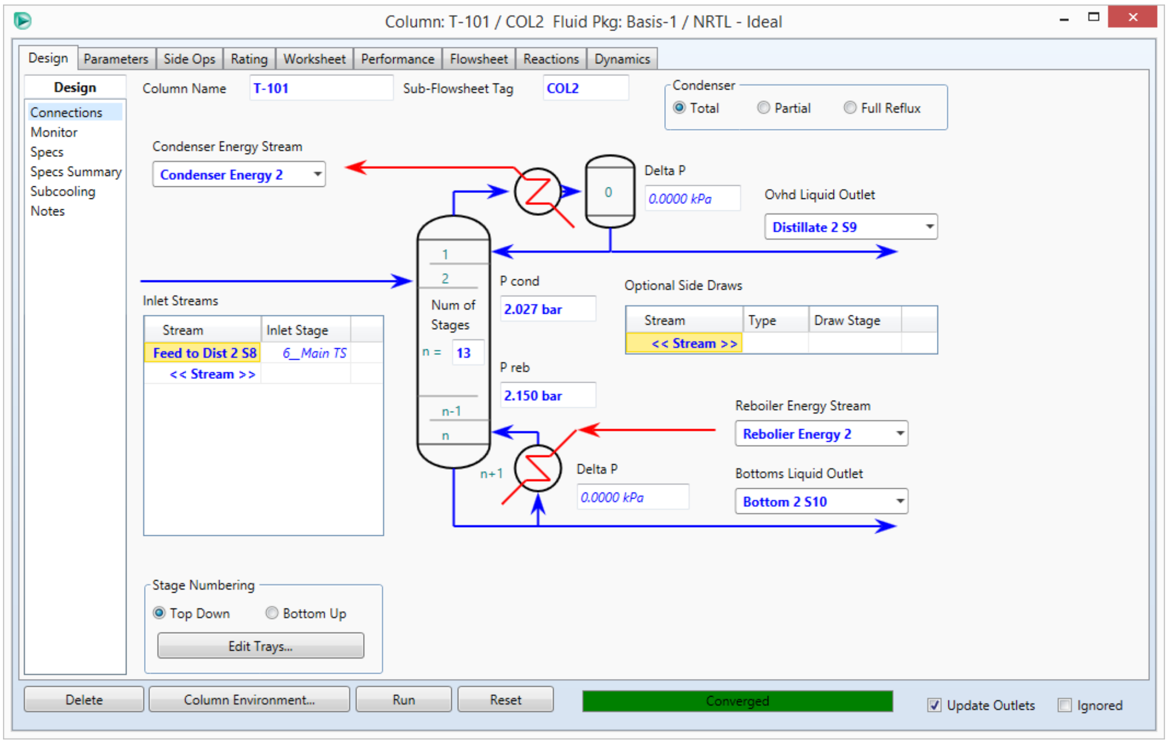


Figure 2.9 Distillation Column 1, Pressure vs Tray Position



Column: T-101 / COL2 Fluid Pkg: Basis-1 / NRTL - Ideal

Column Name: T-101

Sub-Flowsheet Tag: COL2

Condenser: ● Total ○ Partial ○ Full Reflux

Condenser Energy Stream: Condenser Energy 2

Delta P: 0.0000 kPa

Ovhd Liquid Outlet: Distillate 2 S9

P cond: 2.027 bar

Num of Stages: n = 13

P reb: 2.150 bar

Inlet Streams

Stream	Inlet Stage
Feed to Dist 2 S8	6_Main TS
<< Stream >>	

Optional Side Draws

Stream	Type	Draw Stage
<< Stream >>		

Reboiler Energy Stream: Rebolier Energy 2

Delta P: 0.0000 kPa

Bottoms Liquid Outlet: Bottom 2 S10

Stage Numbering: ● Top Down ○ Bottom Up

Converged

☑ Update Outlets ☐ Ignored

Figure 2.10 Distillation Column 2 Design

2.4 Polymerization Section

In this section ethylene is converted to Polyethylene using a fluidized bed reactor in gas phase polymerization. The product being produced is Linear Low Density Polyethylene (LLDPE). There are no by-products of this reaction and we can achieve 100% ethylene conversion for this reaction.

2.4.1 Feed Preparation

Feed for polymerization are monomer and co-monomer along with catalyst. The monomer i.e ethylene has been prepared in monomer preparation section. The co-monomer is 1-butene that will be purchased from market. H_2 will be used as reaction terminator. The catalyst being used is Ti, V, $CrCO_3$ and Nitrogen is used as an inert gas that also bring in the catalyst. All the feed streams are compressed to 20 bar and heated to 57^oC before being sent to reactor.

2.4.2 Polymerization

The reaction mechanism that this reaction follows is Co-Polymerization. The reactor being used is a fluidized bed reactor.

2.4.2.1 Reaction Mechanism

Ethylene polymerization can be envisioned as occurring at the interface between the solid catalyst and the polymer matrix, where the active centers are located. From gas-state monomer to solid-state polymer, ethylene experiences a dramatic physicochemical transition within a very short time. The polymerization environment changes with the composition of catalyst, polymerization process, reactant composition, reactor operating conditions, and extent of polymerization. Although intensive research activity has been focused on Ziegler-Natta catalyst systems since their discovery in the early 1950s, no definitive chemical reaction mechanisms have been developed to fully describe the kinetic behavior of ethylene homo/copolymerization, due to the complexity of the systems employed. Nevertheless, the key elementary reactions have been established, which include formation of active centers, insertion of monomer into the growing polymer chains, chain-transfer reactions, and catalyst deactivation. Most of the proposed mechanisms are based on information about polymerization rate, molecular weight and its distribution, polymer chain microstructure, and active center concentrations. Since commercial production of LLDPE and HDPE consists of a copolymerization process, copolymerization mechanisms are required to understand kinetic behavior and polymer properties. If one assumes that all of the active centers perform the same reaction mechanisms, but with different reaction rates for each elementary reaction, then elementary reactions which are commonly adopted in modeling studies can be summarized as in Table 2, where C, is the catalyst potential active center; P^*_0 is the active center without polymer chain; $P^*_{m,n,i}$ is the active center with m units of monomer 1 and n units of monomer 2, with the third subscript i denoting the chain terminal monomer type bonded to the active center; $q'_{m,n}$ is a dead polymer chain with a terminal double bond; and $q_{m,n}$ is a dead polymer chain without terminal double bond.

For simplification of notation, no subscript is shown corresponding to the type of active center. The reactions shown in Table 2 should be considered to occur at each type of active center. The mechanisms in Table 2 are summarized based on Ti-based catalysts. Reaction mechanisms for chromium oxide based catalysts are a subset of those in Table 2.

Table 2: Summary of elementary reactions for ethylene and α-olefins co-polymerization.

Reaction	Description
Activation	
$C_p \xrightarrow{K_{aS}} P_0^*$	Spontaneous activation
$C_p + [A] \xrightarrow{K_{aA}} P_0^*$	Activation by aluminum alkyl (A)
$C_p + [E] \xrightarrow{K_{aE}} P_0^*$	Activation by electron donor (E)
$C_p + [H_2] \xrightarrow{K_{aH}} P_0^*$	Activation by hydrogen (H_2)
$C_p + [M_1] \xrightarrow{K_{aM1}} P_0^* + [M_1]$	Activation by monomer 1 (M_1)
$C_p + [M_2] \xrightarrow{K_{aM2}} P_0^* + [M_2]$	Activation by monomer 2 (M_2)
Initiation	
$P_0^* + [M_1] \xrightarrow{K_{i1}} P_{1,0,1}^*$	Initiation of M_1 by normal active center
$P_0^* + [M_2] \xrightarrow{K_{i2}} P_{0,1,2}^*$	Initiation of M_2 by normal active center
$P_{H,0}^* + [M_1] \xrightarrow{K_{iH1}} P_{1,0,1}^*$	Initiation of M_1 by active center with H
$P_{H,0}^* + [M_2] \xrightarrow{K_{iH2}} P_{0,1,2}^*$	Initiation of M_2 by active center with H
$P_{A,0}^* + [M_1] \xrightarrow{K_{iA1}} P_{1,0,1}^*$	Initiation of M_1 by active center with A
$P_{A,0}^* + [M_2] \xrightarrow{K_{iA2}} P_{0,1,2}^*$	Initiation of M_2 by active center with A
$P_{E,0}^* + [M_1] \xrightarrow{K_{iE1}} P_{1,0,1}^*$	Initiation of M_1 by active center with E
$P_{E,0}^* + [M_2] \xrightarrow{K_{iE2}} P_{0,1,2}^*$	Initiation of M_2 by active center with E
Propagation	
$P_{m,n,1}^* + [M_1] \xrightarrow{K_{p11}} P_{m+1,n,1}^*$	Propagation of chain type 1 with M_1
$P_{m,n,1}^* + [M_2] \xrightarrow{K_{p12}} P_{m,n+1,1}^*$	Propagation of chain type 1 with M_2
$P_{m,n,2}^* + [M_1] \xrightarrow{K_{p11}} P_{m+1,n,2}^*$	Propagation of chain type 2 with M_1
$P_{m,n,2}^* + [M_2] \xrightarrow{K_{p12}} P_{m,n+1,2}^*$	Propagation of chain type 2 with M_2

Chain transfer	
$P^*_{m,n,i} \xrightarrow{K_{fspi}} P^*_0 + q'_{m,n}$	Spontaneous chain transfer or β-elimination
$P^*_{m,n,i} + [H_2] \xrightarrow{K_{fHi}} P^*_{H,0} + q'_{m,n}$	Chain transfer to hydrogen (H_2)
$P^*_{m,n,i} + [A] \xrightarrow{K_{fAi}} P^*_{A,0} + q'_{m,n}$	Chain transfer to aluminum alkyl (A)
$P^*_{m,n,i} + [E] \xrightarrow{K_{fEi}} P^*_{E,0} + q'_{m,n}$	Chain transfer to electron donor (E)
$P^*_{m,n,i} + [M_1] \xrightarrow{K_{fM1i}} P^*_{1,0,1} + q'_{m,n}$	Chain transfer to M_1
$P^*_{m,n,i} + [M_2] \xrightarrow{K_{fM2i}} P^*_{0,1,2} + q'_{m,n}$	Chain transfer to M_2
Deactivation	
$P^*_{m,n,i} \xrightarrow{K_{dspi}} C_d + q_{m,n}$	Spontaneous deactivation
$P^*_{m,n,i} + [Z] \xrightarrow{K_{dZi}} C_d + q_{m,n}$	Deactivation by impurities or poison (Z)
$P^*_{m,n,i} + [A] \xrightarrow{K_{dAi}} C_d + q_{m,n}$	Deactivation by aluminum alkyl (A)
$P^*_{m,n,i} + [E] \xrightarrow{K_{dEi}} C_d + q_{m,n}$	Deactivation by electron donor (E)
$P^*_{m,n,i} + [H_2] \xrightarrow{K_{dHi}} C_d + q_{m,n}$	Deactivation by hydrogen (H_2)
$P^*_{m,n,i} + [M_j] \xrightarrow{K_{dMij}} C_d + q_{m,n}$	Deactivation by monomers
Other possible reactions	
$P^*_{1,0,1} + q'_{r,s} \xrightarrow{K^*_{p1}} P^*_{r+1,s,1}$	Formation of short-chain branches
$P^*_{0,1,2} + q'_{r,s} \xrightarrow{K^*_{p2}} P^*_{r,s+1,2}$	Formation of short-chain branches
$P^*_{m,n,1} + q'_{r,s} \xrightarrow{K^*_{p1}} P^*_{m+r,n+s,1}$	Formation of long-chain branches (rare)
$P^*_{m,n,2} + q'_{r,s} \xrightarrow{K^*_{p2}} P^*_{m+r,n+s,2}$	Formation of long-chain branches (rare)

2.4.2.2 Fluidized Bed Reactor

The reactor used for polymerization is fluidized bed reactor which operates at 90°C and 20 bar. A single pass conversion of 3.3% is achieved with a residence time of 2 minutes. An overall conversion of 100% is achieved. The reaction is high exothermic and huge amount of heat is generated. The heat being generated is dissipated via flue gases.

The top outlet streams that contain the gases are sent to cyclone to separate any solid particles present. The bottom streams that contains the polymer and 1-butene is passed through degasser to let the gases escape and polymer is sent to extruder for further processing.

2.4.2.3 Effects of various factors on single pass conversion

The effects of superficial gas velocity

Industrial fluidized bed polyethylene reactors are operated at superficial gas velocities ranging from three to six times the minimum fluidization velocity. The major effect of an increase in the superficial velocity, Ug, is a reduction in the time required for a given quantity of gas to pass through the bed. Figure 2.11 shows the effect of the superficial gas velocity on the percent ethylene conversion. It shows that high gas velocities reduce the conversion of monomer per pass through the reactor and can lead to a greater elutriation of small particles from the bed. Also, the actual ethylene conversion is in the same trend with the chart. Elutriated particles are prevented from passing out from the reactor and into the gas recycle system using a velocity reduction zone at the top of the reactor, where entrained particles are given the opportunity to drop back into the bed. Particle return may also be aided by a cyclone.

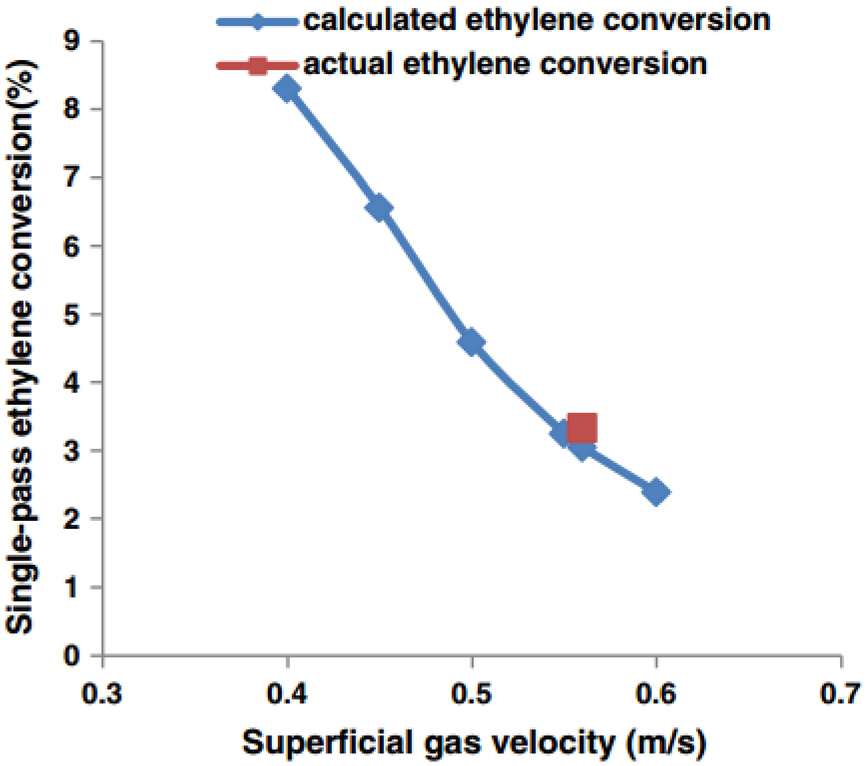


Figure 2.11 Effect of superficial gas velocity on single pass ethylene conversion

The effect of bed height

There is a highly active reaction zone in the top of the reactor; the ethylene conversion decreases by increasing the bed height. It is clear from Figure 2.12 that single-pass ethylene conversion decreased with increasing bed height. According to the parametric study of the system, this situation can be avoided by controlling the gas feed velocity.

In terms of polyethylene production, it can be enhanced by decreasing the gas feed velocity.

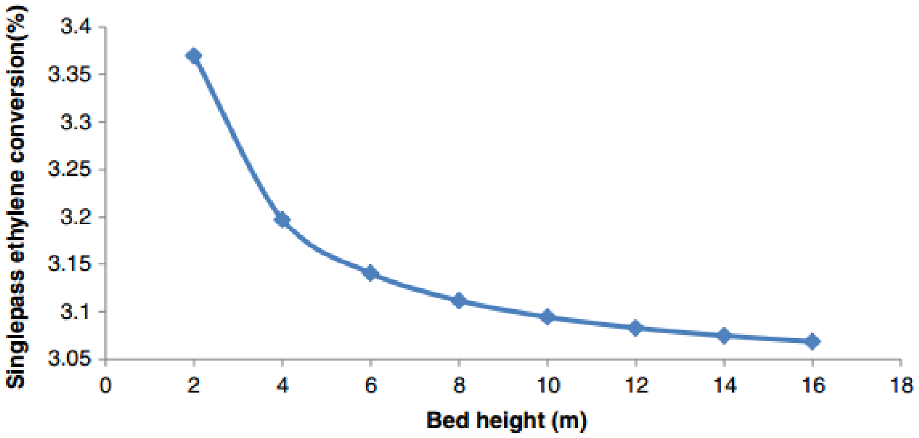


Figure 2.12 Effect of bed height on ethylene single-pass conversion

The effect of feed catalyst properties

Figure 2.13 shows the effect of the catalyst feed rate on the ethylene conversion. It indicates that as the catalyst feed rate increases, the ethylene conversion and particle distribution increase and lead to higher polymerization rates.

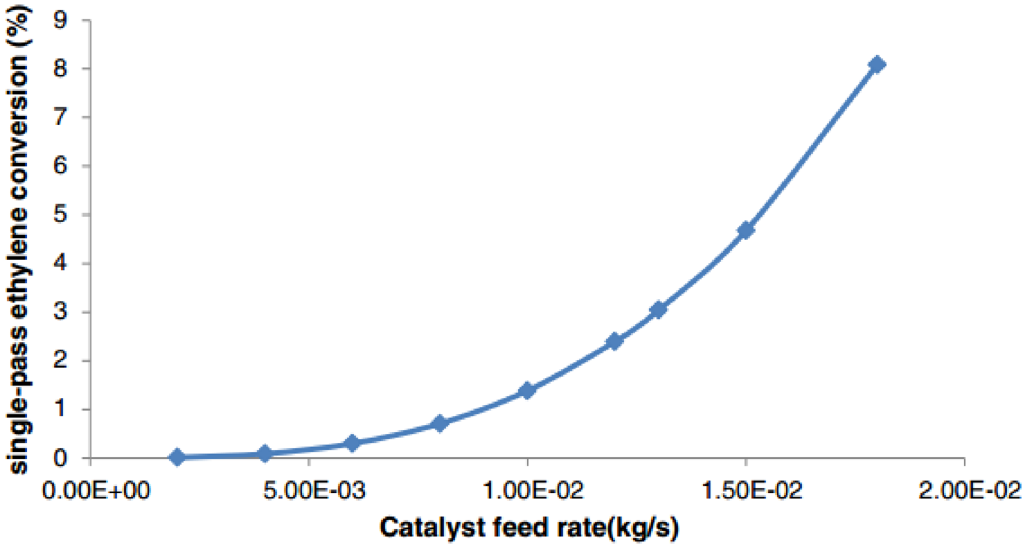


Figure 2.13 Effect of initial catalyst size on particle size distribution in the bed

Figure 2.14 shows that as Ug decreases from 6Umf to 3Umf, the safe regime, in which the reactor can be operated without a danger of particle melting, decreases accordingly. High gas velocities are required to reduce the risk of particle melting, agglomeration, and subsequent reactor shutdown. However, high gas velocities reduce the conversion of monomer per pass through the reactor and can lead to greater elutriation of small particles from the bed. Elutriated particles are prevented from passing out from the reactor and into the gas recycle system using a velocity reduction zone at the top of the reactor where entrained particles are given the opportunity to drop back into the bed. Particle return may also be aided by a cyclone.

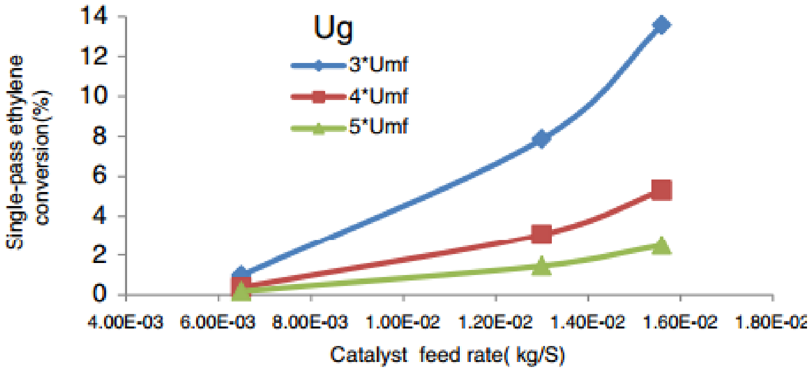


Figure 2.14 Effect of superficial gas velocity and catalyst feed rate on ethylene single pass conversion.

Figure 2.15 shows the effects of catalyst feed rate and bubble size on the single-pass conversion of ethylene. As expected, higher catalyst feed rates lead to higher polymerization rates and to higher conversion. The effects of bubble size on conversion are less obvious. Smaller bubbles have a lower velocity through the bed compared with larger bubbles. As a result, smaller bubbles lead to a larger bubble fraction, δ, in the bed and to a reduction in the volume of the emulsion phase for a given expanded bed height. Therefore, the residence time for both the solid phase and the catalyst decreases with decreasing bubble size, reducing the quantity of catalyst in the reactor for a given catalyst feed rate. This reduction in the quantity of catalyst tends to reduce Rp, the rate of polymerization, thereby reducing the rate of heat generation in the emulsion phase.

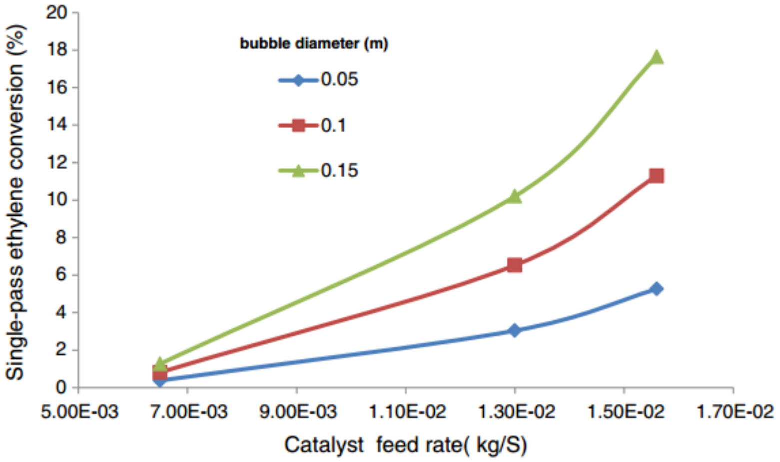


Figure 2.15 Effect of initial bubble dia and catalyst feed rate on single pass conversion

2.4.3 Cyclone and Degasser

The top (S13) and bottom (S14) streams of reactor are sent to cyclone and degassers respectively to separate the solid particles from gases. This process helps remove gases from the polymer take off stream and solids from the flue gases from reactor top that have to be recycled. A mixed stream of gases (S17) from both cyclone and degasser are passed through a filter to remove any solid particle still present and cooled down (S17a) to optimum membrane operation temperature (35^{o}C).

2.4.4 Membrane Separation and Purging

A Cellulose Acetate – Silica Nanocomposite membrane has been applied to gaseous recycle stream (s17b). It separates hydrogen and nitrogen from the stream in fair amount. The permeate (s18) is compressed and 5% of it is purged (s19) in the air, rest(s20) is heated and sent to reactor as recycle stream. Purging is done in order to introduce fresh nitrogen in reactor which carries catalyst. The reject (s21) is compressed, heated and sent back to reactor.

Chapter – 3 **Material Balance**

3.1 Monomer Section:

Name	S1 Feed	S1a Feed to pump	S1b Feed to heater
Temperature (ºC)	25.0000	48.3300	50.2800
Pressure (Bar)	1.0140	1.0140	41.5400
Mass Flow Rate (kg/hr)	1000.0000	1455.0000	1455.0000
Molar Flow (kgmole/hr)	22.3878	33.9886	33.9886
Frac (Ethanol)	0.95	0.8842	0.8842
Frac (H2O)	0.05	0.1158	0.1158
Frac (Ethylene)	0	0	0
Frac (diE-Ether)	0	0	0
Frac (Hydrogen)	0	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0	0
Frac (AceticAcid)	0	0	0

Name	S2 Reactor feed	S3 Reactor top	S4
Temperature (ºC)	424.3000	206.4652	206.4652
Pressure (Bar)	42.6100	42.6096	42.6096
Mass Flow Rate (kg/hr)	1455.0000	1310.0000	145.0000
Molar Flow (kgmole/hr)	33.9886	47.9573	7.0779
Frac (Ethanol)	0.8842	0.1740	0.0869
Frac (H2O)	0.1158	0.3869	0.9099
Frac (Ethylene)	0	0.4384	0.0020
Frac (diE-Ether)	0	0.0005	0
Frac (Hydrogen)	0	0.0002	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0	0.0010
Frac (AceticAcid)	0	0	0.0001

Name	**S5**	**S6**	**S4b feed to separator**
Temperature (ºC)	25.0000	-55.0000	25.0000
Pressure (Bar)	20.5200	20.4912	1.0135
Mass Flow Rate (kg/hr)	1311.0000	596.2000	145.1000
Molar Flow (kgmole/hr)	47.9723	21.1783	7.0779
Frac (Ethanol)	0.1739	0.0000	0.0869
Frac (H2O)	0.3868	0.0013	0.9099
Frac (Ethylene)	0.4385	0.9997	0.0020
Frac (diE-Ether)	0.0005	0	0
Frac (Hydrogen)	0.0002	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0	0.0010
Frac (AceticAcid)	0	0	0.0001

Name	**Separator top**	**Separator Bottom**	**S7**
Temperature (ºC)	25.0000	25.0000	186.6579
Pressure (Bar)	1.0135	1.0135	20.5326
Mass Flow Rate (kg/hr)	0.4204	144.7000	714.5000
Molar Flow (kgmole/hr)	0.0150	7.0629	26.7909
Frac (Ethanol)	0.0144	0.0871	0.3084
Frac (H2O)	0.0304	0.9118	0.6916
Frac (Ethylene)	0.9541	0	0
Frac (diE-Ether)	0.0009	0	0
Frac (Hydrogen)	0.0001	0	0
Frac(Methane)	0.0001	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0.0010	0
Frac (AceticAcid)	0	0.0001	0.0001

Name	**S8**	**S9**	**10**
Temperature (ºC)	50.0000	96.2058	121.3685
Pressure (Bar)	2.1305	2.0271	2.1498
Mass Flow Rate (kg/hr)	859.2000	455.6000	403.6000
Molar Flow (kgmole/hr)	33.8538	11.6036	22.2503
Frac (Ethanol)	0.2622	0.7573	0.0040
Frac (H2O)	0.7375	0.2426	0.9956
Frac (Ethylene)	0	0	0
Frac (diE-Ether)	0	0	0
Frac (Hydrogen)	0	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0.0002	0	0.0003
Frac (AceticAcid)	0.0001	0	0.0001

Name	**S3a**	**S7a**	**S1c**
Temperature (ºC)	196.0377	83.5084	114.0000
Pressure (Bar)	1.0135	1.0135	
Mass Flow Rate (kg/hr)	1311.0000	859.2011	1455.0000
Molar Flow (kgmole/hr)	47.9700	33.8538	33.9886
Frac (Ethanol)	0.1739	0.2622	0.8842
Frac (H2O)	0.3868	0.7375	0.1158
Frac (Ethylene)	0.4385	0	0
Frac (diE-Ether)	0.0005	0	0
Frac (Hydrogen)	0.0002	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0.0002	0
Frac (AceticAcid)	0	0.0001	0

Name	**S4a**	**To cond 1**	**Reflux**
Temperature (ºC)	70.0000	30.95	-55
Pressure (Bar)		20.49	20.49
Mass Flow Rate (kg/hr)	145.0000	1043.0000	447.2000
Molar Flow (kgmole/hr)	7.0779	37.0700	15.8800
Frac (Ethanol)	0.0869	0.0040	0.0040
Frac (H2O)	0.9099	0.0007	0.0007
Frac (Ethylene)	0.0020	0.9937	0.9938
Frac (diE-Ether)	0	0.0011	0.0011
Frac (Hydrogen)	0	0.0004	0.0004
Frac(Methane)	0	0.0001	0.0001
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0.0010	0	0
Frac (AceticAcid)	0.0001	0	0

Name	**To reb**	**Boil up**	**To cond 2**
Temperature (ºC)	184.3	186.7	97.58
Pressure (Bar)	20.53	20.53	2.027
Mass Flow Rate (kg/hr)	1691.0000	976.6000	864.0000
Molar Flow (kgmole/hr)	56.0900	29.3000	22.6400
Frac (Ethanol)	0.4258	0.5420	0.7184
Frac (H2O)	0.5742	0.4580	0.2816
Frac (Ethylene)	0	0	0
Frac (diE-Ether)	0	0	0
Frac (Hydrogen)	0	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0	0
Frac (AceticAcid)	0	0	0

Name	**Reflux**	**To reb**	**Boilup**
Temperature (ºC)	96.36	119.4	121.4
Pressure (Bar)	2.027	2.15	2.15
Mass Flow Rate (kg/hr)	397.0000	915.3000	511.8000
Molar Flow (kgmole/hr)	10.4000	49.0300	26.7900
Frac (Ethanol)	0.7184	0.0207	0.0346
Frac (H2O)	0.2816	0.9767	0.9609
Frac (Ethylene)	0	0	0
Frac (diE-Ether)	0	0	0
Frac (Hydrogen)	0	0	0
Frac(Methane)	0	0	0
Frac(Ethane)	0	0	0
Frac (AcetAldehyde)	0	0.0026	0.0044
Frac (AceticAcid)	0	0.0001	0.0001

3.2 Polymer Section

Name	**S11**	**S12**	**S13**
Temperature (°C)	57	57	100
Pressure (Bar)	20	20	20
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0.5985	0	0.0088
Frac 1-Butene	0.2620	0	0.0524
Frac Hydrogen	0.1405	0	0.1879
Frac Nitrogen	0	0.9985	0.7318
Frac Polyethylene	0	0	0.0181
Frac Catalyst	0	0.0015	0.0010

Name	**S14**	**S15**	**S16**
Temperature (°C)	100	100	100
Pressure (Bar)	20	19	1
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0	0.0089	0
Frac 1-Butene	0.2491	0.0534	0
Frac Hydrogen	0.0083	0.1916	0
Frac Nitrogen	0	0.7461	0
Frac Polyethylene	0.7426	0	0.9455
Frac Catalyst	0	0	0.0545

Name	**S16a**	**S16b**	**S14a**
Temperature (ºC)	100	100	100
Pressure (Bar)			19
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0	0	0
Frac 1-Butene	0	0	0.9677
Frac Hydrogen	0	0	0.0323
Frac Nitrogen	0	0	0
Frac Polyethylene	0	1	0
Frac Catalyst	1	0	0

Name	**S14b**	**S17=S14a+S15**	**S17a**
Temperature (ºC)	100	100	35
Pressure (Bar)		19	18.5
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0	0.0068	0.0068
Frac 1-Butene	0	0.2712	0.2712
Frac Hydrogen	0	0.1536	0.1536
Frac Nitrogen	0	0.5684	0.5684
Frac Polyethylene	1	0	0
Frac Catalyst	0	0	0

Name	**S17b**	**S18 permeate**	**S19 purge**
Temperature (ºC)	35	35	35
Pressure (Bar)	6	1	20
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0.0068	9.46E-07	9.46E-07
Frac 1-Butene	0.2712	2.67E-05	2.67E-05
Frac Hydrogen	0.1536	0.2602	0.2602
Frac Nitrogen	0.5684	0.7398	0.7398
Frac Polyethylene	0	0	0
Frac Catalyst	0	0	0

Name	**S20**	**S21 reject**	**S21a**
Temperature (ºC)	35	35	25
Pressure (Bar)	20	6	21
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	9.46E-07	0.0149	0.0245
Frac 1-Butene	2.67E-05	0.5911	0.9755
Frac Hydrogen	0.2602	0.0279	0
Frac Nitrogen	0.7398	0.3661	0
Frac Polyethylene	0	0	0
Frac Catalyst	0	0	0

Name	**S21b**	**S6a**	**S6b**
Temperature (ºC)	57	15	57
Pressure (Bar)	20.5	20	20
Mass Flow Rate (kg/hr)	1	1	1
Frac Ethylene	0.0245	1	1
Frac 1-Butene	0.9755	0	0
Frac Hydrogen	0	0	0
Frac Nitrogen	0	0	0
Frac Polyethylene	0	0	0
Frac Catalyst	0	0	0

Chapter – 4 **Energy Balance**

4.1 Mixer1:

S1 Feed			
Component	**m**	**Cp (25°C)**	**H**
Ethanol	21.26842	7.193125	3824.66
H2O	1.119391	34.28929	959.5777
Ethylene	0	6.557188	0
diE-Ether	0	43.95569	0
Hydrogen	0	26.9251	0
Methane	0	26.61315	0
Ethane	0	11.53995	0
AcetAldehyde	0	25.88831	0
AceticAcid	0	16.8601	0
Total	22.38781	199.8219	4784.238

S9 Recycle			
Component	**m**	**Cp (96.20°C)**	**H**
Ethanol	8.78768	23.656829	20000.07682
H2O	2.81556	33.981657	9204.723694
Ethylene	0.00010	17.082738	0.164509977
diE-Ether	0.00023	65.0033	1.449336469
Hydrogen	0.00000	27.431405	1.57099E-05
Methane	0.00000	27.985836	5.04509E-05
Ethane	0.00000	22.656003	2.77209E-05
AcetAldehyde	0.00000	31.954123	3.56329E-26
AceticAcid	0.00000	30.114397	0.000109345
Total	11.60357	279.86629	29206.41

S1a Mixer Out			
Component	**m**	**Cp (48ºC)**	**H**
Ethanol	30.05314	12.76045	18534.15
H2O	3.93513	34.13616	6492.181
Ethylene	0.00010	10.11805	0.049044
diE-Ether	0.00023	50.98457	0.572216
Hydrogen	0.00000	27.11761	7.82E-06
Methane	0.00000	26.94272	2.45E-05
Ethane	0.00000	15.21787	9.37E-06
AcetAldehyde	0.00000	27.73577	1.53E-26
AceticAcid	0.00000	21.23833	3.91E-05
Total	33.98859953	226.2515	25026.95

4.2 Heater1:

S1c			
Component	**m**	**Cp (114°C)**	**H**
Ethanol	30.05314	27.52562	94304.36
H2O	3.935131	33.97899	15243.14
Ethylene	0.0001	19.5539	0.223568
diE-Ether	0.000232	70.07478	1.855114
Hydrogen	5.97E-09	27.52018	1.87E-05
Methane	1.88E-08	28.49927	6.11E-05
Ethane	1.27E-08	25.38309	3.69E-05
AcetAldehyde	1.14E-29	33.6684	4.37E-26
AceticAcid	3.81E-08	33.37621	0.000145
Total	33.9886	299.5804	109549.6

S2 Reactor Feed					
Component	**m**	**Cp (424°C)**	**ml**	**H**	**Total**
Ethanol	30.05314	79.21027	25424.95	1010053	1035478
H2O	3.93513	38.70323	8881.591	64621.86	73503.45
Ethylene	0.00010	52.41494	0.048442	2.230487	2.278929
diE-Ether	0.00023	146.4074	0.032047	14.4258	14.45785
Hydrogen	0.00000	26.64107	1.35E-05	6.75E-05	8.1E-05
Methane	0.00000	48.40722	9.6E-06	0.000386	0.000396
Ethane	0.00000	69.67262	6.23E-06	0.000377	0.000383
AcetAldehyde	0.00000	76.31882	6.65E-27	3.69E-25	3.75E-25
AceticAcid	0.00000	87.01483	1.53E-05	0.001406	0.001422
Total	33.9886	624.7904	34306.62	1074692	1108999

4.3 Cooler1:

S3a Cooler Feed					
Component	**m**	**Cp (196ºC)**	**H**	**ml**	**Total**
Ethanol	8.3441	44.09266	72124.95	7059.109	79184.06
H2O	18.5537	34.35049	124940.5	41875.69	166816.1
Ethylene	21.03619	30.12374	124226.9	10160.48	134387.4
diE-Ether	0.022545	92.48228	408.7377	3.111183	411.8488
Hydrogen	0.008972	27.73419	48.77785	20.24879	69.02664
Methane	0.001792	31.74765	11.1542	0.915457	12.06965
Ethane	0.000896	37.69318	6.620887	0.438508	7.059395
AcetAldehyde	0.000269	42.59802	2.245885	0.157076	2.402961
AceticAcid	0.001544	48.15353	14.57918	0.620857	15.20004
Total	47.97	388.9757	321784.4	59120.77	380905.2

S5 Column Feed					
Component	**m**	**Cp (25ºC)**	**H**	**ml**	**Total**
Ethanol	8.344501	7.193125	1500.576	7059.447778	8560.024
H2O	18.55459	34.28929	15905.59	41877.70346	57783.29
Ethylene	21.0372	6.557188	3448.621	10160.96531	13609.59
diE-Ether	0.022546	43.95569	24.7755	3.111332172	27.88683
Hydrogen	0.008972	26.9251	6.039288	20.24976287	26.28905
Methane	0.001792	26.61315	1.192461	0.915501088	2.107962
Ethane	0.000896	11.53995	0.258511	0.438529194	0.69704
AcetAldehyde	0.000269	25.88831	0.17407	0.157083063	0.331153
AceticAcid	0.001544	16.8601	0.651008	0.620886452	1.271894
Total	47.9723	199.8219	20887.88	25606.43533	46494.31

4.4 Cooler2:

S4a Cooler Feed			
Component	**M**	**Cp (70ºC)**	**H**
Ethanol	0.615366	17.7805	765.9064
H2O	6.440283	34.03961	15345.73
Ethylene	0.0144	13.32755	13.43442
diE-Ether	0.00024	57.39739	0.963326
Hydrogen	9.08E-07	27.27318	0.001733
Methane	1.01E-06	27.35376	0.001934
Ethane	6.29E-07	18.60281	0.000819
AcetAldehyde	0.006906	29.57397	14.29652
AceticAcid	0.000698	25.27398	1.235458
Total	7.077896	250.6228	16141.57

S4b Cooler out			
Component	**m**	**Cp (25ºC)**	**H**
Ethanol	0.615366	7.193125	110.6602
H2O	6.440283	34.28929	5520.818
Ethylene	0.0144	6.557188	2.360631
diE-Ether	0.00024	43.95569	0.263474
Hydrogen	9.08E-07	26.9251	0.000611
Methane	1.01E-06	26.61315	0.000672
Ethane	6.29E-07	11.53995	0.000181
AcetAldehyde	0.006906	25.88831	4.469578
AceticAcid	6.3E-08	16.8601	0.294345
Total	7.077198	199.8219	5638.868

4.5 Cooler3:

s7a Cooler feed					
Component	**m**	**Cp (83ºC)**	**H**	**ml**	**Total**
Ethanol	8.876401	20.83618	15444.9	7509.435	18448.67
H2O	24.96769	34.0017	70893.94	56352.08	93434.77
Ethylene	0.0001	15.28049	0.127742	0.048352	0.147083
diE-Ether	0.000232	61.33843	1.187123	0.031982	1.199916
Hydrogen	5.95E-09	27.35883	1.36E-05	1.34E-05	1.9E-05
Methane	1.87E-08	27.66112	4.33E-05	9.57E-06	4.71E-05
Ethane	1.27E-08	20.69763	2.2E-05	6.22E-06	2.45E-05
AcetAldehyde	0.007175	30.77938	18.44189	4.190497	20.11809
AceticAcid	0.002243	27.77455	5.201749	0.901568	5.562377
Total	33.85384	265.7283	86363.8	13130.99	91616.19

S8 Cooler out			
Component	**M**	**Cp (50ºC)**	**H**
Ethanol	8.8764	13.1525	5837.3432
H2O	24.9677	34.1272	42603.8094
Ethylene	0.0001	10.3688	0.0519
diE-Ether	0.0002	51.4828	0.5966
Hydrogen	0.0000	27.1304	0.0000
Methane	0.0000	26.9708	0.0000
Ethane	0.0000	15.4798	0.0000
AcetAldehyde	0.0072	27.8733	9.9994
AceticAcid	0.0022	21.5504	2.4166
Total	33.85384	228.1358	48454.217

4.6 Mixer2:

S3 Mixer in					
Component	**m**	**Cp (206ºC)**	**H**	**ml**	**Total**
Ethanol	8.344285	46.04899	79333.42	7059.265	82510.08
H2O	18.55413	34.44289	131943.3	41876.68	150787.8
Ethylene	21.0229	31.37034	136162.8	10154.06	140732.2
diE-Ether	0.022532	95.21577	442.957	3.109459	444.3562
Hydrogen	0.008971	27.7384	51.37752	20.24773	60.489
Methane	0.001791	32.26428	11.93264	0.914995	12.34439
Ethane	0.000895	39.22694	7.252157	0.438228	7.44936
AcetAldehyde	0.000269	43.85384	2.435196	0.157083	2.505883
AceticAcid	0.001544	50.00112	15.94392	0.620861	16.22331
Total	47.95732	400.1626	347971.4	59115.49	374573.4

Separator top					
Component	**m**	**Cp (25ºC)**	**H**	**ml**	**Total**
Ethanol	0.000216	7.193125	0.03883	0.182677	0.221507
H2O	0.000455	34.28929	0.390149	1.027219	1.417368
Ethylene	0.0143	6.557188	2.34422	6.906976	9.251196
diE-Ether	1.36E-05	43.95569	0.014917	0.001873	0.01679
Hydrogen	9.02E-07	26.9251	0.000607	0.002035	0.002642
Methane	9.91E-07	26.61315	0.000659	0.000506	0.001166
Ethane	6.16E-07	11.53995	0.000178	0.000301	0.000479
AcetAldehyde	1.4E-105	25.88831	9.1E-103	8.2E-103	1.7E-102
AceticAcid	6.3E-08	16.8601	2.66E-05	2.53E-05	5.19E-05
Total	0.014987	199.8219	2.789587	8.121613	10.9112

S3a Cooler feed					
Component	**m**	**Cp (196ºC)**	**H**	**ml**	**Total**
Ethanol	8.3441	44.09266	72124.95	7059.109	79184.06
H2O	18.5537	34.35049	124940.5	41875.69	166816.1
Ethylene	21.03619	30.12374	124226.9	10160.48	134387.4
diE-Ether	0.022545	92.48228	408.7377	3.111183	411.8488
Hydrogen	0.008972	27.73419	48.77785	20.24879	69.02664
Methane	0.001792	31.74765	11.1542	0.915457	12.06965
Ethane	0.000896	37.69318	6.620887	0.438508	7.059395
AcetAldehyde	0.000269	42.59802	2.245885	0.157076	2.402961
AceticAcid	0.001544	48.15353	14.57918	0.620857	15.20004
Total	47.97	388.9757	321784.4	59120.77	380905.2

4.7 Mixer3:

S7 Column bottom			
Component	M	Cp (186^{o}C)	H
Ethanol	8.261251	42.30409	65234.08
H2O	18.52786	34.27608	118539.4
Ethylene	1.81E-15	28.98373	9.79E-12
diE-Ether	5.57E-06	90.00133	0.093541
Hydrogen	1.67E-22	27.72597	8.65E-19
Methane	1.55E-18	31.30291	9.06E-15
Ethane	6.29E-20	36.30756	4.26E-16
AcetAldehyde	0.000269	41.49165	2.082986
AceticAcid	0.001544	46.48566	13.40103
Total	26.79093	378.879	183789.1

Sep bot			
Component	**M**	**Cp (25^{o}C)**	**H**
Ethanol	0.61515	7.193125	110.6213
H2O	6.439828	34.28929	5520.428
Ethylene	0.0001	6.557188	0.016411
diE-Ether	0.000226	43.95569	0.248557
Hydrogen	5.95E-09	26.9251	4.01E-06
Methane	1.87E-08	26.61315	1.25E-05
Ethane	1.27E-08	11.53995	3.67E-06
AcetAldehyde	0.006906	25.88831	4.469578
AceticAcid	0.000698	16.8601	0.294318
Total	7.062909	199.8219	5636.078

4.8 Fixed Bed Reactor:

S2 Reactor Feed					
Component	**m**	**Cp (424^{o}C)**	**ml**	**H**	**Total**
Ethanol	30.05314	79.210274	25424.95	1010053	1035478.368
H2O	3.93513	38.703229	8881.591	64621.86	73503.44845
Ethylene	0.00010	52.414936	0.048442	2.230487	2.278928552
diE-Ether	0.00023	146.40737	0.032047	14.4258	14.45785136
Hydrogen	0.00000	26.641073	1.35E-05	6.75E-05	8.09554E-05
Methane	0.00000	48.407216	9.6E-06	0.000386	0.000395572
Ethane	0.00000	69.672622	6.23E-06	0.000377	0.000382834
AcetAldehyde	0.00000	76.31882	6.65E-27	3.69E-25	3.75336E-25
AceticAcid	0.00000	87.014829	1.53E-05	0.001406	0.001421694
Total	33.9886	624.79037	34306.62	1074692	1108998.556

S3 Reactor Out Top					
Component	**m**	**Cp (206^{o}C)**	**ml**	**H**	**Total**
Ethanol	8.34428	46.04899	7059.265	79333.41537	86392.68047
H2O	18.55413	34.44289	41876.68	131943.253	173819.9293
Ethylene	21.02290	31.37034	10154.06	136162.8484	146316.9067
diE-Ether	0.02253	95.21577	3.109459	442.9569819	446.0664408
Hydrogen	0.00897	27.7384	20.24773	51.37752027	71.62524796
Methane	0.00179	32.26428	0.914995	11.93264329	12.84763811
Ethane	0.00090	39.22694	0.438228	7.252157497	7.690385234
AcetAldehyde	0.00027	43.85384	0.157083	2.435196046	2.592279109
AceticAcid	0.00154	50.00112	0.620861	15.94392071	16.56478183
Total	47.9573157	400.1626	59115.49	347971.4152	407086.9032

S4 Reactor Out Bot			
Component	**M**	**Cp (206ºC)**	**H**
Ethanol	0.61537	46.04899	5850.604
H2O	6.44028	34.44289	45798.53
Ethylene	0.01440	31.37034	93.26884
diE-Ether	0.00024	95.21577	4.713452
Hydrogen	0.00000	27.7384	0.005198
Methane	0.00000	32.26428	0.006727
Ethane	0.00000	39.22694	0.005092
AcetAldehyde	0.00691	43.85384	62.52841
AceticAcid	0.00070	50.00112	7.20913
Total	7.077896	400.1626	51816.87

4.9 Separator:

S4b Sep feed				
Component	**M**	**Cp (25ºC)**	**H**	**Total**
Ethanol	0.615366	7.193125	110.6602	520.5998
H2O	6.440283	34.28929	5520.818	14535.72
Ethylene	0.0144	6.557188	2.360631	6.955328
diE-Ether	0.00024	43.95569	0.263474	0.033087
Hydrogen	9.08E-07	26.9251	0.000611	0.002049
Methane	1.01E-06	26.61315	0.000672	0.000516
Ethane	6.29E-07	11.53995	0.000181	0.000308
AcetAldehyde	0.006906	25.88831	4.469578	4.033414
AceticAcid	6.3E-08	16.8601	0.294345	0.280726
Total	7.077198	199.8219	5638.868	15067.62

Sep top					
Component	**m**	**Cp (25ºC)**	**H**	**ml**	**Total**
Ethanol	0.000216	7.193125	0.03883	0.182677	0.221507
H2O	0.000455	34.28929	0.390149	1.027219	1.417368
Ethylene	0.0143	6.557188	2.34422	6.906976	9.251196
diE-Ether	1.36E-05	43.95569	0.014917	0.001873	0.01679
Hydrogen	9.02E-07	26.9251	0.000607	0.002035	0.002642
Methane	9.91E-07	26.61315	0.000659	0.000506	0.001166
Ethane	6.16E-07	11.53995	0.000178	0.000301	0.000479
AcetAldehyde	1.4E-105	25.88831	9.1E-103	8.2E-103	1.7E-102
AceticAcid	6.3E-08	16.8601	2.66E-05	2.53E-05	5.19E-05
Total	0.014987	199.8219	2.789587	8.121613	10.9112

Sep bot			
Component	**m**	**Cp (25ºC)**	**H**
Ethanol	0.61515	7.193125	110.6213
H2O	6.439828	34.28929	5520.428
Ethylene	0.0001	6.557188	0.016411
diE-Ether	0.000226	43.95569	0.248557
Hydrogen	5.95E-09	26.9251	4.01E-06
Methane	1.87E-08	26.61315	1.25E-05
Ethane	1.27E-08	11.53995	3.67E-06
AcetAldehyde	0.006906	25.88831	4.469578
AceticAcid	0.000698	16.8601	0.294318
Total	7.062909	199.8219	5636.078

4.10 Distillation Column1:

S5 Column feed					
Component	**m**	**Cp (25ºC)**	**H**	**ml**	**Total**
Ethanol	8.344501	7.193125	1500.576	7059.448	8560.024
H2O	18.55459	34.28929	15905.59	41877.7	57783.29
Ethylene	21.0372	6.557188	3448.621	10160.97	13609.59
diE-Ether	0.022546	43.95569	24.7755	3.111332	27.88683
Hydrogen	0.008972	26.9251	6.039288	20.24976	26.28905
Methane	0.001792	26.61315	1.192461	0.915501	2.107962
Ethane	0.000896	11.53995	0.258511	0.438529	0.69704
AcetAldehyde	0.000269	25.88831	0.17407	0.157083	0.331153
AceticAcid	0.001544	16.8601	0.651008	0.620886	1.271894
Total	47.9723	199.8219	20887.88	25606.44	46494.31

Column top to condenser					
Component	**M**	**Cp (30.95ºC)**	**H**	**ml**	**Total**
Ethanol	0.14667	8.629025	39.17211	124.0866	163.2587
H2O	0.02520	34.24539	26.70426	56.86556	83.56981
Ethylene	36.83830	7.475731	8523.419	17792.9	26316.32
diE-Ether	0.03949	45.76061	55.93453	5.450127	61.38465
Hydrogen	0.01564	26.97666	13.05437	35.28894	48.34331
Methane	0.00314	26.68607	2.589751	1.601635	4.191386
Ethane	0.00157	12.48127	0.60613	0.76791	1.37404
AcetAldehyde	0.00000	26.34653	3.4E-38	2.43E-38	5.83E-38
AceticAcid	0.00000	17.98	4.28E-09	3.09E-09	7.37E-09
Total	37.07	206.5813	8661.48	18016.96	26678.44

Column bottom to re-boiler			
Component	**M**	**Cp (184.3°C)**	**H**
Ethanol	23.88285	41.85019	184208.2
H2O	32.20472	34.25867	203336.5
Ethylene	0.00000	28.69437	2.78E-25
diE-Ether	0.00000	89.37438	2.04E-06
Hydrogen	0.00000	27.72324	2.83E-25
Methane	0.00000	31.19409	6.81E-35
Ethane	0.00000	35.95836	6.88E-38
AcetAldehyde	0.00036	41.217	2.742165
AceticAcid	0.00207	46.06551	17.56651
Total	56.09	376.3358	387565

Reboil					
Component	**M**	**Cp (186.7°C)**	**H**	**ml**	**Total**
Ethanol	15.88057	42.31218	125451.5	13434.96	138886.5
H2O	13.41890	34.27639	85872.97	30286.47	116159.4
Ethylene	0.00000	28.98888	1.48E-25	1.32E-26	1.62E-25
diE-Ether	0.00000	90.01252	1.92E-06	1.58E-08	1.93E-06
Hydrogen	0.00000	27.72601	1.5E-25	6.52E-26	2.15E-25
Methane	0.00000	31.30486	6.97E-35	6.09E-36	7.58E-35
Ethane	0.00000	36.31379	7.09E-38	5.12E-39	7.6E-38
AcetAldehyde	0.00000	41.49657	1.78E-08	1.34E-09	1.91E-08
AceticAcid	0.00052	46.49316	4.537629	0.210146	4.747775
Total	29.3	378.9244	211329	43721.64	255050.7

Reflux			
Component	**M**	**Cp (-55ºC)**	**H**
Ethanol	0.06283	-13.1789	45.54333
H2O	0.01079	35.20175	-20.8965
Ethylene	15.78079	-6.48401	5627.755
diE-Ether	0.01692	18.87033	-17.559
Hydrogen	0.00665	26.06788	-9.54109
Methane	0.00134	26.37251	-1.94586
Ethane	0.00067	-1.33704	0.049429
AcetAldehyde	0.00000	20.58903	-2E-38
AceticAcid	0.00000	1.583684	-2.9E-10
Total	15.88	107.6853	5623.406

4.11 Distillation Column2:

S8 Column feed			
Component	**M**	**Cp (50ºC)**	**H**
Ethanol	8.8764	13.1525	5837.3432
H2O	24.9677	34.1272	42603.8094
Ethylene	0.0001	10.3688	0.0519
diE-Ether	0.0002	51.4828	0.5966
Hydrogen	0.0000	27.1304	0.0000
Methane	0.0000	26.9708	0.0000
Ethane	0.0000	15.4798	0.0000
AcetAldehyde	0.0072	27.8733	9.9994
AceticAcid	0.0022	21.5504	2.4166
Total	33.85384	228.1358	48454.217

Column top to condenser					
Component	**M**	**Cp (97ºC)**	**H**	**ml**	**Total**
Ethanol	16.2637	23.9591	38023.4495	13759.1099	51782.56
H2O	6.3757	33.9804	21140.5522	14389.9293	35530.48
Ethylene	0.0002	17.2759	0.3008	0.0862	0.38702
diE-Ether	0.0004	65.3977	2.5083	0.0542	2.56258
Hydrogen	0	27.4388	0	0	5.15E-05
Methane	0	28.0231	0.0001	0	0.000107
Ethane	0	22.8673	0.0001	0	6.19E-05
AcetAldehyde	0	32.0837	0	0	7.88E-26
AceticAcid	0	30.3670	0.0487	0.0066	0.055291
Total	22.64	281.3929	59166.86	28149.186	87316.05

Column bottom to re-boiler			
Component	**M**	**Cp (119.4^{o}C)**	**H**
Ethanol	1.0133	28.6803	3470.0739
H2O	47.8862	33.9841	194307.8341
Ethylene	0	20.2912	0
diE-Ether	0	71.5989	0
Hydrogen	0	27.5441	0
Methane	0	28.6686	0
Ethane	0	26.2067	0
AcetAldehyde	0.1252	34.2043	511.1480
AceticAcid	0.0053	34.3621	21.5904
Total	49.03	305.5402	198310.646

Reboil					
Component	**m**	**Cp (121.4^{o}C)**	**H**	**ml**	**Total**
Ethanol	0.92657	29.11	3273.98	783.8814	4057.858
H2O	25.74240	33.99	106212.53	58100.6021	164313.1
Ethylene	0	20.56	0	0	7.95E-26
diE-Ether	0	72.16	0	0	6.17E-09
Hydrogen	0	27.55	0	0	1.51E-25
Methane	0	28.73	0	0	1.06E-25
Ethane	0	26.51	0	0	9.72E-26
AcetAldehyde	0.11800	34.40	492.87	68.9201	561.7896
AceticAcid	0.00302	34.73	12.73	1.2141	13.9463
Total	26.79	307.7448	109992.11	58954.618	168946.7

Reflux			
Component	**M**	**Cp (96.36ºC)**	**H**
Ethanol	7.47097	23.690786	17055.056
H2O	2.92876	33.981507	9590.1068
Ethylene	0.00008	17.104432	0.1350991
diE-Ether	0.00018	65.047584	1.1317431
Hydrogen	0	27.43224	1.266E-05
Methane	0	27.989994	4.073E-05
Ethane	0	22.679729	2.285E-05
AcetAldehyde	0	31.968642	3.003E-26
AceticAcid	0.00001	30.142758	0.0219219
Total	10.4	280.03767	26646.452

4.12 Shell & Tube Heat Exchanger:

S1b			
Component	**m**	**Cp (50.28^{o}C)**	**H**
Ethanol	30.05314	13.21815	19973.57
H2O	3.935131	34.12567	6752.049
Ethylene	0.0001	10.41073	0.052499
diE-Ether	0.000232	51.56621	0.602094
Hydrogen	5.97E-09	27.13253	8.14E-06
Methane	1.88E-08	26.97557	2.55E-05
Ethane	1.27E-08	15.5237	9.94E-06
AcetAldehyde	1.14E-29	27.89637	1.6E-26
AceticAcid	3.81E-08	21.60271	4.14E-05
Total	33.9886	228.4516	26726.27

S1c			
Component	**m**	**Cp (114^{o}C)**	**H**
Ethanol	30.05314	27.52562	94304.36
H2O	3.935131	33.97899	15243.14
Ethylene	0.0001	19.5539	0.223568
diE-Ether	0.000232	70.07478	1.855114
Hydrogen	5.97E-09	27.52018	1.87E-05
Methane	1.88E-08	28.49927	6.11E-05
Ethane	1.27E-08	25.38309	3.69E-05
AcetAldehyde	1.14E-29	33.6684	4.37E-26
AceticAcid	3.81E-08	33.37621	0.000145
Total	33.9886	299.5804	109549.6

S4			
Component	**M**	**Cp (206.465ºC)**	**H**
Ethanol	0.615366	46.04899	5850.604
H2O	6.440283	34.44289	45798.53
Ethylene	0.0144	31.37034	93.26884
diE-Ether	0.00024	95.21577	4.713452
Hydrogen	9.08E-07	27.7384	0.005198
Methane	1.01E-06	32.26428	0.006727
Ethane	6.29E-07	39.22694	0.005092
AcetAldehyde	0.006906	43.85384	62.52841
AceticAcid	0.000698	50.00112	7.20913
Total	7.077896	400.1626	51816.87

S4a			
Component	**M**	**Cp (70ºC)**	**H**
Ethanol	0.615366	17.7805	765.9064
H2O	6.440283	34.03961	15345.73
Ethylene	0.0144	13.32755	13.43442
diE-Ether	0.00024	57.39739	0.963326
Hydrogen	9.08E-07	27.27318	0.001733
Methane	1.01E-06	27.35376	0.001934
Ethane	6.29E-07	18.60281	0.000819
AcetAldehyde	0.006906	29.57397	14.29652
AceticAcid	0.000698	25.27398	1.235458
Total	7.077896	250.6228	16141.57

4.13 Fluidized Bed Reactor:

Name	**S6b**	**Cp**	**H**
Temperature (^oC)	**57**		
Pressure (Bar)	20		
Ethylene	21.15793	0	310533.5
1-Butene	0	92.73	
Hydrogen	0	0	0
Nitrogen	0	0	0
Polyethylene	0	39.43	0
Total	21.15793		310533.5

Name	**S12**	**Cp**	**H**
Temperature (^oC)	**57**		
Pressure (Bar)	20		
Ethylene	0	44.47555	0
1-Butene	0	92.73	
Hydrogen	0	27.39382	0
Nitrogen	35.47457	32.13554	376198.1
Polyethylene	0	39.43	0
Total	35.47457		376198.1

Name	**S14**	**Cp**	**H**
Temperature (^oC)	**100**		
Pressure (Bar)	20		
Ethylene	0	48.31754	0
1-Butene	3.596711	102.405	
Hydrogen	6.7133	27.10316	67867.97
Nitrogen	0	32.81464	0
Polyethylene	0.006003	35.88	80.34227
Total	10.31601		67948.32

Name	**S13**	**Cp**	**H**
Temperature (ºC)	**100**		
Pressure (Bar)	20		
Ethylene	0.2125	48.31754	3829.769
1-Butene	0.634714	102.405	
Hydrogen	127.553	27.10316	1289495
Nitrogen	35.47643	32.81464	434226.6
Polyethylene	0.000123	35.88	1.639447
Total	163.8768		1727553

Chapter – 5 **Equipment Designing**

This chapter contains all the details and designing factors calculated for equipment being used in the process.

5.1 Mixer

Mass flow rate of feed= m1= 1000kg/h

Mass flow rate of feed= m2= 455.6kg/h

Mass flow rate of mixing tank = m1 + m2 = 1455.6kg/h

Ethanol:

Mass flow rate of ethanol = 1000(.979) + 455.6(.89)

= 1384.48 kg/h

Water:

Mass flow rate of water = 1000(.0202) + 455.6 (.11)

= 70.116 kg/h

Mass concentration of ethanol= $X_{ethanol}$ = 1384.84/1455.6

= 0.95

Mass concentration of water= X_{H20} = 70.12/1455.6

= .05

Density of mixture:

$\rho_{mix} = (\rho_{ethanol} * X_{ethanol}) + (\rho_{H2o} * X_{H20})$

$= (798 * 0.95) + (1000 * .05)$

$\rho_{mix} = 799.5$ kg/h

We know that:

Mass flow rate= Density * vol. flow rate

$G = \rho_{mix} * V_o$

$V_o = G / \rho_{mix}$

Also

$Tr = Vr / V_o$

Let

Tr= 1.5hr

So

$Vr = Tr * V_o$

$Vr = 1.5 * 1.82$

$Vr = 2.73m^3$

(eq. 1)

Giving 5% allowance as safety factor:

Volume of the mixer = 2.73 * (2.73*.05)

$= 2.87m^3$

Volume of cylindrical vessel is given as :

$Vr = ∏/4 * D^2 * H$

$Vr= ∏/4 * D^{2\,*}\ 2D$ (H=2D)

$Vr= ∏/2 * D^3$

(eq.2)

Solving eq.1 and eq.2 simultaneously we get:

$2.87 = ∏/2 * D^3$

D = 1.22m

Since H= 2D

H= 2 (1.22)

=2.44m

Designing Parameters for mixing tank

No. of units	1
Tank Volume(m^3)	2.73
Height (m)	2.44
Diameter(m)	1.22

5.2 Pump

Shaft work of pump in Kw is given as:

$$Wo = Hm_V\rho / 10^3$$

Where:

H = Total dynamic head

m_V = Volumetric flow rate

ρ = *Density*

To calculate pressure head we have equation

$$H = P_2 - P_1 / \rho$$

P_2 = outlet pressure (n/m^2)

P_1 = Inlet pressure (n/m^2)

H= 4154000 – 10400/ 799.5

H= 5068.91 (Nm/ Kg)

Wo = 5068.91 * 0.3 * 799.5/ 10

Wo = 12.2 Kw

5.3 Heat Exchanger:

Tube Side:

Component	Molar Composition
Ethanol	88.42%
Water	11.58%

$\rho_{mix} = 799.5 kg/m^3$

Molar weight= 42.76

Mass flow rate= 33.98 kgmole/hr

Mass flow rate= 1455 kg/hr

1. Temperature Limits

Tube side: $50.28^{O}C$ to $114\ ^{O}C$

Shell side: $206\ ^{O}C$ to $70\ ^{O}C$

LMTD:

$T_{LMTD} = (T1 - t_2) - (T_2 - t_1)\ /\ \ln\ (T_1 - t_2)/\ (T_2 - t_1)$

Where:

T_1 = Temp of hot fluid in from shell side

T_2 = Temp of hot fluid out from shell side

t_1 = Temp of cold fluid in from tube side

t_2 = Temp of cold fluid out from tube side

$T_{LMTD} = (206 - 114) - (70 - 50.28)/\ \ln\ (206 - 114)/\ (70 - 50.28)$

$T_{LMTD} = 46.9^{o}C$

Correction factor:

$R = T_1 - t_2/\ t_2 - t_1 = 0.534$

$S = t_2 - t_1/\ T_2 - t_1 = 0.575$

From Figure 5.1 by process heat transfer by kern

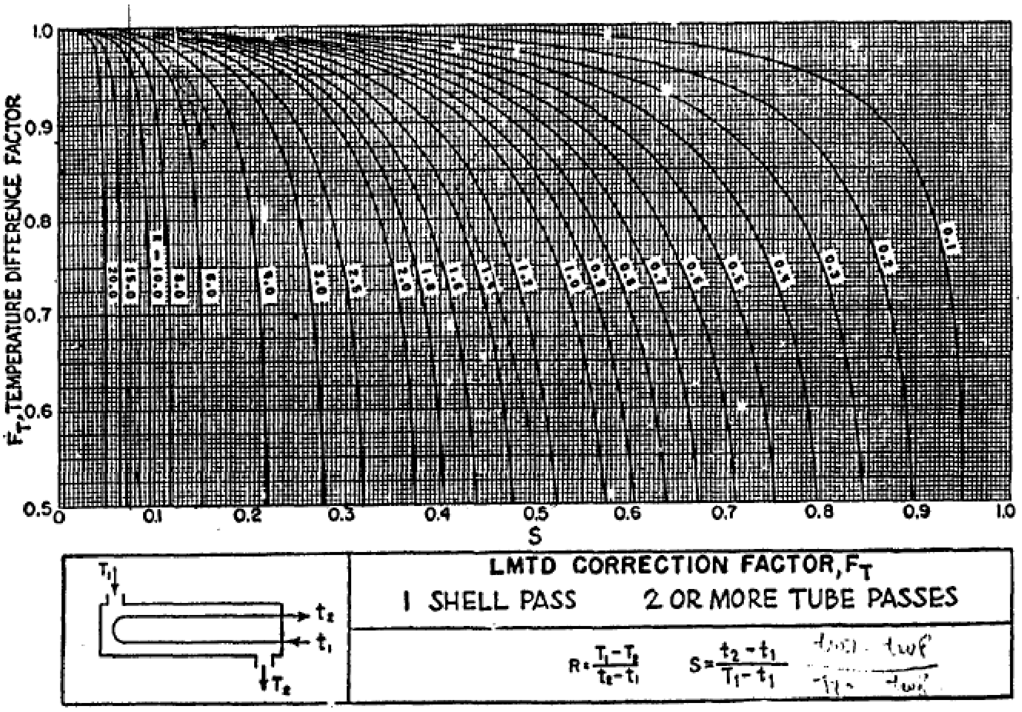


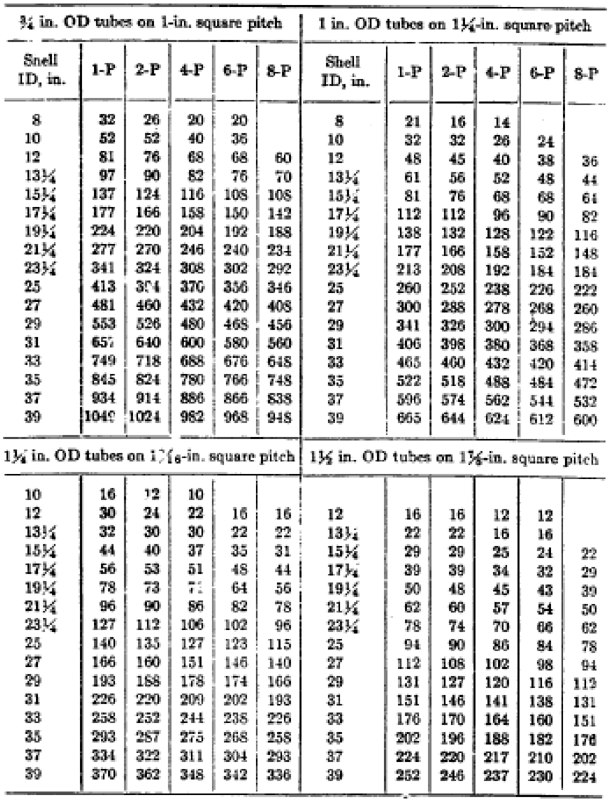
Figure 5.1 LMTD correction factors for 1 – 2 exchangers

$f_{(t)} = .90$

$T_{LMTD} = 88 * .90 = 42.2\ ^{o}C$

Using the following tables from process heat transfer by kern,

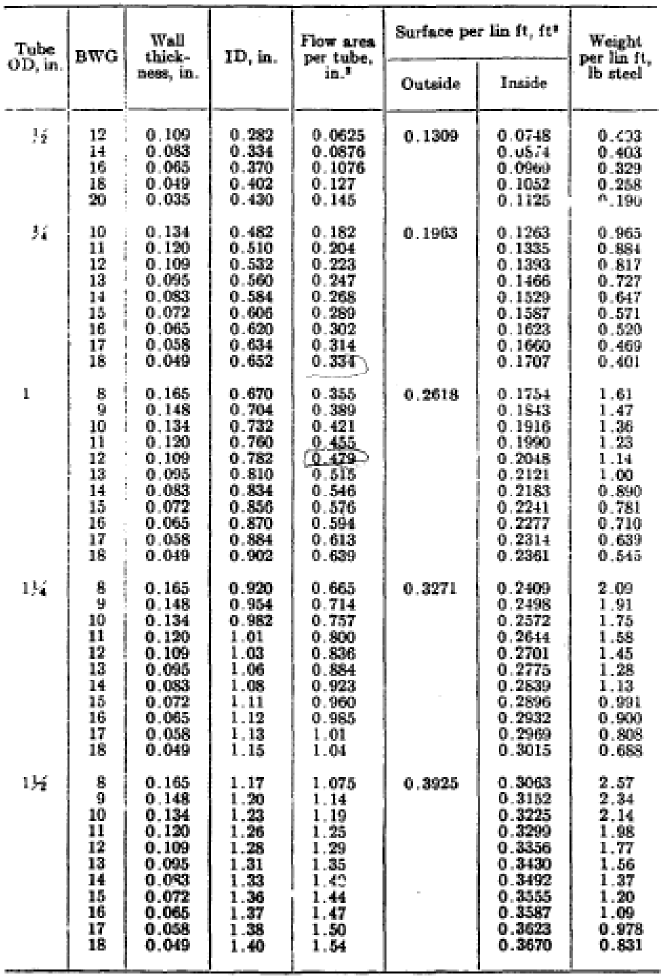
Table 5.1 Tube-Sheet Layouts (Square Pitch)



¾ in. OD tubes on 1-in. square pitch						1 in. OD tubes on 1¼-in. square pitch					
Shell ID, in.	1-P	2-P	4-P	6-P	8-P	Shell ID, in.	1-P	2-P	4-P	6-P	8-P
8	32	26	20	20		8	21	16	14		
10	52	52	40	36		10	32	32	26	24	
12	81	76	68	68	60	12	48	45	40	38	36
13¼	97	90	82	76	70	13¼	61	56	52	48	44
15¼	137	124	116	108	108	15¼	81	76	68	68	64
17¼	177	166	158	150	142	17¼	112	112	96	90	82
19¼	224	220	204	192	188	19¼	138	132	128	122	116
21¼	277	270	246	240	234	21¼	177	166	158	152	148
23¼	341	324	308	302	292	23¼	213	208	192	184	184
25	413	304	370	356	346	25	260	252	238	226	222
27	481	460	432	420	408	27	300	288	278	268	260
29	553	526	480	468	456	29	341	326	300	294	286
31	657	640	600	580	560	31	406	398	380	368	358
33	749	718	688	676	648	33	465	460	432	420	414
35	845	824	780	766	748	35	522	518	488	484	472
37	934	914	886	866	838	37	596	574	562	544	532
39	1049	1024	982	968	948	39	665	644	624	612	600

1¼ in. OD tubes on 1$\frac{9}{16}$-in. square pitch						1½ in. OD tubes on 1⅞-in. square pitch					
10	16	12	10								
12	30	24	22	16	16	12	16	16	12	12	
13¼	32	30	30	22	22	13¼	22	22	16	16	
15¼	44	40	37	35	31	15¼	29	29	25	24	22
17¼	56	53	51	48	44	17¼	39	39	34	32	29
19¼	78	73	71	64	56	19¼	50	48	45	43	39
21¼	96	90	86	82	78	21¼	62	60	57	54	50
23¼	127	112	106	102	96	23¼	78	74	70	66	62
25	140	135	127	123	115	25	94	90	86	84	78
27	166	160	151	146	140	27	112	108	102	98	94
29	193	188	178	174	166	29	131	127	120	116	112
31	226	220	209	202	193	31	151	146	141	138	131
33	258	252	244	238	226	33	176	170	164	160	151
35	293	287	275	268	258	35	202	196	188	182	176
37	334	322	311	304	293	37	224	220	217	210	202
39	370	362	348	342	336	39	252	246	237	230	224

Table 5.2 Heat Exchanger and Condenser Tube Data



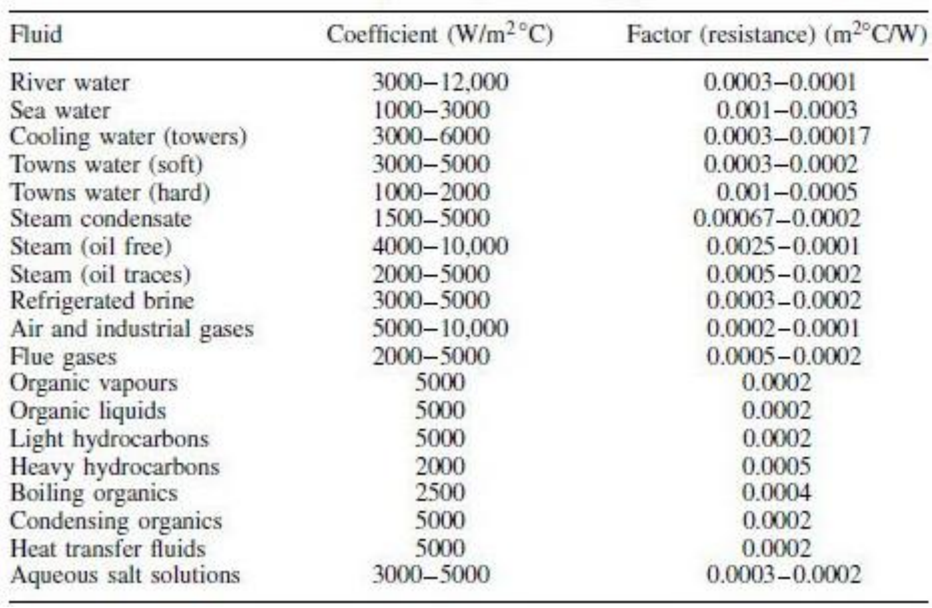
Tube OD, in.	BWG	Wall thickness, in.	ID, in.	Flow area per tube, in.^{2}	Surface per lin ft, ft^2		Weight per lin ft, lb steel
					Outside	Inside	
½	12	0.109	0.282	0.0625	0.1309	0.0748	0.493
	14	0.083	0.334	0.0876		0.0874	0.403
	16	0.065	0.370	0.1076		0.0969	0.329
	18	0.049	0.402	0.127		0.1052	0.258
	20	0.035	0.430	0.145		0.1125	0.190
¾	10	0.134	0.482	0.182	0.1963	0.1263	0.965
	11	0.120	0.510	0.204		0.1335	0.884
	12	0.109	0.532	0.223		0.1393	0.817
	13	0.095	0.560	0.247		0.1466	0.727
	14	0.083	0.584	0.268		0.1529	0.647
	15	0.072	0.606	0.289		0.1587	0.571
	16	0.065	0.620	0.302		0.1623	0.520
	17	0.058	0.634	0.314		0.1660	0.469
	18	0.049	0.652	0.334		0.1707	0.401
1	8	0.165	0.670	0.355	0.2618	0.1754	1.61
	9	0.148	0.704	0.389		0.1843	1.47
	10	0.134	0.732	0.421		0.1916	1.36
	11	0.120	0.760	0.455		0.1990	1.23
	12	0.109	0.782	0.479		0.2048	1.14
	13	0.095	0.810	0.515		0.2121	1.00
	14	0.083	0.834	0.546		0.2183	0.890
	15	0.072	0.856	0.576		0.2241	0.781
	16	0.065	0.870	0.594		0.2277	0.710
	17	0.058	0.884	0.613		0.2314	0.639
	18	0.049	0.902	0.639		0.2361	0.545
1¼	8	0.165	0.920	0.665	0.3271	0.2409	2.09
	9	0.148	0.954	0.714		0.2498	1.91
	10	0.134	0.982	0.757		0.2572	1.75
	11	0.120	1.01	0.800		0.2644	1.58
	12	0.109	1.03	0.836		0.2701	1.45
	13	0.095	1.06	0.884		0.2775	1.28
	14	0.083	1.08	0.923		0.2839	1.13
	15	0.072	1.11	0.960		0.2896	0.991
	16	0.065	1.12	0.985		0.2932	0.900
	17	0.058	1.13	1.01		0.2969	0.808
	18	0.049	1.15	1.04		0.3015	0.688
1½	8	0.165	1.17	1.075	0.3925	0.3063	2.57
	9	0.148	1.20	1.14		0.3152	2.34
	10	0.134	1.23	1.19		0.3225	2.14
	11	0.120	1.26	1.25		0.3299	1.98
	12	0.109	1.28	1.29		0.3356	1.77
	13	0.095	1.31	1.35		0.3430	1.56
	14	0.083	1.33	1.40		0.3492	1.37
	15	0.072	1.36	1.44		0.3555	1.20
	16	0.065	1.37	1.47		0.3587	1.09
	17	0.058	1.38	1.50		0.3623	0.978
	18	0.049	1.40	1.54		0.3670	0.831

We have selected the following heat exchanger data for our calculations:

Tube Data		Shell data	
OD	¾ inch	OD	39 inch
ID	0.624 inch	De	0.02513
L (wall thickness)	0.0625 inch	B	12.7 cm
Flow area per tube	0.302 inch^2	Pt	1.25 inch
Surface Area per linear ft.	0.1623 ft^2	Surface Area per linear ft.	0.1693 ft^2
Tube passes	2	Shell passes	1

Heat transfer area:

Table 5.3 Fouling factors



Fluid	Coefficient (W/m^2°C)	Factor (resistance) (m^2°C/W)
River water	3000–12,000	0.0003–0.0001
Sea water	1000–3000	0.001–0.0003
Cooling water (towers)	3000–6000	0.0003–0.00017
Towns water (soft)	3000–5000	0.0003–0.0002
Towns water (hard)	1000–2000	0.001–0.0005
Steam condensate	1500–5000	0.00067–0.0002
Steam (oil free)	4000–10,000	0.0025–0.0001
Steam (oil traces)	2000–5000	0.0005–0.0002
Refrigerated brine	3000–5000	0.0003–0.0002
Air and industrial gases	5000–10,000	0.0002–0.0001
Flue gases	2000–5000	0.0005–0.0002
Organic vapours	5000	0.0002
Organic liquids	5000	0.0002
Light hydrocarbons	5000	0.0002
Heavy hydrocarbons	2000	0.0005
Boiling organics	2500	0.0004
Condensing organics	5000	0.0002
Heat transfer fluids	5000	0.0002
Aqueous salt solutions	3000–5000	0.0003–0.0002

Overall heat transfer co-efficient:

U = 1500 W/m^{2o}C

From table 12.1 Coulson and Richard

Now to calculate surface area we use this equation:

Q= UA(T_{LMTD})

Where:

Q = 699855 Kj/hr

T_{LMTD} = 42.2^{o}C

Putting values in above equation we get:

A = 699855/ 1500*42.2

A= 11.05m^2

<u>Designing of tube:</u>

Tube: Carbon Material

Tube OD= ¾ inch

Tube ID= 0.624 inch

Flow cross section area= 0.302inch^2

Surface Area of one tube= 0.24m^2

Nt= Heat transfer Area/ surface area of one tube

= 11.05/ 0.14

= 79

Tube side Calculations:

Flow area per tube = at^I= 0.302ich^2

Nt= 79

Total area= a_{total}= at^I * Nt/n

a_{total} = 1.95 * 79/2

= 77.02 cm^2 or .0077m^2

For one pass = 0.00385m^2

Tube side heat transfer Co-efficient

Mass Velocity= G= m/at

=1455/.0077

= 1500 kg/hr.m^{2h}

Viscosity = 0.011cp

Reynolds's number= Re= G * Di/μ

= 15000 * .0157/0.0396

Re= 5946

L/D = 25

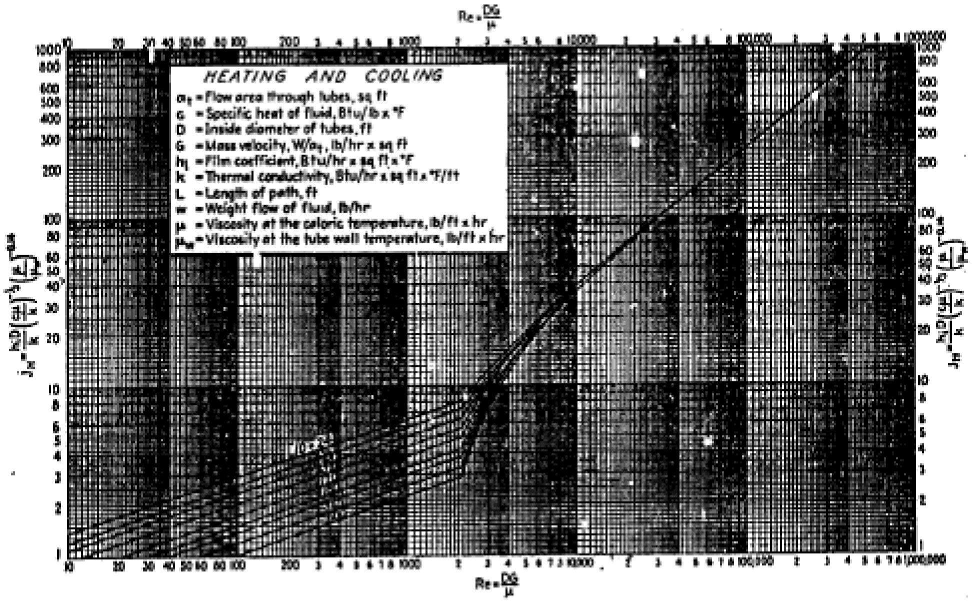


Figure 5.2 Tube Side heat transfer curve

J_H = 24

Heat transfer coefficient = hi = 280× (K/D)×(Cpμ/k)$^{1/3}$ φ_t

K = 0.12 Kj/m.hr.k

Cp= 2.7 Kj/kg.k

µ = 0.088 kg/hr.m

hi = 280 * (0.12/0.0157) * (2.7 * 0.088/0.12)$^{1/3}$* (1)

hi = 2685 kj/hr.m^{2}.^{o}C

hio = hi * ID/OD

= 2865 * 0.0157/0.019

= 2119 kj/hr.m^{2}.^{o}C

<u>Shell side Calculations</u>

Flow area = As = ID × B × C/pt

As = 0.99 × (6.53 ×10^{-3})/0.03175

As = 0.0258m^{2}

Mass velocity = 1000/ 0.0258

= 38759 kg/h.m^{2}

De = 0.02514

µ = 1.26kg/m.hr

Re= G×De/ µ

= 38759×0.02514/1.26

= 773

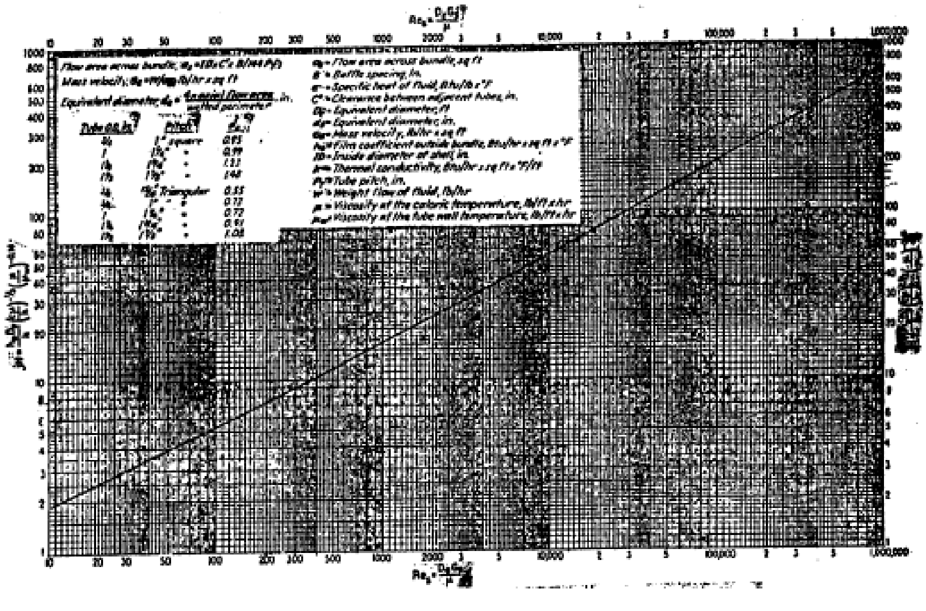


Figure 5.3 Tube Side heat transfer curve

J_H = 10

$h_o = 10 \times (2.24/0.02514) \times (1.26 * 13.1/2.24)^{1/3}(1)$

$= 1728.56$ kj/hr.m^2.ºC

$U_c = h_o \times h_{io}/h_o + h_{io}$

$U_c = 4238$ kj/hr.m^2. ºC

Calculating total surface Area:

$A = N_t \times L \times a^{II}$

$A = 79 \times 5 \times 0.1963$

$A = 64.8$ m^2

$U_D = Q/A \times (T_{LMTD})$

$= 1968/64.8 \times 42$

$= 1291$ kj/hr.m^2. ºC

Dirt Factor:

$R_D = 1/U_D - 1/U_C$

$= 1/1291 - 1/4238$

$= 0.00054$

Pressure Drop Calculations:

Shell side pressure drop

Mass velocity = G = 38759 kg/hr.m^2

Re = 773

Ds =0.99m

f= 0.0025ft^2/in^2 = 0.36m^2/m^2

Do = 0.02154m

s = 1

$\varphi = 1$

B = 0.127m

$N+1 = 12*5/0.127$

$= 424.44$

Equation for pressure drop is:

$\mathbf{\Delta P = fG^2D(N+1)/\ (5.22 \times 10^{10}).\ De.s.\ \varphi}$

Substituting values we get:

$\Delta P = 0.36*38759*0.02514*427.44/(5.22 \times 10^{10})*0.02514*1$

$\Delta P = 4.4$psi (Allowable pressure drop is 10psi)

Tube side pressure drop

Mass velocity = G = 76579 kg/hr.m^2

Re = 3036

ID =0.0221m

L_n= 5m

f= 0.0288m^2/m^2

Do = 0.02154m

s = 1.7

Equation for pressure drop is:

$\Delta P = fG^2L_n / (5.22 \times 10^{10}). ID.s. \varphi$

Substituting values we get:

$\Delta P = 0.0288*76579*5/(5.22 \times 10^{10})*0.02514*1$

$\Delta P = 0.44$psi

$\Delta P_t = (4n/s)* V^2/ 2g$

$= 0.56$psi

$\Delta P = 0.46 +0.56$

$= 1.02$psi

5.4 Fixed Bed Reactor:

Step1

Calculate volumetric flow rate

Temperature of entering stream = 697.3K

Pressure of entering stream = 42.3atm

Flow rate of entering stream = 33.9 kgmol/hr

Molar density = P/RT

= 42.3/0.0821 * 697.3

= 0.738 kgmol/m^3

Average molecular weight of inlet stream = 32kg/kgmol

Average density = PM/RT

=23.3kg/m^3

Volumetric flow rate = Molar rate of stream * Average Mol. Weight/ Density

= 433.9 * 32 / 23.3

= 595m^3/hr

Step2

Calculation of Volume of Catalytic bed

$V_B = (1+E)* V_b$

Where

E = void fraction = 0.4

V_b = Volumetric flow rate/ Space velocity

For 70% conversion and at temperature 697K space velocity is taken to be 333/hr

Space time = 1 / space velocity

= 1*3600/333

= 10.8 sec

V_b = 595/333

=1.78m^3

Substituting values in the above equation we get

V_B= (1+0.4)* 1.78

=2.5 m^3

Step3

Calculation of diameter and length of bed

Suppose

L/D= 3

L= 3D

V_B= 3∏/4(D_B^3)

D_B = 1.02m

L_B = 3.06m

Step4

Calculation of internal diameter and length of reactor

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

Length of reactor = 3.36m

Internal dia of reactor= Length of reactor/3

=1.122m

Step5

Calculation of volume of reactor

V = ∏/4D^2L

= ∏/4 (1.122$^{)2}$(3.36)

= 3.32m^3

Step6

Calculation of thickness of reactor

t = P_iD_i/(4jf-1.2Pi) +C_c

P_i = Pressure Design factor =1.25 * operating pressure

= 1.25*4284

=5356KPa

D_i = 1.02m

J = joint efficiency = 0.85 (Double welded and support)

f = Stress factor = 3.08×10^4

C_c = corrosion allowance= 2m

Putting the values we get

t = 5356*1.02/ (4*3.08×10^{4*}0.85-1.2(5356)) + 2

t= 0.00205m

Step7

Calculation of outer diameter of reactor

D_o= D_i + 2t

= 1.02+ 2(0.00205)

=1.2041m

Step8

Calculation of volume of steel required

$V_s = \prod/4 * (D_o^2 – D_i^2)* L + 2* \prod/4 * D^2*t$

Putting values in the above equation we get

$V_s = 0.0246\ m^3$

Step9

Calculation of mass of steel required

Density of steel = ρ=8000kg/m^3

Volume of steel= V = 0.0246

Mass of steel = Density * volume

=196.8kg

Step10

Calculation of weight of catalyst

Bulk density of catalyst = 650 kg/m^3

Volume of catalyst = 2.5m^3

Weight of Catalyst = 650 * 2.5

= 1625kg

Step11

Pressure drop in the reactor

To calculate pressure drop Ergun’s Equation is used

$\Delta P/L = 150\varepsilon^2\mu V_s/(1- \varepsilon)^3D_p^2 + 1.75\, \rho\varepsilon V_s/(1- \varepsilon)^3Dp$

L= 3.06m

ε =0.4

D_p = 0.0048m

V_s= volumetric flow rate/ Area

= 3.804/1.1304

= 3.36m/s

μ = 1.08cp

$\rho = 0.897 kg/m^3$

Putting values in above equation we get

$\Delta P/3.06 = 150(0.4)^3(3.36)/(1-0.4)^3(0.0048)^2 + 1.75(0.897)(0.4)(3.36))/(1-0.4)^3(0.0048)$

ΔP = 2atm

Designing Parameters

Reactor Category	Fixed Bed Reactor
Volume of catalytic bed (m^3)	2.5
Volume of reactor (m^3)	3.32
Length of reactor (m)	3.36
Diameter of reactor(m)	1.12
Weight of catalyst (/kg)	1625
Wight of steel (kg)	196.8
Void fraction	0.4
Reactor pressure drop(atm)	2atm

5.5 Fluidized Bed Reactor:

Model assumptions

- The model assumes the following:
- The reactor operates at a steady state, under uniform temperature.
- The reactor is in isothermal operation.
- The gas flows in plug flow, with gas interchange between phases
- The bed is axially divided into N compartments, each one consisting of the bubble, cloud, and emulsion phases.
- Bubbles grow continuously along the reactor height from their initial diameter until they reach the maximum stable bubble diameter.
- The bed volume fraction occupied by bubbles and emulsion depends on the flow regime and changes along the reactor height.
- Solid entrainment and carryover are taken into account by the model. However, particle agglomeration and breakage are not considered.
- Bed voidage is constant from the distributor until Hmf and is equal to 0.5

Operating Temp = 90°C

Operating Pressure = 20 bar

Monomer and comonomer Feed flow rate = 989 kg/hr

Nitrogen feed rate = 497 kg/hr

Catalyst feed rate = 0.746 kg/hr

Monomer = Ethylene

Comonomer = 1-Butene

Treminator = Hydrogen

Catalyst = Ti, V, $CrCO_3\,\rho_g$

Modelling Equaitons:

Bed Voidage at Minimum Fluidization:

$\varepsilon_{mf} = 0.586\Phi^{-00.72}\ (\mu^2/(\rho_g.g(\rho_s-\rho_g)d^3_p))^{0.029}\ (\rho_{g/}\ \rho_s)^{0.021}$

Superficial Velocity at minimum fluidization:

$(1.75/\ \varepsilon^3_{mf})Re^2_{mf} + (150(1 - \varepsilon_{mf})/\ \varepsilon^3_{mf}).Re_{mf} - (d^3_p\ \rho_g(\rho_s-\rho_g)g/\ \mu^2) = 0$

$Re_{mf} = \rho_g.D_p.U_{mf}/\ \mu$

Bubble dia:

$d_B = d_{BM} – (d_{BM} – d_{Bo})e^{– 0.3H/D}$

$d_{BM} = 0.652[A(U_o – U_{mf})]^{0.4}$

$d_{Bo} = 0.00376(U_o – U_{mf})^2$

Bubble Rising Velocity:

$U_b = U_o – U_{mf} + 0.711(g.d_B)^{0.5}$

Fraction of Bubble Phase:

$\delta = (U_o – U_{mf})/U_b$

Height at minimum fluidization conditions:

Height at minimum fluidizing conditions

Height at minimum fluidizing conditions is calculated by

$H_{mf} = H(1- \delta)$

Coefficient of Mass transfer:

$1/K_{be} = (1/K_b + 1/K_e)$

$K_b = 4.5\ U_{mf}/d_B + 10.4\ D_e^{0.5}/d_B^{1.25}$

$Ke = 6.78\ ((\varepsilon_{mf}.D_e.U_b)/d^3_B\ )^{0.5}$

Coefficient of Heat transfer b/w bubble and cloud:

$H_{be} = 4.5\ (U_{mf}\ p_g\ C_{pg}/d_B) + 10.4(p_g k_g C_{pg}/d_B^{2.5})^{0.5}$

Calculated Values:

Density of gaseous mixture = ρ_g =17.05 kg/m^3

Bed Voidage = ε_{mf} = 0.5

Minimum Fluidization Velocity = U_{mf} = 0.57 m/s

Bubble fraction in fluidized bed = δ = 0.214

dia of bubble = d_b = 15 cm

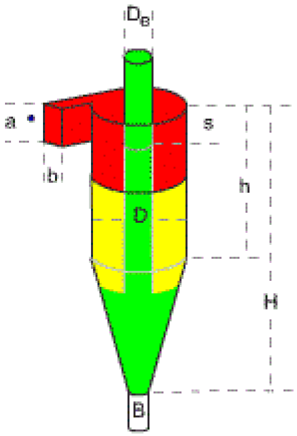
Bed Height 7.29 m

Height of reactor = 10 m

Dia = 3 m

5.6 First Cyclone

For designing we use standard design diameter i.e 203mm



<u>Pressure Drop Calculation</u>

Area of inlet duck = $A_1 = 0.2D_c * 0.5D_c$

$= 4120.9mm^2$

Cyclone surface area = $A_s = \prod \times D \times H$

$= 517.6mm^2$

f_c=friction factor for gases = 0.005

$\Psi = f_c \times A_s / A_1$

$= 0.628$

Where Ψ is a parameter used in graph for finding out pressure drop factor

$R_1/R_e = (203 - 40/2)/101.5$

$=1.80$

From the graph $\Theta = 0.9$

Velocity = $V_1 = 24.529 \times 10^6 / 3600 \times 4120.9$

$=1.653m/s$

Area of the exit pipe= $\prod D^2/4$

$=8087mm^2$

Where 0.5D = 101.5mm

Velocity of pipe at exit point

$V_2 = 24.529 \times 10^6 / 3600 \times 8087$

$=0.8425m/s$

Equation for pressure drop:

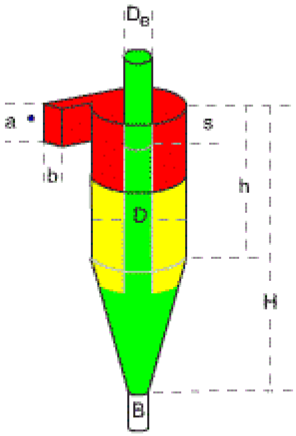
$\Delta P = P_f/D_c \{V_1^2 [1+ 2\Theta^2 (2 R_1/R_e-1)] +2v_2^2\}$

$= 0.0013/203 \{1.653^2[1+2(0.9)^2(2*1.80 - 1)] +2(0.8425)^2$

$\Delta P = 6.3\times10^{-3}$bar

5.7 Second cyclone

For designing we use standard desgn diameter i.e 203mm



Pressure Drop Calculation

Area of inlet duck = $A_1 = 0.2D_c * 0.5D_c$

$= 4120.9\text{mm}^2$

Cyclone surface area = $A_s = \prod \times D \times H$

$= 517.6\text{mm}^2$

f_c=friction factor for gases = 0.005

$\Psi = f_c \times A_s / A_1$

$= 0.628$

Where Ψ is a parameter used in graph for finding out pressure drop factor

$R_1/R_e = (203 - 40/2)/101.5$

$=1.80$

From the graph $\Theta = 0.9$

Velocity = $V_1 = 28.529 \times 10^6 / 3600 \times 4120.9$

$=1.93\text{m/s}$

Area of the exit pipe= $\prod D^2/4$

$=8087\text{mm}^2$

Where 0.5D = 101.5mm

Velocity of pipe at exit point

$V_2 = 24.529 \times 10^6 / 3600 \times 8087$

$=0.97 m/s$

Equation for pressure drop:

$\Delta P = P_f/D_c \{V_1^2 [1+ 2\Theta^2 (2 R_1/R_e-1)] +2v_2^2\}$

$= 0.0013/203 \{1.92^2[1+2(0.9)^2(2*1.80 - 1)] +2(0.97)^2$

$\Delta P = 4.18\times10^{-5}$

5.8 Distillation Column: 1

Selection: Tray Column

Mass flow rate of feed= F= 1456 Kg/hr

Mass flow rate of distillate= D= 1311Kg/hr

Mass flow rate of Bottom= B= 145Kg/hr

Reflux Ratio= R = L/D

Mass flow rate of reflux= L= 447Kg/hr

Mass flow rate of vapor= V= 976Kg/hr

Light key component= Ethylene

Heavy key component= Ethanol

Heavy non-key component= Water

Calculation of column plate:

Minimum no of plates= 26 (Aspen Hysys)

Minimum Reflux Ratio:

$R= 1.5R_{min}$

R= 0.75

$R_{min}= 0.5$

Theoretical No. of plates:

$N-N_{min}/N+1 = 0.75[1-(R-R_{min}/R+1)^{0.566}]$

N= 7.8

Actual No. of plates:

Column efficiency= 30%

No. of actual plates= N/0.3= 26

Column Dia:

Assumption: Column is operating at atmospheric pressure

Flow parameter

$F_{LY}=(L_n/V_n)(p_v/p_L)^{0.5}= 0.028$

P_L (density of liquid water at boiling point)= 958Kg/L

P_v (density of water vapor at boiling point)

Assumption water vapors at boiling point is an ideal gas, then

$P_v=PM/RT = 0.588g/L$

Assumption Plate Spacing= 18 inch= 0.45m

K_v= 0.28

U_c= $K_v(p_L-p_v/p)^{1/2}(6/20)^{0.2}$

=4.28m/s

V= vapor flow rate= 3.32 m/s

Note: Plate Spacing of distillation column (Mc Cabe & Smith 6th Edition)

Cross section Area= V/U_c

= 0.77 m^2

Column area: (Reference Mc Cabe & Smith 7th Edition)

Bubble area= 70% of total column area

Column area= 1.1 m^2

Column Dia= $(4*\text{column area}/3.14)^{0.5}$

D_c= 1.183 m

Liquid flow Arrangement:

Liquid flow rate= $1.9*10^{-4}$ m/s

Using figure 5.55

Cross flow single pass plate is selected

Plate Design:

Column Dia= D_c= 1.183 m

Column Cross Sectional Area= A_c= 0.77m^2

Down Comer Area= $A_d=0.15A_c$= 0.1155 m^2

Net Area= $A_n=A_c-A_D$= 0.654 m^2

Active Area= $A_a=A_c-2\pi d$= 0.539 m^2

Hole Area= $0.1*A_a$= 0.0539 m^2

Weir length

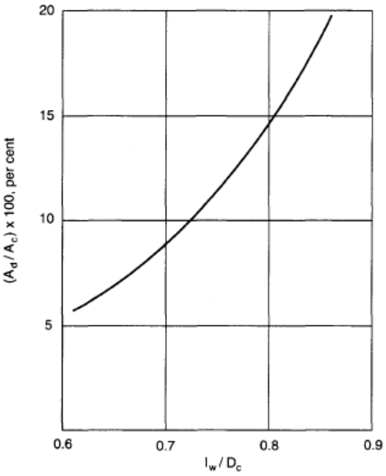


Figure 5.4 Relation b/w downcomer area and Weir Length

A_d/A_c= 0.15

Figure 5.6 Coulson & Richardson 6th volume 3rd Edition

L_w/D_c= 0.8

L_w= 0.946 m

Weir length should be 60 to 85% of column dia which is satisfactory

Weir length= h_w= 50 mm

Hole dia= 5 mm+plate thickness

Plate thickness= 5 mm

Height of column:

Height of column= $H_c=(N_{act}-1)H_s+\Delta H$

N_{act}= No. of actual plates= 26

Tray spacing= H_s= 0.45 m

ΔH=0.9 m

Total thickness of tray= 0.09 m

Height of column= 13 m

5.9 Distillation Column: 2

Selection: Tray Column

Mass flow rate of feed= F= 859 Kg/hr

Mass flow rate of distillate= D= 455Kg/hr

Mass flow rate of Bottom= B= 404Kg/hr

Reflux Ratio= R = L/D

Mass flow rate of reflux= L= 397 Kg/hr

Mass flow rate of vapor= V =794Kg/hr

Light key component= Ethanol

Heavy key component= water

Heavy non-key component= acetic acid, acetaldehyde

Calculation of column plate:

Minimum no of plates= 26 (Aspen Hysys)

Minimum Reflux Ratio:

$R= 1.5R_{min}$

R= 0.85

$R_{min}= 0.566$

Theoretical No. of plates:

$N-N_{min}/N+L = 0.85[1-(R-R_{min}/R+1)^{0.566}]$

N= 4

Actual No. of plates:

Column efficiency= 30%

No. of actual plates= N/0.3= 13

Column Dia:

Assumption: Column is operating at atmospheric pressure

Flow parameter

$F_{LY}=(L_n/V_n)(p_v/p_L)^{0.5}= 0.012$

P_L (density of liquid water at boiling point)= 958Kg/L

P_v (density of water vapor at boiling point)

Assumption water vapors at boiling point is an ideal gas, then

$P_v=PM/RT = 0.588g/L$

Assumption Plate Spacing= 18 inch= 0.45m

K_v= 0.28

U_c= $K_v(p_L-p_v/p)^{1/2}(6/20)^{0.2}$

=4.28m/s

V= vapor flow rate= 2.23 m/s

Note: Plate Spacing of distillation column (Mc Cabe & Smith 6th Edition)

Cross section Area= V/U_c

= 1.48 m^2

Column area: (Reference Mc Cabe & Smith 7th Edition)

Bubble area= 70% of total column area

Column area= 2.1 m^2

Column Dia= $(4*\text{column area}/3.14)^{0.5}$

D_c= 1.64 m

Liquid flow Arrangement:

Liquid flow rate= $1.9*10^{-4}$ m/s

Using figure 5.55

Cross flow single pass plate is selected

Plate Design:

Column Dia= D_c= 1.64 m

Column Cross Sectional Area= A_c= 0.86m^2

Down Comer Area= A_d=0.15A_c= 0.129 m^2

Net Area= A_n=A_c-A_D= 0.731 m^2

Active Area= A_a=A_c-2πd= 0.602 m^2

Hole Area= 0.1*A_a= 0.0602 m^2

Weir length

From Figure 5.4

A_d/A_c= 0.15

Figure 5.6 Coulson & Richardson 6th volume 3rd Edition

L_w/D_c= 0.8

L_w= 1.312 m

Weir length should be 60 to 85% of column dia which is satisfactory

Weir length= h_w= 50 mm

Hole dia= 5 mm+plate thickness

Plate thickness= 5 mm

Height of column:

Height of column= $H_c=(N_{act}-1)H_s+\Delta H$

N_{act}= No. of actual plates= 13

Tray spacing= H_s= 0.6 m

ΔH=1.2 m

Total thickness of tray= 0.1 m

Height of column= 9 m

5.10 Membrane

Feed

Sr.	Component	Volumetric Flow Rate (m^3/s)	Mole Fraction
a	Hydrogen	.414863	xfa = .770819
b	Nitrogen	.110318	xfb = .203669
c	Ethylene	.001312	xfc = .00122
d	1-Butene	.026289	xfd = .024292
	Total	.55278	

Feed flow rate = qf = .55278 m^3/s

Feed Pressure = ph = 600000 Pa

Permeate pressure = pl = 100000 Pa

Stage Cut = ϑ = 0.5

Membrane: Spiral Wound, Cellulose Acetate – Silica nanocomposite membrane.

Thickness = t = 2.54e-5 m

Sr.	Componenet	Permeabilities $m^3(stp).m/(s.m^2.Pa)$
a	Hydrogen	pa = 32.6e-15
b	Nitrogen	pb = 5.96e-15
c	Ethylene	pc = 1.8e-19
d	1-Butene	pd = 1.275e-19

Permeate flow rate = qp = ϑ*qf

Reject flow rate = qr = qf – qp

Using matlab, the following formulas were looped for given conditions and following results were obtained:

Taking initial permeate fraction = 0 (ypa = 0)
Incrementing ypa using a dummy variable h=0.000001

$$\text{Am} = \frac{qp{*}ypa{*}t}{pa{*}\frac{ph}{1-\vartheta}{*}(xfa-(\vartheta{*}\text{yap}))-(\text{pl}{*}\text{ypa})}$$

$$\text{ypb} = \frac{\frac{ph{*}xfb}{1-\vartheta}}{\frac{qp{*}t}{pb{*}Am}} + \frac{\vartheta{*}\text{ph}}{1-\vartheta} + \text{pl}$$

$$\text{ypc} = \frac{\frac{ph{*}xfc}{1-\vartheta}}{\frac{qp{*}t}{pc{*}Am}} + \frac{\vartheta{*}\text{ph}}{1-\vartheta} + \text{pl}$$

$$\text{ypd} = \frac{\frac{ph{*}xfd}{1-\vartheta}}{\frac{qp{*}t}{pd{*}Am}} + \frac{\vartheta{*}\text{ph}}{1-\vartheta} + \text{pl}$$

Applying conditions for

ypa+ypb+ypc+ypd = 1

ypa permeate composition of a
ypb permeate composition of b
ypc permeate composition of c
xoa reject composition of a
xob reject composition of b
xoc reject composition of c
Am membrane area (m^2)

$$\text{xoa} = \frac{xfa}{1-\vartheta}\,\frac{\vartheta{*}\text{ypa}}{1-\vartheta}$$

$$\text{xob} = \frac{xfb}{1-\vartheta}\,\frac{\vartheta{*}\text{ypb}}{1-\vartheta}$$

$$\text{xoc} = \frac{xfc}{1-\vartheta}\,\frac{\vartheta{*}\text{ypc}}{1-\vartheta}$$

$$\text{xod} = \frac{xfd}{1-\vartheta}\,\frac{\vartheta{*}\text{ypd}}{1-\vartheta}$$

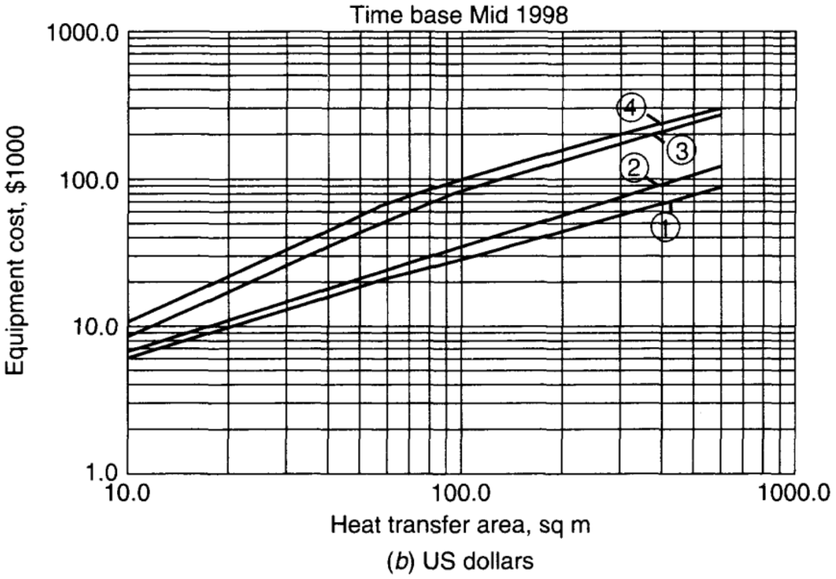
The following results are obtained:

Component	Permeate Mol Fraction	Permeate Flowrate kg/hr	Reject Mol Fraction	Reject Flowrate kg/hr
Hydrogen	0.9016	78.52377	0.6401	55.74874
Nitrogen	9.84E-02	119.9804	0.3089	376.6458
Ethylene	2.48E-08	6.05E-05	0.0024	5.852703
1-Butene	3.50E-07	0.001706	0.0486	237.0345

Am = $660m^2$

Chapter – 6 **Cost Estimation**

Following are the figures and charts used to calculate plant commissioning cost.

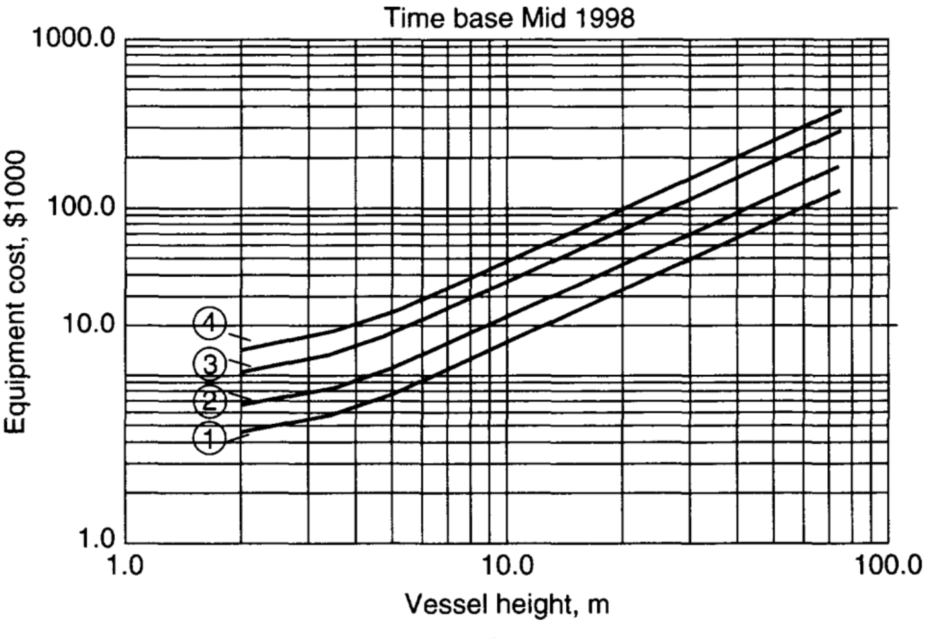


Materials	
Shell	Tubes
① Carbon steel	Carbon steel
② C.S.	Brass
③ C.S.	Stainless steel
④ S.S.	S.S.

Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

Type factors	
Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Figure 6.1 Shell and tube heat exchangers. Time base mid-1998



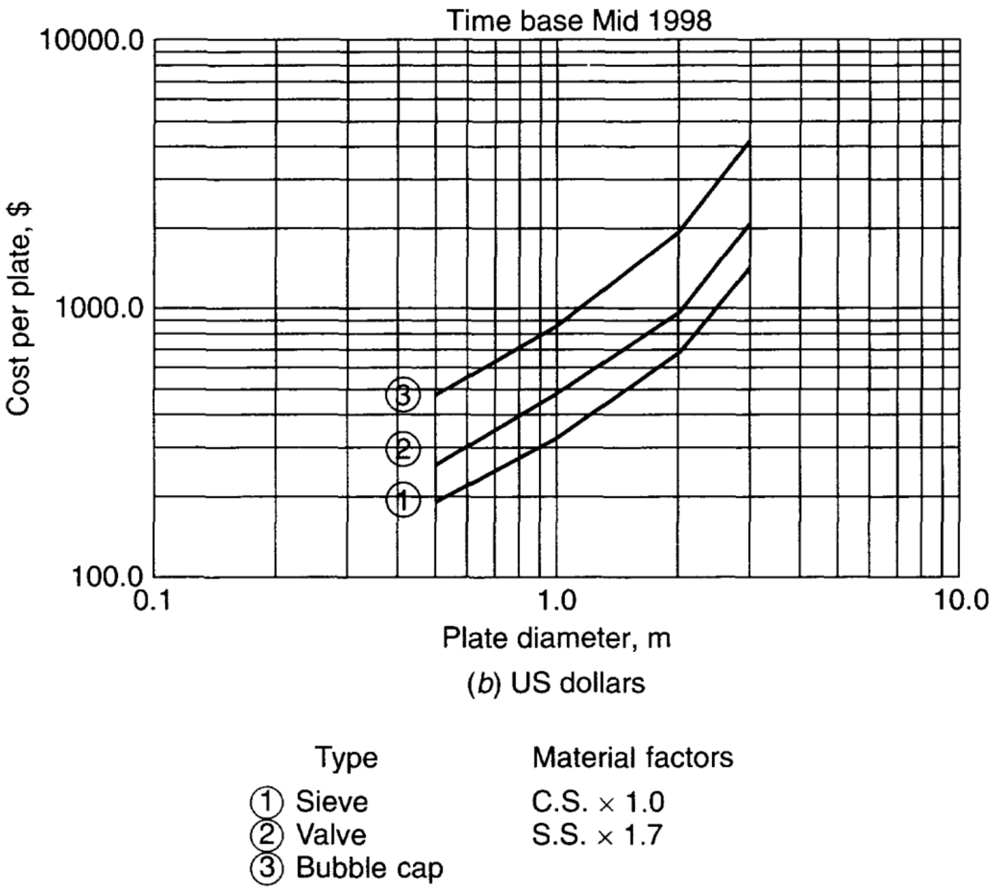
(*b*) US dollars

Diameter, m	
①—0.5	③—2.0
②—1.0	④—3.0

Material factors	
C.S.	× 1.0
S.S.	× 2.0
Monel	× 3.4
S.S. clad	× 1.5
Monel clad	× 2.1

Pressure factors	
1–5 bar	× 1.0
5–10	× 1.1
10–20	× 1.2
20–30	× 1.4
30–40	× 1.6
40–50	× 1.8
50–60	× 2.2

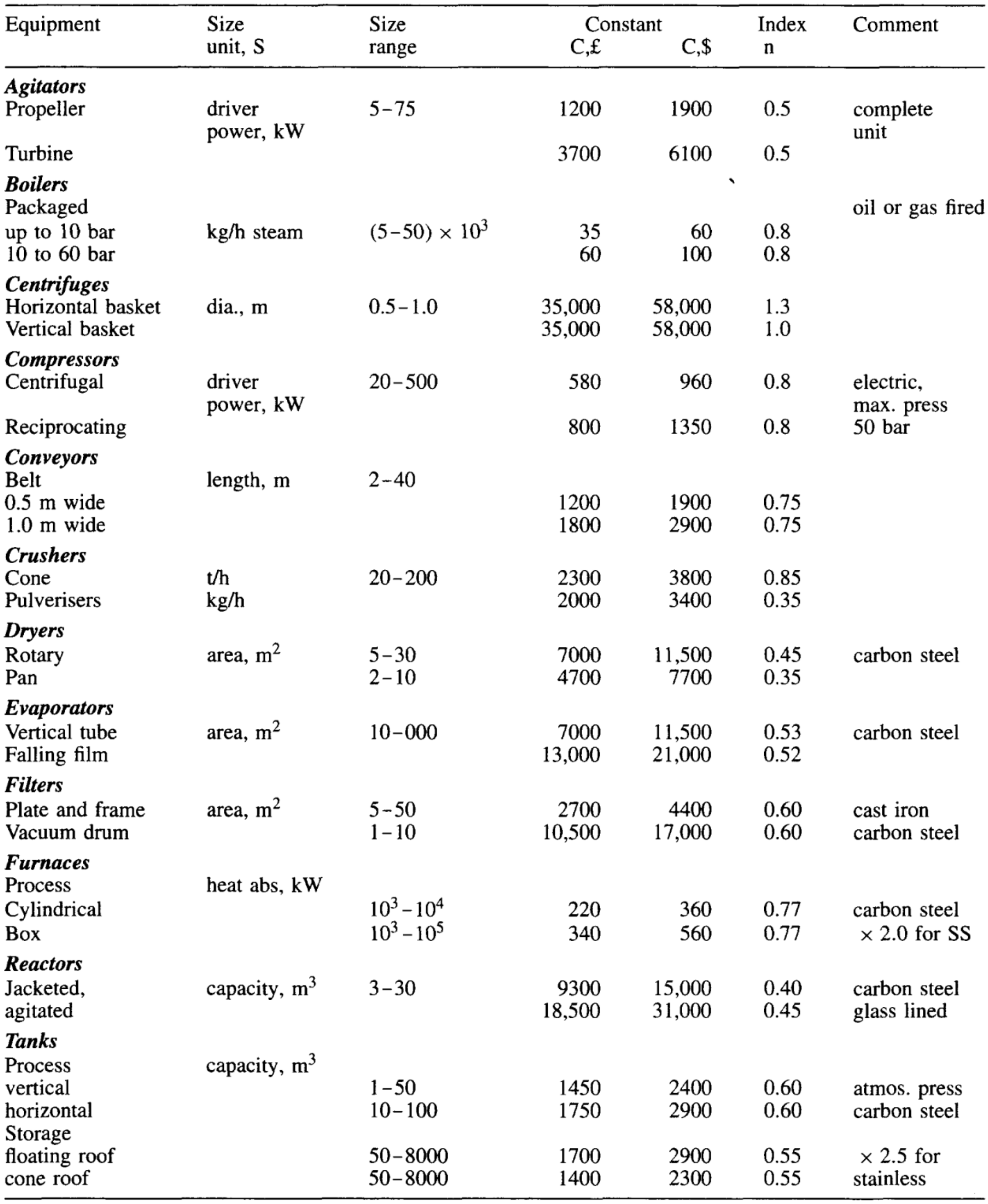
Figure 6.2 Vertical pressure vessels. Time base mid-1998



(*b*) US dollars

Figure 6.3 Column plates. Time base mid-1998

Table 6.1, Purchase cost of miscellaneous equipment Cost. Basis mid 1998



Equipment	Size unit, S	Size range	Constant		Index n	Comment
			C,£	C,$		
Agitators						
Propeller	driver power, kW	5–75	1200	1900	0.5	complete unit
Turbine			3700	6100	0.5	
Boilers						
Packaged						oil or gas fired
up to 10 bar	kg/h steam	$(5-50) \times 10^3$	35	60	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	
Vertical basket			35,000	58,000	1.0	
Compressors						
Centrifugal	driver power, kW	20–500	580	960	0.8	electric, max. press
Reciprocating			800	1350	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	7000	11,500	0.45	carbon steel
Pan		2–10	4700	7700	0.35	
Evaporators						
Vertical tube	area, m^2	10–000	7000	11,500	0.53	carbon steel
Falling film			13,000	21,000	0.52	
Filters						
Plate and frame	area, m^2	5–50	2700	4400	0.60	cast iron
Vacuum drum		1–10	10,500	17,000	0.60	carbon steel
Furnaces						
Process	heat abs, kW					
Cylindrical		10^3-10^4	220	360	0.77	carbon steel
Box		10^3-10^5	340	560	0.77	× 2.0 for 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	0.60	atmos. press
horizontal		10–100	1750	2900	0.60	carbon steel
Storage						
floating roof		50–8000	1700	2900	0.55	× 2.5 for
cone roof		50–8000	1400	2300	0.55	stainless

Mixer 1:

Volume= 2.87 m^3

Height= 2.44 m

Dia= 1.22 m

Bare equipment cost= $500 (figure 2)

Pressure factor= 1

Material factor= 1

Total cost= $500

Mixer 2:

Volume= 2.5 m^3

Height= 2.2 m

Dia= 1.0 m

Bare equipment cost= $435 (figure 2)

Pressure factor= 1.8

Material factor= 1

Total cost= $783

Mixer 3:

Volume= 2.02 m^3

Height= 1.9 m

Dia= 1.01 m

Bare equipment cost= $325 (figure 2)

Pressure factor= 1.2

Material factor= 1

Total cost= $422

Shell & Tube Heat Exchanger:

Heat Transfer area= 230 m^2

Bare equipment cost= $73303 (Figure 1)

Pressure factor= 1.3

Type factor= 0.85

Total Cost= $81000

Distillation Column 1:

Height= 13 m

Dia= 1.183 m

Bare cost= $25000 (Figure 2)

Pressure factor= 1.2

Material factor= 1

Cost= $30000

Plates= 26

Cost of plate= $210 (Figure 3)

Total plates cost= $13000

Total cost of column= $35460

Distillation Column 2:

Height= 9 m

Dia= 1.64 m

Bare cost= $8900 (Figure 2)

Pressure factor= 1

Material factor= 1

Cost= $8900

Plates= 13

Cost of plate= $190 (Figure 3)

Total plates cost= $2470

Total cost of column= $11370

Fixed Bed Reactor:

Height= 3.6 m

Dia= 1.2 m

Bare cost= $5000 (Figure 2)

Pressure factor= 2.2

Material factor= 2

Total cost= $22000

Fluidized Bed Reactor:

Height= 10 m

Dia= 3 m

Bare cost= $25000 (Figure 2)

Pressure factor= 1.2

Material factor= 2

Total cost= $60000

Reboiler1:

Heat transfer area= 15 m^2

Bare cost= $9000 (Figure 1)

Pressure factor= 1.25

Type factor= 1.3

Total cost= $14625

Reboiler2:

Heat transfer area= 25 m^2

Bare cost= $10000 (Figure 1)

Pressure factor= 1

Type factor= 1.3

Total cost= $13000

Condenser1:

Heat transfer area= 25 m^2

Bare cost= $10000 (Figure 1)

Pressure factor= 1

Type factor= 1.25

Total cost= $12500

Condenser2:

Heat transfer area= 15 m^2

Bare cost= $8000 (Figure 1)

Pressure factor= 1

Type factor= 1.3

Total cost= $8000

After multiplying with index of 2.5 we got the following costs

Equipment	**Cost ($)**
Mixer 1	1250
Mixer 2	1958
Mixer 3	1055
Column 1	88650
Column 2	28425
Fixed Bed Reactor	55000
Fluidized Bed Reactor	150000
Cooler 1	130000
Cooler 2	45000
Cooler 3	37500
Heater 1	75000
Membrane	200000
Heater 2	37500
Heater 3	32500
Heater 4	36750
Condenser 1	31250
Condenser 2	20000
Re-boiler 1	36563
Re-boiler 2	32500
Shell and Tube HE	202500
Plate Type HE	112500
Compressor 1	112500
Compressor 2	137500
Pump 1	2667

PCE	$1608568
PPC	$3860563
Fixed Capital	$5404788

Total Investment Required	$5675000
Variable Cost	
Steam	$194491
Cooling Water	$955
Chilled Water	$15091
Raw Material	$4123206
Catalyst	$124625
Total	**$4458368**
Fixed Cost	
Maintenance	$8205
Overhead Cost	$20000
Operating Labor Cost	$10000
Lab Charges	$6000
Capital Charges	$16411
Insurance	$1641
Total	$62257
Direct Production Cost	$4520895
Annual Operating Cost	$452100
Polymer Produced T/y	$5288
Selling Price $/T	$1450
Total Revenue/year	$7667600
Total Profit/year	$2694605
Pay Back Time (years)	2.1

Conclusion

As the oil prices fluctuate and the oil reservoirs are decreasing day by day and the demand for petroleum products goes on increasing, under such circumstances we think that an alternative for petroleum is required. Keeping this approach in mind we developed a process which does not use any petroleum sources rather than that we extract our major raw material which is ethanol from sugar cane. The process produces 612 kg/hr of LLDPE from 1000kg/hr of ethanol. The process that we have developed is more efficient and give greater yield of the desired product as compared to that of the processes which extract raw material from petroleum sources. Various heat recovery units have been employed to recover as much heat as possible. This makes the process much more efficient and energy losses have been minimized. Moreover, this process develops the product which is environmental friendly that gives us another advantage over the previous process which uses petroleum sources. Since it is a continuous process and run throughout the year hence the production of polyethylene will be in larger quantity and fulfill the desire market as well as costumers needs.

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