PRODUCTION OF 30,000 TPA OF PROPYLENE GLYCOL FROM GLYCEROL

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Production of 30,000 Tons/Year of Propylene Glycol From Glycerol

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This report is submitted to the Department of Chemical Engineering, Wah Engineering College, University of Wah for the partial fulfilments of the requirement for the

Bachelor of Science
In
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Internal Examiner

Supervisor

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Finally, we have high expectations that our work will be constructive and valuable for anyone who is interested in reading this Project.

ABSTRACT

Glycerol supply is now rising significantly, mainly as a result of the increased biodiesel production on a global scale. One ton of glycerol is obtained as a by-product for every nine tones of biodiesel produced. Glycerol's economic value has been reduced due to the excess supply, making it possible to utilize it in a variety of other applications. Many studies have been performed to exploit this excess glycerol as a raw material for the manufacture of new products like propylene glycol. The main objective of this work is to evaluate the potential of the production of propylene glycol (PG) using glycerol that is derived from the biodiesel production process. Propylene glycol market in Pakistan consists almost entirely of imported product and there is no industrial manufacturing unit in the country. This project proposes the manufacture of propylene glycol by the ecofriendly process which will eventually lead Pakistan to be self-sufficient in its production. Material balance calculations were performed with 1 hour of operation as the basis to achieve the necessary production capacity. Material and energy balance were used to design and rate various equipment, which were then matched to common design values from the literature. One of the report's highlights were that the equipment design was also carried out using simulation and design tools such as Aspen Plus. Following the design, we conducted an economic assessment of all of the equipment and estimated our payback period. This project also took into account environmental regulations. A HAZOP analysis was conducted for the raw materials and required commodity, and the project's protection of the plant and employees was prioritized. At the end of the project, readers can find detailed references and appendices to assist them with various standard tables and charts.

Keywords: Propylene Glycol, Biodiesel, Glycerol, Pakistan, Hydrogenation

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CHAPTER NO. 1
INTRODUCTION

1.1 Propylene Glycol:

Propylene glycol $C_3H_8O_2$ (also called 1, 2-Propanediol), is a significant commodity chemical. It is utilised as a precursor in the synthesis of unsaturated polyester resins, medicines, and other products, as well as biodegradable functional fluids including de-icing agents, antifreezes, and coolants. It is a clear, colourless, hygroscopic, viscous liquid with a mildly pleasant flavour that is generally considered as harmless and non-toxic. It is also nearly odorless. Chemical neutrality and nonreactivity make propylene glycol an excellent solvent.

Currently, petroleum-derived propylene is converted into propylene glycol by a method that involves selective oxidation of propylene to propylene oxide and its subsequent hydrolysis. However, due to the limited supply of propylene because of the depletion of the petroleum resource, attempts are made to find sustainable alternatives to propylene. In recent years, glycerol has emerged as a promising alternative for the production of propylene glycol, considering the limited supply of petroleum-derived propylene. Glycerol, a bio-renewable substance, is readily available through two primary routes: the soap industry and the biodiesel production process.

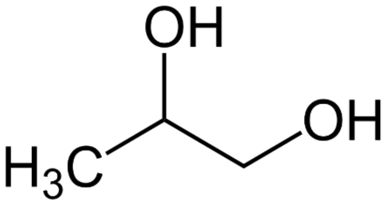


Figure 1-1 Structure of propylene glycol

Firstly, in the soap industry, glycerol is a by-product of the saponification process. When oils or fats are hydrolyzed with an alkali, such as sodium hydroxide, to produce soap, glycerol is released as a valuable co-product. This route provides a significant source of glycerol that can be utilized for the synthesis of propylene glycol. Secondly, the production of biodiesel from vegetable or animal fats via transesterification generates glycerol as a by-product. Bio-renewable glycerol has become a promising contender in this regard. Given the international incentives for the development of biodiesel, it is easily accessible as a by-product of the transesterification of vegetable or animal fats into biodiesel. It could be hydrogenolyzed to produce propylene glycol, offering a different method for producing the propylene glycol. [1]

About 1 kilogram of a crude glycerol by-product is formed for every 9 kg of biodiesel produced, and today's biodiesel manufacturing facilities require ways to boost the revenue from this glycerol. By exploring both the soap industry route and the biodiesel route, we can tap into diverse and abundant sources of glycerol. This not only helps address the challenges posed by the limited availability of petroleum-derived propylene but also promotes the development of a more sustainable and resource-efficient chemical industry.

The Food and Drug Administration (FDA) acknowledge propylene glycol as being harmless and non-toxic. The bio-based propylene glycol industry has grown thanks to environmentally friendly production methods. Due to its chemical neutrality and lack of reactivity, propylene glycol is a remarkably efficient solvent. Moreover, the utilization of glycerol as a feedstock for propylene glycol synthesis offers significant environmental benefits. The bio-based propylene glycol industry has experienced growth due to the adoption of environmentally friendly production methods. By leveraging glycerol from these renewable sources, we contribute to reducing reliance on petroleum resources and minimizing the carbon footprint associated with chemical manufacturing. [2]

1.2 Physical Properties & Thermodynamic Data:

Table 1-1 Physical properties of PG [3]

Properties	**Values**
Taste	Faintly sweet taste
Appearance	Colorless liquid
Odor	Odorless
Formula	$C_3H_8O_2$
Molecular weight	76 g/mol
Density at 25^0C	1.036 g/cm^3
Freezing point	-60^0C
B.P at 101.3 kPa	187.3^0C
Flash point	107^0C
Specific Heat at 25^0C	0.59 Cal/g

Table 1-2 Thermodynamic Properties of Propylene glycol [3]

Properties	**Value**
(Heat of combustion) at 25^0C, kJ/mol	-1822.9
(Heat of Vaporization) at 1atm, Cal/g	167
(Saturated Vapor pressure) mmHg at 25^0C	0.129
(Heat of formation) at 25^0C , kJ/mol (liquid)	-500.30
(Heat of formation) at 25^0C, kJ/mol (Gas)	-421

1.3 Reactions of the Product:

A simplified reaction of propylene glycol from glycerol is given below.

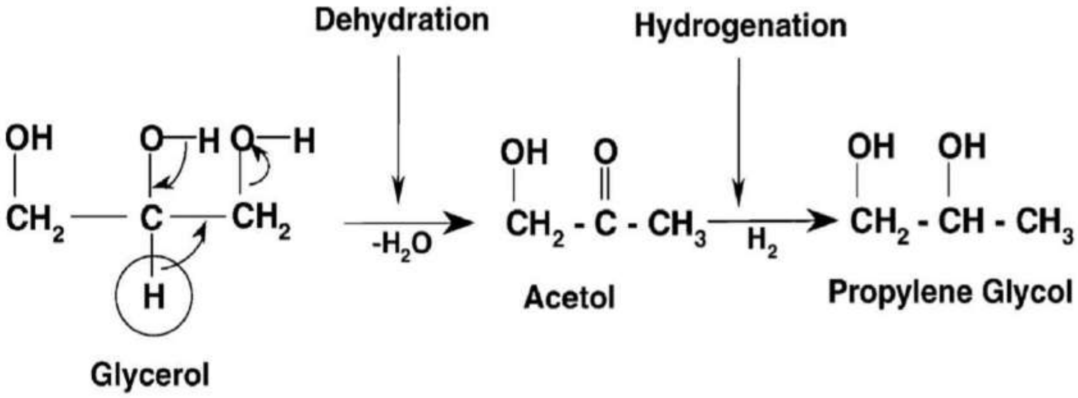


Figure 1-2 Mechanism of Production of Propylene Glycol [1]

The reaction is of two-step reaction. In step one: Glycerol is converted into acetol by dehydration of glycerol is purposed as an intermediate. In step two: Acetol is hydrogenated in the presence of hydrogen and it will convert it into propylene glycol via using copper based catalyst in a single reactor.

1.4 Industrial Applications of Propylene Glycol:

Propylene glycol is used in wide range of manufacturing processes and products. Propylene glycol has a wide range of applications in the pharmaceutical, food and beverage, cosmetics, and automotive antifreeze sectors. Propylene glycol is harmless and non-toxic when consumed or exposed to humans. Following are the applications of propylene glycol are; [4]

1.4.1 Application in Food and Beverages:

Propylene glycol is often used in foods and is generally regarded as safe. The Food and Drug Administration has approved the use of propylene glycol in food at certain or specific amounts, and it is safe for consumption. Up to 97% of spices and flavorings, 24% of baked goods and frosting, 5% of alcoholic drinks, and 1% of nuts and nut goods may include it. The maximum propylene glycol concentrations for dairy products and all other food items are 2.5% and 2%, respectively. [4]

Numerous characteristics of propylene make it advantageous for packaged goods. Food producers to extend the shelf life of their processed goods frequently use it. Baking mixes for dishes like cakes, muffins, biscuits, cupcakes, and pancakes are a few examples of prepackaged goods that contain propylene glycol. [5]

In addition to using propylene glycol as a preservative and flavour enhancer, food manufacturers also utilise it as an emulsifier, a texturizer, and a process aid to improve the look of food. Propylene glycol is utilised in food in a variety of ways, including:

- As an anti-clumping agent, preventing the formation of lumps in food.
- As a solvent, it assists in dissolving and blending components in food flavorings to enhance flavour.
- As a preservative, its antibacterial characteristics make it easier to destroy microorganisms like bacteria and mildew and/or restrict their development.
- As a thickening for food.
- To help keep food moist. [6]

1.4.2 Application in Pharmaceuticals:

Propylene glycol has become widely used as a solvent, extractant, and preservative in a variety of parenteral and non-parenteral pharmaceutical formulations. It's much better general solvent than glycerol and dissolves a wide variety of materials, like corticosteroids, phenols, sulfa drugs medication, barbiturates, vitamins (A and D), most alkaloids, and lots of native anesthetic propylene glycol has become extensively used as a extractant, solvent and preservative in a wide range of parenteral and non-parenteral pharmaceutical formulations. It dissolves a wide range of substances, including corticosteroids, phenols, sulfa drugs, barbiturates, vitamin A and vitamin D, the majority of alkaloids, and many natural anesthetics.

Propylene glycol is used as a solvent and carrier for several medicinal medications that are insoluble in water, such as anxiolytic pills. This implies that it is used to dissolve other compounds (often solids) without altering their basic chemistry or structure.

Additionally, active substances can be synthesized in propylene glycol and administered to the body through it when it is employed as a carrier in medication formulations. It used to retain moisture in medications by absorbing additional water. Various types of medication, such as intravenous (injected) medication, topical treatment, such as creams and gels, and oral medication, such as capsules and tablets, can all include propylene glycol. [4], [7]

1.4.3 Application in Cosmetics:

Propylene glycol is a commonly available component in cosmetic, skin care and personal products. Between 26.4% and 37.8% of registered personal care items include it. The versatile chemical propylene glycol serves a variety of purposes in the product compositions in which it is used. Several of these characteristics include: [4]

- **Humectant:** Humectants would be included in skin and cosmetic care products for their hydrating abilities. As a humectant, propylene glycol draws moisture to the skin, hydrating and moisturizing it as a result.
- **Solvent:** In order to get ingredients in a product formulation to mix and function effectively, propylene glycol is utilised to dissolve the ingredients. Additionally, it serves as the active ingredient's carrier.
- **Emollient:** Emollients are substances that moisturize and soften the skin. They are a great ingredient for skin care treatments that cure dry skin. Due to the fact that it creates an oily coating on the skin and stops water loss, propylene glycol is utilised as an emollient.
- **Viscosity control:** In order to reduce the thickness of cosmetic formulations and products, propylene glycol is utilised or employed. This enhances both how effectively the products distribute throughout the skin and how well they are absorbed.
- **Preservative:** Propylene glycol is typically used as a preservative in cosmetic and skin care products together with other ingredients.

1.4.4 Application in Antifreeze:

Propylene glycol serves as a base for deicing solutions. The antifreeze properties of propylene glycol are enhanced by the fact that it lowers the freezing point of water and water-based liquids. A significant portion of aircraft deicers are made of propylene glycol, which is also used as an antifreeze and dicing solution for vehicles, boats, and airport runways. It could be used widely in water-based paints, to help in maintaining the emulsions stable in cold temperatures.

A 50% water-diluted and heated solution is typically used to remove freezing buildup on commercial aircraft on the ground; while a 100% undiluted cold solution is typically used exclusively on an aircraft's wings and tail surfaces to avoid ice buildup for a certain period before departure. Because propylene glycol is non-toxic, it is also utilised in water pipelines that link hoses and in food processing systems as an antifreeze. [7]

1.5 Handling, Storage and Safety:

Propylene Glycol is a highly pure substance that has to be handled carefully to prevent contamination. It should be handled in a space that is well-ventilated. They may be transported or kept in containers made of lined steel, aluminium, or stainless steel since they are noncorrosive. Carbon steel is also suitable, although it may get somewhat contaminated with iron after prolonged storage.

Due to its hygroscopic nature, propylene glycol should be kept in a tightly closed, light-protected container and kept in a cold, dry environment. Separated from strong oxidants and alkalis, and also floor ventilation is advised. [7]

1.5.1 Precautionary Measures Include:

- Only use with appropriate ventilation.
- Avoid eating, drinking, and smoking in workplaces.
- Prevent inhaling gas, mist, or vapour
- Avoid contact with the skin, eyes, and clothes
- Keep the container.
- Wash hands after handling.

1.6 Shipping of the Product:

Transportation of propylene glycol needs extreme quality average in order to escape from product pollution. Transportation companies should establish they confirm responsibility of these standard, using quality management. Contractual agreements with transportation firms must expressly verify that no transportation is subcontracted until certain controls have been met, guaranteeing the precise degree of standard and product purity.

Aluminum, stainless steel or food level authorized steel with coated are suggested as tank material. It is suggested to use some Food-related technology includes trucks and containers. Although barge tanks may also be manufactured of carbon steel that has been coated with propylene glycol, stainless steel is the optimum material for formation.[8]

1.7 Production and Consumption Data of Product in World:

In 2020, the total amount of propylene glycol produced was 2.72 million metric tonnes. Between 2022 and 2027, the worldwide propylene glycol market is anticipated to expand at a CAGR of 4.4%, reaching a volume of over 3.5 million metric tonnes by 2026. The Asia Pacific region, which accounts for more than 40% of the world's consumption of the substance, is fueling the rise of the propylene glycol market. The area has a sizable market for the commodity, with China continuing to consume the most propylene glycol globally, accounting for over 22% of the entire amount. The propylene glycol consumption by nation is shown in the following pie chart figure 4. [9]

The key players operating in the global PG market are the Dow Chemical Company, BASF (Badische Anilin-Soda-Fabrik), Sumitomo Chemical Co.Ltd., Huntsman International, Archer Daniels Midland Company, Lyle Bio Products & DuPont Tate, China Petrochemical Corporation, AGC Chemicals and other prominent players.

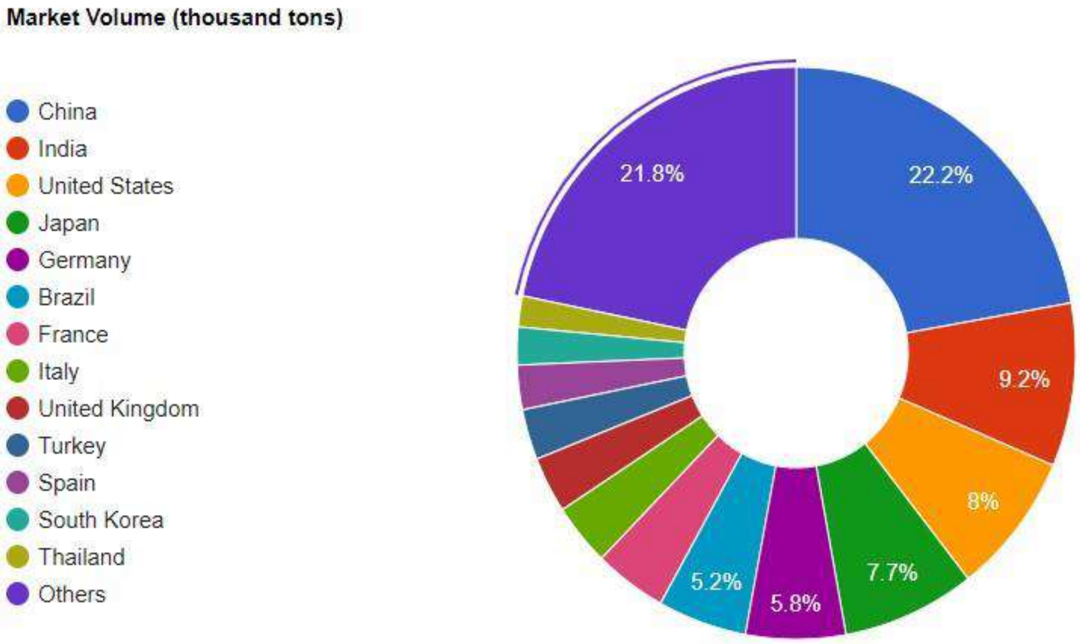


Figure 1-3 Propylene Glycol Consumption Volume according To Countries [10]

1.8 Production and Consumption Data of Product in Pakistan:

Propylene glycol market in Pakistan consist of almost entirely of imported product. Pakistan is one of the largest importer of Propylene glycol. The import volume of propylene glycol is 13k tons in 2021 worth of $23M.

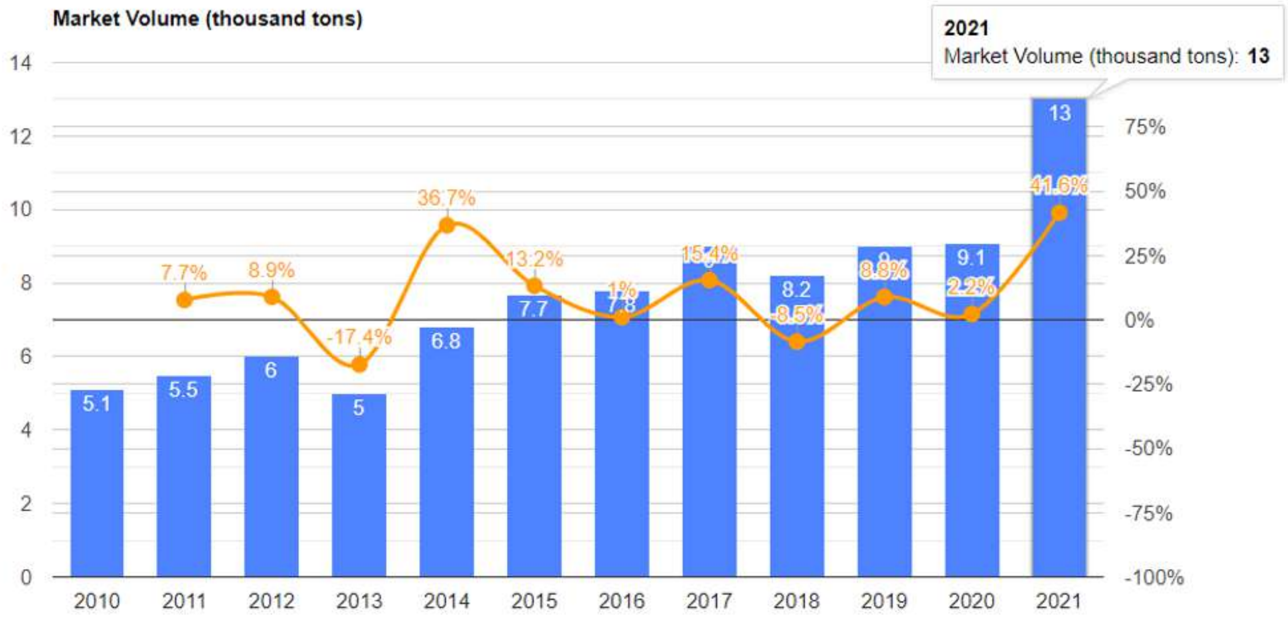


Figure 1-4 Market Volume of Pakistan Propylene Glycol [10]

Consumption of propylene glycol is based on import volume. In 2021, the amount of propylene glycol (propane-1,2-diol) consumed is 100% of import volume as shown in figure. The size of the propylene glycol market in Pakistan rose remarkably to $23M in 2021. Overall, the total consumption indicated a remarkable increase in last five years and is likely to see gradual growth in the near future because the demand of propylene glycol in Pakistan is increasing.

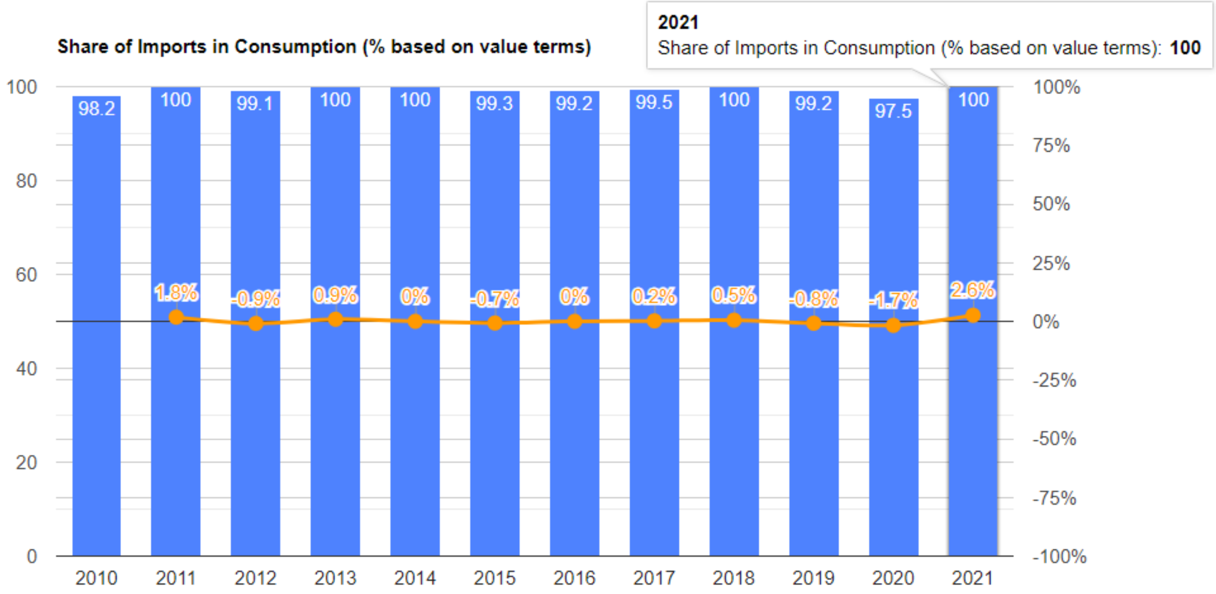


Figure 1-5 Share of Import in Consumption of Propylene Glycol

1.9 Market Assessment:

Industrial-grade propylene glycol is used as a solvent, chemical intermediate, and heat transfer medium in a wide range of goods, including lubricants, deicing fluid, engine coolants, polyester resins, commercial paints, varnishes, and laundry detergents. The demand for industrial-grade propylene glycol is predicted to increase over the course of the projected period because of its rising use in several applications that call for low toxicity and low vapour pressure.

1.10 Future Trend:

At a predicted CAGR of 4.4%, the propylene glycol market is expected to grow from USD 3.8 billion in 2019 to USD 4.7 billion in 2024. During the projected period, the market is anticipated to be driven by APAC's expanding automotive sector and bio-based propylene glycol is environmentally favorable manufacturing method. [11]

- The global market growth is attributed to the rising demand for propylene glycol in developed and developing economies.
- China, India, the US, Japan, and Brazil offer lucrative growth opportunities for the propylene glycol market.
- APAC accounted for the largest share in the propylene glycol market.

Figure 1-6 Propylene Glycol Global Demand [11]

According to estimates, the market for propylene glycol will be valued USD 4.14 billion in 2021 and USD 5.84 billion in 2029. In-depth expert analysis, price analysis, production consumption analysis, as well as market data like market value, growth rate, geographical coverage, market players, and market situation are all included in the market study that the Data Bridge Market Research team has produced. [12]

Figure 1-7 Global Propylene Glycol Market Future Trend [12]

1.11 Project Motivation:

- The project is to produce propylene glycol from glycerol (By-product of biodiesel).
- The motivation of project is to resolve the demand & import problem of propylene glycol because Pakistan is one of the largest importer of propylene glycol and there is no industrial manufacturing unit of propylene glycol in the country.
- Project helps Pakistan to manufacture propylene glycol itself by the ecofriendly process.
- In this Project, we use glycerol as a raw material, which is a by-product of biodiesel. Better carbon usage from the successful conversion of glycerin to propylene glycol and the use of glycerin as a possible petrochemical feedstock would benefit the biodiesel industry.
- Hydrogenation of glycerin is used in this process to produce propylene glycol.
- The most popular option is propylene glycol because of its established market and high demand. Propylene glycol is a major commodity chemical that is used in food, pharmaceutical, oil, anti-freeze industries, etc. as a raw material.

CHAPTER NO. 2
MANUFACTURING PROCESSES

2.1 Production Methods:

Different processes at both lab scale and industrial process prepare propylene glycol. The industrial process includes only two method that are given below:

- Production of propylene glycol from Hydrolysis of Propylene-Oxide.
- Production of propylene glycol from Hydrogenolysis of Glycerol.

2.1.1 Hydrolysis of Propylene Glycol:

Propylene oxide is racemic mixture which is commercially 99.9% pure. It can be used for the production of propylene glycol via hydrolysis of propylene oxide. All commercial manufacturing of propylene glycol involves the non-catalytic hydrolysis of propylene oxide under high pressure, high temperature conditions. Propylene oxide is transformed into a mixture of mono-, di-, and tri-propylene glycols using an excessive amount of water. In a typical product distribution, PG makes up 90% and coproducts 10%. Conditions for hydration reactors are 120-1900C and up to 2170 kPa of pressure (21.41 atm). Following the completion of the hydration reaction, extra water is drained in multi-effect evaporators and drying towers, and high vacuum distillation is used to clean the glycols.

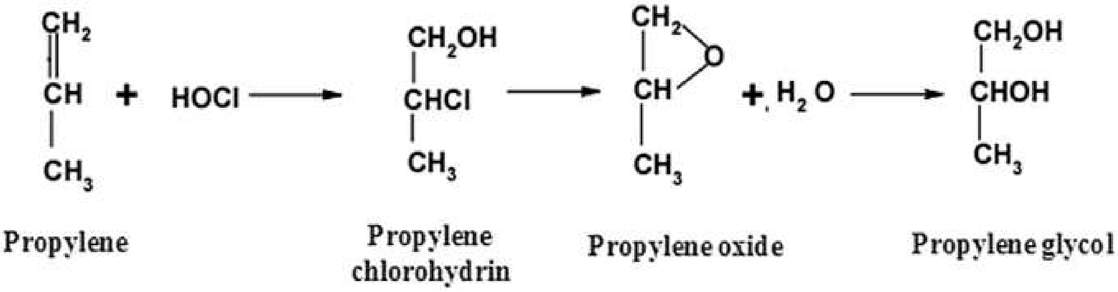


Figure 2-1 Commercially Synthesis of Propylene Glycol from Propylene oxide [13]

Both the peroxidation and the chlorohydrin processes can be used to produce propylene oxide. In the chlorohydrin procedure, propylene chlorohydrin is created by mixing chlorine, propylene, and water. This substance then combines with an inorganic base to produce the oxide.

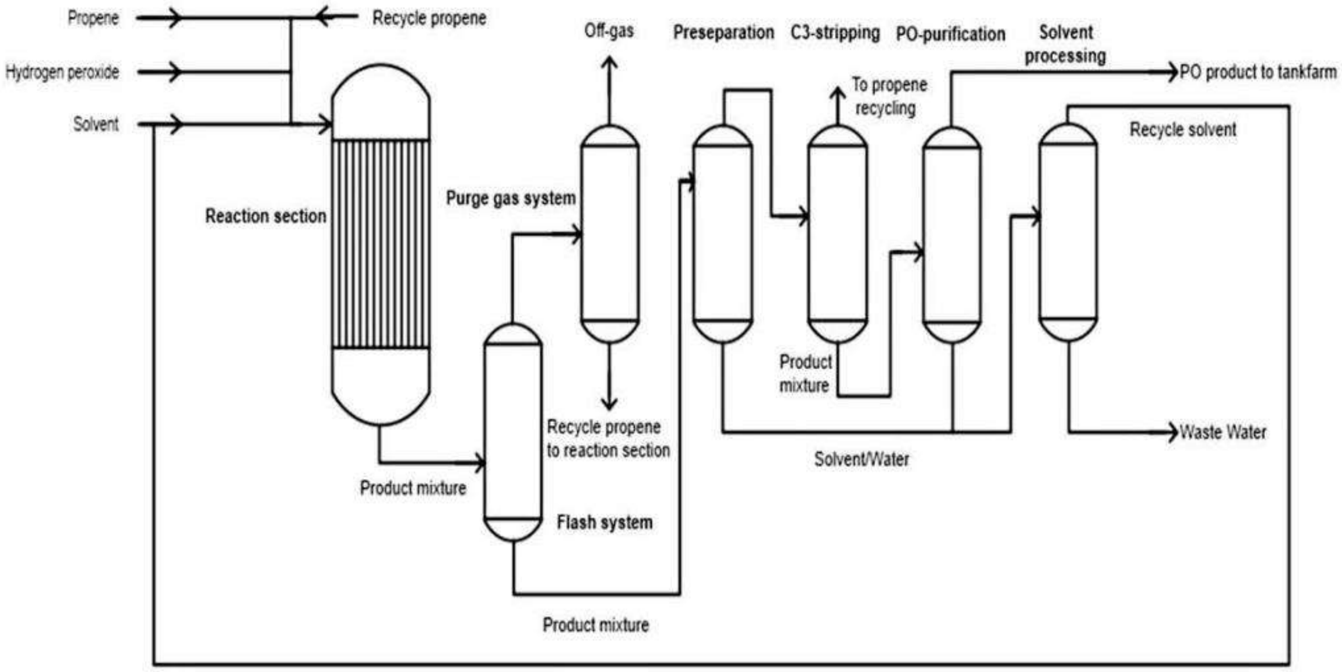


Figure 2-2 Manufacturing Of Propylene Glycol from Propylene Oxide

To produce propylene oxide and t-butyl alcohol or methyl benzyl alcohol, respectively, the peroxidation process transforms either isobutane or ethylbenzene straight into an alkyl hydroperoxide. Since propylene oxide is a relatively low-boiling species (Boiling Point = 34.3^0C), it is crucial to manage the reaction's temperature and employ a significant amount of water to maintain the reaction in the liquid phase. Because propylene oxide is only partially soluble in water, methanol is further added to avoid phase separation. In a quick reaction, propylene oxide and propylene glycol can create di-, tri-, and polypropylene glycols. [13]

2.1.2 Production of Propylene Glycol from Glycerol:

Reaction: Conventional processing of glycerol to propylene glycol involves copper-based catalysts and hydrogen, as documented in multiple United States patents. The hydrogenolysis of glycerol to propylene glycol has long been recognized. These studies confirmed that glycerol could be successfully hydrogenated to produce propylene glycol.

Figure 3 illustrates the unique reaction process for the conversion of glycerol to propylene glycol through a reactive intermediate. An indication that the reaction method for generating propylene glycerol with high yield and selectivity may be completed in two phases is the relatively pure acetol that was extracted from the dehydration of glycerol as the transitory intermediate.

The process for converting glycerol to propylene glycol based on copper catalyst reaction network has advanced to the point of commercial feasibility and solely includes the manufacture of the following main products: In three steps, 1,2-propanediol, ethylene glycol, and acetone. [14]

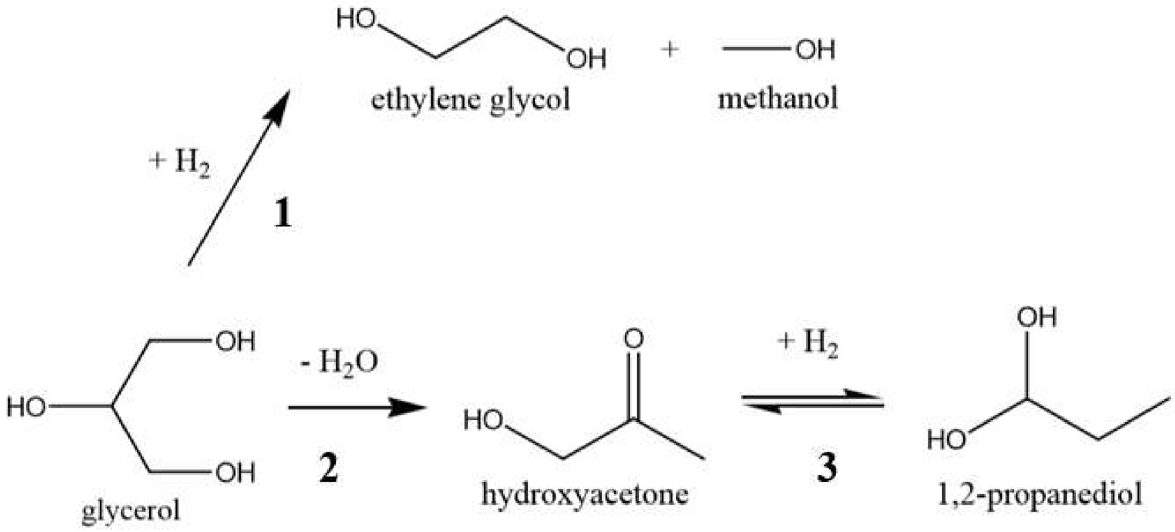


Figure 2-3 Simplified Scheme of Glycerol, Hydrogenolysis Reaction Pathways [15]:

In order to create propylene glycol from glycerin, a hydrogenation procedure is performed (PG). The method provides PG with a purity of at least 98% for industrial applications and has better than 95% selectivity to PG, according to the patent. Figure 11 depicts a process flow diagram.

The process plan consists of a reaction step that turns glycerin into propylene glycol and a fractionation step that yields the finished product. A metal or metal oxide distributed on an inert support serves as a proprietary catalyst. Glycerin is subjected to the hydrogenation process at a temperature of around 190° C. and a pressure of 2.0-8.0 MPa (20-80 atmospheres). Propylene glycol selectivity is greater than 95%, and one-pass glycerin conversion is higher than 70%.

In one example of the invention, the bulk of the glycerin in the feed is transformed into propylene glycol by hydrogenation in a fixed bed reactor at temperatures between 150° C. and 240° C. and pressures between 20 and 80 atmospheres. The feed-effluent heat exchanger is where the reactor's effluent is sent after being split into a vapour phase stream and a liquid phase stream. The condensed liquid from the additional condensation of the vapour phase is returned to the fixed bed reactor. Recycle solvents such water, methanol, or other substances with low boiling points are present in the vapour phase stream. The gas phase separated is cooled down and sent to recycle gas flash drum. The hydrogen-rich gas phase separated is recycled to the reaction section via recycle gas compressor; a small portion is purged as fuel gas. Make-up hydrogen is mixed with the outlet stream of compressor before being sent to the reactor.

The liquid stream from the high pressure separator is cooled down and de-pressurized before entering distillation section. Multiple Distillation columns are used in the purification of propylene glycol. The reactor effluent is passed through three distillation columns. [16]

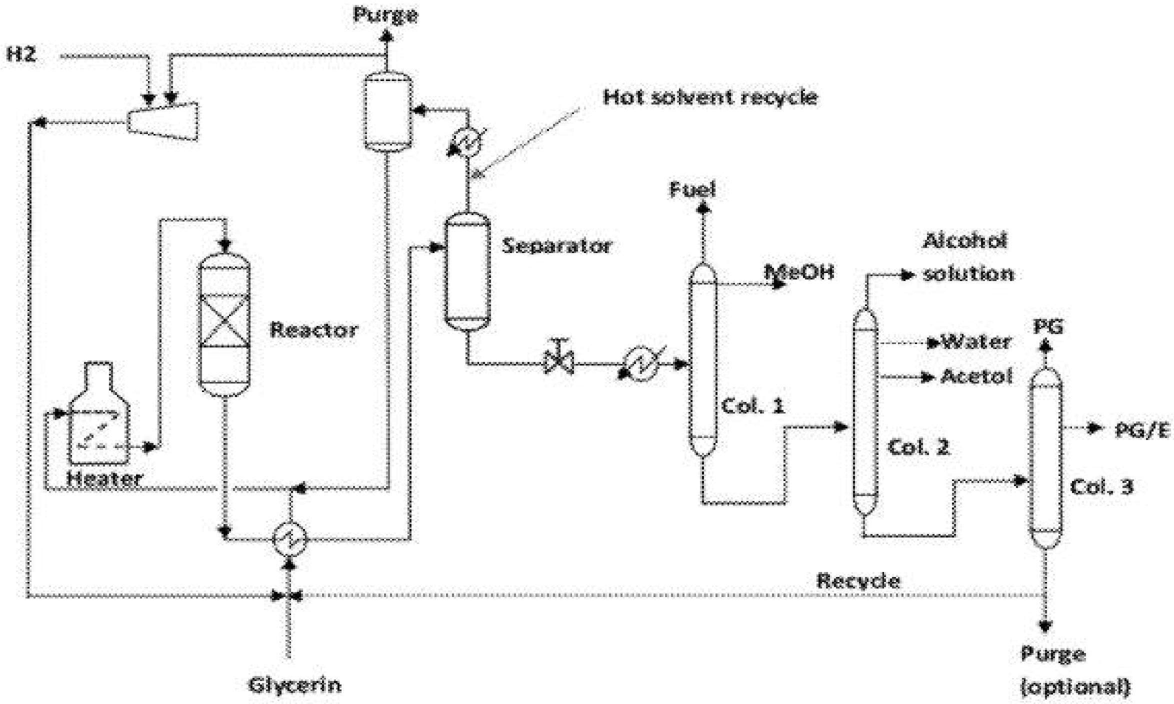


Figure 2-4 General process flowsheet of production of propylene glycol from glycerol [16]

2.2 Comparative Study of Different Process:

Table 2-1 Comparative study of different processes [17] [18]

Production Methods	**PG from Glycerol**	**PG from Propene-Oxide**
Raw Materials	Glycerin, Hydrogen, water	Chlorine, methanol, propylene, water
Temperature	150-240^{o}C	120–190^{0}C
Pressure	20-80 atmospheric	21.5 atmospheric
Selectivity	93.4% of PG	86%
Yield	76%	71%

Conversion	81.5% of Glycerin	83%
Purity	99%	97.5%
Catalyst	Copper based catalyst	H_2SO_4
By-products	ethylene glycol	di-PG, tri-PG and polypropylene glycols
Advantage	• Easy to obtain raw material since it is harvested from biodiesel production. • The price of raw material is also low. • The manufacturing process is simple. • Not harmful to the environment as the raw material is eco-friendly.	• Easy to get the raw material since propylene is produced from petrochemical propylene. • Low temperature range.
Disadvantage	• Requirement of multiple distillation columns to improve purity of product by removing by-products.	• Price of raw material is high. • Complicated manufacturing process due to the need for high temperature and high pressure.

2.3 Process Selection:

We selected production of propylene glycol from glycerol based on several advantages over hydration method including:

1. Less expensive to build than the traditional PG from Propylene Oxide (PO) approach
2. More selective simple conversion of glycerin to PG:
3. Platform for process technologies in renewable resources:
4. Integrated with biodiesel process for optimal carbon resource utilisation:
5. Glycerin is a green substance that comes from a biodegradable source.

2.4 Capacity Selection:

Globally the annual production volume of propylene glycol estimated at 2.72 million metric tons in the year 2021. [19] The annual import volume of propylene glycol in Pakistan in 2021 was 13 K tones per year. The amount of propylene glycol consumed in Pakistan totaled 13 K tons with an increase of 42% in 2021.

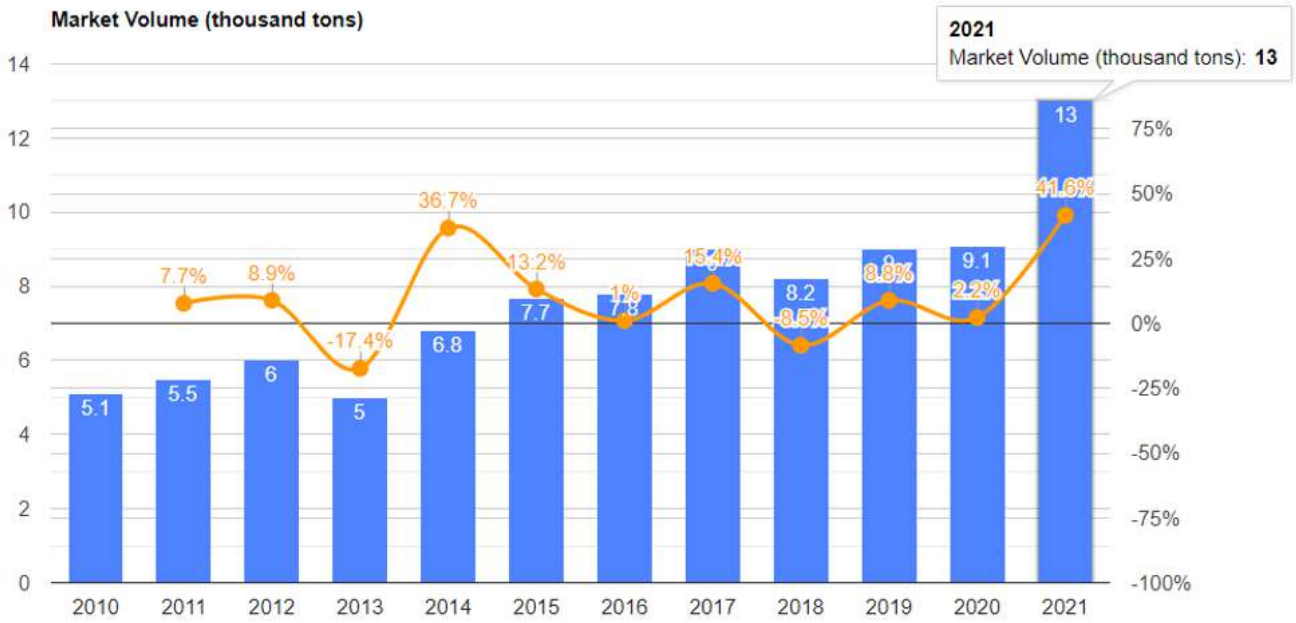


Figure 2-5 Market volume of Pakistan propylene glycol [10]

- Propylene glycol market in Pakistan consist of almost entirely of imported product.
- Based on import data the average growth rate of PG is 8.85% per year from 2011 to 2021 and we do projection based on growth rate from 2022 to 2031 shown in figure 13.

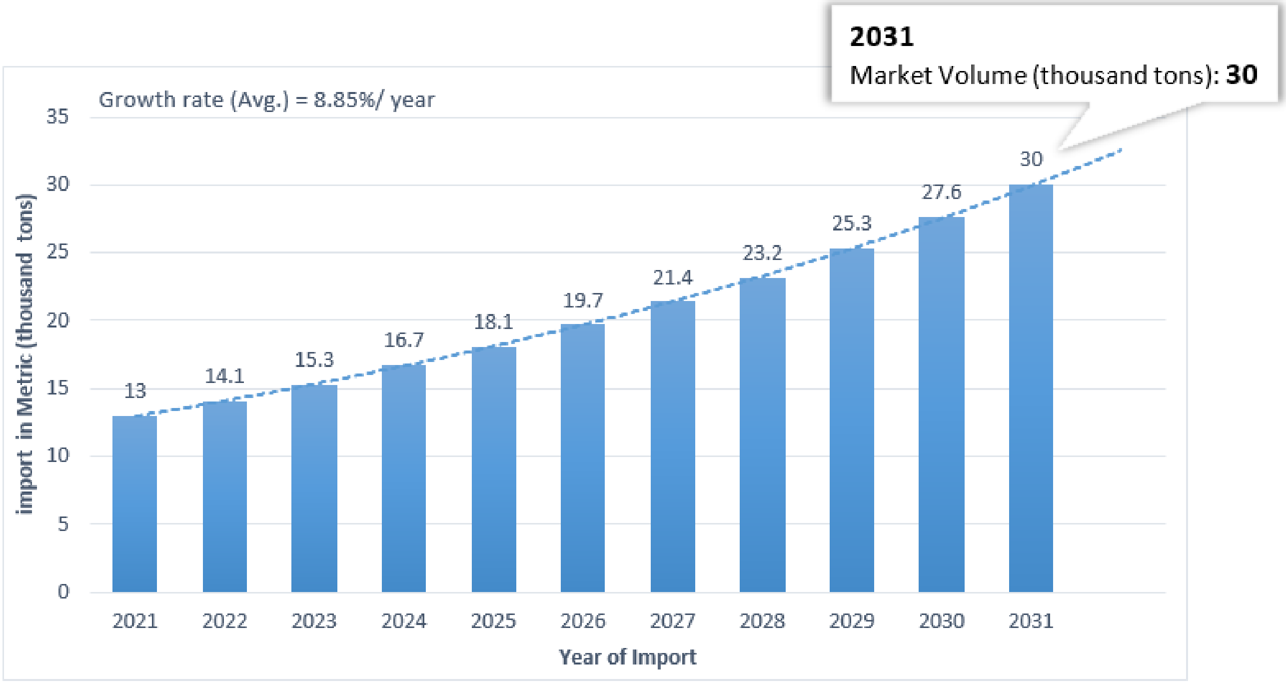
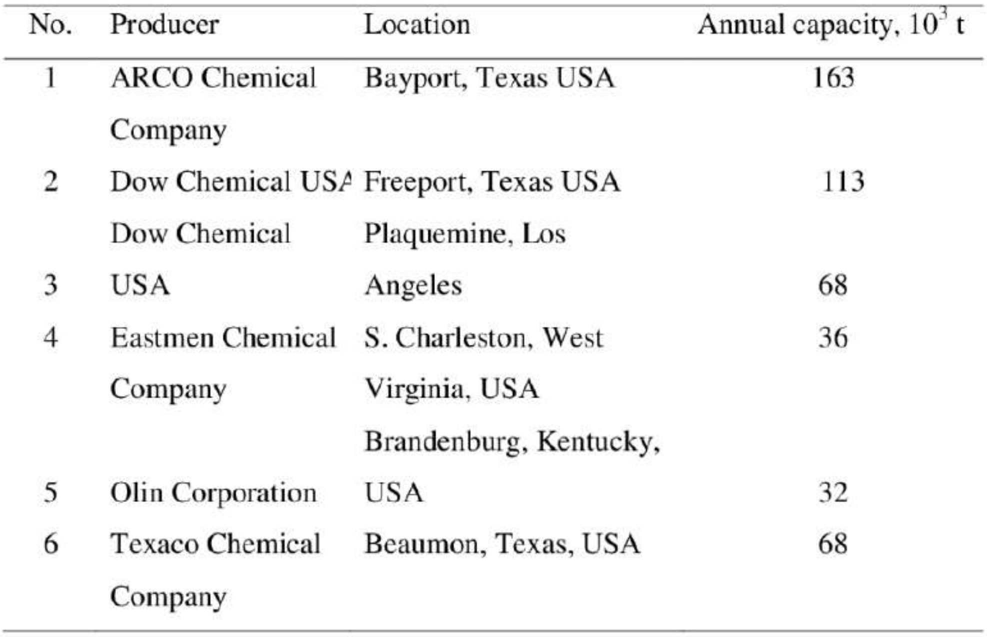


Figure 2-6 Propylene glycol import volume from (2021-2031)

- Therefore, we selected the capacity of plant at approximately **30 k** tones per year.
- The plant capacity is relatively small as compare to world, which leaves room for increased production.

Table 2-2 Data of propylene glycol production capacity abroad [20]



No.	Producer	Location	Annual capacity, 10^3 t
1	ARCO Chemical Company	Bayport, Texas USA	163
2	Dow Chemical USA	Freeport, Texas USA	113
3	Dow Chemical USA	Plaquemine, Los Angeles	68
4	Eastmen Chemical Company	S. Charleston, West Virginia, USA	36
5	Olin Corporation	Brandenburg, Kentucky, USA	32
6	Texaco Chemical Company	Beaumon, Texas, USA	68

2.5 Process Description:

The following process steps are used to turn glycerin into propylene glycol:

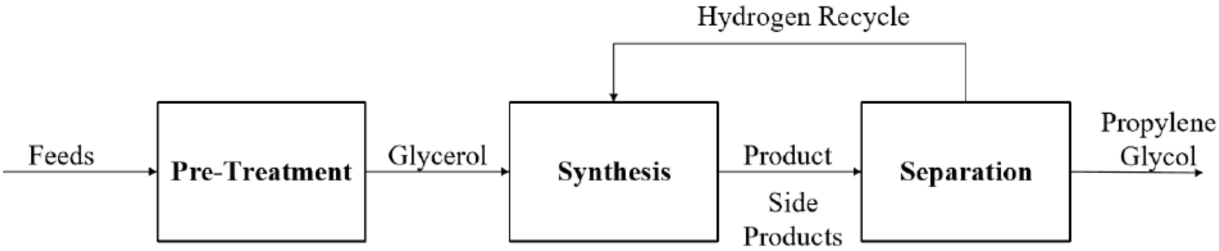


Figure 2-7 BFD for the production of propylene glycol form glycerol

Pre Treatment: In Figure 15, the process flow diagram (PFD) is displayed. Incoming glycerol is a byproduct of the manufacturing of biodiesel, which is refined and has an input stream composition of 84% glycerol, 1% methanol, and 14% water. The glycerol stream is first heated to 150 °C before being combined with recycling streams of unreacted glycerol in M-101. The fixed-bed reactor R-101 receives the ejected glycerol mixture from mixer.

Hydrogen gas comes as a pure gas from an available tank at 50 atm of pressure and mixed with recycled hydrogen gas which is coming from flash separator V-101. The resultant hydrogen gas is then transferred from the bottom to the fixed-bed reactor R-101. [21]

Synthesis: Hydrogenolysis of glycerol to propylene glycol is carried out in R-101 at 220 °C and 50 atm. Due to the exothermic nature of the reaction, it is necessary to provide a quench gas stream. In this case, the recycled hydrogen maintains the reactor temperature at 220 °C. The catalyst provides an 81.5% conversion of glycerol, with a 93.4% selectivity to propylene glycol at the given operating conditions. The reactor effluent contains propylene glycol, unreacted glycerol and other byproducts and hydrogen gas. [17]

$$C_3H_5(OH)_3 + H_2 \rightarrow C_3H_6(OH)_2 + H_2O$$

Separation: The effluent is sent to the V-101 flash separator, where the liquid combination at the bottom and the hydrogen gas on top are separated. The splitter S-101 recycles hydrogen. The resultant propylene glycol mixture then goes to T-101 for separation and purification. Water and C_2 alcohols are taken out of the effluent from the propylene glycol reactor by the fractionation tower T-101. The overhead stream, which is supplied to a utility, has 96 weight percent water. Propylene glycol without water is transferred from T-101's bottoms to T-102, another fractionation tower, where it is separated from unreacted glycerol and other byproducts to produce the required product. Propylene glycol accounts for 92.6 weight percent of the overhead stream of T-102. Unreacted glycerol from the bottoms stream is returned to the start of the operation and combined with fresh feed in M-101.

T-103 will separate propylene glycol from ethylene glycol using the overheads of T-102. Propylene glycol makes up 99.8 weight percent of the overheads, which are then put in a storage tank. The bottoms contain 99.9% by weight of ethylene glycol, which is also sent to storage area. [22]

P-101	**E-101**	**T-101**	**R-101**	**E-102**	**E-106**	**E-105**	**V-101**	**V-102**	**C-101**
P-102/3	**Feed**	**T-102**	Reactor	**E-103/4**	**E-108**	**E-107**	Gas/Liquid	**V-103**	Compressor
P-104/5	Pre-	**T-103**		Heat	**E-110**	**E-109**	Separator	**V-104**	
Pump	Heater	Distillation Column		Exchanger	Reboiler	Condenser		Reflux Drum	

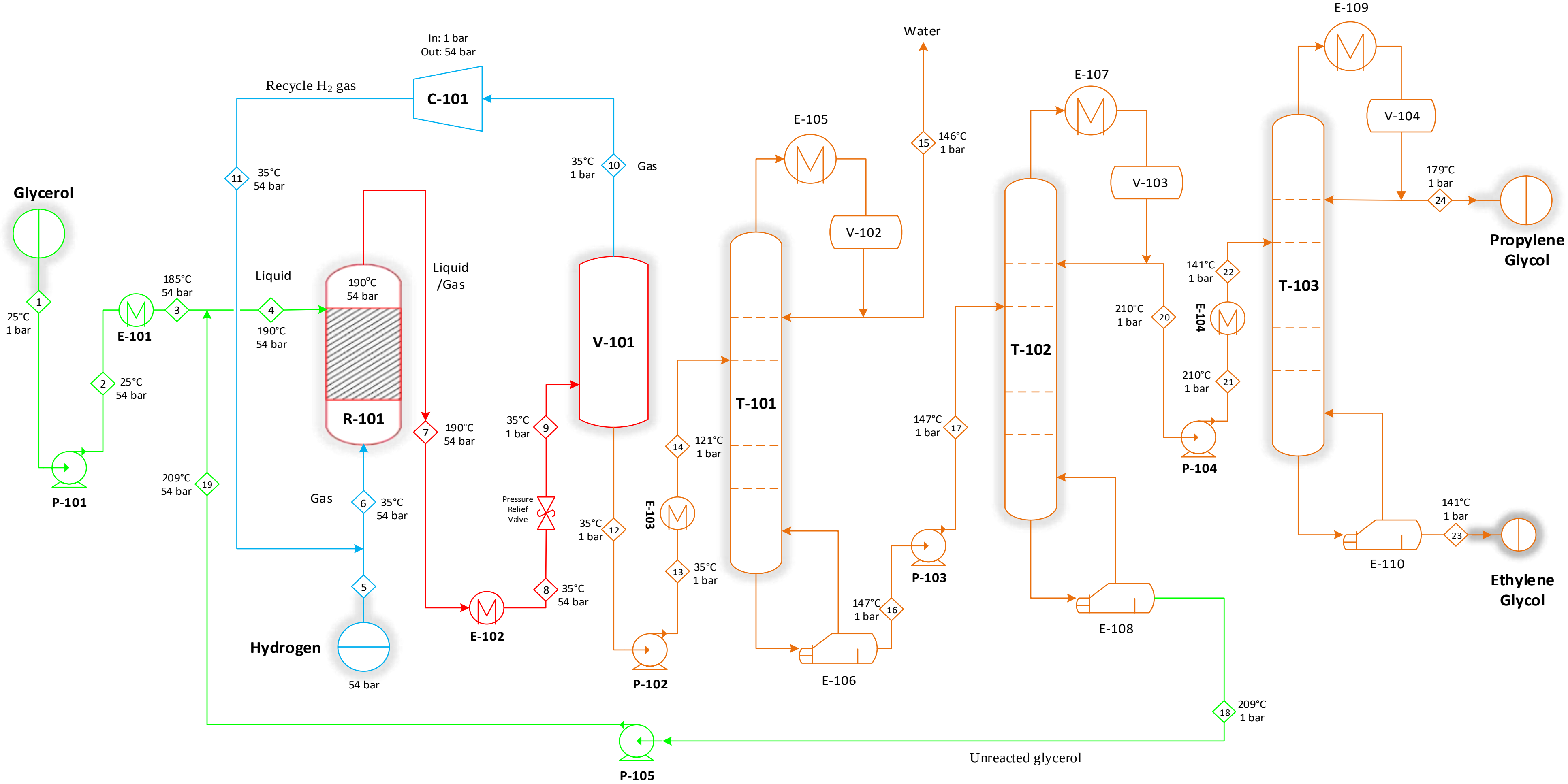


Figure 2-8 Production of Propylene Glycol from Glycerol via Hydrogenolysis Process

CHAPTER NO. 3

MATERIAL BALANCE

3.1 Material Balance:

Material balance is a fundamental concept in chemical engineering that involves the quantitative analysis of the flow and transformation of materials within a chemical process. The goal of material balance is to ensure that the mass of all chemical species entering a process equals the mass of those leaving the process, and that no species accumulate or disappear in the process.

Material balance calculations involve the use of mass balances, which are equations that describe the conservation of mass for a given process. Mass balances are typically expressed in terms of input and output streams, and they account for both the mass of the reactants and the products, as well as any losses due to reactions or other factors.

$$\text{Mass in} - \text{Mass out} + \text{Generation} - \text{Consumption} = \text{Accumulation}$$

If no reaction is occurring then generation, consumption and accumulation (at steady state) is zero then equation becomes;

$$\text{Input} = \text{output}$$

Material balance calculations are used extensively in the design, optimization, and troubleshooting of chemical processes. They are essential for determining the quantities of materials that need to be added to a process, for calculating yields and efficiencies, and for identifying potential sources of waste or inefficiency.

3.2 Plant Capacity:

The capacity of the plant to produce propylene glycol (PG) is 30,000 tons/year

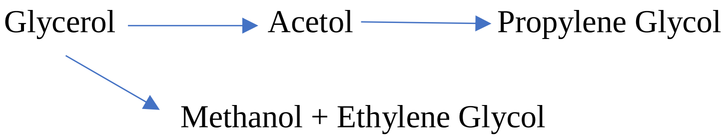
$$\frac{30000\ \text{tons}}{\text{year}} \times \frac{1000\ \text{Kg}}{1\ \text{ton}} \times \frac{1\ \text{year}}{330\ \text{days}} \times \frac{1\ \text{day}}{24\ \text{hours}}$$

$$\text{Production of Propylene Glycol} = 3787.87\ \text{Kg/hr}$$

Molecular Weight of Propylene Glycol = 76.09 Kg/Kg.mol

$$\text{Production of Propylene Glycol} = \frac{3787.87}{76.09} = 49.782\ \text{Kmol/hr}$$

3.3 Overall Reaction:



Reaction 1: Decomposition of Glycerol into Acetol

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

Reaction 2: Acetol reacted with hydrogen and convert it into Propylene glycol.

$$C_2H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

Reaction 3: A side reaction in which glycerol reacted with hydrogen and convert into Methanol and Ethylene Glycol

$$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH$$

Note: All reactions can occur in the presence of catalyst (Cu-ZnO-Al_2O_3)

3.3.1 Assumptions:

- Steady State
- Taking 100 Kg/hr as a basis to start the material balance.

3.3.2 Raw Material Required:

Glycerol = 78.70 Kmol/hr

Hydrogen Needed = 76.54 Kg/hr

3.4 Mixer (M-101):

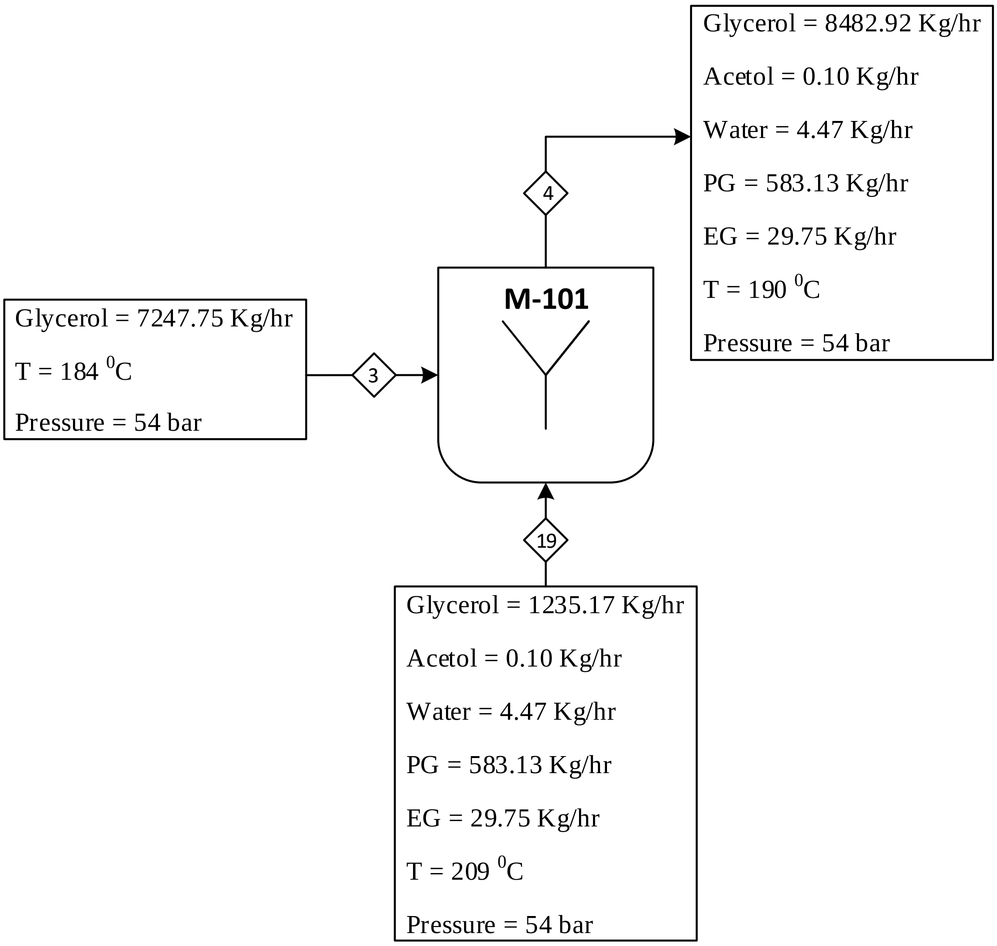


Figure 3-1 Mixer (M-101)

Input Stream 3:

Glycerol ($C_3H_8O_3$) = 7247.75 Kg/hr

Input Stream 19:

Glycerol ($C_3H_8O_3$) = 1235.17 Kg/hr

Acetol ($C_3H_6O_2$) = 0.10 Kg/hr

Water (H_2O) = 4.47 Kg/hr

Propylene Glycol ($C_3H_8O_2$) = 583.13 Kg/hr

Ethylene Glycol ($C_2H_6O_2$) = 29.75 Kg/hr

Formula:

$$input = output$$

Stream 4:

Glycerol = 7247.75+1235.17 Kg/hr

Glycerol = 8482.92

Acetol ($C_3H_6O_2$) = 0.10 Kg/hr

Water (H_2O) = 4.47 Kg/hr

Propylene Glycol ($C_3H_8O_2$) = 583.13 Kg/hr

Ethylene Glycol ($C_2H_6O_2$) = 29.75 Kg/hr

3.5 Mixer (M-102):

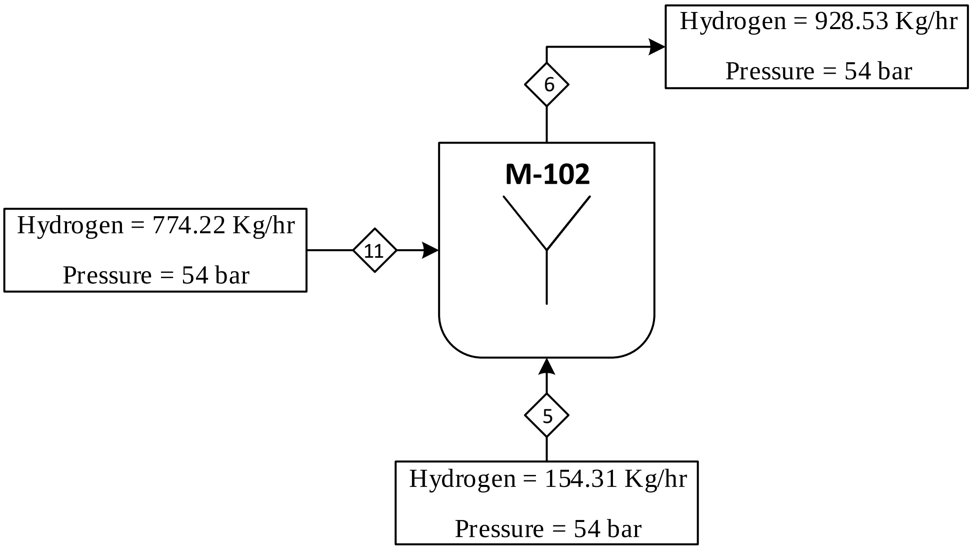


Figure 3-2 Mixer (M-102)

Input Stream 11:

Hydrogen = 774.22 Kg/hr

Input Stream 5:

Hydrogen = 154.31 Kg/hr

Formula:

$$input = output$$

Output Stream 6:

Hydrogen = 774.22 + 154.31

Hydrogen = 928.53 Kg/hr

3.6 Reactor (R-101):

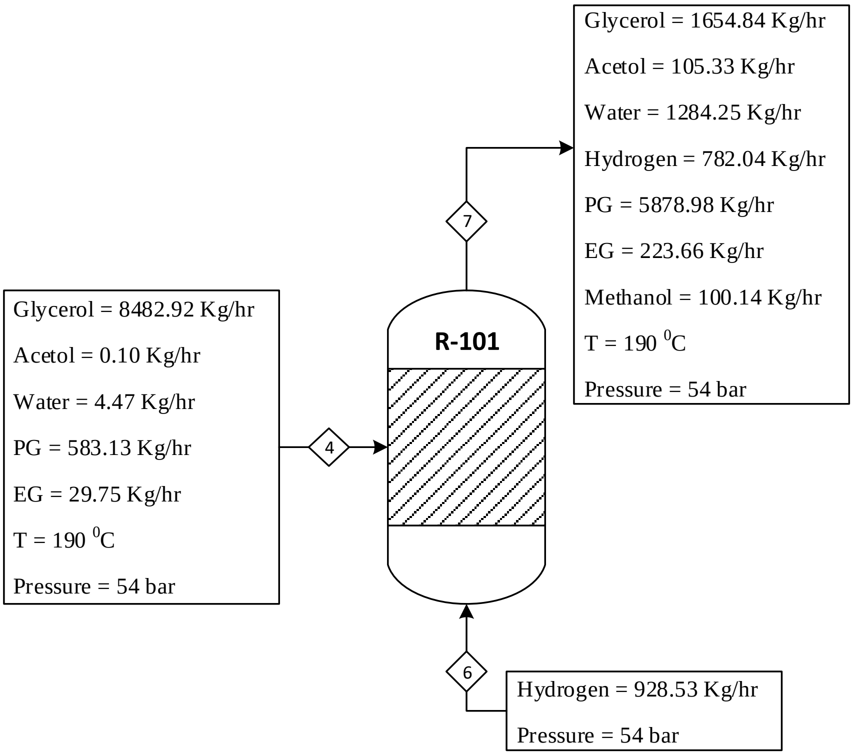


Figure 3-3 Reactor (R-101)

Reaction:

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

$$C_2H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

$$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH$$

Conversion of Glycerol = 81.5%

Conversion of Acetol = 98%

Selectivity = 94.6%

Operating Temperature = 190 °C

Operating Pressure = 54 bar

Hydrogen to Glycerol ratio = 5:1 (in mol)

Raw Material:

Table 3-1 (R-101) feed flow rate

Component	Flow rate Kg/hr	Flow Rate Kmol/hr
Glycerol	8482.92	92.12
Hydrogen	928.53	460.58

Reaction 1:

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

$$\text{Acetol Produced} = 92.12 \times 0.815 \times 0.946 = 71.02\,\frac{\text{Kmol}}{\text{hr}}$$

$$\text{Acetol Produced} = 71.02 \times 74.08 = 5261.18\,\frac{\text{Kg}}{\text{hr}}$$

$$\text{Unreacted Glycerol} = 92.12 - 71.02 = 21.1\,\frac{\text{Kmol}}{\text{hr}} = 21.1 \times 92.09 = 1943.1\ \text{Kg/hr}$$

From unity method;

1 kmol Acetol : 1 Kmol Water

71.02 Kmol Acetol : 71.02 Kmol Water

$$\text{Water Produced} = 71.02\ \text{Kmol/hr}$$

$$\text{Water Produced} = 71.02 \times 18.02 = 1279.78\,\frac{\text{Kg}}{\text{hr}}$$

Reaction 2:

$$C_2H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

$$\text{Propylene Glycol Produced} = 71.02 \times 0.98 = 69.60\ \text{Kmol/hr}$$

$$\text{Propylene Glycol Produced} = 69.60 \times 76.09 = 5295.85\,\frac{\text{Kg}}{\text{hr}}$$

$$\text{Unreacted Acetol} = 71.02 - 69.60 = 1.42\,\frac{\text{Kmol}}{\text{hr}} = 1.42 \times 74.08 = 105.19\ \text{Kg/hr}$$

As from reaction, 1 mol of acetol needed 1 mol of hydrogen to convert into propylene glycol. And hydrogen is supplied 5 time of glycerol which is 460.58 Kmol/hr. so first we divide it with 5 to convert hydrogen into 1 mol.

$$\text{Hydrogen Consumed} = \frac{460.58}{5} \times 0.815 \times 0.946 \times 0.98 = 69.60\,\frac{\text{Kmol}}{\text{hr}}$$

$$\text{Hydrogen Consumed} = 69.60 \times 2.02 = 140.59\,\frac{\text{Kg}}{\text{hr}}$$

$$\text{Unreated Hydrogen} = 460.58 - 69.60 = 390.98\,\frac{\text{Kmol}}{\text{hr}} = 789.77\,\frac{\text{Kg}}{\text{hr}}$$

Reaction 3:

$$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH$$

$$\text{Ethlyene Glycol Produced} = (92.12 \times 0.815 \times 0.946) \times (0.815 \times 0.054)$$

$$\text{Ethylene Glycol} = 3.13\ \text{Kmol/hr}$$

$$\text{Ethylene Glycol} = 3.13 \times 62.04 = 193.91\ \text{Kg/hr}$$

From Unity method;

$$\text{Methanol Produced} = 3.13 \times 32.04 = 100.14\ \text{Kg/hr}$$

$$\text{Total Unreacted Glycerol in overall reaction} = 3.13 + 71.02 - 92.12 = 17.97\ \text{Kmol/hr}$$

$$\text{Total Unreacted Glycerol in overall reaction} = 17.97 \times 92.09 = 1654.82\ \text{Kg/hr}$$

Table 3-2 R-101 Flow rate in Kg/hr

Component	**Stream 3 Kg/hr**	**Stream 4' Kg/hr**	**Stream 4 Kg/hr**	**generation**	**consumption**	**Out Kg/hr**
Glycerol	8,482.92	-	-	-	6,828.09	1,654.84
Acetol	0.10	-	-	5,261.18	5,155.95	105.33
Water	4.47	-	-	1,279.78	-	1,284.25
Hydrogen	-	154.31	928.53	-	146.49	782.04
PG	583.13	-	-	5,295.85	-	5,878.98
EG	29.75	-	-	193.91	-	223.66
Methanol	-	-	-	100.14	-	100.14
Total	**9100.38**	**154.31**	**928.53**	**12130.86**	**12130.53**	**10029.24**

Formula:

$$\text{input} - \text{output} + \text{generation} - \text{consumption} = \text{accumulation}$$

$$(9100.38 + 154.31 + 928.53) - 10029.24 + 12130.86 - 12130.53 = 0$$

3.7 Gas Liquid Separator (V-101):

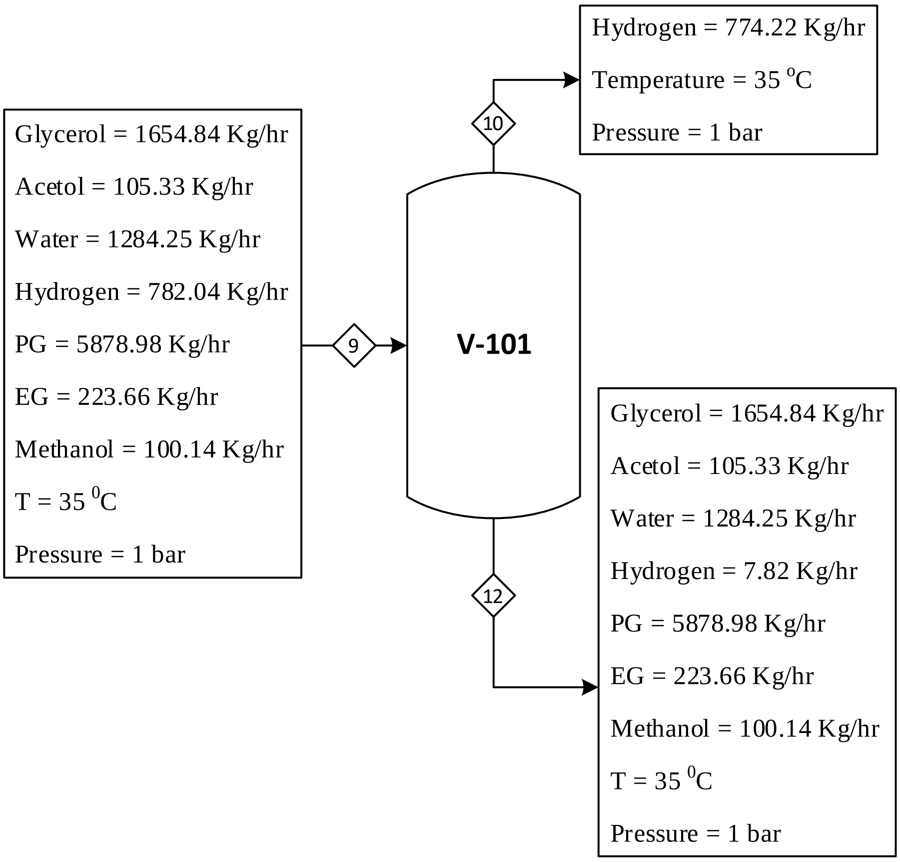


Figure 3-4 Gas Liquid Separator (V-101)

Only hydrogen is present in vapor phase at 35 ^{o}C and 1 bar pressure.

$$\text{Efficiency of Liquid Vapor Separator} = 99\%$$

$$\text{Hydrogen} = 782.04\ \text{Kg/hr} \times 0.99$$

$$\text{Hydrogen Seprated} = 774.22\ \text{Kg/hr}$$

$$\text{Hydrogen} = 782.04 - 774.22 = 7.82\ \text{Kg/hr}$$

3.8 Distillation Column (T-101):

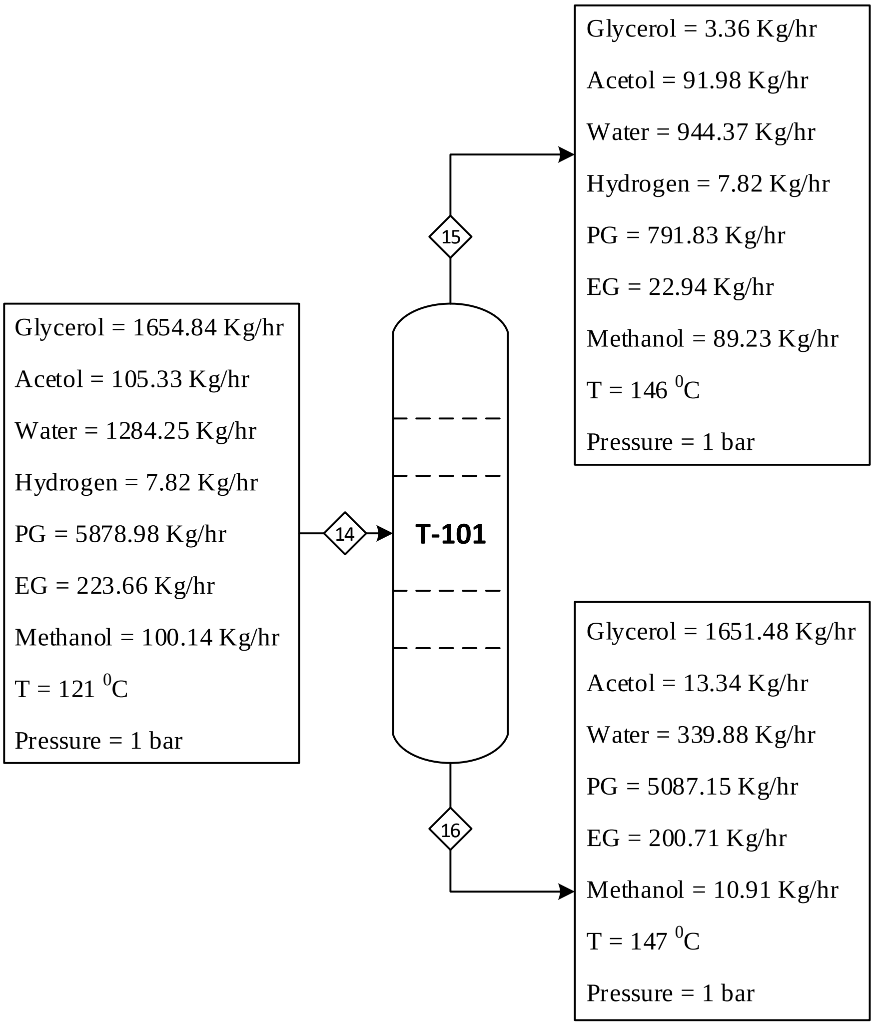


Figure 3-5 Distillation Column (T-101)

Table 3-3 (T-101) Feed in (Kg/hr)/(Kmol/hr)

Component	Feed In Kg/hr	Feed in Kmol/hr	Fraction
Glycerol	1,654.84	17.97	0.10
Acetol	105.33	1.42	0.01
Water	1,284.25	71.27	0.40
Hydrogen	7.82	3.88	0.02
PG	5,878.98	77.26	0.43
EG	223.66	3.61	0.02
Methanol	100.14	3.13	0.02
Total	**9255.02**	**178.53**	**1.00**

Assumptions:

- Hydrogen is lighter than lighter key so its not take part in Bubble point/dew point Calculations
- We assume the Pressure as one atm/pascal (1 bar=101325 pascal) and find Bubble temperature

Antoine Equation:

Table 3-4 Antoine Equation Constant

Component	C1	C2	C3	C4	C5
Glycerol	3.94	1411.53	-200.57		
Acetol	69.01	-5599.60	-7.10	6.22E-06	2
Water	73.65	-7258.20	-7.30	4.17E-06	2
Hydrogen	0.00	0.00	0.00	0.00E+00	0
PG	212.80	-15420.00	-28.11	2.16E-05	2
EG	84.09	-10411.00	-8.20	1.65E-18	6
Methanol	82.72	-6904.50	-8.86	7.47E-06	2

Formula:

$$\mathrm{Ln}\ (\mathrm{P}) = \mathrm{C}_1 + \frac{\mathrm{C}_2}{\mathrm{T}} + \mathrm{C}_3 \times \mathrm{Ln}(\mathrm{T}) + \mathrm{C}_4 \times \mathrm{T}^{\mathrm{C}_5}$$

The unit of Pressure and Temperature is Pascal and degree kelvin, respectively.

Bubble Temperature Calculation:

$$\mathrm{P} = \mathrm{P}_{1(\mathrm{sat})} \times \mathrm{Fraction} + \mathrm{P}_{2(\mathrm{sat})} \times \mathrm{Fraction} \ldots.$$

Where $P_{1\ (sat)}$ is find from the Antoine equation;

Table 3-5 Bubble Temperature Calculation of Feed

Component	Fraction	Temp (K)	P_{sat} Pascal	Total Bubble Pressure Pascal	$K_i=P_i/P$	Xi*ki
Glycerol	0.10	393.98	43.60	4.39	0.00	0.00
Acetol	0.01	393.98	619363.90	4932.44	6.11	0.05
Water	0.40	393.98	203572.12	81263.43	2.01	0.80
Hydrogen	0.02	393.98	0.00	0.00	0.00	0.00
PG	0.43	393.98	8270.52	3579.22	0.08	0.04
EG	0.02	393.98	5882.90	118.79	0.06	0.00
Methanol	0.02	393.98	652690.83	11426.73	6.44	0.11
Total	**1**			**101325**		**1.00**

Where P is the total pressure (101325 Pascal) and P_i is saturation pressure.

Flash Calculation:

To find Fraction in vapor y_i

$$y_i = \frac{Z_i \times K_i}{1 + V(K_i - 1)}$$

Where;

- y_i is the fraction in distillate
- V is find by iteration.
- Z_i is the fraction of feed.

To find fraction in liquid X_i

$$X_i = \frac{y_i}{K_i}$$

Table 3-6 T-101 Flash Calculation

Component	**Fraction**	**Temp (K)**	**P_{sat} Pascal**	**K_i=P_i/P**	**V**	**Y**	**X**	**L**
Glycerol	0.10	420.00	319.72	0.00	0.39	0.001	0.17	0.61
Acetol	0.01	420.00	1082443.63	10.68	0.39	0.02	0.00	0.61
Water	0.40	420.00	436315.99	4.31	0.39	0.75	0.17	0.61
Hydrogen	0.02	420.00	0.00	0.00	0.39	0.00	0.00	0.61
PG	0.43	420.00	24442.63	0.24	0.39	0.15	0.62	0.61
EG	0.02	420.00	17950.44	0.18	0.39	0.01	0.03	0.61
Methanol	0.02	420.00	1284450.9	12.68	0.39	0.04	0.00	0.61
Total	**1**					**1**	**1**	

Where P is the total pressure in Pascal which is 101325 Pascal = 1 bar

Distillate and Bottom Flowrate:

$$\text{Distillate } (\frac{\text{Kmol}}{\text{hr}}) = \text{V} \times \text{Y} \times \text{Total Feed}$$

$$\text{Bottom } \left(\frac{\text{kmol}}{\text{hr}}\right) = \text{L} \times \text{X} \times \text{Total Feed}$$

Table 3-7 Feed in Distillate and Bottom

	Distillate		**Bottom**	
Component	**Kmol/hr in vapor**	**Fraction**	**Kmol/hr in Liquid**	**Fraction**
Glycerol	0.037	0.001	17.933	0.167
Acetol	1.242	0.017	0.180	0.002
Water	52.407	0.737	18.861	0.176

Hydrogen	3.879	0.055	0.000	0.000
PG	10.407	0.146	66.857	0.622
EG	0.370	0.005	3.235	0.030
Methanol	2.785	0.039	0.340	0.003
Total	71.125	1.000	107.408	1.000

Bubble and Dew Temperature Calculation of Distillate and Bottom:

Bubble Temperature calculation of bottom;

Table 3-8 Bubble Temperature Calculation

Component	**Bottom Kmol/hr**	**Fraction**	**Temp (K)**	**Psat in Pascal**	**Total Bubble Pressure (Pascal)**	**$K_i=P_i/P$**	**X_i*K_i**
Glycerol	17.93	0.17	421.0	343.0	57.3	0.003	0.001
Acetol	0.18	0.00	421.0	1105386.3	1853.8	10.909	0.018
Water	18.86	0.18	421.0	448918.7	78833.0	4.430	0.778
PG	66.86	0.00	421.0	25448.5	15840.7	0.251	0.156
EG	3.24	0.62	421.0	18709.0	563.5	0.185	0.006
Methanol	0.34	0.03	421.0	1317501.3	4176.7	13.003	0.041
Total	**107.41**	**1.00**			**101325.0**		**1.0**

Dew Temperature calculation of Distillate;

Table 3-9 Dew Temperature Calculation of Distillate

Component	**Distillate Kmol/hr**	**Fraction**	**Temp (K)**	**P_{sat} Pascal**	**Total Dew Pressure Pascal**	**$K_i=P_i/P$**	**y_i/K_i**
Glycerol	0.04	0.001	419.4	306.5	101325	0.003	0.170
Acetol	1.24	0.017	419.4	1068938		10.55	0.002
Water	52.41	0.737	419.4	428938.9		4.23	0.174
Hydrogen	3.88	0.055	419.4	0.0		0.00	0.000
PG	10.41	0.146	419.4	23859.3		0.24	0.621
EG	0.37	0.005	419.4	17510.8		0.17	0.030
Methanol	2.79	0.039	419.4	1265063.4		12.49	0.003
Total	71.13	1.000			101325		1

Formula used to find total dew pressure.

$$P = \frac{1}{\sum(\frac{\text{fraction}}{P_{\text{sat}}})}$$

3.9 Distillation Column (T-102):

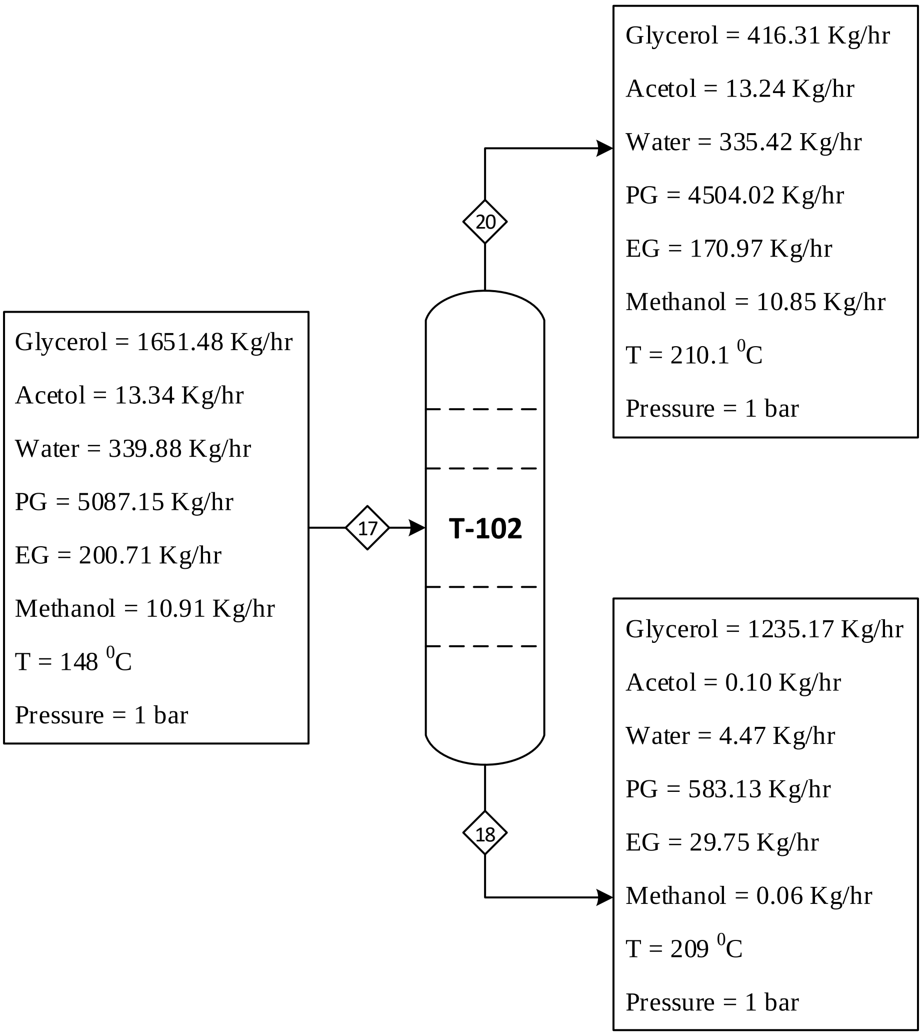


Figure 3-6 Distillation Column T-102

Table 3-10 (T-102) Feed in (Kg/hr)/(Kmol/hr)

Component	Feed In Kg/hr	Feed in Kmol/hr	Fraction
Glycerol	1,651.48	17.93	0.167
Acetol	13.34	0.18	0.002
Water	339.88	18.86	0.176
PG	5,087.15	66.86	0.622
EG	200.71	3.24	0.030
Methanol	10.91	0.34	0.003
Total	**7303.48**	**107.41**	**1.0**

Assumption:

We assume the Pressure as one atm/pascal (1 bar=101325 pascal) and find Bubble temperature

Antoine Equation:

Table 3-11 Antoine Equation Constant

Component	C1	C2	C3	C4	C5
Glycerol	3.94	1411.53	-200.57		
Acetol	69.01	-5599.60	-7.10	6.22E-06	2
Water	73.65	-7258.20	-7.30	4.17E-06	2
Hydrogen	0.00	0.00	0.00	0.00E+00	0
PG	212.80	-15420.00	-28.11	2.16E-05	2
EG	84.09	-10411.00	-8.20	1.65E-18	6
Methanol	82.72	-6904.50	-8.86	7.47E-06	2

Formula:

$$\mathrm{Ln}\ (\mathrm{P}) = \mathrm{C}_1 + \frac{\mathrm{C}_2}{\mathrm{T}} + \mathrm{C}_3 \times \mathrm{Ln}(\mathrm{T}) + \mathrm{C}_4 \times \mathrm{T}^{\mathrm{C}_5}$$

The unit of Pressure and Temperature is pascal and degree kelvin, respectively.

Bubble Temperature Calculation:

$$\mathrm{P} = \mathrm{P}_{1(\mathrm{sat})} \times \mathrm{Fraction} + \mathrm{P}_{2(\mathrm{sat})} \times \mathrm{Fraction} \ldots.$$

Where $P_{1\ (sat)}$ is find from the Antoine equation;

Table 3-12 Bubble Temperature Calculation of Feed

Component	Fraction	Temp (K)	P_{sat} Pascal	Total Bubble Pressure Pascal	$K_i=P_i/P$	Xi*ki
Glycerol	0.167	421.0	343.0	57.3	0.003	0.001
Acetol	0.002	421.0	1105386.3	1853.8	10.909	0.018
Water	0.176	421.0	448918.7	78833.0	4.430	0.778
PG	0.622	421.0	25448.5	15840.7	0.251	0.156
EG	0.030	421.0	18709.0	563.5	0.185	0.006
Methanol	0.003	421.0	1317501.3	4176.7	13.003	0.041
Total	**1.0**			**101325.0**		**1**

Where P is the total pressure (101325 Pascal) and P_i is saturation pressure.

Flash Calculation:

To find Fraction in vapor y_i

$$\mathrm{y_i} = \frac{\mathrm{Z_i} \times \mathrm{K_i}}{1 + \mathrm{V}(\mathrm{K_i} - 1)}$$

Where;

- y_i is the fraction in distillate
- V is find by iteration.
- Z_i is the fraction of feed.

To find fraction in liquid X_i

$$X_i = \frac{y_i}{K_i}$$

Table 3-13 T-102 Flash Calculation

Component	Fraction	Temp (K)	Psat in Pascal	K=pi/p	V	Y	X	L
Glycerol	0.167	482.0	8353.6	0.1	0.80	0.052	0.635	0.20
Acetol	0.002	482.0	3205412.0	31.6	0.80	0.002	6.55E-05	0.20
Water	0.176	482.0	1860475.2	18.4	0.80	0.216	0.012	0.20
PG	0.622	482.0	191434.8	1.9	0.80	0.686	0.363	0.20
EG	0.030	482.0	142456.3	1.4	0.80	0.032	0.023	0.20
Methanol	0.003	482.0	4769532.2	47.1	0.80	0.004	0.000	0.20
Total	1.000					1.0	1.0	

Where P is the total pressure in pascal which is 101325 pascal = 1 bar

Distillate and Bottom Flowrate:

$$\text{Distillate}\ (\frac{\text{Kmol}}{\text{hr}}) = \text{V} \times \text{Y} \times \text{Total Feed}$$

$$\text{Bottom}\ \left(\frac{\text{kmol}}{\text{hr}}\right) = \text{L} \times \text{X} \times \text{Total Feed}$$

Table 3-14 Feed in Distillate and Bottom

	Distillate		Bottom	
Component	Kmol/hr in vapor	Fraction	Kmol/hr in Liquid	Fraction
Glycerol	4.52	0.053	13.4	0.615
Acetol	0.18	0.002	0.0	0.000
Water	18.61	0.217	0.2	0.011
PG	59.19	0.692	7.7	0.351
EG	2.76	0.032	0.5	0.022
Methanol	0.34	0.004	0.0	0.000
Total	85.60	1.000	107.408	1.000

Bubble and Dew Temperature Calculation of Distillate and Bottom:

Bubble Temperature calculation of bottom

Table 3-15 Bubble Temperature Calculation

Component	**Bottom Kmol/hr**	**Fraction**	**Temp (K)**	**Psat in Pascal**	**Total Bubble Pressure (Pascal)**	**$K_i=P_i/P$**	**X_i*K_i**
Glycerol	13.413	0.615	482.0	8874.4	5458.31	0.088	0.054
Acetol	0.001	0.000	482.0	3279060.8	207.83	32.362	0.002
Water	0.248	0.011	482.0	1916534.9	21792.93	18.915	0.215
PG	7.664	0.351	482.0	199768.2	70205.70	1.972	0.693
EG	0.479	0.022	482.0	148479.8	3264.56	1.465	0.032
Methanol	0.002	0.000	482.0	4901911.6	395.68	48.378	0.004
Total	21.807	1.000			101325.00		**1.0**

Dew Temperature calculation of Distillate

Table 3-16 Dew Temperature Calculation of Distillate

Component	**Distillate Kmol/hr**	**Fraction**	**Temp (K)**	**P_{sat} Pascal**	**Total Dew Pressure Pascal**	**$K_i=P_i/P$**	**y_i/K_i**
Glycerol	4.52	0.053	483	8747.10	101325	0.09	0.61
Acetol	0.18	0.002	483	3261278.49		32.19	0.00
Water	18.61	0.217	483	1902969.52		18.78	0.01
Hydrogen	0.00	0.000	483	0.00		0.00	0.00
PG	59.19	0.692	483	197741.12		1.95	0.35
EG	2.76	0.032	483	147016.45		1.45	0.02
Methanol	0.34	0.004	483	4869894.04		48.06	0.00
Total	85.60	1.000			101325		1

Formula used to find total dew pressure.

$$P = \frac{1}{\sum\left(\frac{\text{fraction}}{P_{\text{sat}}}\right)}$$

3.10 Distillation Column (T-103):

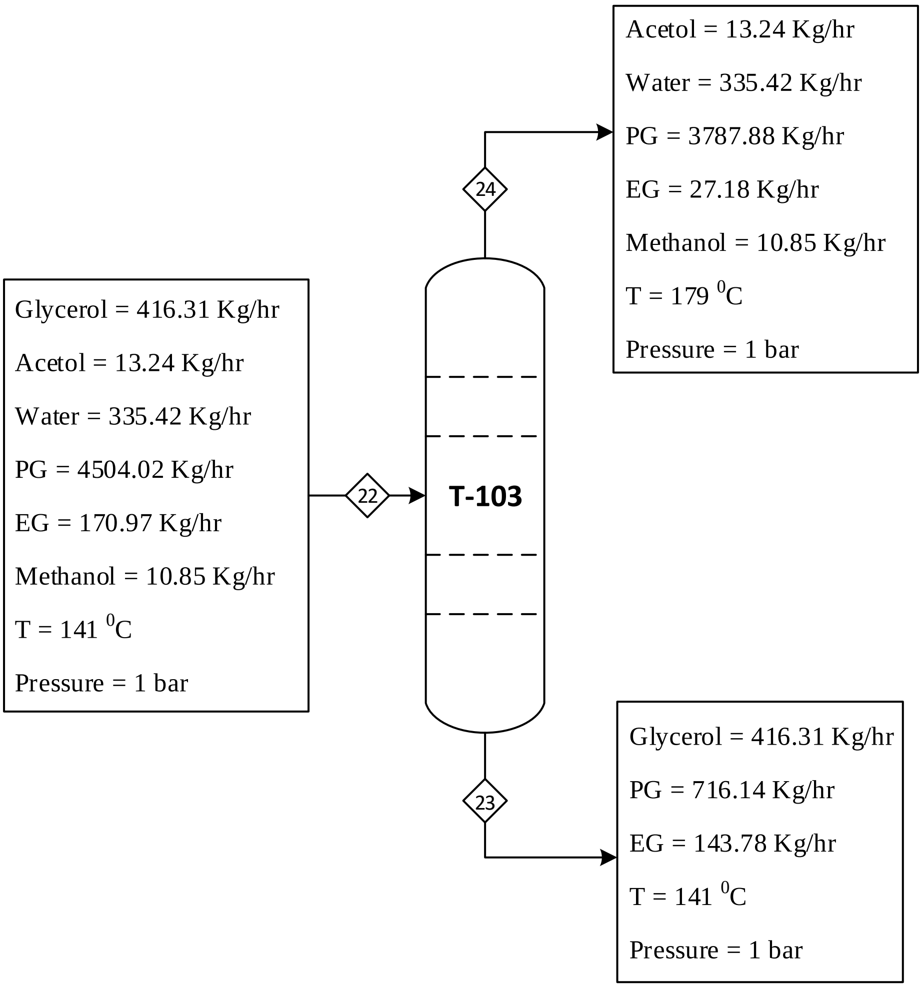


Figure 3-7 Distillation Column (T-103)

Table 3-17 (T-103) Feed in (Kg/hr)/(Kmol/hr)

Component	Feed In Kg/hr	Feed in Kmol/hr	Fraction
Glycerol	416.31	4.52	0.053
Acetol	13.24	0.18	0.002
Water	335.42	18.61	0.217
PG	4,504.02	59.19	0.692
EG	170.97	2.76	0.032
Methanol	10.85	0.34	0.004
Total	**5,450.80**	**85.60**	**1**

Table 3-18 Recoveries (T-103)

T-103 Recoveries			
	top	bot	Total
Glycerol	0.00	1.00	1
Acetol	1.00	0.00	1
Water	1.00	0.00	1
Hydrogen	0.00	0.00	
PG	0.84	0.16	1

EG	0.16	0.84	1
Methanol	1.00	0.00	1.000000

Table 3-19 Flow rates (T-103)

Component	Feed Kmol/hr	Distillate Kmol/hr	Bottom Kmol/hr
Glycerol	4.52	4.52	-
Acetol	0.18	-	0.18
Water	18.61	-	18.61
PG	59.19	9.41	49.78
EG	2.76	2.32	0.44
Methanol	0.34	-	0.34
Total	**85.60**	**16.25**	**69.35**

Assumptions:

- Hydrogen is lighter than lighter key so its not take part in Bubble point/dew point Calculations
- We assume the Pressure as one atm/pascal (1 bar=101325 pascal) and find Bubble temperature

Antoine Equation:

Table 3-20 Antoine Equation Constant

Component	**C1**	**C2**	**C3**	**C4**	**C5**
Glycerol	3.94	1411.53	-200.57		
Acetol	69.01	-5599.60	-7.10	6.22E-06	2
Water	73.65	-7258.20	-7.30	4.17E-06	2
Hydrogen	0.00	0.00	0.00	0.00E+00	0
PG	212.80	-15420.00	-28.11	2.16E-05	2
EG	84.09	-10411.00	-8.20	1.65E-18	6
Methanol	82.72	-6904.50	-8.86	7.47E-06	2

Formula:

$$\mathrm{Ln}\ (\mathrm{P}) = \mathrm{C}_1 + \frac{\mathrm{C}_2}{\mathrm{T}} + \mathrm{C}_3 \times \mathrm{Ln}(\mathrm{T}) + \mathrm{C}_4 \times \mathrm{T}^{\mathrm{C}_5}$$

The unit of Pressure and Temperature is pascal and degree kelvin, respectively.

Bubble Temperature Calculation:

$$\mathrm{P} = \mathrm{P}_{1(\mathrm{sat})} \times \mathrm{Fraction} + \mathrm{P}_{2(\mathrm{sat})} \times \mathrm{Fraction} \ldots.$$

Where $P_{1\ (sat)}$ is find from the Antoine equation

Table 3-21 Bubble Temperature Calculation of Feed

Component	**Fraction**	**Temp (K)**	**P_{sat} Pascal**	**Total Bubble Pressure Pascal**	**$K_i=P_i/P$**	**Xi*ki**
Glycerol	0.053	414	214.78	11.34	0.002	0.0001
Acetol	0.002	414	963073.00	2011.05	9.505	0.020
Water	0.217	414	372219.98	80937.69	3.674	0.799
PG	0.692	414	19514.80	13494.58	0.193	0.133
EG	0.032	414	14242.84	458.53	0.141	0.005
Methanol	0.004	414	1114890.07	4411.82	11.003	0.044
Total	**1**		214.78	**101325**		**1.00**

Where P is the total pressure (101325 Pascal) and P_i is saturation pressure.

Dew Temperature Calculation of Distillate:

Dew Temperature calculation of Distillate

Table 3-22 Dew Temperature Calculation of Distillate

Component	**Distillate Kmol/hr**	**Fraction**	**Temp (K)**	**P_{sat} Pascal**	**Total Dew Pressure Pascal**	**$K_i=P_i/P$**	**y_i/K_i**
Acetol	0.179	0.00	452	1958795.32	101325	19.33	0.0001
Water	18.614	0.27	452	970169.73		9.57	0.028
PG	49.782	0.72	452	75734.36		0.75	0.960
EG	0.438	0.01	452	56796.70		0.56	0.011
Total	69.351	1.00			101325		1

Formula used to find total dew pressure.

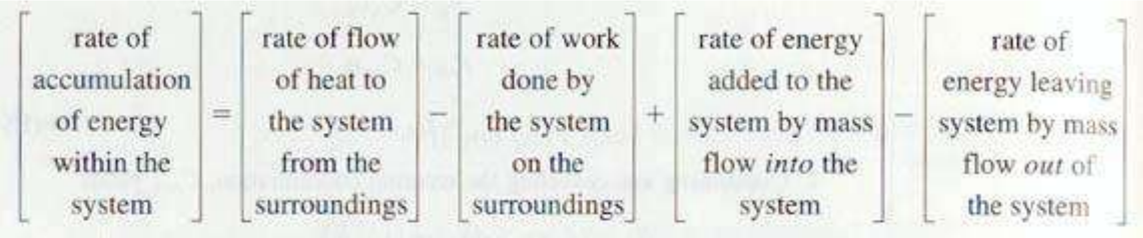
$$P = \frac{1}{\sum\left(\frac{\text{fraction}}{P_{sat}}\right)}$$

CHAPTER NO. 4

ENERGY BALANCE

4.1 Introduction:

An energy balance is a consideration of the energy input, output, and consumption or generation in a process or stage. In establishing an energy balance, all sources of thermal energy are put on the input side, and all items of heat utilization on the output side.



$$\begin{bmatrix}\text{rate of}\\ \text{accumulation}\\ \text{of energy}\\ \text{within the}\\ \text{system}\end{bmatrix} = \begin{bmatrix}\text{rate of flow}\\ \text{of heat to}\\ \text{the system}\\ \text{from the}\\ \text{surroundings}\end{bmatrix} - \begin{bmatrix}\text{rate of work}\\ \text{done by}\\ \text{the system}\\ \text{on the}\\ \text{surroundings}\end{bmatrix} + \begin{bmatrix}\text{rate of energy}\\ \text{added to the}\\ \text{system by mass}\\ \text{flow \textit{into} the}\\ \text{system}\end{bmatrix} - \begin{bmatrix}\text{rate of}\\ \text{energy leaving}\\ \text{system by mass}\\ \text{flow \textit{out} of}\\ \text{the system}\end{bmatrix}$$

Figure 4-1 General Energy Balance Equation

To find heat of formation and specific heat of component at constant pressure, we have use the following table.

Table 4-1 Heat of formation and Specific heat at constant pressure

	Cp Constants (KJ/Kmol.K)				
Component	**A**	**B**	**C**	**D**	**Hf KJ/mol**
Glycerol	8.42E+00	4.44E-01	-3.16E-04	9.38E-08	-525.31
Acetol	8.43E+00	2.35E-01	-1.43E-04	3.36E-08	-366
Water	3.22E+01	1.92E-03	1.06E-05	-3.60E-09	-228.77
Hydrogen	2.71E+01	9.27E-03	-1.38E-05	7.64E-09	0
PG	6.32E-01	4.21E-01	-2.98E-04	8.95E-08	-466
EG	3.57E+01	2.48E-01	-1.50E-04	3.01E-08	-399
Methanol	2.12E+01	7.09E-02	2.59E-05	-2.83E-08	-201.3

Formula Used To Find Specific Heat

$$C_p = a + bT + cT^2 + dT^3$$

The values of a, b, c and d are taken from Appendix D, Coulson and Richardson Chemical Engineering, Volume 6.

To find the value of ΔH, we use this equation

$$\Delta H = a(T_2 - T_1) + \frac{b}{2}(T_2 - T_1)^2 + \frac{c}{3}(T_2 - T_1)^3 + \frac{d}{4}(T_2 - T_1)^4$$

Process involve different reaction; we need also to find the values of ΔH_r which takes place in the equipment. The equation, which we used to find ΔH_r is

$\Delta H_R = (\Delta\hat{H}_F \text{ product} - \Delta\hat{H}_F \text{ reactant}) x\ n$

4.2 Heat Exchanger (E-101):

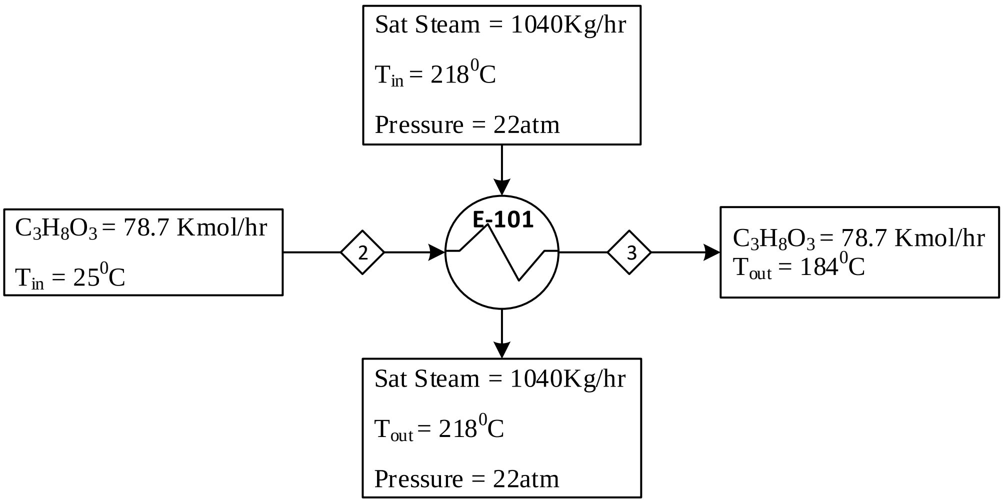


Figure 4-2 Heat Exchanger (E-101)

Calculations:

Formula:

$$Q = \dot{m}C_p\Delta T$$

$$C_p = a + bT + cT^2 + dT^3$$

By solving above formula and putting the value of constant (a,b,c and d taken from Richardson Coulson Vol 6) and temperature (Kelvin), We calculate Enthalpy of the inlet and the outlet streams.

Steam	Feed
Temperature of Steam at inlet = 218 ºC	Temperature of feed at Inlet = 25 ºC
Temperature of Steam at Outlet = 218 ºC	Temperature of feed at Outlet = 184 ºC
Pressure of steam at inlet = 22 bar	Pressure of feed at inlet = 1 bar
Pressure of Steam at outlet = 22 bar	Pressure of feed at outlet = 1 bar

Enthalpy:

Table 4-2 Heat Capacity in/out

Components	Feed 5	Fraction	C_p(at inlet) Kj/kmol.K	Weighted C_p	C_p (at Oultet) Kj/kmol.K	Additive Cp
Glycerol	78.7	1.0	115.2	115.2	154.5	154.5
Total kmol/h	78.7	1.0		115.2		154.5

Enthalpy at inlet:

$T_{in} = 25\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 0\ ℃$

$$Q_{in} = 78.7 \times 115.2 \times 0 = 0\,\frac{KJ}{hr} \qquad\qquad Q_{in} = mC_p\Delta T$$

Enthalpy at Outlet:

$T_{out} = 184\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 159\ ℃$

$$Q_{out} = 78.7 \times 154.5 \times 159 = 1939599\,\frac{KJ}{hr} \qquad\qquad Q_{out} = mC_p\Delta T$$

$\Delta Q = 1939599\ KJ/hr$

Steam Requirement:

$T_{in} = 218℃$

$T_{out} = 218℃$

$\lambda = 1865\,\frac{KJ}{Kg}$

$\Delta Q = 1939599\,\frac{KJ}{hr}$

$m = \frac{Q}{\lambda}$

$$m = \frac{1939599}{1865} = 1040\,\frac{Kg}{hr}$$

4.3 Mixer (M-101):

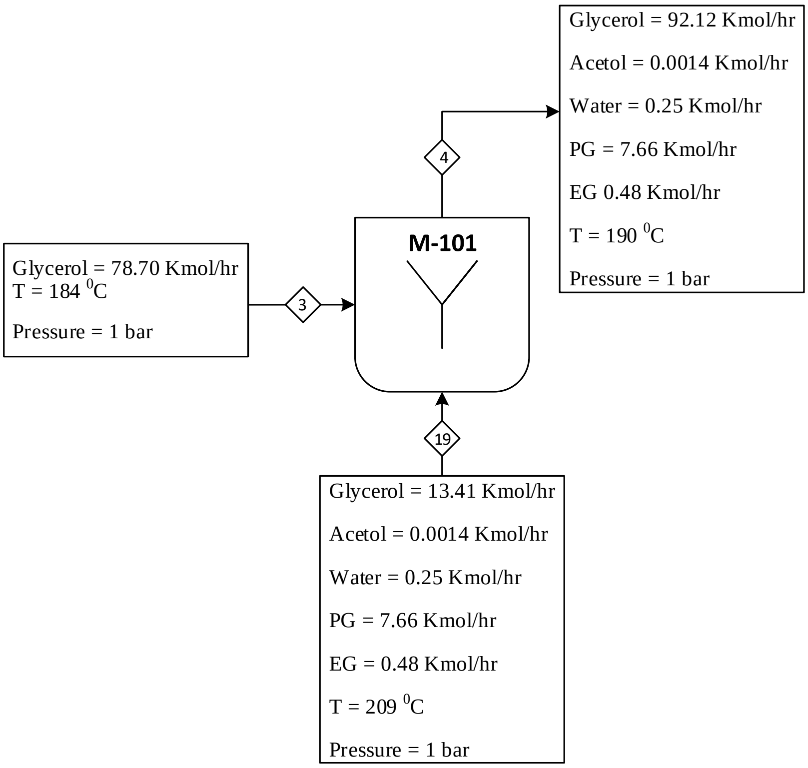


Figure 4-3 Energy Balance on Mixer (M-101)

Input of Stream 1:

Table 4-3 M-101 Enthalpy In

Component	Flow rate Kmol/hr	T_{In} (^{0}C)	T_{ref} (^{0}C)	ΔĤ KJ/mol	ΔH KJ/hr
Glycerol	78.70	184	25	8156.16	641914.0

ΣΔH(2) = 641914.0 KJ/hr

Input of Stream 2:

Table 4-4 M-101 Enthalpy in

Component	Flow rate Kmol/hr	T_{in} (^{o}C)	T_{ref} (^{o}C)	ΔĤ KJ/mol	ΔH KJ/hr
Glycerol	13.41	209	25	10198.24	136785.34
Acetol	0.0014			6187.03	8.55
Water	0.25			6004.48	1488.91
PG	7.66			8320.76	63768.17
EG	0.48			1147.66	5501.16

ΣΔH(15)` = 207552.13 KJ/hr

ΣΔH = 849466.13 KJ/hr

Output of Stream 1:

Table 4-5 M-101 Enthalpy Out

Component	Flow rate Kmol/hr	T_{in} (^{o}C)	T_{ref} (^{o}C)	ΔĤ KJ/mol	ΔH KJ/hr
Glycerol	92.12	190	25	8579.25	790282.74
Acetol	0.0014			5240.02	7.24
Water	0.25			5377.12	1333.35
PG	7.66			6924.29	53065.99
EG	0.48			9962.90	4776.81

ΣΔH = 849466.13 KJ/hr

Sample Calculation of Stream 2:

$$\Delta H = \int_{T1}^{T2} C_p dt$$

$$\Delta \hat{H} = a(T_2 - T_1) + \frac{b}{2}(T_2 - T_1)^2 + \frac{c}{3}(T_2 - T_1)^3 + \frac{d}{4}(T_2 - T_1)^4$$

$$= 8.424(184 - 25) + \frac{0.44422}{2}(184 - 25) + \frac{-3.16 \times 10^{-4}}{3}(184 - 25) + \frac{9.38 \times 10^{-08}}{4}(184 - 25)$$

$$\Delta\hat{H} = 8156.16\,\frac{KJ}{mol}$$

$$\Delta H = 8156.16 \times 78.70 = 641914\,\frac{Kj}{hr}$$

4.4 Reactor (R-101):

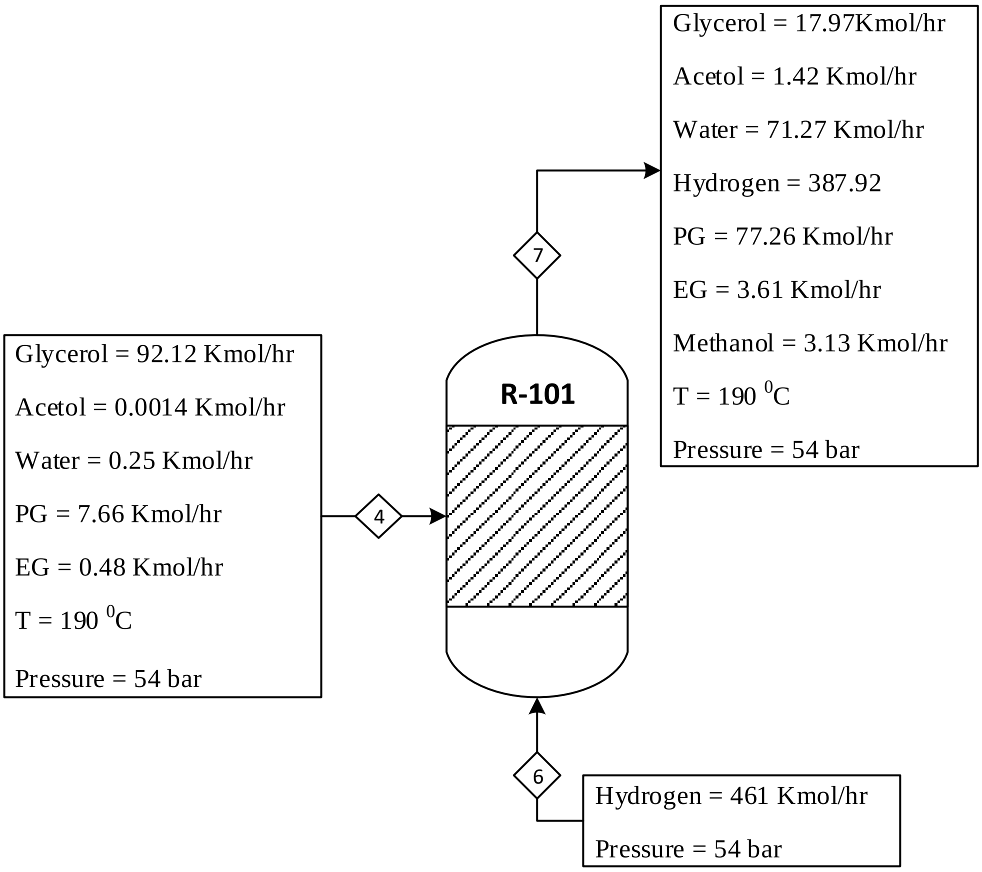


Figure 4-4 Energy Balance on Reactor (R-101)

Reaction Involved:

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

$$C_2H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

$$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH$$

Reaction Temperature = 190 °C

Reference Temperature = 25 °C

Pressure = 54 bar

Heat of Reaction:

Table 4-6 Heat of Formation of Component

	Cp Constant (Kj/Kmol.K)				
Component	**A**	**B**	**C**	**D**	**ΔH_f KJ/mol**
Glycerol	8.42E+00	4.44E-01	-3.16E-04	9.38E-08	-525.31
Acetol	8.43E+00	2.35E-01	-1.43E-04	3.36E-08	-366
Water	3.22E+01	1.92E-03	1.06E-05	-3.60E-09	-228.77
Hydrogen	2.71E+01	9.27E-03	-1.38E-05	7.64E-09	0
PG	6.32E-01	4.21E-01	-2.98E-04	8.95E-08	-466
EG	3.57E+01	2.48E-01	-1.50E-04	3.01E-08	-399
Methanol	2.12E+01	7.09E-02	2.59E-05	-2.83E-08	-201.3

Formula Used:

$$\Delta H_{reaction} = \sum \Delta H_{f(product)} - \sum \Delta H_{f(reactant)}$$

$$\Delta\hat{H} = a(T_2 - T_1) + \frac{b}{2}(T_2 - T_1)^2 + \frac{c}{3}(T_2 - T_1)^3 + \frac{d}{4}(T_2 - T_1)^4$$

Where ΔH_f, heat of formation (KJ/mol) is, $\Delta\hat{H}$ is enthalpy (KJ/Kmol) and T_2 and T_1 is reaction and reference temperature respectively.

For Reaction 1:

Table 4-7 ΔHr of Reaction 1

Component	**Flow rate Kmol/hr**	**$\Delta\hat{H}$ KJ/Kmol**	**ΔH KJ/hr**	**$\Delta\hat{H}r$ 25^{o}C KJ/mol**	**$\Delta\hat{H}r$ KJ/Kmol**	**$\Delta\hat{H}r$ 190 ^{o}C KJ/Kmol**	**ΔHr 190 ^{o}C KJ/hr**
Glycerol	71.0	22507.0	1598454.0	-69.46	-69460	-73319.4	**-5.21E+06**
Acetol	71.0	12984.9	922190.3				
Water	71.0	5662.7	402169.6				

$$\Delta H_r(1) = -521 \times 10^6 \text{ KJ/hr}$$

For Reaction 2:

Table 4-8 ΔHr of Reaction 1

Component	**Flow rate Kmol/hr**	**$\Delta\hat{H}$ KJ/Kmol**	**ΔH KJ/hr**	**$\Delta\hat{H}r$ 25^{o}C KJ/mol**	**$\Delta\hat{H}r$ KJ/Kmol**	**$\Delta\hat{H}r$ 190 ^{o}C KJ/Kmol**	**ΔHr 190 ^{o}C KJ/hr**
Acetol	69.6	12984.9	903746.5	-100	-100000	-97617	**-6.79E+06**

Hydrogen	69.6	4798.5	333973.1				
PG	69.6	20166.7	1403599.4				

$\Delta H_r(2) = -6.79 \times 10^6\ \text{KJ/hr}$

For Reaction 3:

Table 4-9 ΔHr of Reaction 3

Component	**Flow rate Kmol/hr**	**ΔĤ KJ/Kmol**	**ΔH KJ/hr**	**ΔĤr 25ºC KJ/mol**	**ΔĤr KJ/Kmol**	**ΔĤr 190 ºC KJ/Kmol**	**ΔHr 190 ºC KJ/hr**
Glycerol	4.1	22507.0	91243.7	-74.99	-74990	-75859.4	**-3.08E+05**
Hydrogen	4.1	4798.5	19453.1				
Methanol	4.1	8301.7	33655.1				
EG	4.1	18134.5	73517.2				

$\Delta H_r(3) = -3.08 \times 10^5\ \text{KJ/hr}$

Total heat of reaction $\Delta H_r = -12308790.9\ \text{KJ/hr}$

Enthalpy of Reactant:

Table 4-10 (R-101) Enthalpy of reactant

Components	**Feed in Stream (3,4) Kmol/hr**	**ΔĤ KJ/Kmol**	**ΔH KJ/hr**
Glycerol	92.12	22507	2073249
Acetol	0.0014	12985	18
Water	0.248	5663	1404
Hydrogen	460.58	4798	2210073
PG	7.6637	20167	154553
EG	0.4795	18134	8695
Methanol	0	8302	0

$$\sum \Delta H_{\text{input}} = 4447991\,\frac{\text{KJ}}{\text{hr}}$$

Enthalpy of Product:

Table 4-11 (R-101) Enthalpy of Product

Components	Product Stream 5 Kmol/hr	$\Delta\hat{H}$ KJ/Kmol	ΔH KJ/hr
Glycerol	17.97	22507	404447
Acetol	1.42	12985	18462
Water	71.27	5663	403574
Hydrogen	387.92	4798	1861402
PG	77.26	20167	1558152
EG	3.61	18134	65376
Methanol	3.13	8302	25948

$$\sum \Delta H_{\text{product}} = 4337359.82 \ \frac{\text{KJ}}{\text{hr}}$$

Heat Balance:

$$\text{Output} = \text{input} + \text{generatioin} - \text{consumption}$$

$$Q = \Delta H_{\text{Product}} - \Delta H_{\text{feed}} + \text{Generation}$$

$$Q = 4337359.82 - 4447991 + \ 12308790.9 \frac{\text{KJ}}{\text{hr}}$$

$$Q = 1.22 \times 10^7 \frac{\text{Kj}}{\text{hr}}$$

Cooling Water Requirement:

Water Temperature at inlet $= 25°\text{C}$

Water Temperature at outlet $= 45°\text{C}$

Specific Heat of Water $C_p = 4.178 \frac{\text{KJ}}{\text{kg. K}}$

$$Q = 1.22 \times 10^7 \frac{\text{KJ}}{\text{hr}}$$

$$m = \frac{Q}{C_p \Delta T}$$

$$m = \frac{1.22 \times 10^7}{4.178 \times (45 - 25)}$$

$$m = 1.46 \times 10^5 \frac{\text{Kg}}{\text{hr}}$$

4.5 Waste Heat Boiler (E-102):

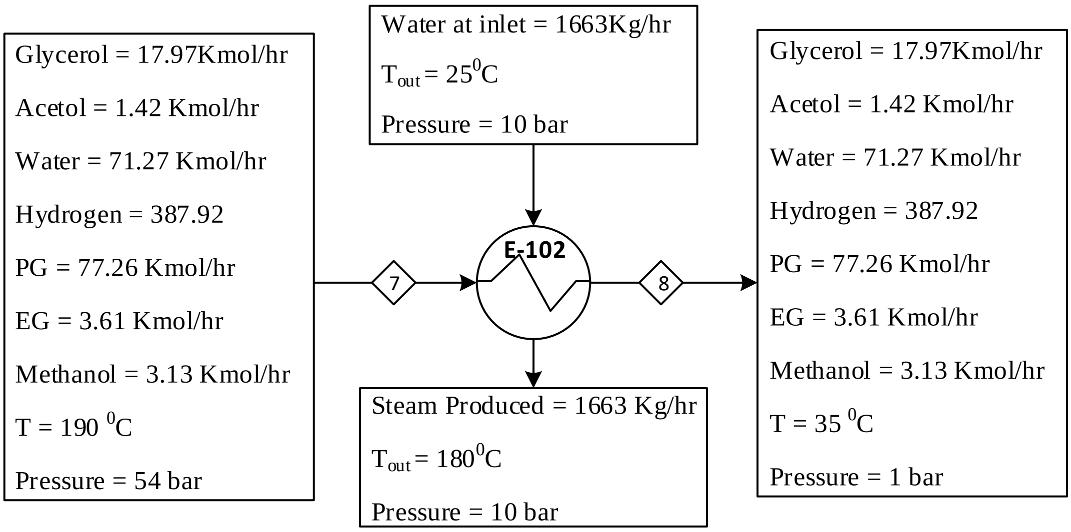


Figure 4-5 Energy Balance on (E-102)

Calculations:

Formula:

$$Q = \dot{m} C_p \Delta T$$

$$C_p = a + bT + cT^2 + dT^3$$

By solving above formula and putting the value of constant (a,b,c and d taken from Richardson Coulson Vol 6) and temperature (Kelvin), We calculate Enthalpy of the inlet and the outlet streams.

Temperature of Water at inlet = 25 °C	Temperature of feed at Inlet = 190 °C
Temperature of Steam Produced at Outlet = 180 °C	Temperature of feed at Outlet = 35 °C
Pressure of water at inlet = 1 bar	Pressure of feed at inlet = 54 bar
Pressure of Steam Produced at outlet = 10 bar	Pressure of feed at outlet = 1 bar

Enthalpy:

Table 4-12 Specific heat in/out

Components	Feed 5	Fraction	C_p(at inlet) Kj/kmol.K	Weighted C_p	C_p (at Oultet) Kj/kmol.K	Additive Cp
Glycerol	17.97	0.03	155.69	4.97	118.02	3.77
Acetol	1.42	0.00	89.85	0.23	68.17	0.17
Water	71.27	0.13	35.04	4.44	33.73	4.27
Hydrogen	387.92	0.69	29.23	20.16	28.91	19.94
PG	77.26	0.14	140.62	19.31	104.69	14.38
EG	3.61	0.01	121.57	0.78	98.86	0.63

Methanol	3.13	0.01	56.73	0.32	44.63	0.25
Total kmol/h	562.57	1.00		50.21		43.41

Enthalpy at inlet:

$T_{in} = 190\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 165\ ℃$

$Q_{in} = mC_p\Delta T$

$$Q_{in} = 562.57 \times 50.21 \times 165 = 4660244.5\,\frac{KJ}{hr}$$

Enthalpy at Outlet:

$T_{out} = 35\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 10\ ℃$

$Q_{in} = mC_p\Delta T$

$$Q_{out} = 562.57 \times 43 \times 10 = 244222\,\frac{KJ}{hr}$$

$\Delta Q = 4416022\ KJ/hr$

Steam Produced:

$T_{in} = 25℃$

$T_{out} = 180℃$

$\Delta T = 155\ ℃$

$$\lambda = 2006\,\frac{KJ}{Kg}$$

$$C_p = 4.187\,\frac{KJ}{Kg.K}$$

$$\Delta Q = 4416022\,\frac{KJ}{hr}$$

$$m = \frac{Q}{C_p \times \Delta T + \lambda}$$

$$m = \frac{4416022}{4.187 \times 155 \times 2006}$$

$$m = 1663\,\frac{Kg}{hr}$$

4.6 Heat Exchanger (E-103):

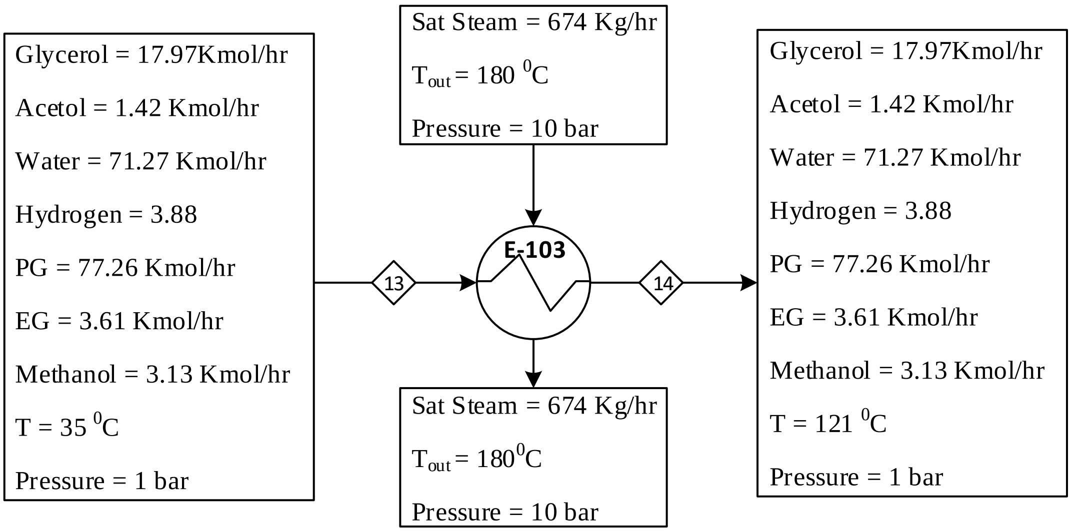


Figure 4-6 Energy Balance on (E-103)

Calculations:

Formula:

$$Q = \dot{m} C_p \Delta T$$

$$C_p = a + bT + cT^2 + dT^3$$

By solving above formula and putting the value of constant (a,b,c and d taken from Richardson Coulson Vol 6) and temperature (Kelvin), We calculate Enthalpy of the inlet and the outlet streams.

Steam	**Feed**
Temperature of Steam at inlet = 180 °C	Temperature of feed at Inlet = 35 °C
Temperature of Steam at Outlet = 180 °C	Temperature of feed at Outlet = 121 °C
Pressure of steam at inlet = 10 bar	Pressure of feed at inlet = 1 bar
Pressure of Steam at outlet = 10 bar	Pressure of feed at outlet = 1 bar

Enthalpy:

Table 4-13 Specific heat in/out

Components	**Feed 5**	**Fraction**	**C_p(at inlet) Kj/kmol.K**	**Weighted C_p**	**C_p (at Oultet) Kj/kmol.K**	**Additive Cp**
Glycerol	17.97	0.101	118.0	11.9	140.1	14.1
Acetol	1.42	0.008	68.2	0.5	80.8	0.6
Water	71.27	0.399	33.7	13.5	34.4	13.7
Hydrogen	3.88	0.022	28.9	0.6	29.1	0.6
PG	77.26	0.433	104.7	45.3	125.8	54.4

EG	3.61	0.020	98.9	2.0	112.1	2.3
Methanol	3.13	0.018	44.6	0.8	51.4	0.9
Total kmol/h	178.5	1.00		74.6		86.7

Enthalpy at inlet:

$T_{in} = 35\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 10\ ℃$

$Q_{in} = mC_p\Delta T$

$$Q_{in} = 178.5 \times 74.6 \times 10 = 133188\,\frac{KJ}{hr}$$

Enthalpy at Outlet:

$T_{out} = 121\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 96\ ℃$

$Q_{out} = mC_p\Delta T$

$$Q_{out} = 178.5 \times 86.7 \times 96 = 1486005\,\frac{KJ}{hr}$$

$\Delta Q = 1352817\ KJ/hr$

Steam Requirement:

$T_{in} = 180℃$

$T_{out} = 180℃$

$$\lambda = 2006\,\frac{KJ}{Kg}$$

$$\Delta Q = 1352817\,\frac{KJ}{hr}$$

$$m = \frac{Q}{\lambda}$$

$$m = \frac{1352817}{2006}$$

$$m = 674\,\frac{Kg}{hr}$$

4.7 Distillation Column (T-101):

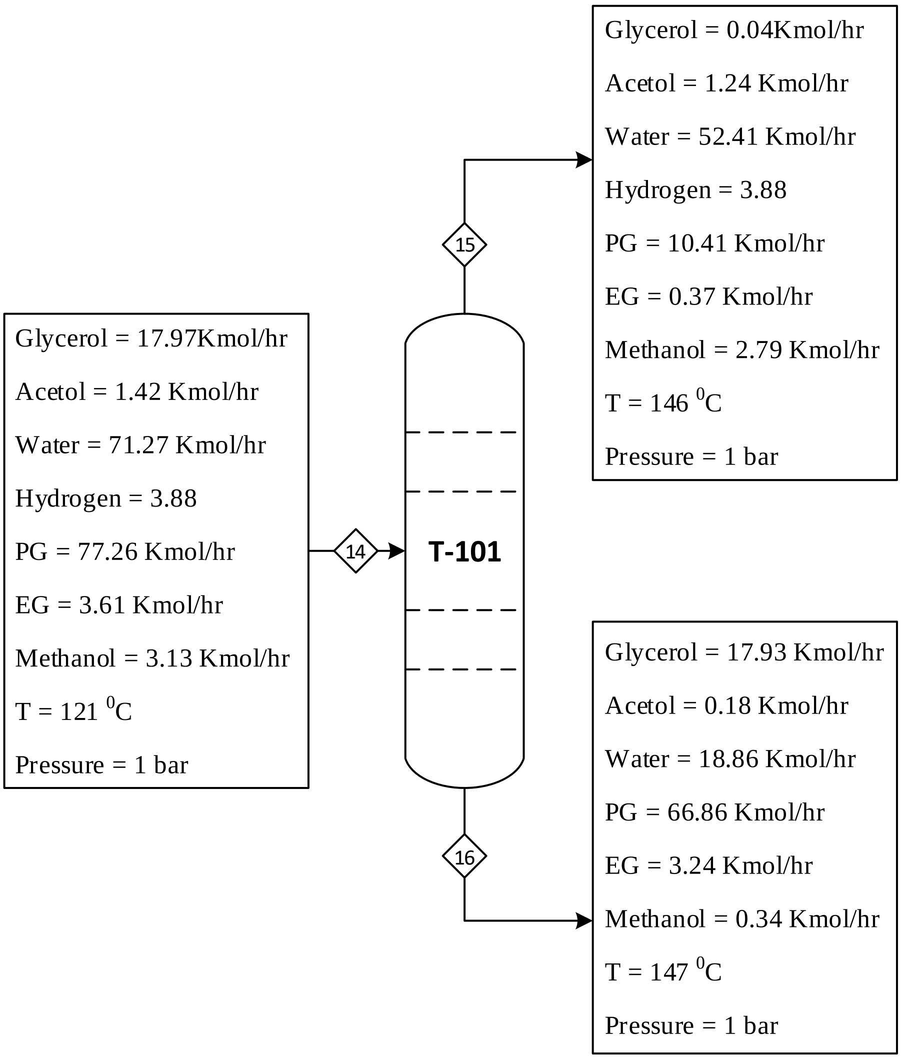


Figure 4-7 Energy Balance on (T-101)

Sample Calculation:

Formulas:

$$C_p = a + bT + cT^2 + dT^3$$

$$\text{Weighted } C_p = C_p \text{ Calculated} \times \text{Fraction of feed}$$

$$Q = mC_p\Delta T$$

$$Q = m\lambda$$

Calculation:

Table 4-14 T-101 Feed at Inlet, Bottom and Distillate

Component	Feed kmol/hr	Fraction	Distillate Kmol/hr	Fraction	Bottom kmol/hr	Fraction
Glycerol	17.97	0.10	0.04	0.00	17.93	0.17
Acetol	1.42	0.01	1.24	0.02	0.18	0.00

Water	71.27	0.40	52.41	0.74	18.86	0.18
Hydrogen	3.88	0.02	3.88	0.05	-	-
PG	77.26	0.43	10.41	0.15	66.86	0.62
EG	3.61	0.02	0.37	0.01	3.24	0.03
Methanol	3.13	0.02	2.79	0.04	0.34	0.00
Total	**178.53**	**1**	**71.13**	**1**	**107.41**	**1**

Total Feed at Inlet = 178.53 Kmol/hr

Total Feed at Distillate = 71.13 Kmol/hr

Total Feed at Bottom = 107.41 Kmol/hr

Heat Capacity:

Temperature at Feed = 121 ^oC

Temperature at Bottom = 147 ^oC

Temperature at Distillate = 146 ^oC

First we convert the temperature into degree kelvin and find the heat capacity at our desired temperature and then find weighted heat capacity by multiplying it with fraction.

Table 4-15 (T-101) Heat Capacity at Inlet, Bottom and Distillate

Component	**C_p of Feed KJ/Kmol. K**	**Weighted C_p**	**C_p (Distillate) KJ/Kmol.K**	**Weighted C_p of Distillate**	**C_p (Bottom) KJ/Kmol.K**	**Weighted C_p of Bottom**
Glycerol	140.14	14.11	146.08	0.07	146.22	24.41
Acetol	80.81	0.64	84.25	1.47	84.33	0.14
Water	34.42	13.74	34.64	25.52	34.65	6.08
Hydrogen	29.12	0.63	29.17	1.59	29.17	-
PG	125.78	54.43	131.44	19.23	131.58	81.90
EG	112.14	2.26	115.73	0.60	115.81	3.49
Methanol	51.38	0.90	53.36	2.09	53.41	0.17
Total		**86.72**		**50.58**		**116.20**

Latent Heat of Vaporization:

We have found latent heat of vaporization of each component from Richardson Coulson Vol 6.

Table 4-16 (T-101) Latent heat of vaporization

Component	Latent Heat of Vaporization KJ/Kmol	Weighted λ of Feed	Weighted λ at Distillate	Weighted λ at Bottom
Glycerol	61,127	6,153	31	10,206
Acetol	30,145	240	526	51
Water	40,683	16,240	29,976	7,144
Hydrogen	904	20	49	-
PG	54,177	23,446	7,927	33,723
EG	52,544	1,061	273	1,583
Methanol	35,278	618	1,381	112
Total		**47777**	**40164**	**52818**

Enthalpy at Distillate:

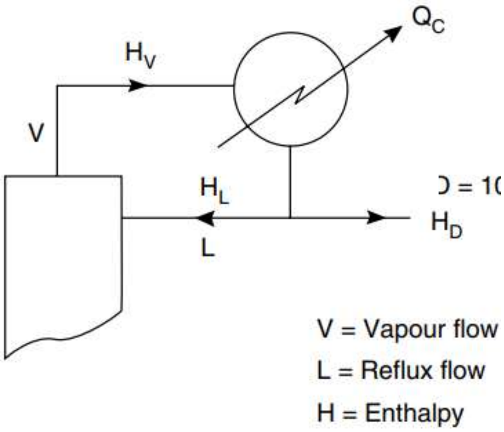


Figure 4-8 (T-101) Distillate

At steady state;

$$\text{input} = \text{output}$$

$$H_v = H_D + H_L + Q_C$$

$$\text{Enthalpy of vapor } H_v = \text{Latent} + \text{sensible heat}$$

$$H_v = mC_p\Delta T + m\lambda$$

$$H_v = 71.13 \times 50.58 \times (146 - 25) + 71.13 \times 40164$$

$$H_v = 3293388 \frac{KJ}{hr}$$

Now

$$\text{Enthalpy of Distillate } H_D = \text{Sensible Heat}$$

$$H_D = mC_p\Delta T$$

$$H_D = 71.13 \times 50.58 \times (146 - 25)$$

$$H_D = 436681\,\frac{KJ}{hr}$$

Here the enthalpy of the liquid is zero so;

$$Q_c = H_v - H_D$$

$$Q_c = 3293388 - 436681$$

$$Q_c = 2856707\,\frac{KJ}{hr}$$

Overall Balance:

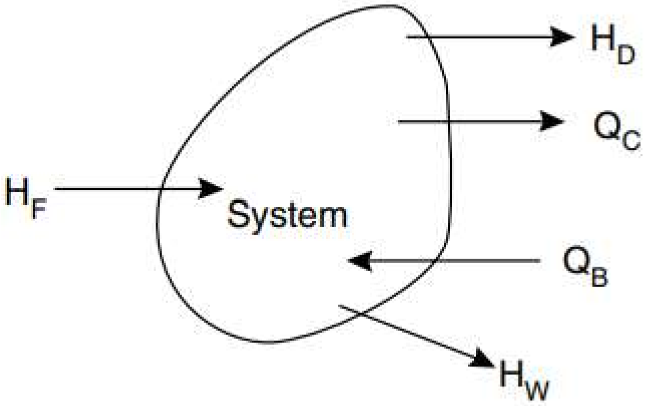


Figure 4-9 Overall System Balance

Where;

- Q_B is reboiler heat input
- H_F is distillation column feed at its bubble point
- Q_C is condenser cooling
- Top and bottom product H_D and H_W, respectively.

Q_B is determined from a balance over complete system;

$$\text{Input} = \text{output}$$

$$Q_B + H_F = Q_C + H_D + H_W$$

$$H_F = \text{latent heat} = m\lambda$$

$$H_F = 178.53 \times 47777$$

$$H_F = 8529805\,\frac{KJ}{hr}$$

Now

$$H_w = \text{Latent heat} + \text{Sensible Heat}$$

$$H_w = m\lambda + mC_p\Delta T$$

$$H_w = 107.41 \times 52818 + 107.41 \times 116.20 \times (147 - 25)$$

$$H_w = 7195746 \frac{KJ}{hr}$$

To find reboiler duty;

$$Q_B = Q_C + H_w + H_D - H_F$$

$$Q_B = 2856707 + 7195746 + 436681 - 8529805$$

$$Q_B = 1959330 \frac{KJ}{hr}$$

Condenser Duty:

Water temperature at inlet = 25 ^oC

Water temperature at outlet = 146 ^oC

Q_C = 2856707 KJ/hr

C_p = 4.18 KJ/Kg.K

ΔT = 121 ^oC

$$m = Q/C_p\Delta T$$

$$m = \frac{2856707}{4.187 \times 121}$$

$$m = 5628 \frac{Kg}{hr}$$

Reboiler Duty:

Steam temperature = 180 ^oC

Steam Pressure = 10 bar

Latent heat of vaporization = 2006 KJ/Kg

Q_B = 1959330 KJ/hr

$$m = \frac{Q}{\lambda}$$

$$m = \frac{1959330}{2006}$$

$$m = 977 \frac{Kg}{hr}$$

4.8 Distillation Column (T-102):

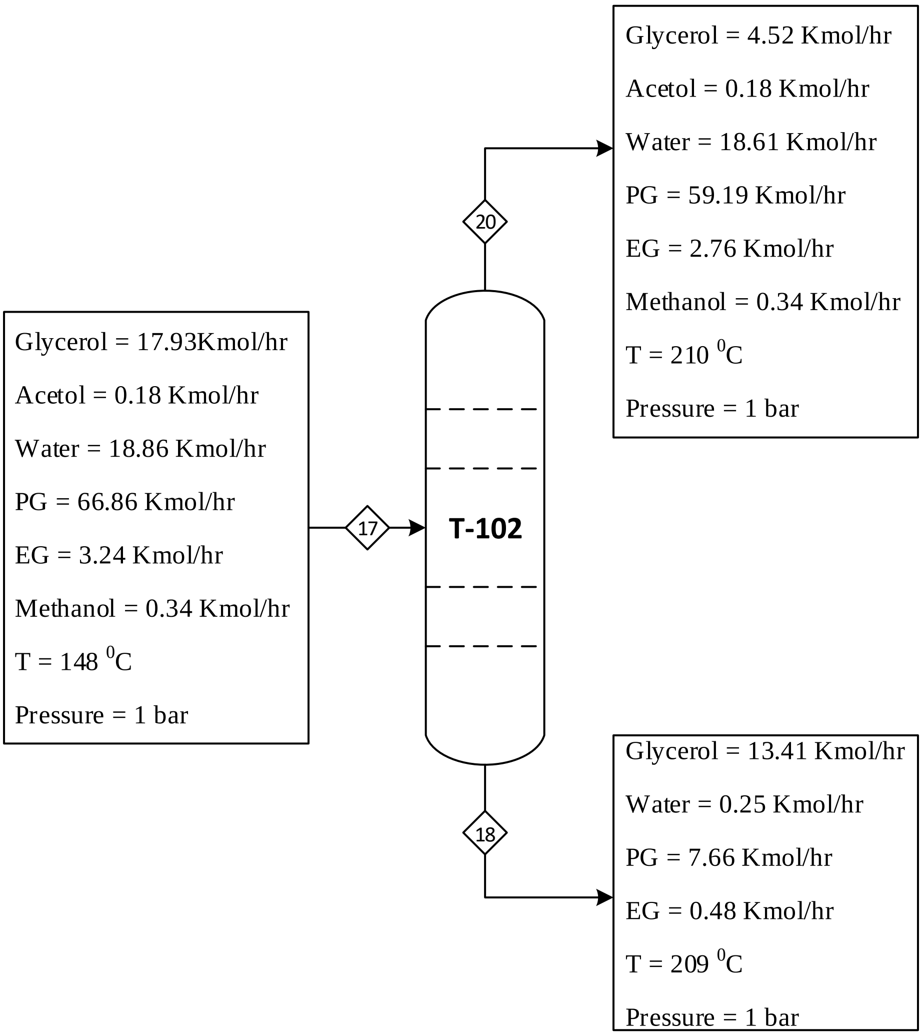


Figure 4-10 Energy Balance on (T-102)

Sample Calculation:

Formulas:

$$C_p = a + bT + cT^2 + dT^3$$

$$\text{Weighted } C_p = C_p \text{ Calculated} \times \text{Fraction of feed}$$

$$Q = mC_p\Delta T$$

$$Q = m\lambda$$

Calculation:

Table 4-17 (T-102) Feed at Inlet, Bottom and Distillate

Component	Feed kmol/hr	Fraction	Distillate Kmol/hr	Fraction	Bottom kmol/hr	Fraction
Glycerol	17.93	0.17	4.52	0.05	13.41	0.62
Acetol	0.18	0.00	0.18	0.00	0.00	0.00

Water	18.86	0.18	18.61	0.22	0.25	0.01
PG	66.86	0.62	59.19	0.69	7.66	0.35
EG	3.24	0.03	2.76	0.03	0.48	0.02
Methanol	0.34	0.00	0.34	0.00	0.00	0.00
Total	**107.41**	**1.0**	**85.60**	**1.0**	**21.81**	**1.0**

Total Feed at Inlet = 107.41 Kmol/hr

Total Feed at Distillate = 85.60 Kmol/hr

Total Feed at Bottom = 21.81 Kmol/hr

Heat Capacity:

Temperature at Feed = 148 ^{o}C

Temperature at Bottom = 209 ^{o}C

Temperature at Distillate = 210 ^{o}C

First we convert the temperature into degree kelvin and find the heat capacity at our desired temperature and then find weighted heat capacity by multiplying it with fraction.

Table 4-18 (T-102) Heat Capacity at Inlet, Bottom and Distillate

Component	**C_p of Feed KJ/Kmol. K**	**Weighted C_p**	**C_p (Distillate) KJ/Kmol.K**	**Weighted C_p of Distillate**	**C_p (Bottom) KJ/Kmol.K**	**Weighted C_p of Bottom**
Glycerol	146.46	24.45	159.88	8.44	159.65	98.19
Acetol	84.47	0.14	92.31	0.19	92.17	0.01
Water	34.66	6.09	35.23	7.66	35.22	0.40
PG	131.81	82.04	144.63	100.02	144.41	50.75
EG	115.96	3.49	124.12	4.00	123.98	2.73
Methanol	53.49	0.17	58.27	0.23	58.18	0.00
Total		**116.39**		**120.54**		**152.08**

Latent Heat of Vaporization:

We have found latent heat of vaporization of each component from Richardson Coulson Vol 6.

Table 4-19 (T-102) Latent heat of vaporization

Component	Latent Heat of Vaporization KJ/Kmol	Weighted λ of Feed	Weighted λ at Distillate	Weighted λ at Bottom
Glycerol	61,127	10,206	3,228	37,597
Acetol	30,145	51	63	2
Water	40,683	7,144	8,846	463
PG	54,177	33,723	37,464	19,040
EG	52,544	1,583	1,692	1,155
Methanol	35,278	112	140	3
Total		**52818.4**	**51432.3**	**58259.3**

Enthalpy at Distillate:

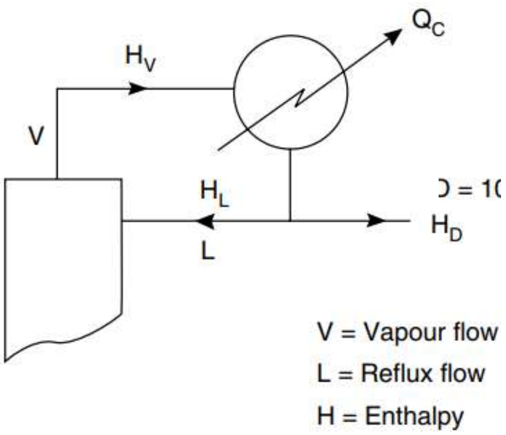


Figure 4-11 (T-101) Distillate

At steady state;

$$\text{input} = \text{output}$$

$$H_v = H_D + H_L + Q_C$$

$$\text{Enthalpy of vapor } H_v = \text{Latent} + \text{sensible heat}$$

$$H_v = mC_p\Delta T + m\lambda$$

$$H_v = 85.6 \times 120.54 \times (210 - 25) + 85.6 \times 51432.3$$

$$H_v = 6312806 \frac{KJ}{hr}$$

Now

$$\text{Enthalpy of Distillate } H_D = \text{Sensible Heat}$$

$$H_D = mC_p\Delta T$$

$$H_D = 58.6 \times 120.54 \times (210 - 25)$$

$$H_D = 1910167 \frac{KJ}{hr}$$

Here the enthalpy of the liquid is zero so;

$$Q_c = H_v - H_D$$

$$Q_c = 6312806 - 1910167$$

$$Q_c = 4402640 \frac{KJ}{hr}$$

Overall Balance:

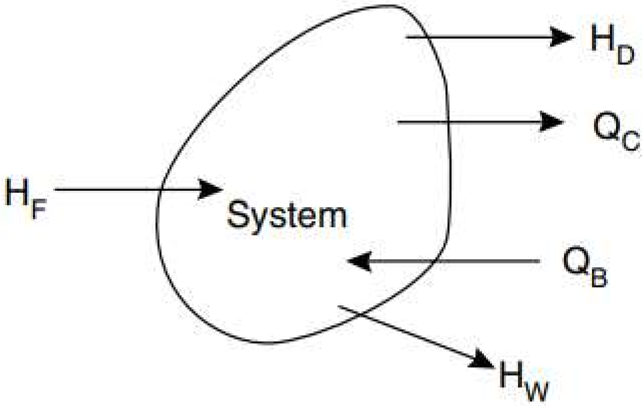


Figure 4-12 Overall System Balance

Where;

- Q_B is reboiler heat input
- H_F is distillation column feed at its bubble point
- Q_C is condenser cooling
- Top and bottom product H_D and H_W, respectively.

Q_B is determined from a balance over complete system;

$$\text{Input} = \text{output}$$

$$Q_B + H_F = Q_C + H_D + H_W$$

$$H_F = \text{latent heat} = m\lambda$$

$$H_F = 107.41 \times 52818.4$$

$$H_F = 5673098 \frac{KJ}{hr}$$

Now

$$H_w = \text{Latent heat} + \text{Sensible Heat}$$

$$H_w = m\lambda + mC_p\Delta T$$

$$H_w = 21.81 \times 58259.3 + 21.81 \times 152.08 \times (209 - 25)$$

$$H_w = 1880688\,\frac{KJ}{hr}$$

To find reboiler duty;

$$Q_B = Q_C + H_w + H_D - H_F$$

$$Q_B = 4402640 + 1880688 + 1910167 - 6312806$$

$$Q_B = 2520397\,\frac{KJ}{hr}$$

Condenser Duty:

Reference temperature = 25 ^{o}C

Water temperature at outlet = 210 ^{o}C

Q_C = 4402640 KJ/hr

C_p = 4.18 KJ/Kg.K

ΔT = 185 ^{o}C

$$m = Q/C_p\Delta T$$

$$m = \frac{4402640}{4.187 \times 185}$$

$$m = 5772\,\frac{Kg}{hr}$$

Reboiler Duty:

Steam temperature = 218 ^{o}C

Steam Pressure = 22 bar

Latent heat of vaporization = 1865 KJ/Kg

Q_B = 2520397 KJ/hr

$$m = \frac{Q}{\lambda}$$

$$m = \frac{2520397}{1865}$$

$$m = 1351\,\frac{Kg}{hr}$$

4.9 Heat Exchanger (E-104):

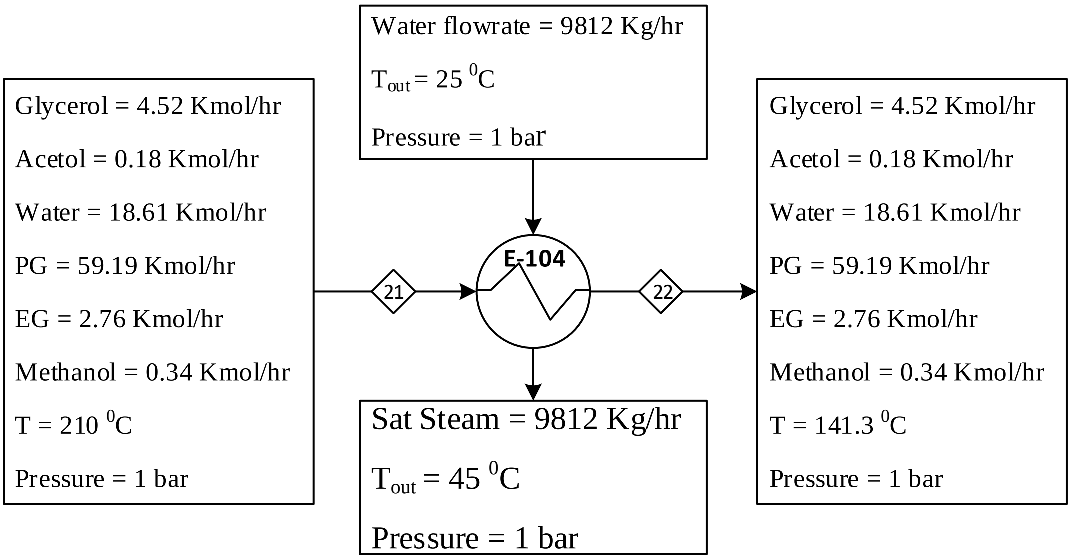


Figure 4-13 Energy Balance on (E-104)

Calculations:

Formula:

$$Q = \dot{m} C_p \Delta T$$

$$C_p = a + bT + cT^2 + dT^3$$

By solving above formula and putting the value of constant (a,b,c and d taken from Richardson Kulson Vol 6) and temperature (Kelvin), We calculate Enthalpy of the inlet and the outlet streams.

Water	**Feed**
Temperature of water at inlet = 25 ^{o}C	Temperature of feed at Inlet = 210 ^{o}C
Temperature of water at Outlet = 45 ^{o}C	Temperature of feed at Outlet = 141.3 ^{o}C
Pressure of steam at inlet = 1 bar	Pressure of feed at inlet = 1 bar
Pressure of Steam at outlet = 1 bar	Pressure of feed at outlet = 1 bar

Enthalpy:

Table 4-20 Heat Capacity in/out

Components	**Feed 5**	**Fraction**	**C_p(at inlet) Kj/kmol.K**	**Weighted C_p**	**C_p (at Oultet) Kj/kmol.K**	**Additive Cp**
Glycerol	4.52	0.1	159.9	8.4	144.9	7.7
Acetol	0.18	0.0	92.3	0.2	83.6	0.2
Water	18.61	0.2	35.2	7.7	34.6	7.5
Hydrogen	0.00	0.0	29.3	0.0	29.2	0.0

PG	59.19	0.7	144.6	100.0	130.3	90.1
EG	2.76	0.0	124.1	4.0	115.0	3.7
Methanol	0.34	0.0	58.3	0.2	53.0	0.2
Total kmol/h	85.60	1.0		120.5		109.4

Enthalpy at inlet:

$T_{in} = 210\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 185.1\ ℃$

$Q_{in} = mC_p\Delta T$

$$Q_{in} = 85.60 \times 120.5 \times 185.1 = 1910167\,\frac{KJ}{hr}$$

Enthalpy at Outlet:

$T_{out} = 141\ ℃$

$T_{ref} = 25\ ℃$

$\Delta T = 116\ ℃$

$Q_{out} = mC_p\Delta T$

$$Q_{out} = 85.60 \times 109.4 \times 116 = 1088539\,\frac{KJ}{hr}$$

$\Delta Q = -821628\ KJ/hr$

Here negative sign show the requirement of cooling.

Cooling Water Requirement:

$T_{in} = 25℃$

$T_{out} = 45℃$
$\Delta T = 20℃$

$$C_p = 4.187\,\frac{KJ}{Kg.K}$$

$$\Delta Q = 821628\ \frac{KJ}{hr}$$

$$m = \frac{Q}{C_p\Delta T}$$

$$m = \frac{821628}{4.187 \times 20}$$

$$m = 9812\,\frac{Kg}{hr}$$

4.10 Distillation Column (T-103):

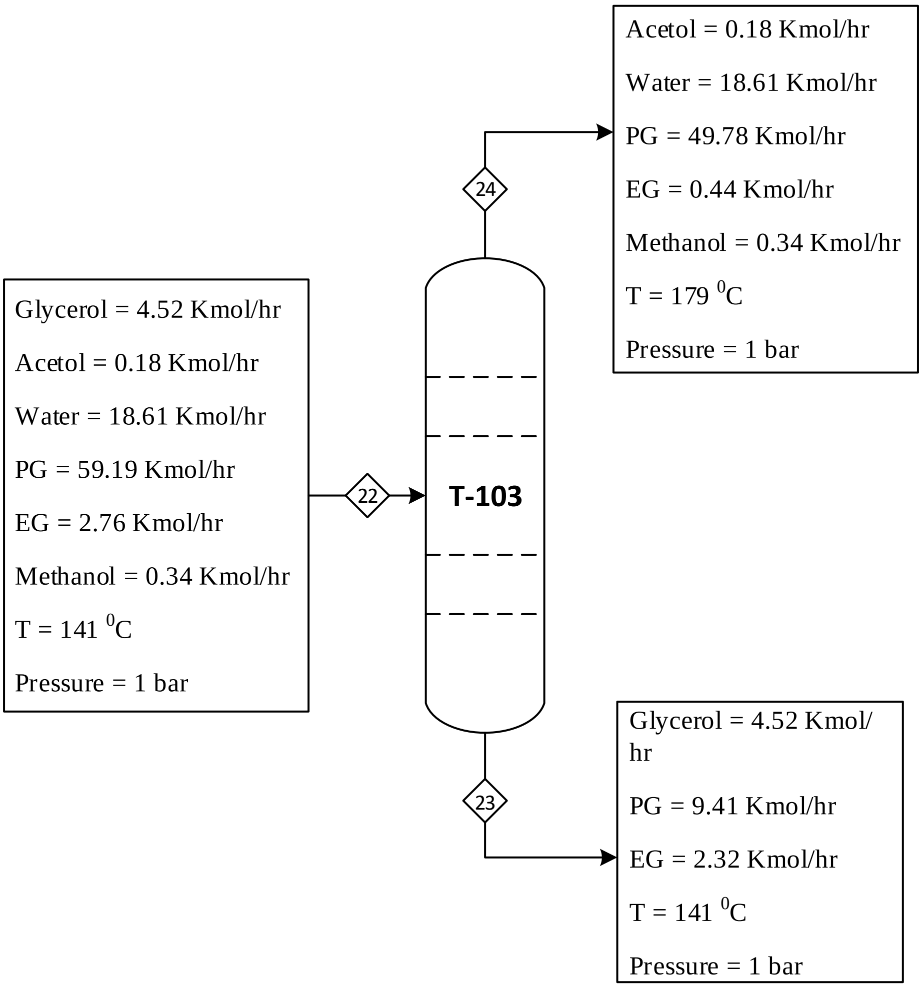


Figure 4-14 Energy Balance on (T-103)

Sample Calculation:

Formulas:

$$C_p = a + bT + cT^2 + dT^3$$

$$\text{Weighted } C_p = C_p \text{ Calculated} \times \text{Fraction of feed}$$

$$Q = mC_p\Delta T$$

$$Q = m\lambda$$

Calculation:

Table 4-21 (T-103) Feed at Inlet, Bottom and Distillate

Component	Feed kmol/hr	Fraction	Distillate Kmol/hr	Fraction	Bottom kmol/hr	Fraction
Glycerol	4.52	0.05	-	-	4.52	0.28
Acetol	0.18	0.002	0.18	0.003	-	-
Water	18.61	0.22	18.61	0.27	-	-

PG	59.19	0.69	49.78	0.72	9.41	0.58
EG	2.76	0.03	0.44	0.01	2.32	0.14
Methanol	0.34	0.004	0.34	0.005	-	-
Total	**85.60**	**1.00**	**69.35**	**1.0**	**16.2**	**1.0**

Total Feed at Inlet = 85.60 Kmol/hr

Total Feed at Distillate = 69.35 Kmol/hr

Total Feed at Bottom = 16.2 Kmol/hr

Heat Capacity:

Temperature at Feed = 141 ^oC

Temperature at Bottom = 179 ^oC

Temperature at Distillate = 141 ^oC

First we convert the temperature into degree kelvin and find the heat capacity at our desired temperature and then find weighted heat capacity by multiplying it with fraction.

Table 4-22 (T-103) Heat Capacity at Inlet, Bottom and Distillate

Component	**C_p of Feed KJ/Kmol. K**	**Weighted C_p**	**C_p (Distillate) KJ/Kmol.K**	**Weighted C_p of Distillate**	**C_p (Bottom) KJ/Kmol.K**	**Weighted C_p of Bottom**
Glycerol	144.90	7.65	153.29	-	144.90	40.31
Acetol	83.57	0.17	88.45	0.23	83.57	-
Water	34.60	7.52	34.94	9.38	34.60	-
PG	130.32	90.12	138.33	99.30	130.32	75.48
EG	115.02	3.70	120.11	0.76	115.02	16.40
Methanol	52.96	0.21	55.87	0.27	52.96	-
Total		**109.38**		**109.94**		**132.19**

Latent Heat of Vaporization:

We have found latent heat of vaporization of each component from Richardson Coulson Vol 6.

Table 4-23 (T-103) Latent heat of vaporization

Component	**Latent Heat of Vaporization KJ/Kmol**	**Weighted λ of Feed**	**Weighted λ at Distillate**	**Weighted λ at Bottom**

Glycerol	61,127	3,228	-	17,005
Acetol	30,145	63	78	-
Water	40,683	8,846	10,919	-
	904	-	-	-
PG	54,177	37,464	38,890	31,378
EG	52,544	1,692	332	7,494
Methanol	35,278	140	172	-
Total		**51432.3**	**50390.7**	**55877.5**

Enthalpy at Distillate:

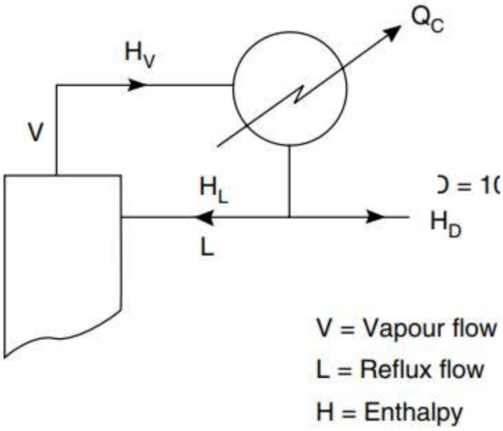


Figure 4-15 (T-103) Distillate

At steady state;

$$\text{input} = \text{output}$$

$$H_v = H_D + H_L + Q_C$$

$$\text{Enthalpy of vapor } H_v = \text{Latent} + \text{sensible heat}$$

$$H_v = mC_p\Delta T + m\lambda$$

$$H_v = 69.35 \times 109.94 \times (179 - 25) + 69.35 \times 50390.7$$

$$H_v = 4667334\,\frac{KJ}{hr}$$

Now

$$\text{Enthalpy of Distillate } H_D = \text{Sensible Heat}$$

$$H_D = mC_p\Delta T$$

$$H_D = 69.35 \times 109.94 \times (179 - 25)$$

$$H_D = 1172704\,\frac{KJ}{hr}$$

Here the enthalpy of the liquid is zero so;

$$Q_c = H_v - H_D$$

$$Q_c = 4667334 - 1172704$$

$$Q_c = 3494631 \frac{KJ}{hr}$$

Overall Balance:

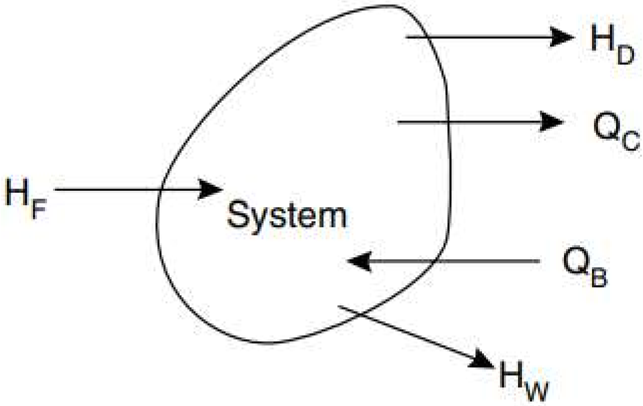


Figure 4-16 Overall System Balance

Where;

- Q_B is reboiler heat input
- H_F is distillation column feed at its bubble point
- Q_C is condenser cooling
- Top and bottom product H_D and $H_{W,}$ respectively.

Q_B is determined from a balance over complete system;

$$\text{Input} = \text{output}$$

$$Q_B + H_F = Q_C + H_D + H_W$$

$$H_F = \text{latent heat} = m\lambda$$

$$H_F = 85.60 \times 51432.3$$

$$H_F = 4402640 \frac{KJ}{hr}$$

Now

$$H_w = \text{Latent heat} + \text{Sensible Heat}$$

$$H_w = m\lambda$$

$$H_w = 16.2 \times 55877.5$$

$$H_w = 908009 \frac{KJ}{hr}$$

To find reboiler duty;

$$\mathrm{Q_B = Q_C + H_w + H_D - H_F}$$

$$\mathrm{Q_B = 3494631 + 908009 + 1172704 - 4402640}$$

$$\mathrm{Q_B = 1172704\,\frac{KJ}{hr}}$$

Condenser Duty:

Reference temperature = 25 ^{o}C

Water temperature at outlet = 179 ^{o}C

Q_C = 3494631 KJ/hr

C_p = 4.18 KJ/Kg.K

ΔT = 154 ^{o}C

$$\mathrm{m = Q/C_p\Delta T}$$

$$\mathrm{m = \frac{3494631}{4.187 \times 154}}$$

$$\mathrm{m = 5515\,\frac{Kg}{hr}}$$

Reboiler Duty:

Steam temperature = 180 ^{o}C

Steam Pressure = 10 bar

Latent heat of vaporization = 2006 KJ/Kg

Q_B = 1172704 KJ/hr

$$\mathrm{m = \frac{Q}{\lambda}}$$

$$\mathrm{m = \frac{1172704}{2006}}$$

$$\mathrm{m = 585\,\frac{Kg}{hr}}$$

CHAPTER NO. 5
EQUIPMENT DESIGN

5.1 Design of Multi-Tube Packed Bed Reactor (R-101):

5.1.1 Glycerol Synthesis:

Hydrogenolysis of glycerol is a chemical reaction in which glycerol is converted to propylene glycol using hydrogen gas and a catalyst. The process involves breaking the C-O bond of the glycerol molecule and forming a C-C bond between two of the resulting fragments.

This reaction is typically carried out at high pressures (around 54 bar) and temperatures (around 190°C) in the presence of a catalyst. The hydrogen gas is usually supplied in excess to drive the reaction towards completion.

5.1.2 Selection of Multi-tube Packed Bed Reactor:

Multi-tube packed bed reactors are widely used in the chemical and petrochemical industries for carrying out a range of catalytic reactions. These reactors are designed to provide high surface area contact between the reactants and the catalyst, which promotes efficient reaction kinetics and maximizes conversion and selectivity.

The selection of a multi-tube packed bed reactor depends on several factors, including the nature of the reaction, the required conversion and selectivity, the reaction conditions, and the economics of the process.

Here are some key considerations when selecting a multi-tube packed bed reactor:

i. Reactor Size and Configuration:

The size and configuration of the reactor should be selected to optimize the reaction conditions and ensure efficient heat and mass transfer. The number and diameter of the tubes, as well as the length and arrangement of the packing, can affect the performance of the reactor.

ii. Catalyst Selection:

The choice of catalyst depends on the specific reaction and the desired selectivity and activity. The catalyst should have high surface area, good stability, and resistance to deactivation under the reaction conditions.

iii. Operating Conditions:

The operating conditions, including temperature, pressure, and flow rate, can affect the reaction kinetics, selectivity, and catalyst life. The reactor should be designed to provide optimal conditions for the reaction, while minimizing any undesirable side reactions or catalyst deactivation.

iv. Safety Considerations:

Multi-tube packed bed reactors can pose safety risks due to the high pressure and temperature conditions. The reactor should be designed with appropriate safety features, such as relief valves and pressure gauges, to ensure safe operation.

v. Economic Factors:

The selection of a multi-tube packed bed reactor also depends on the economics of the process. The capital and operating costs, as well as the expected yields and product quality, should be evaluated to ensure the viability of the process.

vi. Temperature Control:

Temperature control is a critical aspect of operating a multi-tube packed bed reactor, especially for exothermic reactions. Failure to control temperature can result in decreased conversion and selectivity, catalyst deactivation, and even reactor runaway. For moderate exothermic reactions, temperature control can be achieved through various means, such as:

- **Heat removal through a cooling fluid:**

This involves passing a cooling fluid, such as water, through a heat exchanger that is in contact with the reactor. This can help to remove excess heat generated by the reaction and maintain the desired temperature.

- **Controlled flow rate:**

By adjusting the flow rate of reactants or cooling fluid, the temperature of the reactor can be controlled. Increasing the flow rate of cooling fluid can help to decrease the reactor temperature, while increasing the flow rate of reactants can help to increase the temperature.

- **Catalyst dilution:**

By diluting the catalyst with an inert material, the heat generated by the reaction can be spread out over a larger volume, reducing the temperature rise.

5.1.3 Why we select Packed Bed Reactor:

The reaction that is occurred in reactor is three phase reaction. In which glycerol (liquid phase) is feed from the top of the reactor and hydrogen (gas phase) is feed from bottom of the reactor and reaction is proceed under the packing of catalyst known as Cu-ZnO-Al_2O_3 (solid phase). The reaction conversion can be achieved up to 85.1% with the selectivity of 94.6%.

5.1.4 Design Calculation (R-101):

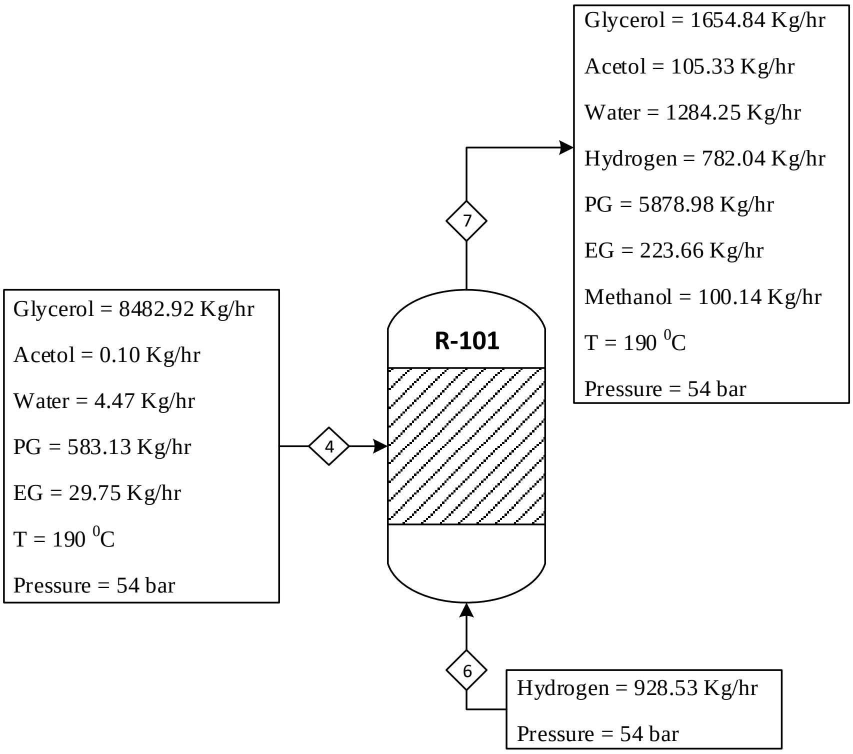


Figure 5-1 Design (R-101)

Reaction:

The reaction that can be occur in the reactor is given below.

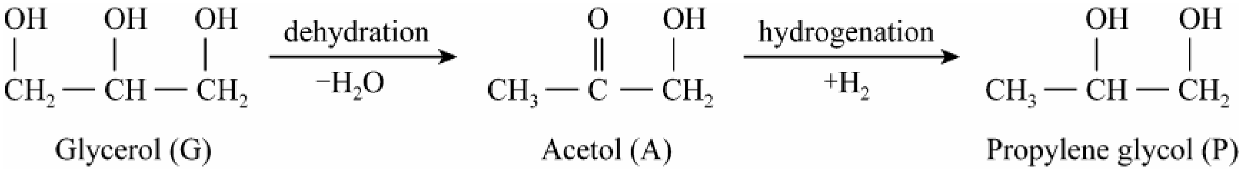


Figure 5-2 Overall Reaction

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

$$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

Rate equation is given by;

$$r_1 = \frac{k_1 b_G C_G}{1 + b_G C_G + b_A C_A + b_P C_P}$$

$$r_2 = \frac{k_2 b_A C_A b_H P_H}{(1 + b_G C_G + b_A C_A + b_P C_P)(1 + \sqrt{b_H P_H})^2}$$

Where;

$$C_G = C_{Go}(1 - X_G)$$

$$C_A = C_{Ao}\frac{(1 + X_G)}{(1 + \varepsilon X_G)}$$

$$C_A = \frac{C_{Go}X_G}{1+\varepsilon X_G}$$

$$Cp = \frac{F_{Pf}}{V_f}$$

So both of the rate equation will become;

$$r_1 = \frac{k_1 b_G C_{Go}(1-X_G)}{1+b_A\frac{C_{Go}X_G}{1+\varepsilon X_G}+b_G C_{Go}(1-X_G)+b_P C_P}$$

$$r_2 = \frac{k_2 b_A\frac{C_{Go}X_G}{1+\varepsilon X_G}b_H P_H}{(1+b_A\frac{C_{Go}X_G}{1+\varepsilon X_G}+b_G C_{Go}(1-X_G)+b_P C_P)(1+\sqrt{b_H P_H})^2}$$

Where;

$$C_{Go} = \frac{F_{Go}}{V_o} = \frac{92.12}{41.008} = 2.25\frac{Kmol}{m^3} = 2246.26\frac{mol}{m^3}$$

$$C_p = \frac{F_{Pf}}{V_f} = \frac{77.26}{413.86} = 0.1866\frac{Kmol}{m^3} = 186.68\frac{mol}{m^3}$$

$$k_i = k_i^{\circ}\exp(-\frac{E_i}{R_g T})$$

$$b_j = b_j^{\circ}\exp(\frac{Q_j}{R_g T})$$

Table 5-1 Estimated Kinetic Parameter

Parameters	**Pre-exponential Factor (mol/g.s)**	**Activation Energy (KJ/mol)**
k_1	15400	86.56
k_2	7160	57.8
b_G	0.00222	36.42
b_A	0.00873	25.94
b_P	0.0058	25.77
b_H	0.0000186	36.24

After Calculation;

Table 5-2 Calculated Parameter

Parameter	**Value**	**Units**
k_1	2.64E-06	mol/gs
k_2	0.0022	mol/g.s
b_G	28.53	m3/mol

b_A	7.37	m3/mol
b_P	4.68	m3/mol
b_H	0.23	MPa^{-1}

Where;

Pressure = 54.71 bar, Temperature = 190°C, R = 0.008314 KJ/mol.K

Weight of bed:

Reaction 1:

Where;

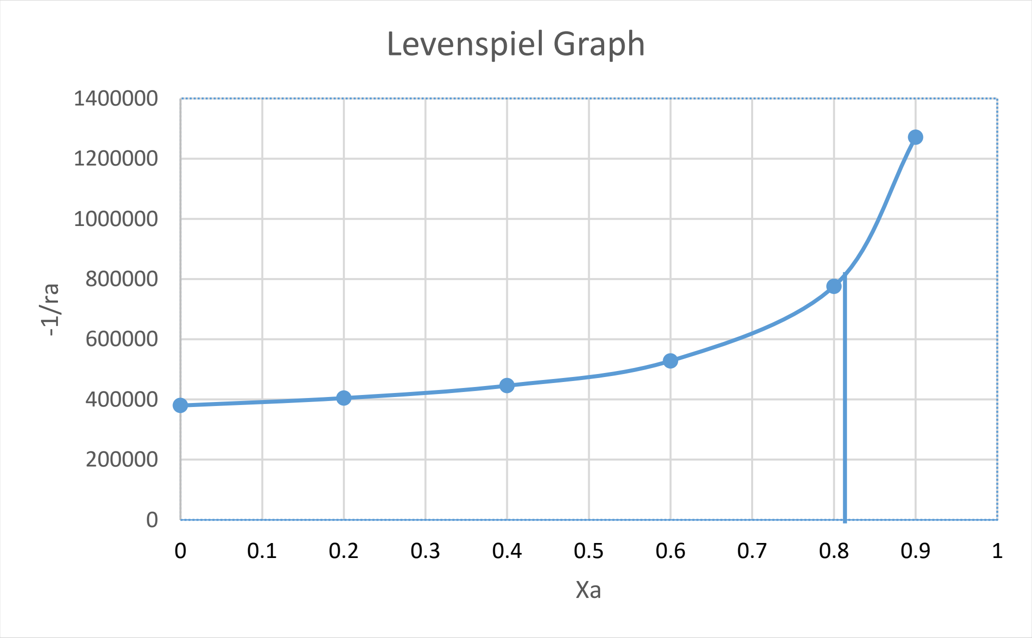
Xa = 81.5%

$\frac{W}{Fao}$ =373322424.7 g.s/Kmol (Through Simpson Five Point Rule)

F_{AO} = 92.12 Kmol/hr OR 8482.92 Kg/hr

W = 9552.4 Kg

Table 5-3 Levenspiel Graph-1



Reaction 2:

Where;

Xa = 81.5%

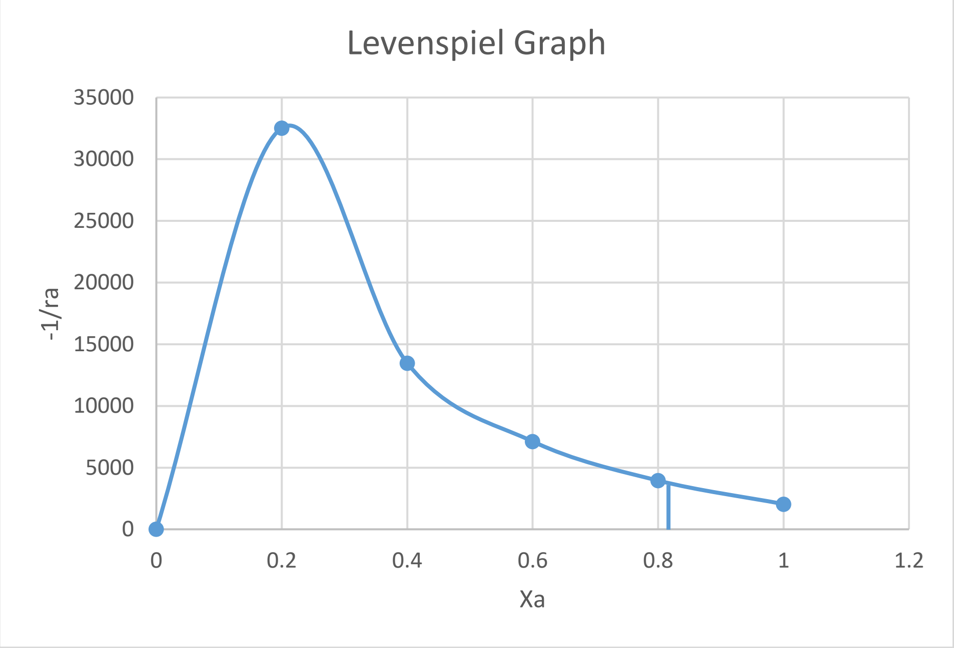
$\frac{W}{Fao}$ =1310353590.67 g.s/Kmol (Through Simpson Five Point Rule)

$$F_{A0} = 92.12 \text{ Kmol/hr OR } 8482.92 \text{ Kg/hr}$$

W = 363.99 Kg

Total Weight = 9916.44 Kg

Table 5-4 Levenspiel Graph-2



Volume of Catalyst:

Where

Bulk density of catalyst = 2500Kg/m3

$$\text{Volume of catalyst} = \frac{\text{Weight of Bed}}{\text{Density}}$$

$$= \frac{9916.44}{2500} = 4.0 \text{ m}^3$$

Volume of Reactor:

Porosity = 0.29

For Volume of Reactor

$$\text{Volume of Reactor} = \frac{\text{Vcatalyst}}{1 - \varepsilon} = \frac{4.0}{1 - 0.29} = 5.6 \text{ m}^3$$

Space Time:

For space time we have

$$\text{Vo} = \frac{\text{Total mass flow rate}}{\text{Weighted Density}} = \frac{10028.9}{222.52} = 45.07 \, {}^{\text{m}^3}\!/_{\text{hr}}$$

$$\tau = \frac{\text{Volume of reactor}}{\text{Vo}} = \frac{5.6}{45.07} = 0.124\ \text{hr}$$

Tube Diameter:

$$\text{length of tube} = 16\text{ft} = 4.87\text{m}$$

To prevent deviations from plug flow assumptions;

$$^{\text{Dt}}/_{\text{Dp}} > 15$$

$\text{Dt} = \text{diameter of tube} = 8\ \text{cm} = 0.08\text{m}$

$\text{Dp} = \text{diameter of particle} = 0.00034\text{m}$

By putting values;

$$\frac{\text{Dt}}{\text{Dp}} = \frac{0.08}{0.00034} = 235.29 > 15$$

Volume of one tube:

For volume of one tube

$$\text{Volume of one tube} = \frac{\pi}{4} \times \text{Dt}^2 \times \text{L} = 0.02\ \text{m}^3$$

Number of tube:

$$\text{Nt} = \frac{\text{Total Volume}}{\text{Volume of one Tube}} = 228$$

Length of reactor:

$$\text{Length of tube} = 16\text{ft}$$

$$\text{For top domb} = 20\%\ \text{allowance} = 0.2 \times 16 = 3.2\text{ft}$$

$$\text{For bottom domb} = 20\%\ \text{allowance} = 0.2 \times 16 = 3.2\text{ft}$$

$$\text{Total length} = 22.4\text{ft} = 6.83\text{m}$$

Diameter of Shell:

For diameter of Shell;

$$\text{Nt} = \frac{\left((\text{Ds} - \text{K}_1)^2 \frac{\pi}{4} + \text{K}_2\right) - \text{P}_t(\text{D}_s - \text{K}_1)(\text{nK}_3 + \text{K}_4)}{1.223\text{P}_t^2}$$

Where;

$\text{N}_t = 228 = \text{No of tubes}$

$\text{P}_t = 1\ \text{inch square pitch} = 0.0254\text{m}$

$\text{Length of tube} = 16\text{ft} = 4.87\text{m}$

For this pitch

$K_1 = 1.08$ $K_2 = -0.9$

$K_3 = 0.69$ $K_4 = -0.8$

$n = 1$ (Tube passes)

Solving above equation for D_S will give us;

$$D_s = 2.24\text{m}$$

Pressure Drop:

For pressure drop we have the relation;

$$\frac{\Delta P}{L} = \frac{150\mu G(1-\varepsilon)^2}{\rho d_p^2 \varepsilon^3} + \frac{1.75G^2(1-\varepsilon)}{\rho d_p \varepsilon^3}$$

$$G = \text{Mass velocity} = \frac{\text{Mass Flow Rate}}{\text{Area of Reactor}} = 1.117\,\frac{\text{Kg}}{\text{m}^2\text{s}}$$

$$\text{Area of Reactor} = \frac{\text{Volume of Reactor}}{\text{Diameter of Reactor}} = 2.49\text{m}^2$$

Table 5-5 Components

Component	**Flow rate**	**Fraction**	**Viscosity Pa.s**	**Weighted Viscosity**
Glycerol	92.11558887	0.164173718	0.0003	4.92521E-05
Acetol	0.001382123	2.4633E-06	2.66E-04	6.56039E-10
Water	0.247967035	0.000441941	1.41E-04	6.23249E-08
Hydrogen	460.5779443	0.820868588	0.00E+00	0
Propylene Glycol	7.663745188	0.013658769	5.71E-04	7.79312E-06
Ethylene Glycol	0.479459618	0.000854521	5.72E-04	4.88629E-07
Total	561.0860872	1		5.75968E-05

$\text{Weighted Viscosity} = 5.76 \times 10^{-5}\ \text{Pa. sec}$

$$\text{Weighted Density} = 222.52$$

$$\Delta P = 0.586\ \text{bar}$$

Cooling Water Requirement:

For cooling Water we have, ($Q = mC_p\,\Delta T$) where;

$$Q = \text{Heat Load} = -4.57 \times 10^6\,\frac{\text{KJ}}{\text{hr}}$$

$$C_p = 4.178\,\frac{\text{KJ}}{\text{Kg. K}}$$

$$\Delta T = T_2 - T_1 = 25 - 45 = 20℃$$

$$m = 5.68 \times 10^4\,\frac{\text{Kg}}{\text{hr}}$$

<table>
<tr><th colspan="2">SPECIFICATION SHEET</th></tr>
<tr><th colspan="2">Identification</th></tr>
<tr><td>Item</td><td>Reactor</td></tr>
<tr><td>Item no.</td><td>R-101</td></tr>
<tr><td>No. of required</td><td>1</td></tr>
<tr><td>Operation</td><td>Continuous</td></tr>
<tr><td>Type</td><td>Multi tube packed bed Reactor</td></tr>
<tr><td>Catalyst</td><td>Cu-ZnO-Al_2O_3</td></tr>
<tr><th colspan="2">Function</th></tr>
<tr><td colspan="2">Hydrogenolysis of Glycerol to Propylene Glycol</td></tr>
<tr><th colspan="2">Chemical Reactions</th></tr>
<tr><td colspan="2">$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$
$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$</td></tr>
<tr><td>Weight of bed</td><td>10181.12 Kg</td></tr>
<tr><td>Volume of Catalyst</td><td>4.1 m^3</td></tr>
<tr><td>Volume of Reactor</td><td>5.74 m^3</td></tr>
<tr><td>Space Time</td><td>0.127 hr</td></tr>
<tr><td>Diameter of tube</td><td>0.08 m</td></tr>
<tr><td>Number of Tube</td><td>235</td></tr>
<tr><td>Diameter of shell</td><td>2.25 m</td></tr>
<tr><td>Length of reactor</td><td>6.83 m</td></tr>
<tr><td>Pressure drop</td><td>0.57 bar</td></tr>
</table>

5.2 Design of Gas-Liquid Separator (V-101):

The vapor liquid separators are used to separate two phase inlets into pure vapors and pure liquid. It basically helps in recovering valuable products and improves product purity. If two phase separators are used after flashing a hot liquid across a valve, it is called a flash separator.

5.2.1 Types of Separators:

1. **Vertical separator:**

- Used where vapor flow is large as compared to liquid flow.
- Good separation efficiency.
- By rule of thumb it is commonly preferable in oil refineries.
- 50% LL must be retained in the separator during operation.

2. **Horizontal separator:**

- Used when the liquid content of the incoming stream is high.

3. **L/D ratio specification:**

- (L/D) ratio is 2 for the case of knockout drum.
- If length to diameter (L/D) ratio lies between 3 and 5, then it will be vertical separator.
- If length to diameter (L/D) ratio is greater than 5 then it will be horizontal separator.

Reference: R. Harry Silla- Chemical Process Engineering

5.2.2 Phenomenon:

The vapor & liquid mixture is separated by gravity and impaction in the separator. The mixture enters the separator and strikes the splash plate where it loses its momentum. Most of the liquid flows downwards and vapors along with liquid drop flow upward. As the vapor rises, large drops settle to the bottom of separator by gravity. Normal separation efficiency is 95% which can be increased to 99.9% by using a mist eliminator. Vortex formation must be prevented to reduce gas entrainment in the liquid by using a vortex breaker at the bottom.

Splash plate:

It is used to cause the initial bulk separation of liquid and gas. It provides a means to cause a sudden and rapid change of momentum (velocity and direction) of the entering stream. If it is not present then the vapors will escape very rapidly without contacting with liquid to establish equilibrium.

Vortex breaker:

A vortex breaker is normally installed on the liquid outlet to prevent formation of vortex when the liquid outlet valve is open. The formation of a vortex at the liquid outlet may result in withdrawal and entrainment of gas with the exiting liquid. This causes the loss of valuable vapors, pump damage and abnormal liquid level readings.

Mist eliminator:

Mist elimination or demisting can be defined as the mechanical separation of liquids from gases. Mesh usually consists of 0.011inch diameter wires to form a pad of 4 to 6 inches thick

& pressure drop is less than 1inch of water.

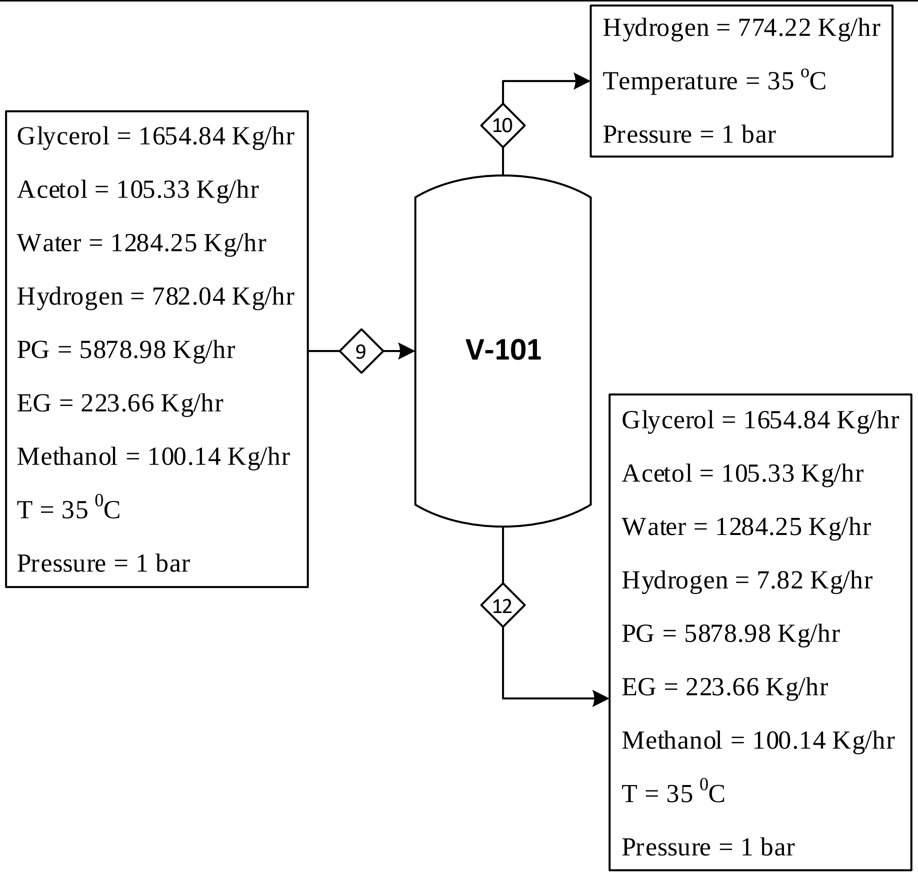


Figure 5-3 Gas Liquid Separator Design (V-101)

5.2.3 Design Steps:

1. Calculate vapor velocity.
2. Calculate cross-sectional area.
3. Calculate diameter.
4. Calculate vapor height.
5. Calculate volume.
6. Calculate liquid height.
7. Calculate total length.
8. Check L/D ratio.

Operating Conditions:

Design Pressure = 1 atm Design Temperature = 35°C

Mass flow rate of liquid = 9255 kg/hr

Mass flow rate of vapor = 774 kg/hr

Volumetric flow rate liquid = 9.08 m3/hr

Volumetric flow rate of vapor =9717 m3/hr

Density of liquid = ρ_l = 1018.88 kg/m3

Density of vapor= ρ_v = 0.0796 kg/m3

Calculation of vapor velocity:

Select K_v value and put in the equation given below:

$K_v = 0.14$ m/s

Maximum vapor velocity (Shouder Brown Equation):

$U_{max} = \left[\frac{K_V(\rho_L - \rho_V)}{\rho_V}\right]^{0.5}$

$U_{max} = 3.6850$ m/s

Calculation of cross-sectional area:

$A = \frac{Q_v}{V_v}$

$A = \frac{2.6991}{3.6850} = 0.7324\ m^2$

Calculate Diameter:

$D = \sqrt{\frac{4 \times A}{\pi}}$

Put the value of A in above equation.

$D = \sqrt{\frac{4 \times 0.7324}{3.14}}$

D = 0.9659 m

Selection of surge time:

(Times, t lies from 2 to 5 min) Let us use t = 4 min.

Height of Separator:

Vapor height h_v:

$h_v = 1.5D + 1.5$

$h_v = 1.5\ (0.9659) + 1.5$

$h_v = 2.949$ m

Liquid height hL:

$h_L = (Q\ L \times t)/A$

$h_L = (0.00252 * 4)/\ 0.7324$

$h_L = 0.0138$ m

Total height:

$h = h_L + h_v$

h = 0.0138 + 2.949

$h = 2.9627\ m \approx 3\ m$

Check L/D ratio:

$L/D = 3/0.9659 = 3.067$

$L/D = 3 < 5$

So, we can use Vertical separator.

Specification Sheet:

Specification Sheet	
Identification	Gas-Liquid Separator V-101
Types	Phase Separator
Function	
Separation of hydrogen gas	
No. Required	1
Operating Pressure	1 atm
Operating Temperature	35^o C
Area	$0.7324\ m^2$
Diameter	0.9659 m
Length	3 m
Material of Construction	Stainless Steel

5.3 Design of Distillation Column (T-101):

5.3.1 Distillation:

In industry it is common practice to separate a liquid mixture by distilling the components, which have lower boiling points when they are in pure condition from those having higher boiling points. This process is accomplished by partial vaporization and subsequent condensation.

“Process in which a liquid or vapor mixture of two or more substances is separated into its component fractions of desired purity, by the application and removal of heat”.

5.3.2 Types of distillation columns:

There are many types of distillation columns, each designed to perform specific types of separations, and each design differs in terms of complexity.

- Batch columns
- Continuous columns

- **Batch Columns:**

In batch operation, the feed to the column is introduced batch-wise. That is, the column is charged with a 'batch' and then the distillation process is carried out. When the desired task is achieved, a next batch of feed is introduced.

- **Continuous Columns:**

In contrast, continuous columns process a continuous feed stream. No interruptions occur unless there is a problem with the column or surrounding process units. They are capable of handling high throughputs and are the more common of the two types. We shall concentrate only on this class of columns.

5.3.3 Choice between Plate and Packed Column:

Vapor liquid mass transfer operation may be carried either in plate or packed column. These two types of operation are quite different. The relative merits of plate over packed column are as follows:

1. Plate column are designed to handle wide range of liquid flow rates without flooding.
2. If a system contains solid contents; it will be handled in plate column, because solid will accumulate in the voids, coating the packing materials and making it ineffective.
3. Dispersion difficulties are handled in plate column when flow rate of liquid are low as compared to gases.
4. For large column heights, weight of the packed column is more than plate column.
5. If periodic cleaning is required, man holes will be provided for cleaning. In packed columns packing must be removed before cleaning.
6. For non-foaming systems the plate column is preferred.
7. Design information for plate column is more readily available and more reliable than that for packed column.
8. Inter stage cooling can be provided to remove heat of reaction or solution in plate column.
9. When temperature change is involved, packing may be damaged.

Our mixture which is to be processed is “Acrylonitrile, Acetonitrile”. I’ve selected plate column because:

- System is non-foaming.
- Temperature is high i.e. 80C.

5.3.4 Choice of Plate Type:

There are three main types, sieve tray, bubble cap, valve tray. I’ve selected sieve tray because:

1. They are lighter in weight and less expensive. It is easier and cheaper to install.
2. Pressure drop is low as compared to bubble cap trays.
3. Peak efficiency is generally high.
4. Maintenance cost is reduced due to the ease of cleaning.

5.3.5 Selection Criteria of Trays:

Cost:

Cost of plate depends upon material of construction used.

For mild steel, the ratio of cost between plates is

Sieve plate	:	Valve plate	:	Bubble-Cap Plate
3	:	1.5	:	1.0

Capacity:

Sieve tray > Valve tray > Bubble-cap tray

Operating Range:

It is the range of liquid and vapor flow rates which must be above the weeping conditions and below the flooding conditions. Operating range flexibility comparison is

Bubble cape tray > Valve tray > Sieve tray

For good design, sieve plate gives satisfactory operating range.

Pressure drop:

Bubble-cap tray > Valve tray > Sieve tray

5.3.6 Main Components of Distillation Columns:

Column internals such as trays/plates and/or packing which are used to enhance component separations.

- A reboiler to provide the necessary vaporization for the distillation process. The liquid removed from the reboiler is known as the bottoms product or simply, bottoms.
- A condenser to cool and condense the vapor leaving the top of the column. The condensed liquid that is removed from the system is known as the distillate or top product.
- A reflux drums to hold the condensed vapor from the top of the column so that liquid (reflux) can be recycled back to the column. The condensed liquid is stored in a holding vessel known as the reflux drum. Some of this liquid is recycled back to the top of the column and this is called the reflux.

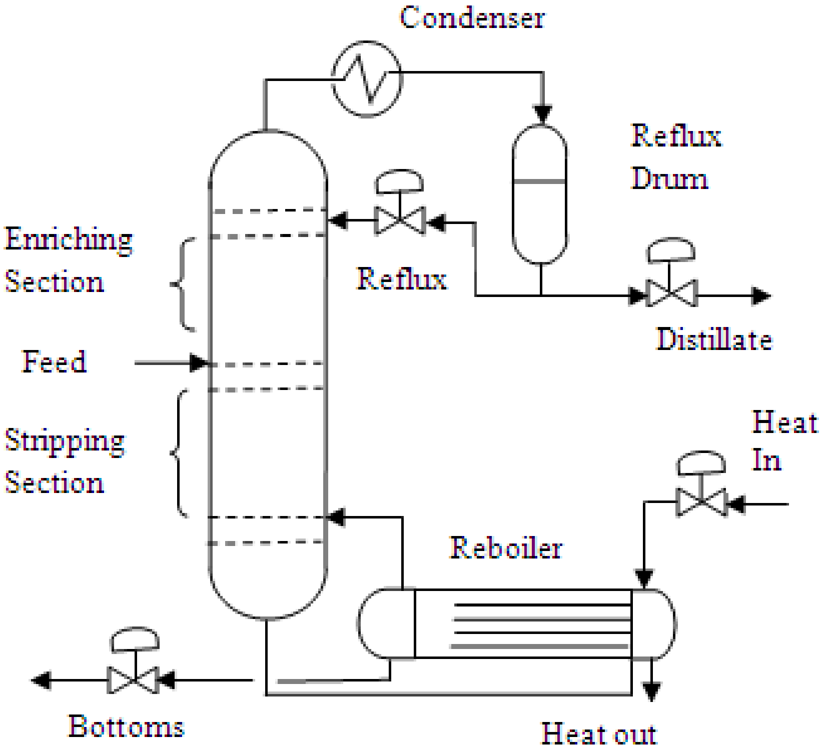


Figure 5-4 Main components of distillation column

A schematic of a typical distillation unit with a single feed and two product streams is shown above.

5.3.7 Factors Affecting Distillation Column Operation:

Vapor Flow Conditions:

Adverse vapor flow conditions can cause:

Foaming: Foaming refers to the expansion of liquid due to passage of vapor or gas. Although it provides high interfacial liquid-vapor contact, excessive foaming often leads to liquid buildup on trays. In some cases, foaming may be so bad that the foam mixes with liquid on the tray above. Whether foaming will occur depends primarily on physical properties of the liquid mixtures, but is sometimes due to tray designs and condition. Whatever the cause, separation efficiency is always reduced.

Entrainment: Entrainment refers to the liquid carried by vapor up to the tray above and is again caused by high vapor flow rates. It is detrimental because tray efficiency is reduced: lower volatile material is carried to a plate holding liquid of higher volatility. It could also contaminate high purity distillate. Excessive entrainment can lead to flooding.

Weeping/Dumping:

This phenomenon is caused by low vapor flow. The pressure exerted by the vapor is insufficient to hold up the liquid on the tray. Therefore, liquid starts to leak through perforations. Excessive weeping will lead to dumping. That is the liquid on all trays will crash (dump) through to the base of the column (via a domino effect) and the column will have to be re-started. Weeping is indicated by a sharp pressure drop in the column and reduced separation efficiency.

Flooding: Flooding is brought about by excessive vapor flow, causing liquid to be entrained in the vapor up the column. The increased pressure from excessive vapor also backs up the liquid in the down comer, causing an increase in liquid holdup on the plate above. Depending on the degree of flooding, the maximum capacity of the column may be severely reduced. Flooding is detected by sharp increases in column differential pressure and significant decrease in separation efficiency.

Reflux Conditions: Minimum trays are required under total reflux conditions, i.e. there is no withdrawal of distillate. On the other hand, as reflux is decreased, more and more trays are required.

Feed Conditions: The state of the feed mixture and feed composition affects the operating lines and hence the number of stages required for separation. It also affects the location of feed tray.

State of Trays and Packings: Remember that the actual number of trays required for a particular separation duty is determined by the efficiency of the plate. Thus, any factors that cause a decrease in tray efficiency will also change the performance of the column. Tray efficiencies are affected by fouling, wear and tear and corrosion, and the rates at which these occur depends on the properties of the liquids being processed. Thus appropriate materials should be specified for tray construction.

Column Diameter: Vapor flow velocity is dependent on column diameter. Weeping determines the minimum vapor flow required while flooding determines the maximum vapor flow allowed, hence column capacity. Thus, if the column diameter is not sized properly, the column will not perform well.

5.3.8 Design Steps of Distillation Column:

- Calculation of Minimum Reflux Ratio R_m.
- Calculation of optimum reflux ratio.
- Calculation of theoretical number of stages.

- Calculation of actual number of stages.
- Calculation of diameter of the column.
- Calculation of weeping point.
- Calculation of pressure drop.
- Calculation of thickness of the shell.
- Calculation of the height of the column.

5.3.9 Process Design:

Temperature of feed = 124^o C

Temperature of top product = 146^o C

Temperature of bottom product = 147^o C

P = 1 atm

Table 5-6 Components Flowrate

Components	**flow rate(feed) Kmol/hr**	**x_f**	**flowrate(D) Kmol/hr**	**x_d**	**Flowrate(W) Kmol/hr**	**x_w**
Glycerol	17.9	0.102	0.036	0.00054	17.9	0.166
Acetol	1.42	0.008	1.24	0.018	0.180	0.0016
Water	71.2	0.408	52.4	0.779	18.86	0.175
PG	77.2	0.442	10.40	0.154	66.85	0.622
EG	3.60	0.020	0.36	0.0054	3.23	0.030
Methanol	3.12	0.017	2.78	0.041	0.34	0.003
Total	174.6	1	67.2	1	107.40	1

Heavy Key Component = Ethylene Glycol

Light Key Component = Methanol

Relative Volatility:

Methanol = 2.998

Ethylene Glycol = 1

Calculation of Minimum Reflux Ratio R_m:

Using Underwood equation,

$$\frac{\alpha_A x_{fA}}{\alpha_A - \theta} + \frac{\alpha_B x_{fB}}{\alpha_B - \theta} = 1 - q$$

As feed is entering on its boiling point so, q = 1

By trial, θ = 2.71

Using eq. of min. reflux ratio,

$$\frac{\alpha_A x_{dA}}{\alpha_A-\theta}+\frac{\alpha_B x_{dB}}{\alpha_B-\theta}=R_m+1$$

Putting all values $R_m = 0.82$

Actual Reflux Ratio:

The rule of thumb is:

$$R = (1.2 \text{ ------- } 1.5)\, R_{min}$$

$$R = 1.5\, Rmin$$

$$R = 1.23$$

Calculation of Minimum no. of Plates:

The minimum no. of stages N_{min} is obtained from Fenske relation which is,

$$N_{min}=\frac{\log\left[\left(\frac{x_B}{x_C}\right)_D\left(\frac{x_C}{x_B}\right)_B\right]}{\log\left(\alpha_{BC}\right)_{ave}}$$

$$N_{min} = 6$$

Theoretical no. of Plates:

Gilliland related the number of equilibrium stages and the minimum reflux ratio and the no. of equilibrium stages with a plot that was transformed by Eduljee into the relation;

$$N-N_{min}\Big/N+1=.75\left[1-\left(R-R_{min}\Big/R+1\right)^{0.566}\right]$$

From which the theoretical no. of stages to be,

$$N= 11.$$

One plates is removed for reboiler, so N = 11-1 = 10

Location of feed Plate:

The Kirkbride method is used to determine the ratio of trays above and below the feed point.

$$\log\left(N_D\Big/N_B\right)=.206\log\left[\left(B\Big/D\right)\left(x_{HK}\Big/x_{LK}\right)\left(\left(x_{LK}\right)_B\Big/\left(x_{HK}\right)_D\right)^2\right]$$

From which,

Number of Plates above the feed tray = N_B = 7

Number of Plates below the feed tray = N_D = 8

Calculation of actual number of stages:

Tray Efficiency:

We Take Colum Efficiency 70%

Actual Stages = 10 /0.70 = 15 plates

Determination of the Column Diameter:

Top Conditions	Bottom Conditions
$L_n = D \times R_{min}$ L_n = 55.3649 kgmol/hr $V_n = L_n + D$ V_n =230.018 kgmol/hr Average molecular wt. = 67.99 g/mol T = 146 ^oC ρ_V = 0.840Kg/m^3 ρ_L = 140.23 Kg/m^3	$L_m = L_n + F$ L_m = 230.02 kgmol/hr $V_m = L_m - B$ = 122.61 kgmol/hr Average molecular wt. = 28.90g/mol T = 147 ^oC ρ_V = 1.971 Kg/m^3 ρ_L = 571.69 Kg/m^3

Because liquid and vapor flow rates are greater at bottom so based upon bottom flow rates

Flow Parameter:

Rectifying Section:

$$F_{LV} = \left(\frac{L_n}{V_n}\right)\left(\frac{\rho_v}{\rho_L}\right)^{0.5}$$

F_{LV} = Liquid Vapor Factor = 0.018

Capacity Parameter:

Assume tray Spacing = 0.6m

K = 0.075 from Graph between FLV and K

Flooding velocity is find by formula as follows,

Surface Tension = 42.95dynecm^{-1}

$$\left(\frac{\rho L - \rho v}{\rho v}\right)^{0.5} \quad \left(\frac{\sigma}{20}\right)^{0.2}$$

As a rule of thumb, 80 – 85% of flooding velocity is mostly used so we choose 80

Vnf = K × × = 1.125m/s

Vn = 0.80 × 1.125 = 0.90ms^{-1}

Stripping Section:

$$F_{LV} = \left(\frac{L_m}{V_m}\right)\left(\frac{\rho_v}{\rho_L}\right)^{0.5}$$

F_{LV} = Liquid Vapor Factor = 0.11

Capacity Parameter:

Assume tray Spacing = 0.6m

K = 0.09 from Graph between FLV and K

Flooding velocity is find by formula as follows,

Surface Tension = 31.16dynecm^{-1}

$\left(\frac{\rho L - \rho v}{\rho v}\right)^{0.5} \left(\frac{\sigma}{20}\right)^{0.2}$ As a rule of thumb, 80 – 85% of flooding velocity is mostly used so we choose 80%

$\left(\frac{\rho L - \rho v}{\rho v}\right)^{0.5} \left(\frac{\sigma}{20}\right)^{0.2}$ Vnf = 1.67m/s

Vn = 0.80 × 1.67 = 1.33ms^{-1}

Tray Selection:

We have selected single cross flow sieve tray with segmental down comer. For this type of tray,

Column dia = 1.16 m

Column Area = 1.811m^2

Down Comer Area = 0.12Ac = 0.217m^2

Net area = 1.594 m^2

Weir Length = $(A_d/A_c) \times 100$ = 12 %

L_w/D_c = 0.76 by using graph 11.39

L_w = 1.16 × 0.76 =0.88 m

Tower Diameter:

Let flooding = 80% (Correct trial)

$F^* = 0.8$

$U_n^* = U_{nf} \times F^* = 1.18$ m/Sec

U_n^* = flooding velocity based upon net area.

Net area $A_n = A_T - A_d = 0.88\ A_T$

$$A_T = \frac{A_n}{0.88} = \frac{Q_V}{0.88U_n{}^*} = 1.11m^2$$

$A_T = \frac{\pi}{4} D^2 = 1.11\ m^2$

D = 1.16m

Flooding Check:

$U_n = \frac{Q_V}{A_n} = \frac{Q_V}{0.88A_T} = 1.05\ m/Sec$

Now; $F = \left(\frac{U_n}{Uf}\right)100 = \left(\frac{1.05}{1.39}\right)100 = 80\%$

Now following information are available,

Tower area = $A_T = 1.11\ m^2$

Net area = $A_n = 0.88\ A_T = 0.9776\ m^2$

Active area = $A_a = 0.76\ A_T = 0.84\ m^2$

Down comer area = $A_d = 0.12\ A_T = 0.133\ m^2$

Hole area = $A_h = 0.1\ A_T = 0.11\ m^2$

Calculation of Entrainment:

As $F_{LV} = 0.06$ and F = 80%

From Figure 11.29 of Coulson 6, we calculate

$\psi = 0.045$

ψ = Fractional Entrainment factor

Since $\psi < 0.045$, so now process is satisfactory

Tray Pressure Drop:

$h_t = hd + (h_w + h_{ow}) + h_r$

$h_w = 50\ mm$

Dry Tray Pressure Drop:

$h_d = 51\ (U_h/Co)^2\ (\rho_V/\rho_L)$

h_d = Dry tray drop.

U_h = Hole velocity = Q_v/A_h

$U_h = \frac{Q_V}{A_h} = \frac{2.45}{.232} = 42.46\ m/sec$

Using Fig. 11.34 of Coulson 6. We find “C_o“

C_o = Orifice Coefficient = 0.84

$$h_d = 51\left(\frac{U_h}{C_O}\right)^2\left(\frac{\rho_V}{\rho_L}\right)$$

h_d = 499 mm

Weir Crest:

$h_{ow} = 750\ (L_w/\rho_L * l_w)^{2/3}$

l_w = weir length

l_w = 0.88 m

$$h_{ow} = 750\ \left(\frac{.0053}{1.54}\right)^{2/3}$$

h_{ow} = 0.015 mm

Residual Head (Hr):

$$hr = \left(\frac{12.5 \times 10e3}{\rho_L}\right) = 21.86 \text{ mm}$$

So,

$h_t = h_d + (h_w + h_{ow}) + h_r$

h_t = 521.34 mm

Total Pressure Drop:

$\Delta Pt = (9.81 \times 10e\text{-}3)\ Ht \times \rho_L$

$= 9.81 \times 10e\text{-}3 \times 78.5 \times 648.8$

= 0.23psi

Estimation of Weep point:

$$\overline{U}_{h(min)} = \frac{K_2 - [\,0.90 - (25.4 - d_h)}{(\rho_V)^{0.5}}$$

h_w = 50 mm

h_{ow} = 0.015 mm

$h_w + h_{ow}$ = 50.01 mm

From graph,

K_2 = 30

$\bar{U}h(min)$ = 8.93 m/sec

Total no. of holes:

Total no. of holes $= \left(\frac{Ah}{ah}\right)$

Total no. of holes = 5160

Height of Distillation Column:

No. of plates = 15

Tray spacing = 0.6 m

Tray thickness = 0.006 mm/plate

Total thickness of trays = 0.006 $\times$ 15 = 0.09 m

Total height of column = 8.89m

SPECIFICATION SHEET	
Identification	
Item	Distillation Column (T-101)
Type	Sieve Tray
Function	
Separation of Water & Methanol from propylene glycol	
Material Balance	
Feed In	174.65kmol/hr
Top Product	67.24 kmol/hr
Bottom Product	107.40kmol/hr
Operating Condition	
Pressure	1atm
Number of trays	15
Reflux Ratio	1.23
Tray spacing	0.6m
Height of column	8.89m
Diameter of column	1.16m
Pressure drop per tray	0.2 psi
Tray thickness	0.006m
Hole diameter	0.006m
Weir height	0.05m
Weir length	0.76m
Active area	$0.28m^2$
Number of holes	5160 holes
Percentage flooding	80%

SPECIFICATION SHEET	
Identification	
Item	Distillation Column (T-102)
Type	Sieve Tray
Function	
Separation of Unreacted glycerol from PG,EG	
Material Balance	
Feed In	7303.48kg/hr.
Top Product	5450.80kg/hr.
Bottom Product	1852.68kg/hr.
Operating Condition	
Pressure	1atm
Number of trays	36
Reflux Ratio	2.28
Tray spacing	0.3m
Height of column	11.5m
Diameter of column	2.13m
Pressure drop per tray	0.0092atm / 0.13psi
Tray thickness	0.005m
Hole diameter	0.005m
Weir height	0.05m
Weir length	1.72m
Active area	2.49m^2
Number of holes	12678 holes
Percentage flooding	85%

SPECIFICATION SHEET	
Identification	
Item	Distillation Column (T-103)
Type	Sieve Tray
Function	
Separation of Ethylene glycol from propylene glycol	
Material Balance	
147.67	147.67 kmol/hr
Top Product	69.34kmol/hr
Bottom Product	78.33kmol/hr
Operating Condition	
Pressure	1atm
Number of trays	13
Reflux Ratio	1.21
Tray spacing	0.6m
Height of column	6.9m
Diameter of column	1.05m
Pressure drop per tray	0.16 psi
Tray thickness	0.006m
Hole diameter	0.006m
Weir height	0.05m
Weir length	0.88m
Active area	0.39m^2
Number of holes	6270 holes
Percentage flooding	75%

5.4 Design of Shell & Tube Heat Exchanger (E-101):

Shell and tube heat exchanger:

A shell and tube heat exchanger transfers heat from one fluid to another through a barrier or a wall. The heat transfer occurs between two fluids that are flowing in separate channels, with one fluid flowing inside a set of tubes and the other flowing around the outside of the tubes in a shell.

The basic structure of a shell and tube heat exchanger consists of a cylindrical shell that encases a bundle of tubes, with each end of the tube connected to a tube sheet. One fluid flows through the tubes, while the other fluid flows around the outside of the tubes in the shell. The two fluids are kept separate by the tube sheet, which prevents them from mixing.

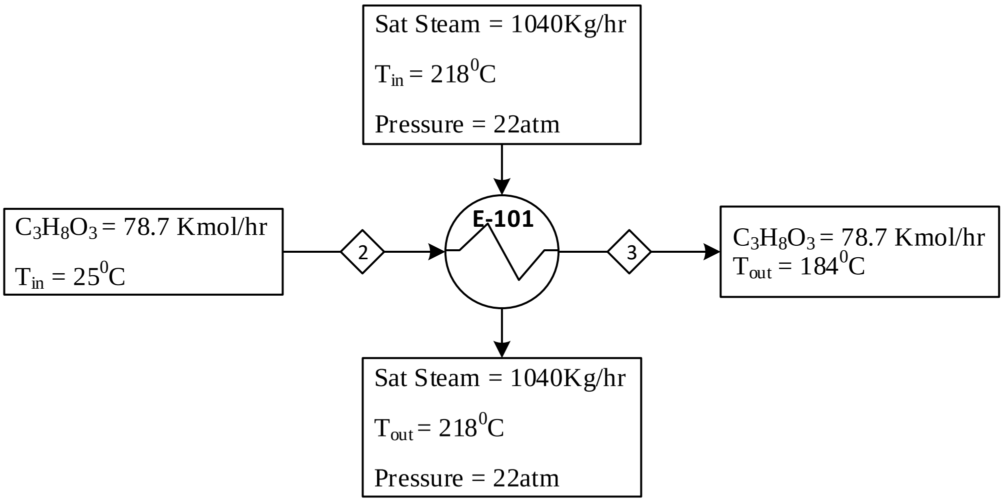


Figure 5-5 Design shell and tube heat exchanger (E-101)

Design Calculations:

Process conditions required:

For the exchanger, the following data must be known

Cold fluid: t_1, t_2, w, c, s, μ, k **Hot fluid:** T_1, T_2, W, c, s, μ, k

Steam is more corrosive than glycerol that's why steam is placed in the tube side.

Shell side (Glycerol)	**Tube side (steam)**
ID = 12 in	Number and Length = 76, 16'
Baffle Spacing (B) = 3 in.	OD, BWG, Pitch = 3/4 in, 16, 1 in square.
Passes = 1	Passes = 2
C = 0.32 Btu/lb.F at avg Temp.	C = 0.44 Btu/lb.°F
K = 0.292 Btu/h.lb.°F	K = 0.0207 Btu/h.lb.°F
μ = 18.3 lb/ft.h	μ = 0.04 lb/ft.h
W = 15979 lb/h	W = 2297 lb/h

Energy Balance:	**Energy Balance:**
$Q = WC(T_1-T_2)$	$Q = wc\ (t_2-t_1)$ Q = 1843735 Btu/hr
Q = 1843735 Btu/hr	

LMTD Calculation:

$$LMTD = \frac{(T2-t1)-(T1-t2)}{\ln(T2-t1)/(T1-t2)}$$

$$LMTD = \frac{(424-76.73)-(424-364.73)}{\ln((424-76.73)/(424-364.73)} = 163^{o}F$$

From Table U_D (range = 6-50)

$U_D = 40$ Btu/(h.ft2.F)

$A = Q/(U_D\Delta T_{(cf)}) = \frac{1843735}{(40)(163)} = 283\ ft^2$

Shell Side Calculation (Glycerol):

Flow Area, as

a_s = (area of shell - area of tube)as = 0.632 ft^2

$a_s = ((13.25)^2/4 - 106*Pi*(0.75)^2/4)$

Mass Velocity, Gs:

$Gs = W/as = \frac{15979}{0.632}$

Gs = 25283.2 $lb/h.ft^2$

Reynolds Number, Re:

De = 0.060ft

$Re = De * Gs/\mu = 99$

Factor from fig: 28 (kern)

$J_H = 3$ from fig

$\phi s = 1.4$

Film heat transfer coefficient outside, ho:

$ho = J_H\ (K/D)(C\mu/k)^{1/3}\ \phi s$

$$ho = 5\left(\frac{0.22}{0.060}\right)\left(\frac{0.27*15.3}{0.292}\right)(1.4)$$

ho = 39.6 Btu/hr. ft^2 °F

Tube (Steam) side calculation:

Flow Area, a_t

a_t’ = 0.302 in (from the able)

$a_t = \frac{Nt*at'}{(n)(144)}$ = 0.11 ft^2

Mass Velocity, G_s:

$G_t = W/a_t = \frac{2297.2}{0.11}$

G_t = 20884 lb/h.ft^2

Reynolds Number, Re:

D = 0.052 ft

Re = $D * Gt/\mu$ = 26105

Film heat transfer coefficient inside:

hi = 1500 for steam (from kern methodology for special cases)

ϕt is Approximately = 1

Hio = hi * ID/OD

Hio = 1224 Btu/hr. ft^2 ˚F

Clean overall coefficient, U_c

$U_c = h_o * h_{io/}\ h_{io\,+}\ h_o = \frac{39.6*1224}{1224+39.6}$ = 38 Btu/hr. ft^2 ˚F

Uc = 38 Btu/hr. ft^2 ˚F

External area = a’’ = 0.1963 surface per linear ft, ft^2

A = $Nt * L * a'' = 106 * 16 * 0.1963$ = 327 ft^2

Design overall coefficient, U_D:

Calculated U_d

U_D = Q/A Δt = 35 Btu/hr. ft^2 ˚F

Dirt factor R_d :

R_d = $Uc - Ud/Uc * Ud = \frac{38-35}{38*35}$ = 0.0024 h.ft^2 F/Btu

Pressure calculation for Shell & Tube:	
Shell side	**Tube side**
f = 0.007 ft^2/in^2 at Re	f = 0.00022 ft^2/in^2 at Re
N + 1 = 12L/B = 64	s = 1.0(V/p) = 0.00080
S = 1.259	L = 16 ft
Ds = 1.10 ft	n = 2
$D_e = 0.060$	D = 0.0625ft
$\phi_s = 1.58$	Gt = 20884 $lb/h.ft^2$
G_s = 25283.2 $lb/h.ft^2$	$\Delta P_t = fG^2Ln/5.22*10^{10}D\phi = 3.1 * ½$
$\Delta P_s = fG^2Ds(N+1)/5.22*10^{10}D_es\phi$	**= 1.55 psi**
= 0.61 Psi	

Specification Sheet		
Identification		
Item	Heat Exchanger (E-101)	
Type	Shell & Tube Heat Exchanger	
Function		
Pre-heating the feed		
Heat Duty	1843735 Btu/hr	
Actual Surface area	327 ft^2	
Uc calculated	38.3 Btu/hr.ft^2.°F	
U$_D$ calculated	35 Btu/hr.ft^2.°F	
Fouling Factor	0.0024 hr.ft^2.°F/Btu	
Fluid allocation	**Shell side**	**Tube Side**
Fluid Name	Feed	Water
Fluid quantity (Total)	15979 lb/hr	2297 lb/hr
Temperature (in / out)	(77 to 365) °F	424 °F
Thermal Conductivity	K = 0.292 Btu/hr.lb.°F	K=0.0207Btu/hr.lb.°F
Viscosity	μ = 18.3 lb/ft.hr	μ = 0.04 lb/ft.hr
Pressure Drop	**0.61 psi**	**1.55 psi**
Tube no: 106 **OD:** ¾ in. **BWG:** 16 **Pitch:** 1in Triangular		
Shell ID: 13.25 in. **TEMA type**: AES		

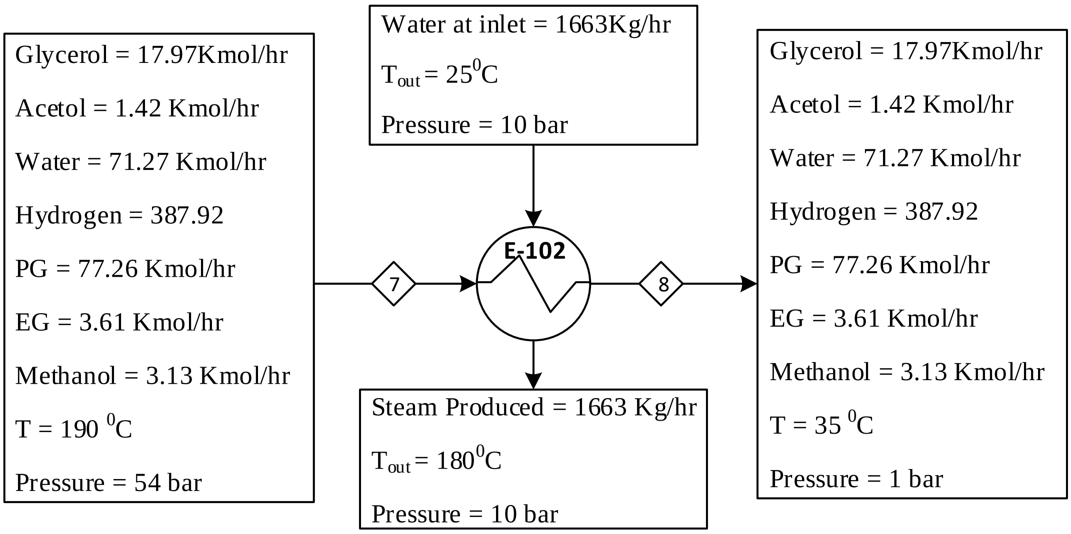
5.5 Design of Waste Heat Boiler (E-102):

A waste heat boiler is a device used to recover heat from an industrial process. These boilers can capture the waste heat and convert it into useful energy that can be used for various purposes such as generating steam or electricity. Waste heat boilers are commonly used in industries such as petrochemical, chemical, cement, and steel, where large amounts of waste heat are generated during the production process. These boilers can be customized to fit the specific requirements of the process or engine, and they are designed to handle high temperatures and pressures.

The working principle of a waste heat boiler is simple. The exhaust gases from the process or engine are passed through a heat exchanger where the heat is transferred to a fluid, typically water. The heated fluid then passes through a steam drum where it is converted into steam, which can be used for various purposes. The steam can be used to drive turbines to generate electricity or for heating or other industrial processes.

There are different types of waste heat boilers available, such as fire-tube boilers, water-tube boilers, and heat recovery steam generators (HRSG).

Design Calculations:



Glycerol = 17.97Kmol/hr
Acetol = 1.42 Kmol/hr
Water = 71.27 Kmol/hr
Hydrogen = 387.92
PG = 77.26 Kmol/hr
EG = 3.61 Kmol/hr
Methanol = 3.13 Kmol/hr
T = 190 ^{0}C
Pressure = 54 bar

Water at inlet = 1663Kg/hr
T_{out} = 25^{0}C
Pressure = 10 bar

Steam Produced = 1663 Kg/hr
T_{out} = 180^{0}C
Pressure = 10 bar

Glycerol = 17.97Kmol/hr
Acetol = 1.42 Kmol/hr
Water = 71.27 Kmol/hr
Hydrogen = 387.92
PG = 77.26 Kmol/hr
EG = 3.61 Kmol/hr
Methanol = 3.13 Kmol/hr
T = 35 ^{0}C
Pressure = 1 bar

Figure 5-6 Design of Waste Heat Boiler (E-102)

Process conditions required:

For the exchanger, the following data must be known

Cold fluid: t_1, t_2, w, c, s, μ, k **Hot fluid:** T_1, T_2, W, c, s, μ, k

Process steam is more corrosive than glycerol that's why steam is placed in the tube side.

Shell side (Product stream)	Tube side (steam)
ID =25in	Number and Length= 452, 16'
Baffle Spacing (B) = 12 in.	OD, BWG, Pitch= 3/4 in, 16, 1 in triangular
Passes = 1	Passes = 2

C = 0.32 Btu/lb.^{o}F at avg Temp.	C = 0.44 Btu/lb.^{o}F
K = 0.16 Btu/hr.lb.^{o}F	K = 0.0207 Btu/h.lb.^{o}F
µ = 1.5 lb/ft.hr	µ = 0.04 lb/ft.hr
W= 20110 lb/hr	W= 3461 lb/hr
Energy Balance: Q=WC(T_1-T_2)	Energy Balance: Q=wc(t_2-t_1)
Q = 3950631 Btu/hr	Q = 3950631 Btu/hr

LMTD = $\frac{(T2-t1)-(T1-t2)}{\ln(T2-t1)/(T1-t2)}$

LMTD = 58^{o}F

From Table U_D (range = 5-75)

U_D = 45 Btu/(h.ft_2.F)

A = Q/($U_D \Delta T_{(cf)}$) = 1513.65 ft^2

Shell side calculations:

Flow Area, a_s

C = 0.25 in B = 12 Pt = 1 in

a_s = $(ID * C * B/Pt * 144)$

a_s = 0.52 ft^2

Mass Velocity, G_s

G_s = W/a_s = 38673 lb/h.ft^2

Reynolds Number, Re

De = 0.060ft

Re = De $* Gs/\mu$ = 1546

Factor from fig: 28 (kern)

J_H = 20 from fig

ϕs = 1.1

Film heat transfer coefficient outside, ho

ho = J_H (K/D)$(C\mu/k)^{1/3}$ ϕs

ho = 74 Btu/hr. ft^2 ˚F

Tube Side Calculations:

Flow Area, a_t

a_t’ = 0.302 in (from the able)

$a_t = \frac{Nt*at'}{(n)(144)} = 0.47\ ft^2$

Mass Velocity, G_s

$G_t = W/a_t = 7364.3\ lb/h.ft^2$

Reynolds Number, Re

D = 0.052 ft

Re = $D * Gt/\mu$ = 9280

Film heat transfer coefficient inside:

hi = 1500 for steam (from kern methodology for special cases)

ϕt is Approximately = 1

Hio = hi * ID/OD

Hio = 1224 Btu/hr. ft^2 °F

Clean overall coefficient, U_c

$U_c = h_o*h_{io/}\ h_{io\ +}\ h_o$ = 69 Btu/hr. ft^2 °F

Uc = 69 Btu/hr. ft^2 °F

External area = a’’ = 0.1963 surface per linear ft, ft^2

A = Nt ∗ L ∗ a” = 452 ∗ 16 ∗ 0.1963 = 1419.6 ft^2

Design overall coefficient, **U_D**

$U_D = Q/A\ \Delta t$ = 52 Btu/hr. ft^2 °F

Dirt factor R_d

R_d = $Uc - Ud/Uc * Ud$ = 0.003 h.ft^2 F/Btu

Pressure calculation for Shell & Tube:	
Shell side	**Tube side**

f = 0.0028 ft^2/in^2 at Re N + 1 = 12L/B = 192 Specific gravity: S = 0.45 ΔP_s = $fG^2Ds(N+1)/5.22*10^{10}D_e s\phi$ **= 0.12 Psi**	f = 0.00028 ft^2/in^2 at Re Specific gravity: s = 1.0(V/p) = 0.00080 ΔP_t = $fG^2Ln/5.22*10^{10}D\phi$ = 0.25 * ½ (ΔP_t *1/2 for steam; by kern) **= 0.125 psi**

<table>
<tr><th colspan="4">Specification Sheet</th></tr>
<tr><th colspan="4">Identification</th></tr>
<tr><td colspan="2">Item</td><td colspan="2">Waste Heat Boiler (E-102)</td></tr>
<tr><td colspan="2">Type</td><td colspan="2">Shell & Tube Heat Exchanger</td></tr>
<tr><th colspan="4">Function</th></tr>
<tr><td colspan="4">Heat recovery</td></tr>
<tr><td colspan="2">Heat Duty</td><td colspan="2">3950631 Btu/hr</td></tr>
<tr><td colspan="2">Actual Surface area</td><td colspan="2">1513 ft^2</td></tr>
<tr><td colspan="2">Uc calculated</td><td colspan="2">69 $Btu/hr.ft^2.^oF$</td></tr>
<tr><td colspan="2">U_D calculated</td><td colspan="2">52 $Btu/hr.ft^2.^oF$</td></tr>
<tr><td colspan="2">Fouling Factor</td><td colspan="2">0.003 $h.ft^2.^oF/Btu$</td></tr>
<tr><td>Fluid allocation</td><td>Shell side</td><td colspan="2">Tube Side</td></tr>
<tr><td>Fluid Name</td><td>Hot fluid</td><td colspan="2">Water</td></tr>
<tr><td>Fluid Flowrate</td><td>20110 lb/hr</td><td colspan="2">3461 lb/hr</td></tr>
<tr><td>Temperature</td><td>374 to 113°F</td><td colspan="2">77 to 356°F</td></tr>
<tr><td>Pressure</td><td>54.7 bar</td><td colspan="2">10.1 bar</td></tr>
<tr><td>Viscosity</td><td>µ = 1.72 lb/ft.hr</td><td colspan="2">µ = 0.041 lb/ft.hr</td></tr>
<tr><td>Thermal Conductivity</td><td>K = 0.22 Btu/h.lb°F</td><td colspan="2">K=0.020Btu/h.lb°F</td></tr>
<tr><td>Pressure Drop</td><td>0.12 psi</td><td colspan="2">0.25 psi</td></tr>
<tr><td>Tube no: 534</td><td>OD: ¾ in.</td><td>BWG: 16</td><td>Pitch: 1in Triangular</td></tr>
<tr><td colspan="2">Shell ID: 25 in.</td><td colspan="2">TEMA type: AES</td></tr>
</table>

Specification Sheet		
Identification		
Item	Heat Exchanger (E-103)	
Type	Double Pipe Heat Exchanger	
No of Hairpins	6	
Function		
To increase the temperature of stream		
Heat Duty	1282223 Btu/h	
Actual Surface area	78 ft^2	
U_C calculated	122 Btu/hr.ft^2.^{o}F	
U_D calculated	97.4 Btu/hr.ft^2.^{o}F	
Fouling Factor	0.0020 hr.ft^2.^{o}F/Btu	
Required Length	240 ft	
Fluid allocation	**Annulus**	**Inner Pipe**
Fluid Name	Fluid	Steam
Fluid Flowrates	20404 lb/hr	1486 lb/hr
Temperature	94.73 to 249^{o}F	305 to 305^{o}F
Pressure	1.01 bar	10 bar
Viscosity	μ = 2.02 lb/ft.hr	μ = 0.041 lb/ft.hr
Thermal Conductivity	0.18 Btu/hr.ft^{o}F	0.020 Btu/hr.ft^{o}F
Pressure Drop	**1.37 psi**	**0.94 psi**

5.6 Design of Double Pipe Heat Exchanger (E-104):

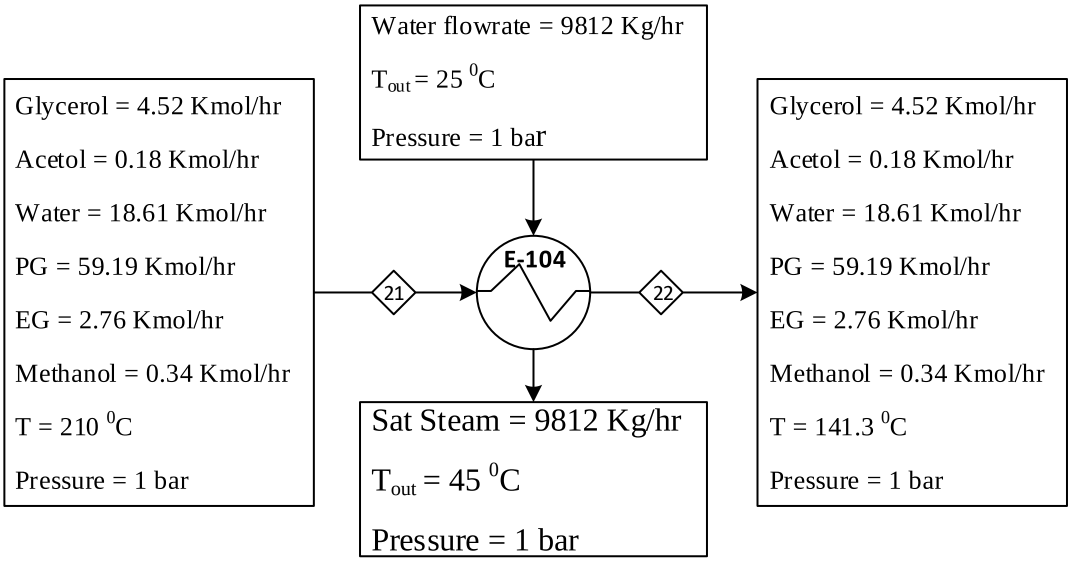


Figure 5-7 Design of Double pipe Heat exchanger (E-104)

Design calculation:

For the exchanger the following data must be known

Hot fluid: T_1, T_2, W, c, s, μ, k

Cold fluid: t_1, t_2, w, c, s, μ, k

Heat balance:

T_1=210 ºC	t_1= 25ºC
T_2 = 141 ºC	t_2 = 45ºC
T_{avg} =175.5ºC	t_{avg} = 35ºC
W_1 = 5450 Kg/hr	w_1 = 9812 Kg/hr
Cp = 2.18 KJ/Kg.K,	cp = 4.2 KJ/Kg.K
$Q = WCp(T_1 – T_2)$	$Q = W\ Cp\ (T_1 – T_2) = w\ cp\ (t_2 – t_1)$
Q= 821628 KJ/hr	Q = 821628 KJ/hr
(778794.3 BTU/hr)	(778794.3 BTU/hr)

LMTD (Log mean temperature difference):

Hot fluid(C)	**Temperatures**	**Cold fluid**(ºC)	**Difference**(ºC)
210	High temperature	45	165
141	Low temperature	25	116

LMTD = $\frac{(T2-t1)-(T1-t2)}{\ln(T2-t1)/(T1-t2)}$

=139.2ºC (282ºF)

Assume U_D=100 Btu/(hr)(ft^2)(ºF)

Area= $Q/U_D\Delta T$

= 27.5 ft^2

As area is less than 200ft^2 double pipe exchanger will be used.

Water is more corrosive than process stream so it is in inner pipe.

Flow area:

Annulus side (process stream)	**Inner pipe (Water)**
Exchanger, IPS =3-by 2-in **Flow area:** ID of outer pipe= 3.068 in D_1 = 0.256 ft OD of inner pipe = 2.38 in D_2 = 0.199 ft a_a= л(D_1-D_2)/4 a_a = 0.0206 ft^2 **Equivalent dia:** De = (D_1-D_2)/D_1 De = 0.13 ft	**Flow area:** D = 2.067 in D = 0.172 ft a_p= лD^2/4 ap =0.0233 ft^2
Mass velocity:	
G_a = w/a_a G_a = 583447.2816 lb/hr.ft^2	G_p = W/a_p G_p = 928560.5 lb/hr.ft^2
Reynold number:	
Re= (De×G)/µ Re= 33760.5	Re= (D×G) /µ Re=82496.08
j_H:	
j_H=100 (from Fig.24)	j_H=210 (from Fig.24)

<table>
<tr><td colspan="2">Prandtl number:</td></tr>
<tr><td>At T_{avg}:
K = 0.169 Btu/hr ft.°F
Cp=0.5207 Btu/lb°F
μ=1.316 lb/(ft)(hr)
$(C\times\mu/K)^{(1/3)}$ = 1.593857909</td><td>At t_{avg}:
K = 0.352Btu/hrft.°F
Cp=1.003 Btu/lb°F
μ=1.936 lb/(ft)(hr)
$(C\times\mu/K)^{(1/3)}$= 1.766938</td></tr>
<tr><td colspan="2">Overall heat transfer coefficient:</td></tr>
<tr><td>$h_{o=}\ j_H(k/De)(cu/k)^{1/3}(u/u_w)^{0.14}$
353.7 Btu/hr.ft^2.°F</td><td>$h_{i=}\ j_H(k/De)(cu/k)^{1/3}(u/u_w)^{0.14}$
795.5328 Btu/hr.ft^2.°</td></tr>
<tr><td></td><td>hio=hi×(ID/OD)
661.3466</td></tr>
</table>

Clean overall coefficient:

Clean overall coefficient, U_c

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

230.4635942 Btu/hr.ft^2.°F

Design overall coefficient:

Design overall coefficient, U_D

$1/U_D=1/U_C+Rd$

U_D= 55 Btu/hr. ft ^{2}(°F)

Required surface:

Required surface:

A= Q/UD*ΔT

A= 39.5 ft^2

External surface area per ft length (from Table) = (0.622 ft^2/ft)

Required length = 63.5 ft

20 ft hair pin have 40 ft length,

So, Number of Hairpins = 63.5/32

1.98 ft

So, use 2 hair fin.

Actual design coefficient:

Actual design coefficient is,

U_D=Q/ A′×Δt

U_D= 55.4 Btu/hr. ft ^{2}(F)

Rd=(U_C-U_D)/($U_C U_D$)

Rd=0.0013

Pressure drop calculation:

Annulus side (process stream)	**Inner pipe (Water)**
f = 0.00062 s = 1, ρ=65 $\Delta F_a=4fG^2L/2g\ \rho^2De$ =0.26302 V=G/3600ρ = 2.49336 fps $\Delta F_1=3(V^2/2g)$ = 0.0401 $\Delta P_a=(\Delta F_a+\Delta F1)\ \rho/144$ **= 0.136853062 psi** **Allowable pressure = 10 psi**	f = 0.000129 s = 1 ρ=62.5 $\Delta F_p=4fG^2L/2g\ \rho^2D$ = 0.0757 $\Delta P_p=\Delta F_p\ \rho/144$ **0.36254 psi**

SPECIFICATION SHEET	
IDENTIFICATION	
Item	Heat Exchanger (E-104)
Type	Double pipe heat exchanger
No of Hairpins	2
Function	
To decrease temperature of process stream	
Heat Duty	778794.3 Btu/hr
Actual surface area	40 ft^2
U_C Calculated	230.4 Btu/hr.ft^2.°F
U_D Calculated	55 Btu/hr. ft^2.°F
Fouling Factor	0.0013 hr.ft^2.°F/Btu
Required Length	80 ft

Fluid Allocation	**Annulus side**	**Inner pipe**
Fluid Name	Process stream	water
Fluid Flowrates	5450 Kg/hr	9812 Kg/hr
Temperature	210 to 141°C	25 to 45°C
Viscosity	0.55 cp	0.8 cp
Thermal Conductivity (k)	K = 0.169 Btu/hr.ft.°F	K = 0.352Btu/hr.ft.°F
Pressure Drop	**0.136 psi**	**0.362507 psi**

CHAPTER NO. 6
MECHANICAL DESIGN

6.1 Introduction:

Mechanical design of a reactor involves the design and selection of the mechanical components, structures, and systems necessary for the safe and efficient operation of the reactor. The design process typically involves several stages, including conceptual design, detailed design, and fabrication.

The mechanical design of a reactor typically includes the following components

- Shell: The shell of the reactor is the main vessel that holds the reactants and products. The design of the shell includes considerations such as the material of construction, thickness, and shape.
- Head: The head of the reactor is the closure that seals the top of the shell. The design of the head includes considerations such as the type of closure, pressure rating, and sealing mechanism.
- Agitator: The agitator is a mechanical component that is used to mix the reactants inside the reactor. The design of the agitator includes considerations such as the type of impeller, speed, torque, and power requirements.
- Heat Transfer System: The heat transfer system is responsible for controlling the temperature inside the reactor. The design of the heat transfer system includes considerations such as the type of heat exchanger, flow rate, and heat transfer coefficient.
- Instrumentation and Control System: The instrumentation and control system is responsible for monitoring and controlling the operating parameters of the reactor. The design of the instrumentation and control system includes considerations such as the type of sensors, controllers, and communication systems.
- Support Structure: The support structure is the framework that holds the reactor and its components in place. The design of the support structure includes considerations such as the material of construction, load-bearing capacity, and stability.

The mechanical design of a reactor involves the design and selection of the mechanical components, structures, and systems necessary for the safe and efficient operation of the reactor. The design process involves several stages, including conceptual design, detailed design, and fabrication, and should consider factors such as the material of construction, pressure rating, temperature control, mixing requirements, and instrumentation and control systems.

6.2 Material Selection:

Stainless Steel 18Cr/8Ni Mo $2\frac{1}{2}$ percent (316)

- High-strength and high-temperature scaling resistance.
- This alloy has a higher resistance to corrosion at high temperatures.

6.3 Minimum Practical Wall Thickness:

The minimum practical wall thickness is the smallest thickness that can provide the required strength and stiffness while ensuring that the component is safe and reliable. It is important to note that the minimum practical wall thickness must also meet any applicable codes and standards for the particular application.

Vessel Diameter:

$$2 \text{ to } 2.5 \text{ (meter)}$$

Minimum Thickness:

$$9\text{mm}$$

Because the vessel’s diameter is 2.24m, so the shell’s minimum thickness is 9mm

6.4 Wall Thickness:

Material = Stainless Steel

Diameter = D_i = 2.24m = 2240mm

Corrosion Allowance = 2mm

Maximum Allowance Stress = S = 115 N/mm^2

Joint Efficiency (double Welded) = E = 1

P_i = Maximum Allowable Pressure (we take 10% above the operating gauge pressure)

$$P_i = (54 - 1) \times 1.1$$

$$P_i = 58.3 \text{ bar or } 5.83 \text{ N/mm}^2$$

$$\text{Wall thickness} = t = \frac{P_i D_i}{2SE - P_i} = \frac{2240 \times 5.83}{2 \times 115 \times 1 - 5.83}$$

$$t = 58.255\text{mm or } 59\text{mm}$$

Adding corrosion allowance of 2mm;

$$t = 59 + 2 = 61\text{mm}$$

Outer dia of reactor;

$$D_o = D_i + 2e$$

$$D_o = 2.24 + 2(0.061) = 2.362\text{m or } 2.4\text{m}$$

6.5 Thickness of Head:

Heads of various forms close the ends of a cylindrical vessel. The principal types used are:

- Flat plates and formed flat heads
- Hemispherical heads
- Ellipsoidal heads

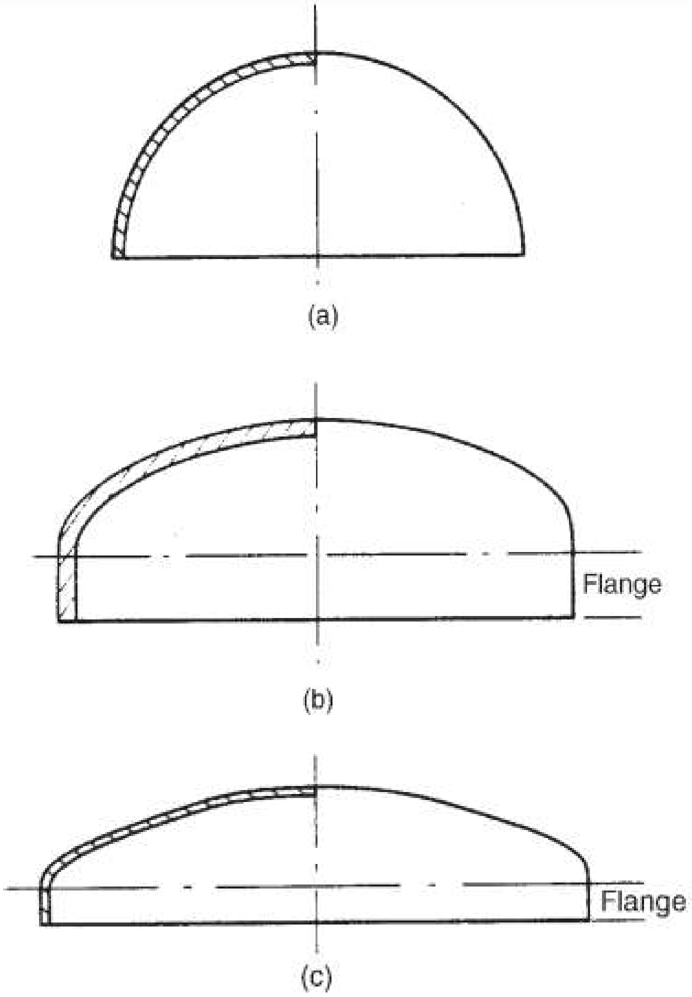


Figure 6-1 Types of Head

Domed heads refer to hemispherical, ellipsoidal, and tori spherical heads as a group. Large diameters are produced from formed sections, which are made by pressing or spinning. Dished ends are a term used to describe Tori spherical heads.

6.6 Thickness of Head:

Torispherical Head:

A torispherical head is a type of end cap or closure used on a pressure vessel, such as a tank or reactor. It is made by forming two curved shapes, a toroidal section and a spherical section, together to create a head that resembles a rounded dome.

Torispherical heads are commonly used in the industry because they are efficient and economical to manufacture. The manufacturing process involves cold pressing or hot forming, which allows for the production of a high-quality head without the need for expensive tooling. Additionally, the torispherical shape provides a smooth and rounded surface that distributes pressure more evenly, reducing stress concentration and increasing the vessel's strength.

Another reason torispherical heads are economical is that they require less material than other head designs. This is because the torispherical shape distributes pressure more evenly across the surface, reducing the amount of stress concentration at the edge of the head. This means that less material is required to create a torispherical head that can withstand the same pressure as a flatter head.

In addition to their economic advantages, torispherical heads are also desirable because they are easy to install and maintain. The shape of the head allows for easy access to the vessel, which makes cleaning, inspection, and maintenance easier.

Overall, torispherical heads are a popular choice in the industry due to their efficient manufacturing process, reduced material costs, improved strength, and ease of maintenance. Their versatility and cost-effectiveness make them a practical choice for many pressure vessel applications.

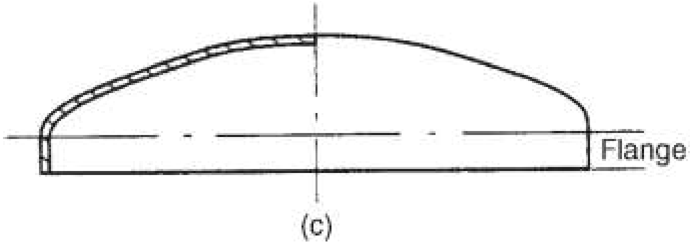


Figure 6-2 Torispherical Head

$$t = \frac{0.885 \times P_i R_c}{SE - 0.1P_i}$$

Where;

$$R_c = D_i = 2.24m = 2240mm$$

$$\text{knuckle radius} = 6\% \text{ of } R_c = 134.4mm$$

By putting the values;

$$t = \frac{0.885 \times 5.83 \times 134.4}{115 \times 1 - 0.1 \times 5.83} = 6.1mm$$

6.7 Vessel Support:

The vessel's size, shape, and weight, as well as the design temperature and pressure, as well as the position and arrangement of the vessel determine the technique used to support a vessel. Some of the forms of vessel support are as follows.

- Saddle support (for horizontal vessels).
- Brackets support (for vertical vessels).
- Skirt support (for vertical vessels, especially if the length is long and the wind influence is significant)

We have chosen Bracket support by considering our conditions;

6.8 Dead Weight:

$$W_v = 240C_w D_m (H_v + 0.8D_m)t$$

Where;

W_v = Total Weight of shell excluding external fittings such as plates

C_w = A factor to account for the weight of nozzles, man ways, internal supported. Which can be taken as=1.08 for the vessels with only a few internal fittings.

T = Thickness of shell = 59mm = 0.0059m

D_m = Mean Diameter = $(D_i + t \times 10^{-3}) = 2.24m$

Height of vessel = 6.83m

By putting the values

$$\mathrm{W_v = 39.81N}$$

6.9 Wind Load:

$$\mathrm{Wind\ Pressure = 1030N/m^2}$$

$$\mathrm{Total\ dia = D_i + 2t = 2.24 + 2 \times 0.0059}$$

$$\mathrm{Total\ dia = 2.25m}$$

$$\mathrm{F = PD = 1030 \times 2.25 = 2323.3\frac{N}{m}}$$

6.10 Stress Calculations:

Longitudinal Stress:

$$\mathrm{\sigma_h = \frac{P_iD_i}{2t}}$$

$$\mathrm{\sigma_h = \frac{5.83 \times 2240}{2 \times 6.1} = 1070.4\frac{N}{mm^2}}$$

Circumferential Stress:

$$\mathrm{\sigma_L = \frac{P_iD_i}{4t}}$$

$$\mathrm{\sigma_L = \frac{5.83 \times 2240}{4 \times 6.1} = 535.2\frac{N}{mm^2}}$$

Dead Weight Stress:

$$\mathrm{\sigma_w = \frac{w}{\pi(D_i + t)t}}$$

$$\mathrm{\sigma_w = \frac{40}{3.14(2240 + 6.1)6.1} = 9.29 \times \frac{10^{-4}N}{mm^2}}$$

Radial Stress:

$$\mathrm{\sigma_l = \frac{P_i}{2} = \frac{5.83}{2} = 2.915\frac{N}{mm^2}}$$

Bending Moment:

$$\mathrm{M_x = F \times H}$$

$$\mathrm{M_x = 2323.3 \times 3.415}$$

$$\mathrm{M_x = 7934.1N}$$

Bending Stress:

$$\sigma_b = \frac{M_x}{l_v}\left(\frac{D_i}{2} + t\right)$$

Where;

$$l_v = \frac{P_i(D_o^4 - D_i^4)}{\pi(D_i + t) \times t}$$

$$l_v = \frac{5.83(2250^4 - 2240^4)}{3.14(2240 + 6.1) \times 6.1} = 6.1 \times 10^7$$

$$\sigma_b = 0.146\mathrm{N/mm^2}$$

CHAPTER NO. 7

PUMPS & COMPRESSOR

7.1 Pump and Compressor:

An industrial pump is a machine used to move fluids or gases through pipes and channels in an industrial setting. These pumps are designed to handle high volumes of liquids or gases, making them ideal for use in large industrial applications such as oil refineries, chemical plants, and water treatment facilities. Industrial pumps come in different types such as centrifugal, positive displacement, diaphragm, and others, each with its specific advantages and use cases. The most common types of industrial pumps include water and sewage pumps, process and transfer pumps, and air compression and vacuum pumps. These pumps are often made of durable materials such as stainless steel or cast iron to endure the rigors of heavy daily use.

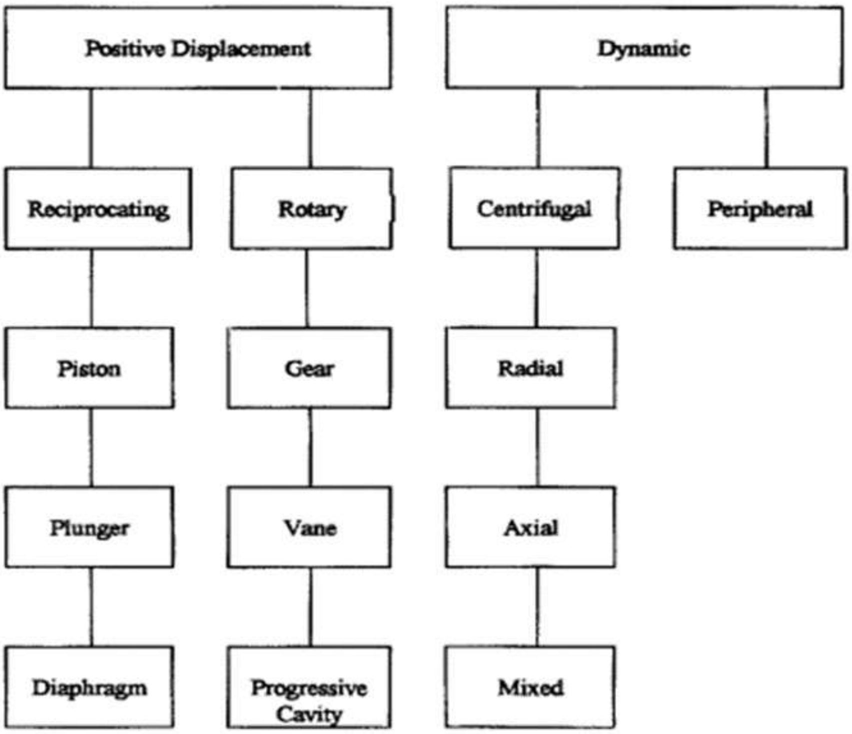


Figure 7-1 Pump Classification Chart

7.2 Types of Pumps:

Centrifugal Pump:

Centrifugal pumps operate by applying a centrifugal force to fluids, many times with the assistance of impellers. These pumps are typically used in moderate to high-flow applications with low-pressure head, and are very common in chemical process industries. There are three types of centrifugal pumps radial, mixed, and axial flow pumps. In radial pumps, pressure is developed completely through a centrifugal force, while in axial pumps pressure is developed by lift generated by the impeller. Mixed flow pumps develop flow through a centrifugal force and the impeller.

Reciprocating Pump:

Reciprocating pumps compress liquid in small chambers via pistons or diaphragms. These pumps are typically used in low-flow and high-head applications. Piston pumps may have single or multiple stages and are generally not suitable for transferring toxic or explosive material. Diaphragm pumps are more commonly used for toxic or explosive materials.

Rotary lobe pumps:

Rotary lobe pumps are positive-displacement type pumps that use two or more lobes rotating around parallel shafts in the pump's body to move liquids. They are widely used in the hygienic processing industries, including food & beverage processing and biopharmaceutical manufacturing.

Peripheral pumps:

Peripheral pumps work by using a spinning impeller to create centrifugal force that moves water from the inlet of the pump to the outlet. Unlike other centrifugal pumps, peripheral pumps have a single impeller that is mounted on the side of the pump housing, creating a peripheral velocity.

7.3 Selection of Pump:

- Rotary pumps are commonly used for pumping high-viscosity liquids
- Widely used in industries
- Easy to maintain and compact design
- high power density and operational reliability

Capacity = 15979 lb/hr

Capacity = 25.36 gpm

SG = 1.263

$$H = \frac{P * 2.31}{SG}$$

Head = 1451.443 psi = 3348.8 ft

Advantages:

- Simple in operation and cheap.
- Fluid is delivered at uniform pressure without shocks or pulsation.
- There are no valves involved in pump operation
- they are much smaller than other pumps of equal capacity.
- Maintenance costs are lower than other types of pumps.

7.4 Pump Sizing Calculation Steps:

Pump sizing steps are:

- Locate the process equipment
- Estimate Z1and Z2.
- Estimate Frictional pressure losses ED and ES
- Calculate Pump Work.
- Calculate Pump shaft horsepower & estimate its Efficiency.
- Calculate electric-motor horsepower & estimate its Efficiency.
- Select a standard electric-motor horsepower.
- Calculate NPSH

7.5 Pump Calculations:

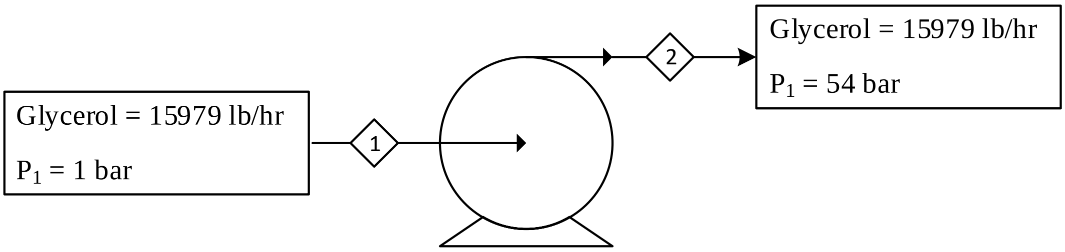


Figure 7-2 Pump (P-101)

The inlet pressure is = P_1 = 1 bar = 100 kpa

The outlet pressure is = P_2 = 54 bar = 5400 kpa

Locate the process equipment:

Locate the process equipment according to the rule of thumb in Appendix B Table 1. As we need to pump the liquid into the heat exchanger, our process equipment is a heat exchanger, a height of about 4 ft or 1.22 m.

Z_1 & Z_2

Z_1 with respect to pump = 0

Z_2 = 4 ft

Frictional pressure losses ED and ES:

So, ES & ED is equal t 0.35 from Appendix B Table 2.

Pump Work Calculation:

$$W = \frac{g}{g_c}(Z_1 - Z_2) + \frac{P_1 - P_2}{\rho} - (E_s - E_D)$$

W **=** 4114.38 Nm/kg

Efficiency of pump:

Ep = 50 % from Appendix B Table 3

Power Calculations:

$$P = \frac{mW}{Ep}$$

m = 2.013 kg/sec

W = 414.38 Nm/kg

Power = 18404.99 J/sec or 24.7 hp

Calculate Electric-Motor Horsepower & Estimate its Efficiency:

On the basis of horsepower, the selected motor is Squired cage inductive motor having a power range of 1 to 5000 hp from Appendix B Table 4.

The efficiency of the motor is selected to be = 0.91

The power of the motor is calculated as:

$P_E = P_p/\eta$

$P_E = 24.7/0.91 = 27$ hp

Net Positive Suction Head NPSH:

$$NPSH = \left(\frac{1}{g}\right)\left(\frac{P_a - P_v}{\rho} - h_{fs}\right) - Z_a$$

$Z_a = 0$

Absolute pressure at the surface of reservoir = P_a = 102642.22 Pa

Vapor pressure of glycerol = P_v = 14418.54 Pa

Friction losses in suction line = h_{fs} = 0

Density of glycerol = 1260 kg/m^3

NPSH = 7.2 m

Specification Sheet 01	
Pump No.	P-101
Type	Rotary pump
Function	To increase the pressure
Feed Flow Rate.	15979 lb/hr
Inlet Pressure	1.01 bar
Outlet Pressure	54.7 bar
Power of Shaft pump	24.7
Power of electric motor	27
NPSH	7. 2 m

Specification Sheet 02	
Pump No.	P-102
Type	Rotary pump
Function	To increase the pressure
Feed Flow Rate.	16022 lb/hr
Inlet Pressure	1.01 bar
Outlet Pressure	1.5 bar
Power of Shaft pump	1.9 hp
Power of electric motor	2.2 hp
NPSH	2.5 m

Specification Sheet 03	
Pump No.	P-103
Type	Rotary pump
Function	To increase the pressure
Feed Flow Rate.	13311.5 lb/hr
Inlet Pressure	1.01 bar
Outlet Pressure	1.5 bar
Power of Shaft pump	1.5 hp
Power of electric motor	1.7 hp
NPSH	2.5 m

Specification Sheet 04	
Pump No.	P-104
Type	Rotary pump
Function	To increase the pressure
Feed Flow Rate.	8585 lb/hr
Inlet Pressure	1.01 bar
Outlet Pressure	1.5 bar
Power of Shaft pump	1.5 hp
Power of electric motor	1.8 hp
NPSH	2.5 m

Specification Sheet 05	
Pump No.	P-105
Type	Rotary pump
Function	To increase the pressure
Feed Flow Rate.	4506 lb/hr
Inlet Pressure	1.01 bar
Outlet Pressure	1.5 bar
Power of Shaft pump	1.3 hp
Power of electric motor	1.5 hp
NPSH	2.5 m

7.6 Compressor:

Positive-Displacement Compressors:

Reciprocating compressors consist of direct-acting and diaphragm types. The direct-acting compressor consists of one or more cylinders, each with a piston or plunger that moves back and forth. A gas enters or leaves a cylinder through valves that are activated by the difference in pressure in the cylinder and intake or discharge. When the pressure in the cylinder drops below the inlet pressure, a valve opens allowing gas to flow into the cylinder.

Dynamic Compressors:

Dynamic compressors, like fans, are divided into two classes, centrifugal and axial, according to the direction of gas flow through the machine.

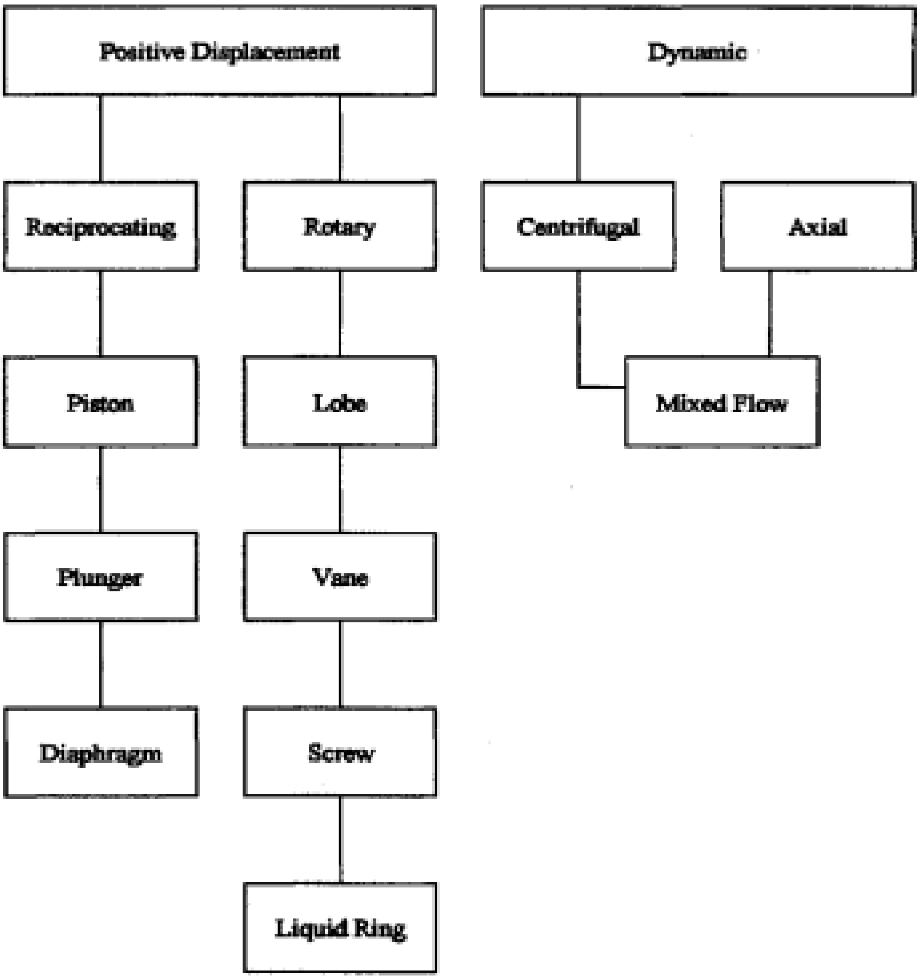


Figure 7-3 Characteristics of compressor

7.7 Design of Compressor:

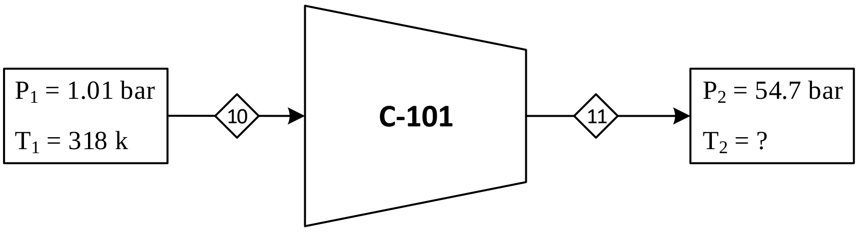


Figure 7-4 Compressor (C-101)

P_1 = 1 atm = 1.01 bar

P_2 = 54 atm = 54.7 bar

T_1 = 45 C = 318 k

T_2 = ?

Molar mass of hydrogen = 2.016 kg/kmol

Mass flow rate = 774.2 kg/hr

Density = 42 kg/m^3

Volumetric flow rate = 18.433 m^3/hr

7.8 Compressor Selection:

Centrifugal compressor:

- Widely used in industries
- Provide high pressure
- Barrel-type centrifugal is preferred for hydrogen compression on an industrial scale
- Easier access for maintenance and repair

7.9 Compressor Calculations:

T_{max} = 505 k

Polytrophic efficiency for centrifugal pump = 70-85%

E_p = 0.75

K = C_p/C_p-R = 1.3

$\frac{n-1}{n} = \frac{(k-1)/k}{Ep} = 0.35$

Find no. of stages by ratio equation (Harry Silla)

$P_2/P_1 = P_3/P_2 = P_4/P_3 = \ldots\ldots = P_{Ns+1}/P_{Ns}$

Ns = no. of stages

By using;

$(P_{Ns+1}/P_1) = (P_2/P_1)^{Ns}$

Now we have the value of P_2/P_1

$P_2/P_1 = 3.78$ bar

Now for P_3

$P_3 = 3.78 * 3.78 = 14.2884$ bar

$P_4 = 14.3 * 3.78 = 54.01$ bar

At stage three pressure is very close to our discharge pressure.

$T_2 = T_1(P_2/P_1)^{(n-1)/n}$

$T_2 = 506.4$ k

$W_p = \frac{NsZRT}{n-1/n} ((P_{Ns+1}/P_1\ )^{1/Ns*(n-1)/n} - 1)$

$W_p = 30716.2$ kJ/kgmol

Actual work required = Polytropic work/$E_s.E_g.E_B.E_p$

$E_s = 0.98$, $E_g = 0.97$, $E_B = 0.98$, $E_p = 0.66$ from index B table 5

Work required

W = 499.5 j/kmol

m = 387.1 kmol/hr

Power calculation:

Power = W*m = 259 hp

Specification Sheet 01	
Compressor No.	C-101
Type	Centrifugal compressor
Function	To increase the pressure
Volumetric Flow Rate.	18.433 m3/hr
Inlet Pressure	1.01 bar
Outlet Pressure	54.7 bar
Inlet temp.	318 k
Outlet temp.	506 k
Work required	499.5 J/kmol
Power	259 hp

CHAPTER NO. 8

COST ESTIMATION

8.1 Working Capital:

Working capital is an important component of cost estimation for businesses, particularly in the context of project management. Working capital refers to the amount of money that a business needs to have on hand in order to fund its day-to-day operations.

When estimating the cost of a project, it is important to consider the project's working capital requirements. This includes estimating the amount of cash required to cover the cost of inventory, accounts receivable, and other current assets needed to support the project.

8.2 Cost Estimation:

Cost estimation is an essential part of chemical engineering, as it helps to determine the economic feasibility of a process or project. It involves the process of estimating the cost of all the materials, equipment, labor, and other expenses required for a chemical process or plant.

The cost estimation process involves identifying all the equipment and materials needed for a specific process, determining the labor required, and calculating the components' cost. This includes the cost of raw materials, energy, utilities, maintenance, and other expenses.

8.3 Cost Indexes:

Cost indexes are widely used in business and government to adjust prices for inflation, to make cost estimates for future projects, and to track changes in the relative prices of goods and services over time. They are also used by economists to study trends in the economy and to analyze the impact of various economic policies on prices and inflation.

The current cost is calculated using the cost index as follows:

$$\frac{\text{Present cost}}{\text{index at present time}} = \frac{\text{(Original cost)}}{\text{index value at time of original cost}}$$

Some common use cost indexes are the following as:

1. Marshal-and-Swift all-industry and process-industry equipment index.
2. Engineering News-record construction index.
3. Nelson-Farrar Rebery construction index.
4. Chemical Engineering Plant Cost Index.

8.3.1 Cost of Reactor:

Material of construction = Stainless Steel

Length = 6.8 m

Diameter = 2.2 m

Material Factor = 2

Pressure Factor = 2.2

Volume of Reactor = 5.3 m^3

Bare Cost = $ 15000

Purchase equipment cost inn 2004 = $ 66000

$$\text{Present Cost} = \text{Original Cost} \times \frac{\text{Index at Present Time}}{\text{Index value at the time of original cost}}$$

Cost Index in 2022 = 808.7

Cost Index in 2004 = 444.2

Purchased equipment cost in (2022) = $ 119801

8.3.2 Cost of Liquid-Gas Separator:

Material of construction = Stainless Steel

Height = 4 m

Diameter = 0.96 m

Material Factor = 2

Pressure Factor = 1.8

Bare Cost = $10030

Purchase equipment cost in 2004 = $ 36108

Cost Index in 2022 = 808.7

Cost Index in 2004 = 444.2

Purchased equipment cost in (2022) = $ 65737.3

8.3.3 Cost of Distillation column (T-101):

Height of column = 8.89m

Diameter of column = 1.16m

Number of plates = 15

Pressure = 1 bar

Material = Carbon steel

Bare cost = $12000

From Appendix C Graph 01

Purchased cost in 2004 = (bare cost *Material Factor *Pressure factor)

= ($12000 × 1.0 × 1.0)

Purchased cost in 2004 = $12000

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$21850

Cost for Sieve Trays:

Cost of plate = $\$300$

From Appendix C Graph 02

Cost of total plates = $\$300\ \times 15$

Cost of total plates = $\$4500$

Total cost of distillation column = $\$21850 + 4500$

Total cost of distillation column = $\$26350$

Cost of Condenser (E-106):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 12m^2

Bare cost is = \$8000

From Appendix C Graph 03

Purchased cost in 2004 = Bare cost*material factor*pressure factor

Purchased cost in 2004 = (\$8000 $\times$ 1.0 $\times$ 0.85)

= (\$6800)

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$12380

Cost of Reboiler (E-107):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 89.9m^2

Bare cost is = \$32000

From Appendix C Graph 03

Purchased cost in 2004 = ($\$32000 \times 1.0 \times 0.85$)

= ($\$27200$)

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$49520

8.3.4 Cost of Distillation column (T-102):

Height of column = 11.5m

Diameter of column = 2.13m

Number of plates = 36

Pressure = 1 bar

Material of construction = Carbon steel

Bare cost = $\$25000$

From Appendix C Graph 01

Purchased cost in 2004 = ($\$25000 \times 1.0 \times 1.0$)

Purchased cost in 2004 = $\$25000$

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$45520

Cost for Sieve Trays:

Cost of plate = $\$400$

Cost of total plates = $\$400 \times 36$

Cost of total plates = $\$14400$

From Appendix C Graph 02

Total cost of distillation column = $\$45520 + 14400$

Total cost of distillation column = $\$59920$

Cost of Condenser (E-108):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 36m^2

Bare cost is = \$19000

From Appendix C Graph 03

Purchased cost in 2004 = $(\$19000 \times 1.0 \times 0.85)$

= $(\$16200)$

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$29450

Cost of Reboiler (E-109):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 23.9m^2

Bare cost is = \$15000

From Appendix C Graph 03

Purchased cost in 2004 = $(\$15000 \times 0.85 \times 1.0)$

= $(\$12750)$

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$23220

8.3.5 Cost of Distillation Column (T-103):

Height of column = 6.9m

Diameter of column = 1.05m

Number of plates = 13

Pressure = 1 bar

Material = Carbon steel

Bare cost = (\$10000)

From Appendix C Graph 01

Purchased Cost in 2004= ($\$10000 \times 1.0 \times 1.0$)

Purchased Cost in 2004= $\$10000$

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$18210

Cost for Sieve Trays:

Cost of plate = $\$200$

Cost of total plates = $\$200 \times 13$

Cost of total plates = $\$2600$

From Appendix C Graph 02

Total cost of distillation column = $\$18210 + 2600$

Total cost of distillation column = $\$20800$

Cost of Condenser (E-110):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 17m^2

Bare cost is = \$12000

From Appendix C Graph 03

Purchased cost in 2004 = ($\$12000 \times 0.85 \times 1.0$)

= ($\$10200$)

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$18570

Cost of Reboiler (E-111):

Material: CS

Pressure 1 bar = pressure factor = 1

Type factor U-Tube = 0.85

Heat transfer area = 15.5m^2

Bare cost is = \$10000

From Appendix C Graph 03

Purchased cost in 2004 = $(\$10000\ \times 0.85 \times 1.0) = (\$8500)$

Cost index in 2004 = 444.2

Cost index in 2022 = 808.7

Cost in 2022 = $Equipment\ cost\ \left(\frac{cost\ index\ in\ 2022}{cost\ index\ in\ 2004}\right)$

= \$15480

8.3.6 Cost Shell & Tube Heat Exchanger (E-101):

Heat transfer area = 30.3 m^2

Cost in 2004 = \$ 18000

From Appendix C Graph 03

Pressure Factor (F_{BM}) = 1.5

Type factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = (18000) × (1.5) = \$ 27000

Cost Index in 2004 = 230

Cost Index in 2022 = 519

Cost in 2022 = $C_{BM}\ (\frac{Cost\ index\ in\ 2022}{Cost\ index\ in\ 2004})$ = \$ 60,926

8.3.7 Cost Shell & Tube Heat Exchanger (E-102):

Heat transfer area = 140.5 m^2

Cost in 2004 = \$ 31,000

From Appendix C Graph 03

Pressure factor = 1.5

Type factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = (31,000) × (1.5) = $ 46,000

Cost Index in 2004 = 230

Cost Index in 2022 = 519

Cost in 2022 = C_{BM} ($\frac{Cost\ index\ in\ 2022}{Cost\ index\ in\ 2004}$) = $ 103800

8.3.8 Cost Double pipe Heat Exchanger (E-103):

Heat transfer area = 72 m^2

Cost in 2004 = $ 3400

From Appendix C Graph 03

Cost Index in 2004 = 230

Cost Index in 2022 = 519

Cost in 2022 = C_{BM} ($\frac{Cost\ index\ in\ 2022}{Cost\ index\ in\ 2004}$)

= $ 7702

Purchase cost of equipment

in 2022 = $ 7702

8.3.9 Cost Double pipe Heat Exchanger (E-104):

Heat transfer area = 3.71 m^2

Cost in 2004 = $ 1800

From Appendix C Graph 03

Cost Index in 2004 = 444

Cost Index in 2022 = 808

Cost in 2022 = C_{BM} ($\frac{Cost\ index\ in\ 2022}{Cost\ index\ in\ 2004}$)

Purchase cost of equipment in 2022 = $ 3277

8.3.10 Pump Cost (P-101):

Pump capacity = 10^{-3} m^3/s

Cost in 2002 = $1080

From Appendix C Graph 04

Material factor = 1

Pressure factor = 2

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 2100

Cost Index in 2002 = 172

Cost Index in 2022 = 349   from graph D

Cost in 2022 = (1400) x (349/172)

Purchase cost of equipment in 2022 = $ 4260

8.3.11 Pump Cost (P-102):

Pump capacity = $10^{-2.1}$ m^3/s

Cost in 2002 = $ 3000

From Appendix C Graph 04

Material factor = 1

Pressure factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 3000

Cost Index in 2002 = 172

Cost Index in 2022 = 349

Cost in 2022 = (3000) (349/172)

Purchase cost of equipment in 2022 = $ 6100

8.3.12 Pump Cost (P-103):

Pump capacity = $10^{-2.2}$ m^3/s

Cost in 2002 = $2900

From Appendix C Graph 04

Material factor = 1

Pressure factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 2900

Cost Index in 2002 = 172

Cost Index in 2022 = 349

Cost in 2022 = (2900) (349/172)

Purchase cost of equipment in 2022 = $ 5890

8.3.13 Pump Cost (P-104):

Pump capacity = $10^{-2.4}$ m^3/s

Cost in 2002 = $2700

From Appendix C Graph 04

Material factor = 1

Pressure factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 2700

Cost Index in 2002 = 172

Cost Index in 2022 = 349

Cost in 2022 = (2700) (349/172)

Purchase cost of equipment in 2022 = $ 5480

8.3.14 Pump Cost (P-105):

Pump capacity = $10^{-2.5}$ m^3/s

Cost in 2002 = $ 2500

From Appendix C Graph 04

Material factor = 1

Pressure factor = 1

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 2500

Cost Index in 2002 = 172

Cost Index in 2022 = 349

Cost in 2022 = (2500) (349/172)

Purchase cost of equipment in 2022 = $ 5070

8.3.15 Compressor Cost (C-101):

Power = 163 kW

Cost in 2004 = $ 80000

From Appendix C Graph 05

Bare Module Cost Factor (F_{BM}) = 2.5

Bare Module Equipment Cost (C_{BM}) = Cost in 2004 × F_{BM}

Bare Module Equipment Cost (C_{BM}) = $ 200000

Cost Index in 2004 = 146

Cost Index in 2020 = 320

Cost in 2020 = (200000) (320/146)

Purchase cost of equipment in 2020 = $ 438000

8.4 Fixed Capital Investment:

8.4.1 Direct Cost:

Direct Cost			
Items	**Range**	**%**	**Cost, $**
Purchased equipment		100	$ 1,080,324
Installation	25 - 55% of Purchased Equipment Cost	40	$ 432,129.5
Instrumentation & Control	6 - 30% of Purchased Equipment Cost	20	$ 216,064.8
Piping	40 - 80% of Purchased Equipment Cost	60	$ 648,194.3
Electricity	10 - 15% of Purchased Equipment Cost	12.5	$ 135,040.5
Building	15% of Purchased Equipment Cost	15	$ 162,048.6
Land	4 - 8% of Purchased Equipment Cost	6	$ 64,819.4
Service Facility	30 - 80% of Purchased Equipment Cost	55	$ 594,178.1
Yard Improvement	10 - 20% of Purchased Equipment Cost	15	$ 162,048.6
Insulation cost	8 - 9% of Purchased Equipment Cost	8	$ 86,425.9
Total Direct Cost			$ 2,500,949.6

8.4.2 Indirect Cost:

Indirect Cost			
Items	Range	%	Cost, $
Engr. & supervision	8 % of Total direct cost	8	200076.0
Contractor fee	2 – 8 % of Total direct cost	5	125047.5
Construction expenses	10 % of Total direct cost	10	250095.0
Contingences	Direct plant cost 8%	8	200076.0
Total Indirect Cost			775294.4

8.5 Fix Capital Investment:

FCI =Direct Cost +Indirect Cost

FCI =$ 3,276,244.00

8.6 Working Capital Investment:

WCI =15%FCI

WCI = 0.15×FCI

WCI = $491,436.60

8.7 Total Capital Investment:

Total Capital Investment =WCI +FCI

Total Capital Investment = $3,767,680.60

Total Capital Investment = $3.77 M

8.8 Direct Operational Cost:

8.8.1 Variable Cost:

Raw Material Cost	
Hydrogen Cost	
H_2 cost	2 $/kg
H_2 Flow Rate	154 kg /hr
H_2 require per hour	308 $/hr
H_2 Cost	2439360 $/yr
Glycerol Cost	
Glycerol cost	0.49 $/kg
Glycerol Flow Rate	7248 kg /hr
Glycerol require per hour	3551.5 $/hr
Glycerol Cost	28128038.4 $/yr
Cu-Zn Al2O3	
Catalyst cost	1.8 $/kg
Catalyst Required	9916 kg
Cost	17849 $/yr
Total	30585247.2 $/yr

8.8.2 Utility Cost:

Utilities Cost	
Cooling Water Cost	
Flow Rate of Water	172727 kg /hr
Price per kg	0.00008 $/kg

Cost of water	13.81 $/hr
Cost of Water	109439.8272 $/yr
Steam Cost	
Flow Rate of Steam	3162 kg /hr
Price per kg	0.0044 $/kg
Cost of steam	13.91 $/hr
Cost of Steam	110189.4$/yr
Total Variable Cost =Raw Materials +Utilities +	Miscellaneous
Total Variable Cost	$30804876

8.8.3 Fixed Cost:

Fixed Cost		
Function	% FCI	Cost ($)
Maintenance	7	229337.08
Operating Labor	10	327624.40
Laboratory Cost	20	655248.80
Supervision	15	491436.60
Clerical Labor	50	1638122.00
Capital Charges	10	327624.40
Insurance	1	32762.44
Local Taxes	2	65524.88
Royalties	1	32762.44
Total		3800443.04

Direct Cost = Variable Cost + Fixed Cost

Direct Cost = $34,605,319

8.9 Overhead Cost:

Overhead Cost = 30% of Direct Production Cost

Overhead Cost = $10,381,596

8.10 Manufacturing Cost:

Manufacturing Cost = Overhead Cost + Direct Production Cost

Manufacturing Cost = $44,986,915

8.11 General Expenses:

General Expenses		
Function	Percentage of Manufacturing Cost	Cost ($)
Administration	2%	$8,997.38
Distribution and Marketing	2%	$8,997.38
Research and Development	5%	$22,493.46
Total		$40,488.22

8.12 Total Production Cost:

Total Production Cost = Manufacturing Cost +General Expenses

Total Production Cost = $45,027,403.51

8.13 Total Production Rate:

Production Rate = 30000 t/year

Total Production Cost = $45,027,403.51/year

Production Cost = $1,501/t

Production Cost = $1.5/kg

8.14 Profitability Analysis:

8.14.1 Selling Price:

Selling Price ($/ton) = $1,570/ ton

Total income = $47,100,000

Production Cost = $1501/ton

8.14.2 Profit:

Profit = Selling price - production cost = 69.09 $/ton

Profit per year = $2,072,596/year

8.15 Depreciation:

FCI = V = $3,276,244

Salvage value = Vs = 5% of FCI

Salvage value = $163,812

Number of years = 20

Depreciation = $155,621.59/yr

8.16 Gross Profit:

Gross Profit = Profit - Depreciation

Gross Profit = $1,916,975/year

8.17 Net Profit:

Net Profit = Gross Profit –Income Taxes

Income Taxes = 35 % of Gross Profit

Income Taxes = $670,941/year

Net Profit = $1,246,033/year

8.18 Rate of Return:

$$\text{Rate of Return} = \frac{\text{Net Profit}}{\text{Total Initial Investment}}$$

Rate of return = 0.33

8.19 Payback Period:

$$\text{Payback Period} = \frac{1}{\text{Rate of Return}}$$

$$\text{Payback Period} = \frac{1}{0.33}$$

Payback Period = 3.02

CHAPTER NO. 9

INSTRUMENTATION AND PROCESS CONTROL

9.1 Introduction:

Instrumentation and process control play a critical role in ensuring safe and efficient operations in chemical process plants. Process control technology involves the use of sensors, controllers, and software to measure and monitor various parameters such as temperature, pressure, flow, and composition of the fluids being processed. This data is then used to regulate the process and make adjustments to maintain optimal operating conditions, ensure product quality, and reduce waste.

In chemical process plants, instrumentation is used to measure and monitor various process variables, such as temperature, pressure, and flow rates. This information is then transmitted to a central control system where it is analyzed and used to adjust the process variables to ensure the desired output. Additionally, safety systems are integrated into the control system to provide alerts and activate emergency shutdown procedures in case of any abnormal conditions or hazardous situations.

Overall, instrumentation and process control are essential components in chemical process plants for ensuring safe, efficient, and profitable operations. The technology allows for precise and accurate control of the process variables, which leads to increased productivity, reduced costs, and improved product quality. Additionally, the use of process control technology minimizes the risk of human error and maximizes safety in the plant. [27]

9.2 Safe Plant Operation:

Safe plant operation is essential to prevent accidents, protect the environment, and ensure the health and safety of employees and surrounding communities. To achieve safe plant operation, several measures need to be put in place:

1. Conduct regular safety audits and risk assessments to identify potential hazards and address them promptly.
2. Ensure that all employees are trained in safety procedures and equipped with the necessary personal protective equipment (PPE).
3. Implement safety protocols and guidelines to prevent accidents and respond promptly in case of emergencies.
4. Regularly maintain equipment and machinery to minimize the risk of malfunctions and breakdowns that can cause accidents.
5. Monitor and control process variables using instrumentation and process control technology to ensure safe and efficient operation.
6. Promote a safety culture among employees by encouraging reporting of safety incidents and addressing safety concerns promptly.
7. Develop and implement emergency response plans and conduct regular drills to ensure that employees know what to do in case of an emergency.
8. Maintain compliance with industry regulations and standards to ensure safe and legal plant operation. [28]

Product Quality: To maintain the product composition within the specified quality standards.

Cost: To operate at the lowest production cost, commensurate with the other objectives.

9.3 Components of the Control System:

Process: A process is any operation or series of operations that results in a desired end result.

Measuring Means: The measuring element is perhaps the most critical of all the components of the control system. If measurements aren't taken correctly, the rest of the device won't work properly. To reflect the desired condition in the process, the measured available is a dozen.

Process Variable: A process variable is a property of the process fluid that has the potential to alter the manufacturing process.

Common process variables include:

- Pressure
- Flow
- Level
- Temperature
- Density
- PH (acidity or alkalinity)
- Mass
- Conductivity

Set Point: A fixed point is a value for a process variable that should be kept constant. Maximum and minimum values can also be used as set points.

Measured Variables: The measured variable is the condition of the process fluid that must be kept at the designated set point.

9.4 Hardware Elements of Control System:

A control system typically consists of several components that work together to regulate and manage various process variables. These components can include:

Sensors: These are devices that detect and measure physical quantities such as temperature, pressure, flow, and level. Sensors are used to monitor the process and provide input to the control system.

Controllers: Controllers receive input from the sensors and provide output to control the process variables. There are different types of controllers such as proportional-integral-derivative (PID) controllers, which adjust the process variables based on set points and feedback from the sensors.

Actuators: These are devices that receive output signals from the controllers and adjust the process variables. For example, an actuator can be used to adjust the flow of a fluid or adjust the position of a valve to control pressure.

Human Machine Interface (HMI): This is the user interface that allows operators to monitor and control the process. The HMI can display process variables, alarms, and trends in real-time, and allow the operator to adjust set points or override control actions.

Communication network: A communication network connects the various components of the control system and allows them to exchange data and commands. This can include wired or wireless networks, such as Ethernet, Modbus, or Profibus.

Software: Control system software can be used to configure and program the controllers, monitor and analyze process data, and provide alerts and notifications in case of any abnormal conditions or alarms.

9.5 Classification of Control Systems:

For instrumentation and control of different sections and equipment of plants, following control loops are most often used.

- Feed-back control loop
- Feed forward control loop
- Ratio control loop
- Split range control loop
- Cascade control loop

Feed Back Control Loop: A monitoring system in which the calculated value of a process variable is compared to the desired value of the process variable and any required actions are taken. The basic control loops framework is known as feedback control. Its operating method is one of its drawbacks. If a certain quantity is entering a process, for example, a monitor will be present to record its value. Any deviations from the set point will be communicated to the final control factor through the controller, allowing the incoming quantity to be adjusted to the desired value (set point).

Feed Forward Control Loop: The value of the disturbance is determined, and then action is taken to avoid the disturbance by altering the value of a process variable. This is a control method that is used to avoid errors in a process variable. Since it anticipates the shift in the process variable until it reaches the process and takes preventive steps, this control mechanism is superior to feedback control. Action is taken after a shift has occurred in a feedback control system.

Ratio Control: The controlling aspect of a control loop keeps a predetermined ratio of one variable to another. This control loop is usually connected to a device in which two separate systems join a vessel for a reaction of some sort. This loop is used to ensure proper process in the process vessel by maintaining the stoichiometric amounts of various streams.

Split Range Loop: This loop controller is pre-programmed with various values that lead to various actions to be taken under various conditions. This loop has the benefit of maintaining proper conditions and avoiding anomalies at very different levels.

Cascade Control Loop: This is a control in which the output of one controlling element changes the set point of another controlling element by the use of two or more control loops. When simple feed forward or feed backward control is insufficient for proper and fast control, this control loop is used. The first loop is usually a feedback control loop. [29]

9.6 Control Scheme of Distillation Column:

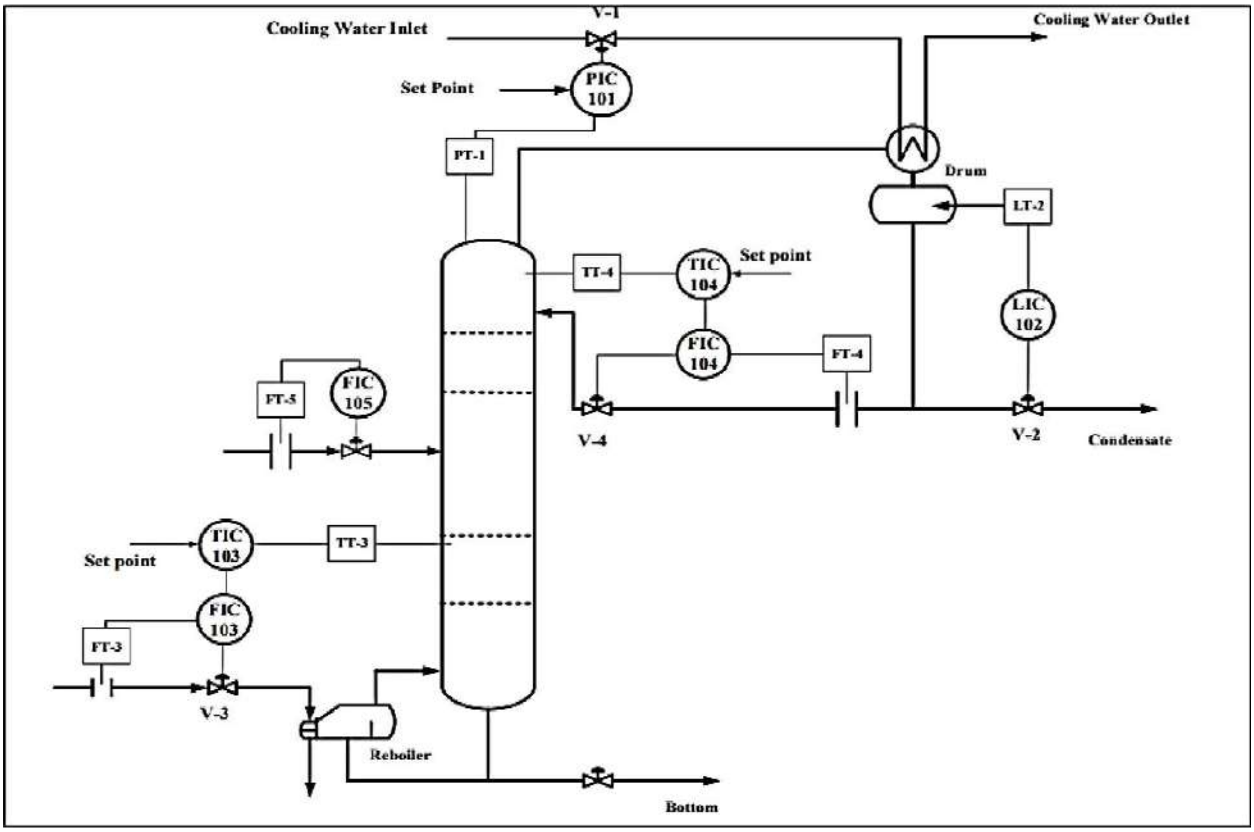


Figure 9-1 Instrumentation and Control of Distillation Column

9.6.1 Objectives:

In distillation column any of following may be the goals to achieve.

- Overhead composition
- Bottom composition
- Constant overhead product rate
- Constant bottom product rate

9.6.2 Manipulated Variables:

In a distillation column, manipulated variables are the process parameters that can be adjusted to control the operation of the column. The main manipulated variables in a distillation column are:

Reflux flow rate: Reflux flow rate is the rate of liquid that is returned from the condenser to the top of the column. By adjusting the reflux flow rate, the liquid holdup in the column and the degree of separation can be controlled.

Reboiler heat input: Reboiler heat input is the amount of heat supplied to the reboiler to generate the required vaporization of the bottom liquid in the column. By adjusting the reboiler heat input, the vaporization rate and temperature in the column can be controlled.

Column pressure: Column pressure is the pressure at which the column operates, and it affects the boiling point of the components in the feed. By adjusting the column pressure, the boiling points of the components can be manipulated, and the separation efficiency can be improved.

Feed flow rate: Feed flow rate is the rate at which the feed is introduced into the column. By adjusting the feed flow rate, the composition of the feed and the degree of separation in the column can be controlled.

Distillate and bottom product flow rates: Distillate and bottom product flow rates are the rates at which the distillate and bottom products are removed from the column. By adjusting the distillate and bottom product flow rates, the composition of the products and the degree of separation in the column can be controlled.

9.7 Control on Distillation Column:

Control Scheme:

Any shift in feed rate must be absorbed by changing the bottom product rate, as the overhead product rate is set. The change in product rate is accomplished by direct level control of the reboiler if the stream rate is set and the feed rate increases, the vapor rate remains roughly constant, and the internal reflux flows must rise. Since an increase in feed rate raises the reflux rate while keeping the vapor rate relatively stable, the purity of the top product rises. The dynamics of the level control system that adjusts it determine the shift in overhead reflux.

Description:

The LC-1 is the level controller. The sensing element (level measuring device) measure the level and sends signal to the controller. Which has a preset value feed to it. It compares the set point and the measured value and send signal to the valve. Which in turn take action on the instruction provided by the controller.

The temperature sensor sense the temperature of the feed and immediately send signal to the controller TC-2 which in turn sends signal to the flow controller. FC-4 that will immediately control the reflux rate.

Feed Control:

Increase the flow rate of the feed if the rate is less than set point and decrease the flow rate of the feed if the rate is more than set point.

Table 9-1 Elements of Control Loop for Feed of Distillation Column

Process	Flow rate of Feed Stream
Controller	Automatic(PIC)
Controlled variable	Flow rate
Measuring element	Orifice
Manipulated element	Valve
Regulating element	Valve
Load variable	Leakage and value characteristics friction in pipe

Operation:

If the feed flow increases the (FIC) will send signal by (FT) to the controller. The controller also send signal to the valve which will drive the control valve to close. If the feed flow decreases the (FIC) will send signal by (FT) to the controller. The controller also send signal to the valve which will drive the control valve to open.

Top Pressure Control:

Reason for control distillation column pressure is that any change in the operating pressure will affect the separation efficiency. The pressure of the top section of this distillation column must be 1 bar. We control the top pressure by controlling the flow rate of vapor outlet from the top of the column.

Set point: 1 bar

Operation:

The manometer measures the pressure of the top and the transmitter sends the measured value to the controller to compare it to the set point, if the pressure is increased above 1 bar the flow rate of the cooling water in the condenser must be increased, and if it is decreased below 1 bar decrease the cooling water flow rate.

Table 9-2Elements of Control Loop for Distillation Column Top Section Pressure

Process	Distillation column
Controller	Automatic(P)
Controlled variable	Pressure
Measuring element	Manometer
Manipulated element	Vapor Flow rate
Regulating element	Valve(pneumatic)
Load variable	Feed flow rate of fed temperature, change in the ratio of gas to liquid, valve characteristic

Drum Level Control:

The drum level in the top section is controlled by changing the distillate flow rate using a valve. Set point: 85% of the holdup volume.

Table 9-3 Control Loop Elements for Drum Level Control for Distillation Column

Process	Distillation column
Controller	Automatic(P)
Controlled variable	Drum level
Measuring element	Orifice
Manipulated element	Distillate flow rate
Regulating element	Valve

Load variable	Feed flow rate of fed temperature, change in the ratio of gas to liquid, valve characteristic

Reactor Control:

A control scheme for a multi-tubular packed bed reactor typically involves monitoring and controlling several key variables to ensure optimal reactor performance. Some of the key variables that may be monitored and controlled in a multi-tubular packed bed reactor include:

Feed flow rate and composition:

The feed flow rate and composition can have a significant impact on reactor performance, and may need to be controlled to maintain a consistent feed to the reactor.

Reactor temperature:

The temperature inside the reactor can have a significant impact on the rate of reaction and the selectivity of the product. Temperature control may be achieved by controlling the flow of heating or cooling fluid through the reactor jacket.

Set Point = 190 ^{0}C

Operation:

The temperature sensor measures the temperature inside the reactor and send an electrical signal analog to the value of the temperature. The controller receives this signal and compares it, then gives corrective action. (If temperature is increased than 190 ^{0}C the controller increase the flow rate of the water and vice versa). The transducer converts the value to pneumatic signal to the regulating element. (Water valve)

Pressure:

The pressure inside the reactor can also affect reaction rate and selectivity. Pressure may be controlled by adjusting the flow rate of the reactants or adjusting the pressure of the heating or cooling fluid.

Catalyst activity:

The activity of the catalyst can also be monitored and controlled to ensure optimal reactor performance. This may involve monitoring the catalyst surface area or particle size, and adjusting the catalyst loading or replacement schedule as needed.

Product composition:

The composition of the product stream leaving the reactor can be monitored and controlled to ensure that the desired product is being produced at the desired purity.

A control scheme for a multi-tubular packed bed reactor may involve a combination of feedback and feedforward control strategies, along with automated shutdown procedures in the event of abnormal conditions. A supervisory control system may also be used to coordinate the operation of multiple reactors in a larger process.

CHAPTER NO. 10
HAZOP

10.1 Introduction:

One of the most popular and generally accepted methods of systematic qualitative hazard analysis is the HAZOP survey. It can be extended to a whole factory, a processing unit, or a piece of equipment, and it can be used for both new and existing facilities. Its database consists of the normal types of plant and process data, and it relies on the expertise of engineering and safety experts in the fields in which they work. The end result is therefore accurate in terms of engineering and organizational expectations, but it is not quantitative and does not take into account the implications of dynamic human error sequences.

10.2 Objectives of HAZOP Study:

The objectives of a HAZOP study can be summarized as follows:

1. To identify (areas of the design that may possess a significant hazard potential.
2. To identify and study features of the design that influence the probability of a hazardous incident occurring.
3. To familiarize the study team with the design information available.
4. To ensure that a systematic study is made of the areas of significant hazard potential.
5. To identify pertinent design information not currently available to the team.
6. To provide a mechanism for feedback to the client of the study teams detailed comments.

10.3 Success or Failure of the HAZOP:

The success or failure of the HAZOP depends on several factors:

- The completeness and accuracy of drawings and other data used as a basis for the study.
- The technical skills insights of the team.
- The ability of the team to use the approach as an aid to their imagination in visualizing deviations, causes, and consequences.
- The ability of the team to concentrate on the more serious hazards which are identified.

The process is systematic and it is helpful to define the terms that are used:

1. **Study Nodes:**

The positions where the method parameters are checked for anomalies (on piping and instrumentation drawings and procedures).

2. **Intention:**

In the absence of anomalies at the study nodes, the purpose specifies how the plant should work. Flow sheets, line diagrams, and P&IDs are examples of this type of documentation, which may be descriptive or diagrammatic.

3. **Deviations:**

There are deviations from the aim that are discovered by applying the guide words in a systematic manner (e.g. more pressure).

4. **Causes:**

These are the possible causes of deviations. Once a credible reason for a deviation has been established, it can be viewed as a meaningful deviation. Hardware failures, human errors, an unexpected process state (e.g., composition change), external disturbances (e.g., power outage), and other factors can all contribute to this. [30]

5. Consequences:

These are the outcomes of any anomalies that might occur (e.g. release of toxic materials). In terms of the study's goal, inconsequential effects are eliminated.

6. Guide Words:

These are basic terms that are used to qualify or measure an intention in order to direct and inspire brainstorming and thereby identify deviations. The guide terms mentioned in Table are the most commonly used in a HAZOP; certain companies have created a list unique to their activities to help the team get to the places where issues have already been discovered more quickly.

7. Data Collection:

- Process description.
- Process flow sheets.
- Data on the chemical, physical and toxicological properties of all raw materials intermediates, and products.
- Piping and instrument diagrams (P & ID’s).
- Equipment, piping, and instrument specifications.
- Process control logic diagrams.
- Layout drawings. [31]

Table 10-1 A List of Guide Words and their Meanings

Guide Words	Meaning	Guide Words	Meaning
No	Negation of design intent	Part of	Qualitative decrease
Less	Quantitative decrease	As well as	Qualitative Increase
More	Quantitative increase	Reverse	Logical opposite of the intent
Other than	Complete substitution		

After the nodes and parameters have been defined, each node is investigated using the specialized guide words for each parameter. These guide words and their meanings are key elements of the HAZOP procedure.

10.4 Procedure:

HAZOP studies are typically conducted by a group of experienced people with complementary skills and expertise, led by a team leader who is familiar with the methodology. To identify any hazards, the team analyses the process vessel by vessel, line by line, using the guide terms. The amount of data required for the analysis will be determined by the scope of the investigation. An overview of the process and process flow sheets may be used to create a preliminary report. Flow sheets, piping and instrumentation diagrams, equipment specifications, and layout drawings will be required for a comprehensive, final design report. In general the procedure steps involving HAZOP are:

- Divide the system into sections (i.e. reactor, storage).
- Choose a study node (i.e. line, vessel, pump, operating instructions).
- Describe the design intent.
- Select a process parameter.
- Apply a guide-word.
- Determine causes.
- Evaluate consequences/ problems.
- Recommend action: What? When? Who?
- Record information.
- Repeat procedure

10.5 HAZOP Study of Distillation Column:

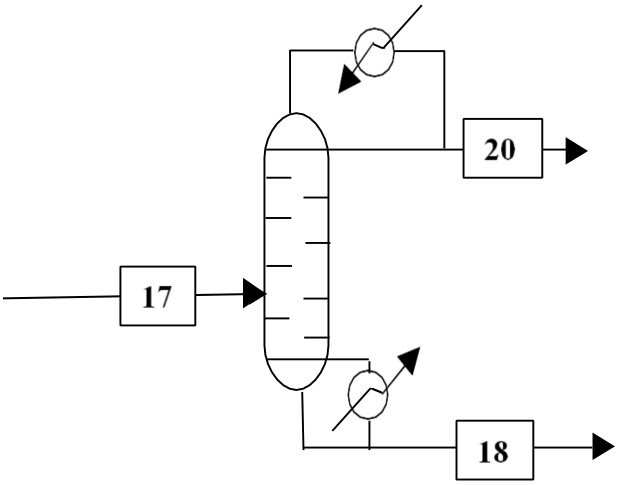


Figure 10-1 HAZOP Study on (T-102)

Table 10-2 HAZOP on Distillation Column (T-102)

Process parameter	**Deviation (guide word)**	**Possible causes**	**Possible consequences**	**Action required**
Flow	No	Pipe broken or plugging	Loss of feed into column (T-102) achieve into desired output.	Schedule inspection
Flow	Low	Pipe partial plugged or leakage.	Level decrease in distillation column. (T-102)	Install check valves
Flow	High	High pressure from source.	Flooding in distillation column. (T-102)	-
Flow	Low	Pipe partial clogged or leakage.	Level decrease in the vessel.	Scheduling inspection.

				Install valve
Temperature	Low	High incoming flow from condenser	Low level inside reboiler	Scheduling inspection
Temperature	Low	High incoming flow from condenser	Low level inside reboiler. Off Specification product.	Scheduling inspection. Install temperature sensors
Flow	No	Condenser line heavy leakage	Reflux drum low level Reflux drum depressurization	Compressor trip indication Level transmitter with low level alarm to be provided
Pressure	More	Valve close	Line over pressure	Compressor failure
Temperature	More	Cooling media fail of Condenser	Level low of reflux drum	Install temperature indicator at condenser outlet
Flow	Less	Leakage in upstream system Reboiler low level	Level low in condenser	Level controller (LLC)
Flow	More	Reboiler high level Leakage in Condenser	Level high in condenser	Level controller (LLC)

CHAPTER NO. 11

ENVIRONMENTAL IMPACT ASSESSMENT

11.1 Introduction:

Environmental Impact Assessment (EIA) is a process of evaluating the likely environmental impacts of a proposed project or development, taking into account interrelated socio-economic, cultural and human-health impacts, both beneficial and adverse. UNEP defines Environmental Impact Assessment (EIA) as a tool used to identify the environmental, social and economic impacts of a project prior to decision-making. It aims to predict environmental impacts at an early stage in project planning and design, find ways and means to reduce adverse impacts, shape projects to suit the local environment and present the predictions and options to decision makers. By using EIA both environmental and economic benefits can be achieved, such as reduced cost and time of project implementation and design, avoided treatment/clean-up costs and impacts of laws and regulations.

11.2 Propylene Glycol:

Propylene glycol (PG) is a synthetic organic compound that has a number of chemical and physical properties, including;

Chemical Properties:

Chemical Formula: $C_3H_8O_2$

Molecular Weight: 76.10 g/mol

Boiling Point: 188.2 °C (370.8 °F)

Melting Point: -60 °C (-76 °F)

Density: 1.036 g/cm^3

Solubility: Soluble in water, alcohol, and some organic solvents pH: Neutral (7)

Physical Properties:

- Colorless, odorless, and slightly viscous liquid
- Low volatility, meaning it has a low tendency to evaporate into the air
- Non-toxic and generally recognized as safe (GRAS) by the U.S. Food and Drug Administration (FDA)

Hygroscopic, meaning it has a strong affinity for water and can absorb moisture from the air. Relatively stable under normal conditions, but can degrade under high heat and pressure, or in the presence of certain chemicals.

Overall, propylene glycol has a range of properties that make it useful for a variety of applications in industries such as food, pharmaceuticals, cosmetics, and e-cigarettes. Its low toxicity, high solubility, and neutral pH make it a safe and effective ingredient in many products, while its hygroscopic and viscosity properties allow it to perform as a humectant and viscosity agent, respectively.

PG is a synthetic organic compound that is derived from propylene oxide, a chemical that is made from propylene, a byproduct of petroleum refining or natural gas processing. PG has a relatively low toxicity and is generally recognized as safe (GRAS) by the U.S. Food and Drug Administration (FDA) when used in small quantities in food, drugs, and cosmetics. [31]

In the food industry, PG is used as a solvent for flavors and colors, and as a humectant to keep foods moist. It is also used in certain medications to help deliver the active ingredients to the body, and as a lubricant in medical devices.

In the electronic cigarette industry, PG is used as a base liquid in e-liquids or vape juice, which is heated to produce an aerosol that can be inhaled. PG is used because it is a good solvent for nicotine and flavors, and produces a satisfying throat hit when inhaled. However, some individuals may be sensitive to PG and experience allergic reactions or irritation in the lungs when inhaling it.

Overall, propylene glycol is a versatile and widely used chemical that has many different applications in various industries.

11.3 Exposure to Propylene Glycol:

Propylene glycol is a common ingredient used in various industries, including food, cosmetics, and pharmaceuticals. It is generally considered safe for human use when used in appropriate amounts.

Exposure to propylene glycol can occur through various sources, including inhalation, ingestion, and skin contact. Inhaling propylene glycol vapor can cause irritation to the eyes, nose, and throat, and prolonged exposure may lead to respiratory irritation and even asthma.

Ingestion of propylene glycol in small amounts is generally considered safe and is often used as a food additive. However, ingesting large amounts may cause gastrointestinal symptoms such as nausea, vomiting, and diarrhea.

Skin contact with propylene glycol can cause irritation, redness, and swelling, particularly in individuals with sensitive skin. However, it is not typically considered a significant skin irritant and is widely used in skincare and cosmetic products.

11.4 Reactivity Profile of Propylene Glycol:

Propylene glycol (PG) is a chemical compound that is commonly used as a solvent, humectant, and preservative in various industries such as food, pharmaceuticals, and cosmetics. Its reactivity profile is as follows:

Chemical Stability: Propylene glycol is a stable compound and is not easily decomposed under normal conditions.

Oxidation: Propylene glycol is not readily oxidized and does not promote oxidation of other compounds.

Acid-Base Reactivity: Propylene glycol is a weak acid, with a pKa of 13.5, and does not react with bases. It can react with strong acids to form esters, but this reaction is slow.

Reduction: Propylene glycol is not readily reduced.

Polymerization: Propylene glycol is not known to undergo significant polymerization under normal conditions.

Reactivity with metals: Propylene glycol is not known to react with most metals, although it can react with aluminum to produce aluminum propylene glycol.

Overall, propylene glycol is a relatively stable compound that does not exhibit significant reactivity under normal conditions. However, it is always important to handle any chemical with care and follow appropriate safety protocols.

11.5 Environmental Impact:

The production of propylene glycol has several potential environmental impacts, including:

Air Pollution: The manufacturing process generates emissions of VOCs, which can contribute to air pollution and have adverse effects on human health and the environment. The combustion of fossil fuels to produce the energy required for the process also releases greenhouse gases such as carbon dioxide and nitrogen oxides, which contribute to climate change.

Water Pollution: The production of propylene glycol generates wastewater that may contain hazardous chemicals and pollutants. If the wastewater is not treated properly, it can contaminate nearby water bodies and have adverse effects on aquatic life.

Land Use: The production of propylene glycol requires land for the construction of manufacturing facilities and storage tanks. This can lead to the conversion of natural habitats and loss of biodiversity.

Waste Generation: The manufacturing process generates solid and hazardous waste, which can pose risks to human health and the environment if not managed properly.

Mitigation Measures To minimize the potential environmental impact of propylene glycol, the following mitigation measures are recommended:

Use of Renewable Energy: The use of renewable energy sources such as solar, wind, and geothermal can reduce greenhouse gas emissions from the manufacturing process.

Wastewater Treatment: Proper wastewater treatment can reduce the amount of pollutants that are released into the environment.

Recycling and Reuse: Recycling and reusing materials and resources can reduce waste generation and the need for virgin materials.

Environmental Monitoring: Regular monitoring of air, water, and soil quality can help detect any potential environmental impacts and allow for timely intervention.

11.6 First Aid:

Move the Person to Fresh Air: If the exposure is due to inhalation, move the person to a well ventilated area with fresh air. If the exposure is due to skin contact, remove any contaminated clothing and rinse the affected area with plenty of water.

Call for Medical Assistance: If the person is experiencing severe symptoms, such as difficulty breathing, dizziness, or loss of consciousness, call for medical assistance immediately. Also, if the exposure is due to ingestion, seek immediate medical attention.

Monitor Breathing and Vital Signs: If the person is conscious and breathing, monitor their vital signs, such as pulse and breathing rate, and observe any changes. If they stop breathing or their pulse stops, start cardiopulmonary resuscitation (CPR) until medical help arrives.

Provide Supportive Care: If the person is conscious and alert, provide supportive care, such as keeping them warm and comfortable, offering they water to drink, and reassuring them.

Seek Medical Advice: Even if the person does not show any immediate symptoms, it is essential to seek medical advice as soon as possible. Some health effects of propylene glycol exposure may not appear until several hours after exposure

11.7 Spillage Disposal:

When it comes to spillage disposal of propylene glycol, it's essential to follow proper guidelines to prevent harm to human health and the environment. Here are some steps you can take:

Contain the spill: Immediately contain the spill to prevent it from spreading. You can use absorbent materials such as sand, clay, or commercial absorbent pads to absorb the spilled propylene glycol.

Ventilate the area: Ensure adequate ventilation in the spill area to reduce the risk of inhaling the vapors. Open windows or use exhaust fans to remove the fumes from the area.

Use protective gear: Wear appropriate personal protective equipment such as gloves, goggles, and respiratory protection to protect yourself from exposure to propylene glycol.

Clean up the spill: Use absorbent materials to clean up the spill completely. Dispose of the used absorbent materials in a sealed container and label it as hazardous waste.

Rinse the area: After cleaning up the spill, rinse the area with water to dilute any remaining propylene glycol. Use a mop or a wet vacuum to remove the rinse water and dispose of it as hazardous waste.

Follow proper disposal procedures: Properly dispose of the hazardous waste in accordance with local, state, and federal regulations. Contact your local hazardous waste disposal facility to obtain proper disposal instructions.

Remember, proper handling, storage, and disposal of propylene glycol is critical to protecting human health and the environment. Always follow safety guidelines and regulations to prevent accidental spills and ensure proper disposal.

11.8 Disposal Methods:

The most common disposal methods for propylene glycol are:

Discharge into a wastewater treatment plant: Propylene glycol can be discharged into a wastewater treatment plant where it can be treated and eventually discharged into a water body. However, it is important to check with the treatment plant beforehand to ensure that they can accept propylene glycol and that it meets their discharge requirements.

Incineration: Propylene glycol can be incinerated at high temperatures in a controlled environment. This method is often used for larger quantities of propylene glycol, such as in industrial settings.

Landfill disposal: Propylene glycol can be disposed of in a landfill, but it is important to check with local regulations and waste management facilities beforehand to ensure that this is allowed and that it is done properly.

Recycling: In some cases, propylene glycol can be recycled and reused in other applications. This method is often used in industrial settings where large quantities of propylene glycol are used.

It is important to handle and dispose of propylene glycol in accordance with local regulations and guidelines to ensure that it does not harm the environment or public health.

11.9 Exposure Control and Personal Protection:

11.9.1 Exposure Control:

- Personal protective equipment (PPE) such as gloves, safety glasses, and protective clothing should be worn when handling propylene glycol to prevent skin and eye irritation or absorption.
- Adequate ventilation is important when working with propylene glycol to avoid inhalation of vapors or mists. Ensure that the work area is well ventilated, and if necessary, wear a respirator or mask.
- Avoid ingestion of propylene glycol by not eating or drinking while working with it and by washing hands thoroughly before eating or drinking.

11.9.2 Personal Protection:

- Avoid skin contact by wearing gloves and protective clothing. If skin contact occurs, wash the affected area with soap and water immediately.
- Protect eyes by wearing safety glasses or goggles. If propylene glycol gets into the eyes, flush them with clean water for at least 15 minutes and seek medical attention if irritation persists.
- Avoid inhalation of vapors or mists by using proper ventilation or wearing a respirator or mask. If propylene glycol is inhaled, move to a well-ventilated area and seek medical attention if necessary.

In case of accidental ingestion, seek medical attention immediately. Do not induce vomiting unless instructed by medical professionals.

11.10 Regulatory Information:

Here is some regulatory information about propylene glycol:

Food and Drug Administration (FDA): The FDA has designated propylene glycol as "generally recognized as safe" (GRAS) for use as a direct food additive. It is approved for use in food as a humectant, solvent, and flavoring agent. It is also used as an ingredient in some medications, including oral, topical, and injectable formulations.

Environmental Protection Agency (EPA): The EPA has classified propylene glycol as a "low toxicity" chemical and has determined that it poses no significant risk to human health or the environment when used as intended.

European Union (EU): The EU has approved propylene glycol as a food additive and it is also used in cosmetics and personal care products. The maximum concentration of propylene glycol that is allowed in food is 10%.

World Health Organization (WHO): The WHO has established a maximum acceptable daily intake (ADI) of propylene glycol of 25 mg/kg of body weight per day. This is based on studies that have shown that propylene glycol is safe for human consumption at levels below this threshold.

Occupational Safety and Health Administration (OSHA): OSHA has established a permissible exposure limit (PEL) of 50 parts per million (ppm) for propylene glycol in the workplace. This is the maximum concentration of propylene glycol that workers can be exposed to over an 8-hour workday without experiencing adverse health effects.

Overall, propylene glycol is considered to be safe for use in a variety of industries when used as intended and in accordance with regulatory guidelines. However, it is important to follow proper handling and storage procedures to prevent accidental exposure or ingestion.

CHAPTER NO. 12
PROCESS SIMULATION

12.1 ASPEN PLUS:

Aspen Plus is a market-leading process modeling tool for conceptual design, optimization, and performance monitoring for the chemical, polymer, specialty chemical, metals and minerals, and coal power industries. Aspen Plus provides;

12.2 Physical Property Models:

- World’s largest database of pure component and phase equilibrium data for conventional chemicals, electrolytes, solids, and polymers.
- Regularly updated with data from U. S. National Institute of Standards and Technology (NIST).

12.3 Comprehensive Library of Unit Operation Models:

- Addresses a wide range of solid, liquid, and gas processing equipment – Extends steady state simulation to dynamic simulation for safety and controllability studies, sizing relief valves, and optimizing transition, startup, and shutdown policies –
- Enables you build your own libraries using Aspen Custom Modeler or programming languages (User-defined models).

12.3.1 Properties Analysis:

- Properties of pure component and mixtures (Enthalpy, density, viscosity, heat capacity etc.)
- Phase equilibrium (VLE, VLLE, azeotrope calculation…etc.)
- Parameters estimation for properties models (UNIFAC method for binary parameters, method for boiling points…etc.)
- Data regression from experimental data.

12.3.2 Process Simulation:

- Pump, compressor, valve, tank, heat exchanger, CSTR, PFR, distillation column, extraction column, absorber, filter, crystallizer…etc.
- A process model can be defined as an engineering system's "blue print." The process model is a complete layout of the engineering system including the following

12.3.3 Chemical Components:

The process model specifies all chemical components of the system from the necessary reactants and products, to steam and cooling water.

12.3.4 Operating Conditions:

- All unit operations in the process model are kept under particular operating conditions (i.e., temperature, pressure, size). These are usually at the discretion of the engineer, for it is the operating conditions of the process that affect the outcome of the system.
- Michigan State University (MSU) has a variety of Aspen packages for different simulations.
- Briefly, here are the programs and capabilities:

Aspen Adsim: Fixed bed adsorption for pressure swing adsorption, etc.

Aspen Chromatography: Fixed bed adsorption, simulated moving bed chromatography. Runs independent of Aspen Plus.

Aspen Custom Modeler: A utility to permit the creation of user unit operations.

Aspen Distil: Aspen's 'Conceptual Engineering Product' for planning for processing schemes. Runs independent of Aspen Plus.

Aspen Dynamics: Unsteady-state simulator.

Aspen Plus: Steady-state process simulator.

Aspen Properties: Modeling of properties and phase equilibria. Incorporated into most other components, though it can be run as a stand-alone subset. All of the phase equilibria and mixture property methods discussed on this site are accessible in either Aspen Plus or Aspen Properties.

Aspen Polymers: Modeling of polymerization reactors and polymer thermodynamics. This package is available within Aspen Plus or Aspen Properties rather than via an external menu.

BatchSep: Batch distillations. Runs independently of Aspen Plus.

12.4 Process Simulation of Production of Propylene Glycol form Glycerol:

- Modeling and Simulation Strategy for SNG synthesis:
- Start Aspen V11.0 and press new to create a blank simulation.
- Add all the components involved in the synthesis of the final product.
- Also define the non-conventional and solid type of components.
- Select the suitable property package and make sure that binary parameters are calculated
- Press Estimate from UNIFAC for missing property parameters.
- Now run the simulation under properties environment.

Blocks and Streams:

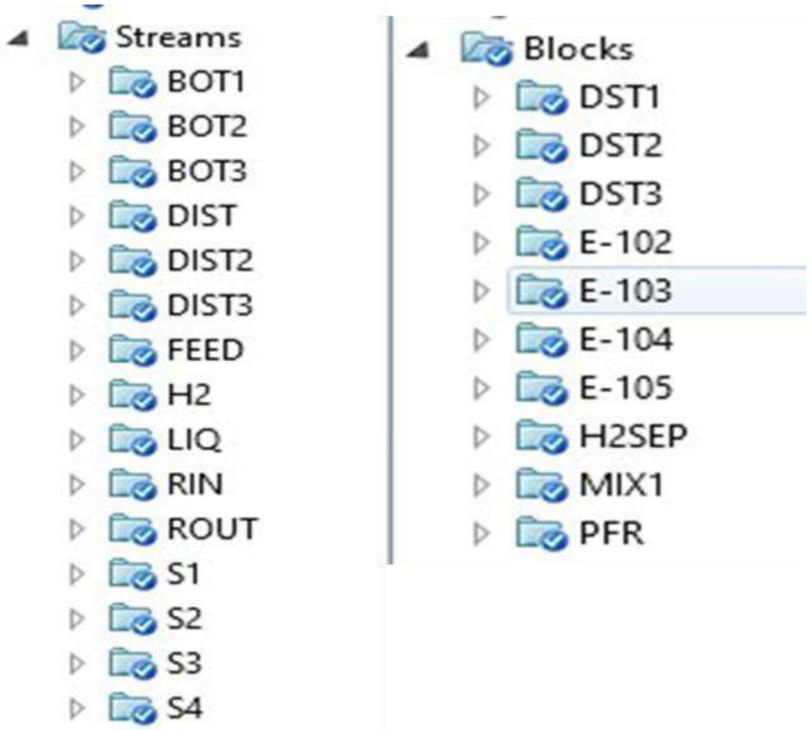
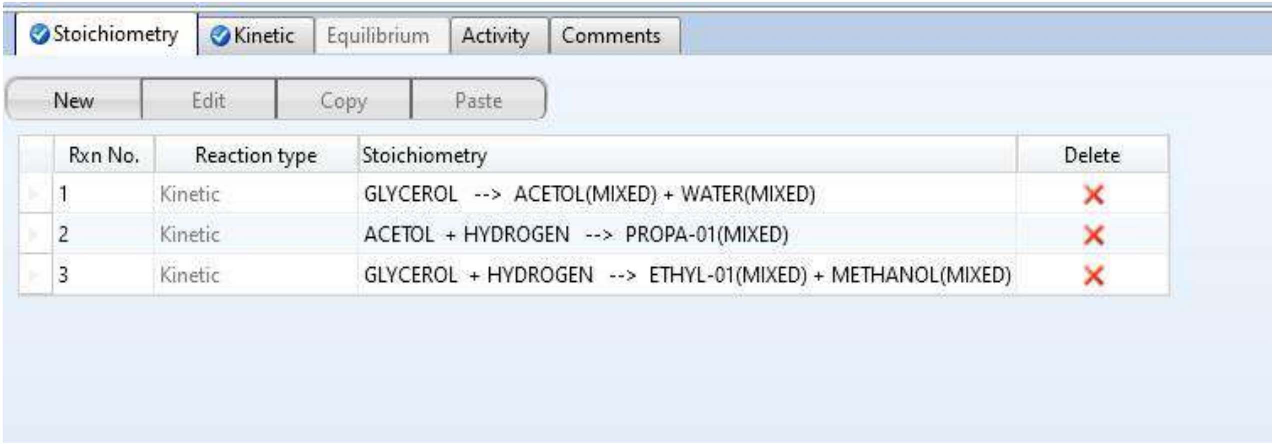


Figure 12-1 Stream Specification

Go to Simulation environment and drag the R-Stoic and Flash2 block from modal pallets to simulate the drying process.

Reactions Specified:

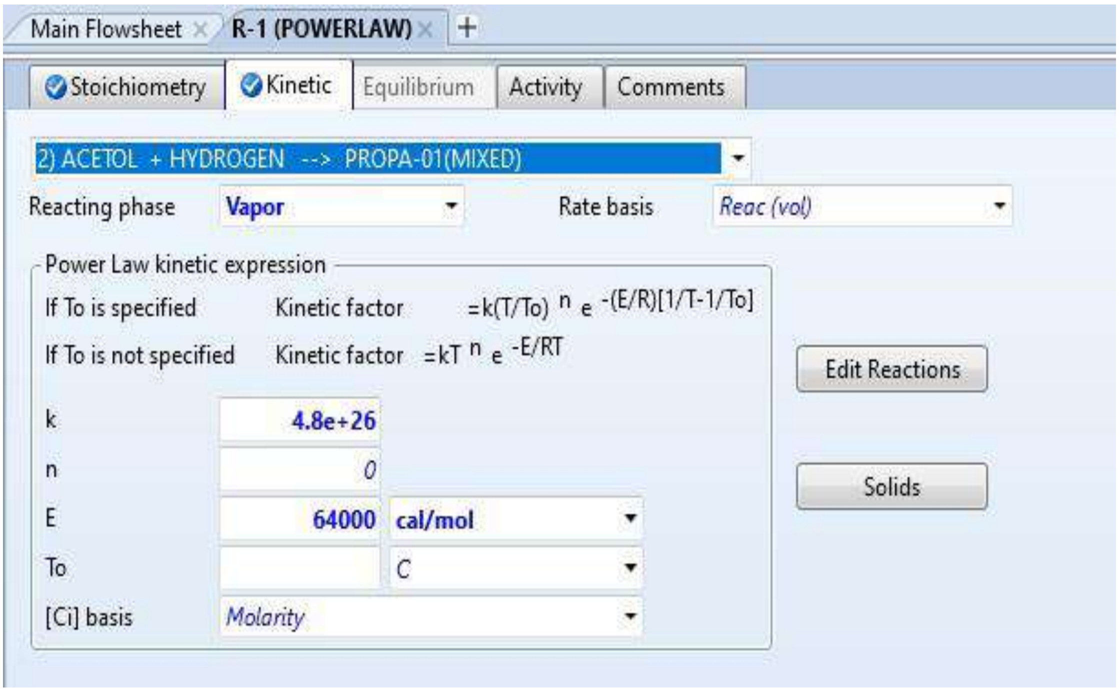


Rxn No.	Reaction type	Stoichiometry	Delete
1	Kinetic	GLYCEROL --> ACETOL(MIXED) + WATER(MIXED)	✕
2	Kinetic	ACETOL + HYDROGEN --> PROPA-01(MIXED)	✕
3	Kinetic	GLYCEROL + HYDROGEN --> ETHYL-01(MIXED) + METHANOL(MIXED)	✕

Figure 12-2 Reaction Specifications

- Model the gasification unit by sequestering the gasification process into decomposition, pyrolysis and gasification. These operations are done by R-Yield, R-Gibbs and R-Plug.

Reaction Kinetics:



2) ACETOL + HYDROGEN --> PROPA-01(MIXED)

Reacting phase: Vapor

Rate basis: Reac (vol)

Power Law kinetic expression

If To is specified Kinetic factor $=k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$

If To is not specified Kinetic factor $=kT^{n} e^{-E/RT}$

k: 4.8e+26

n: 0

E: 64000 cal/mol

To: C

[Ci] basis: Molarity

Figure 12-3 Reaction Kinetics

- The subsequent process includes modelling of tar reformer, water-gas shift reactor and H2 separation by R-Plug block and SEP block. The reactions in R-Plug block were kinetic based power law type of whose kinetic coefficient and activation energy were known.

- The moisture from the synthetic natural gas was kept to an acceptable level by using partial condenser and separator. This was done in SEP block in order to meet the local requirements/characteristics of natural gas to be fed in gas pipelines.

12.5 Results:

Simulation setup:

Title

Global unit set: METCBAR

Global settings

Input mode: Steady-State

Stream class: CONVEN

Flow basis: Mole

Ambient pressure: 1.01325 bar

Ambient temp.: 10 C

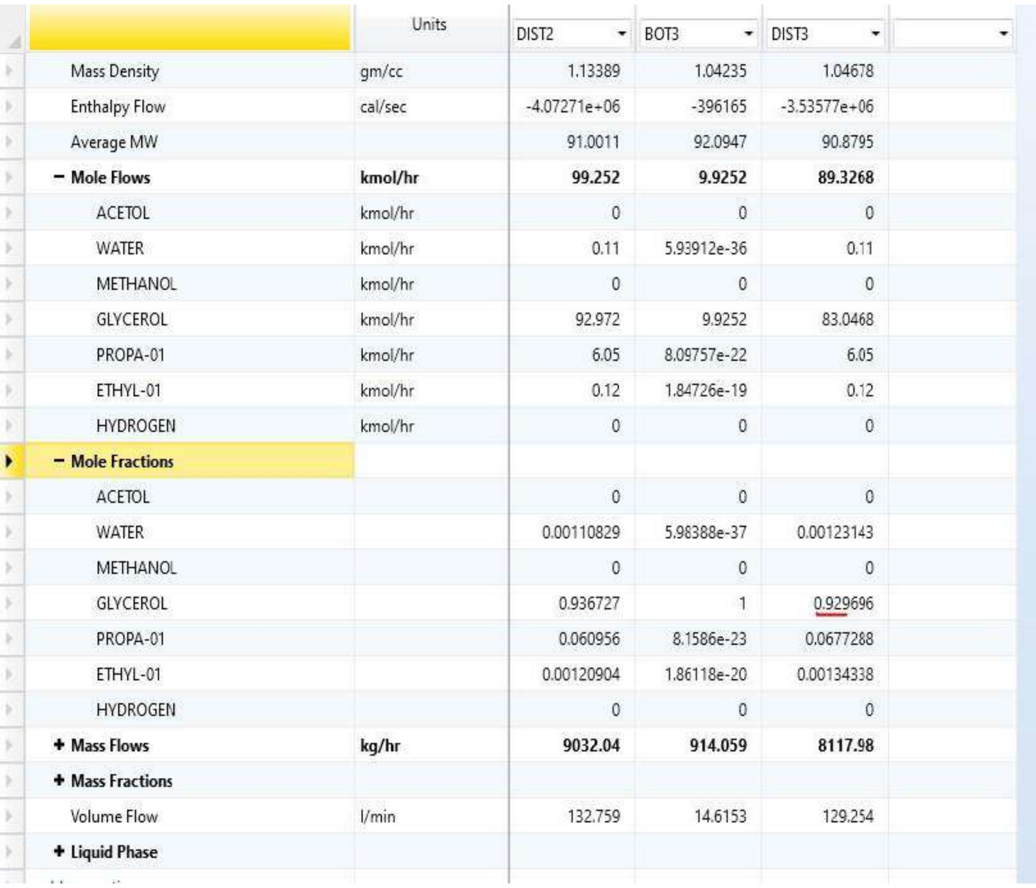
Valid phases:

Free water: No

Operational year: 8766 hr

Figure 12-4 Result of set-up

Product Purity:



	Units	DIST2	BOT3	DIST3	
Mass Density	gm/cc	1.13389	1.04235	1.04678	
Enthalpy Flow	cal/sec	-4.07271e+06	-396165	-3.53577e+06	
Average MW		91.0011	92.0947	90.8795	
− Mole Flows	**kmol/hr**	**99.252**	**9.9252**	**89.3268**	
ACETOL	kmol/hr	0	0	0	
WATER	kmol/hr	0.11	5.93912e-36	0.11	
METHANOL	kmol/hr	0	0	0	
GLYCEROL	kmol/hr	92.972	9.9252	83.0468	
PROPA-01	kmol/hr	6.05	8.09757e-22	6.05	
ETHYL-01	kmol/hr	0.12	1.84726e-19	0.12	
HYDROGEN	kmol/hr	0	0	0	
− Mole Fractions					
ACETOL		0	0	0	
WATER		0.00110829	5.98388e-37	0.00123143	
METHANOL		0	0	0	
GLYCEROL		0.936727	1	0.929696	
PROPA-01		0.060956	8.1586e-23	0.0677288	
ETHYL-01		0.00120904	1.86118e-20	0.00134338	
HYDROGEN		0	0	0	
+ Mass Flows	**kg/hr**	**9032.04**	**914.059**	**8117.98**	
+ Mass Fractions					
Volume Flow	l/min	132.759	14.6153	129.254	
+ Liquid Phase					

Figure 12-5 Results Summary

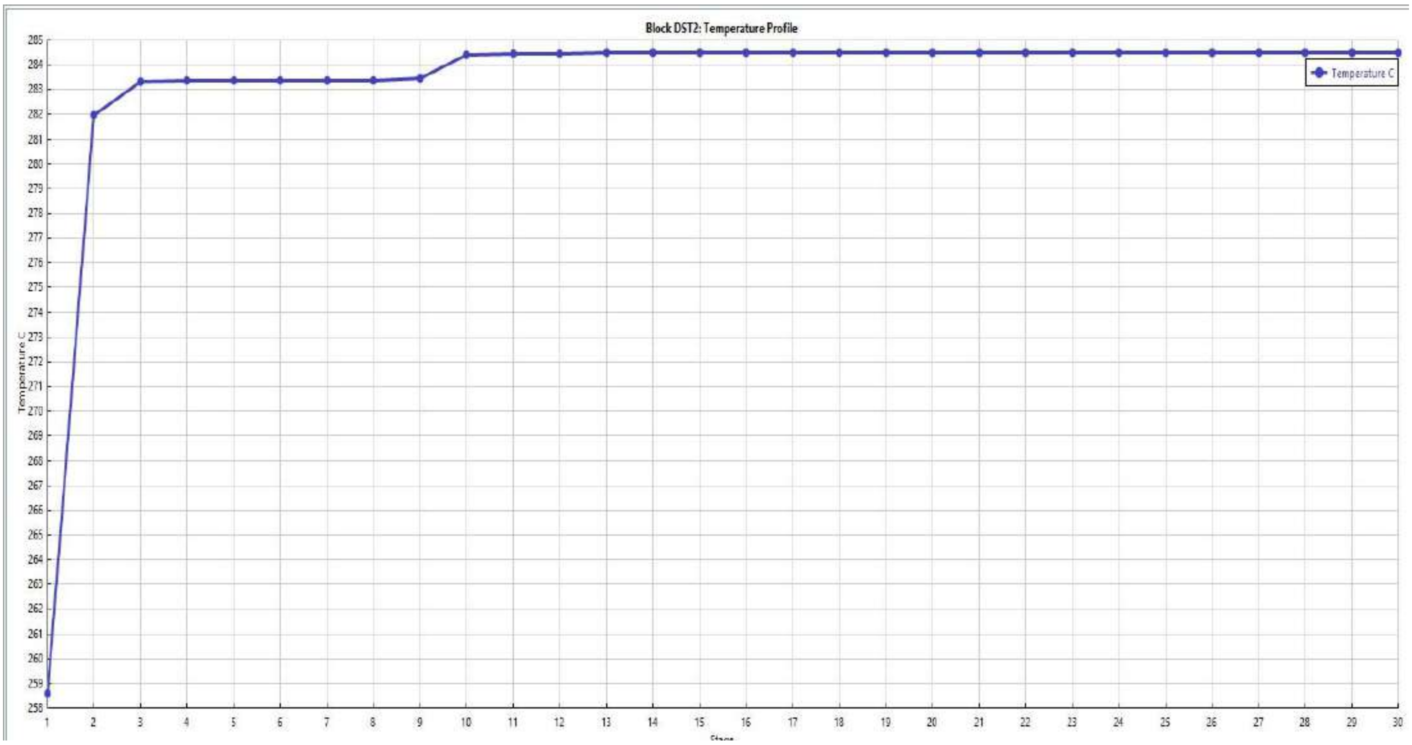


Figure 12-6 Temperature profile in distillation column

12.6 Simulation Flowsheet:

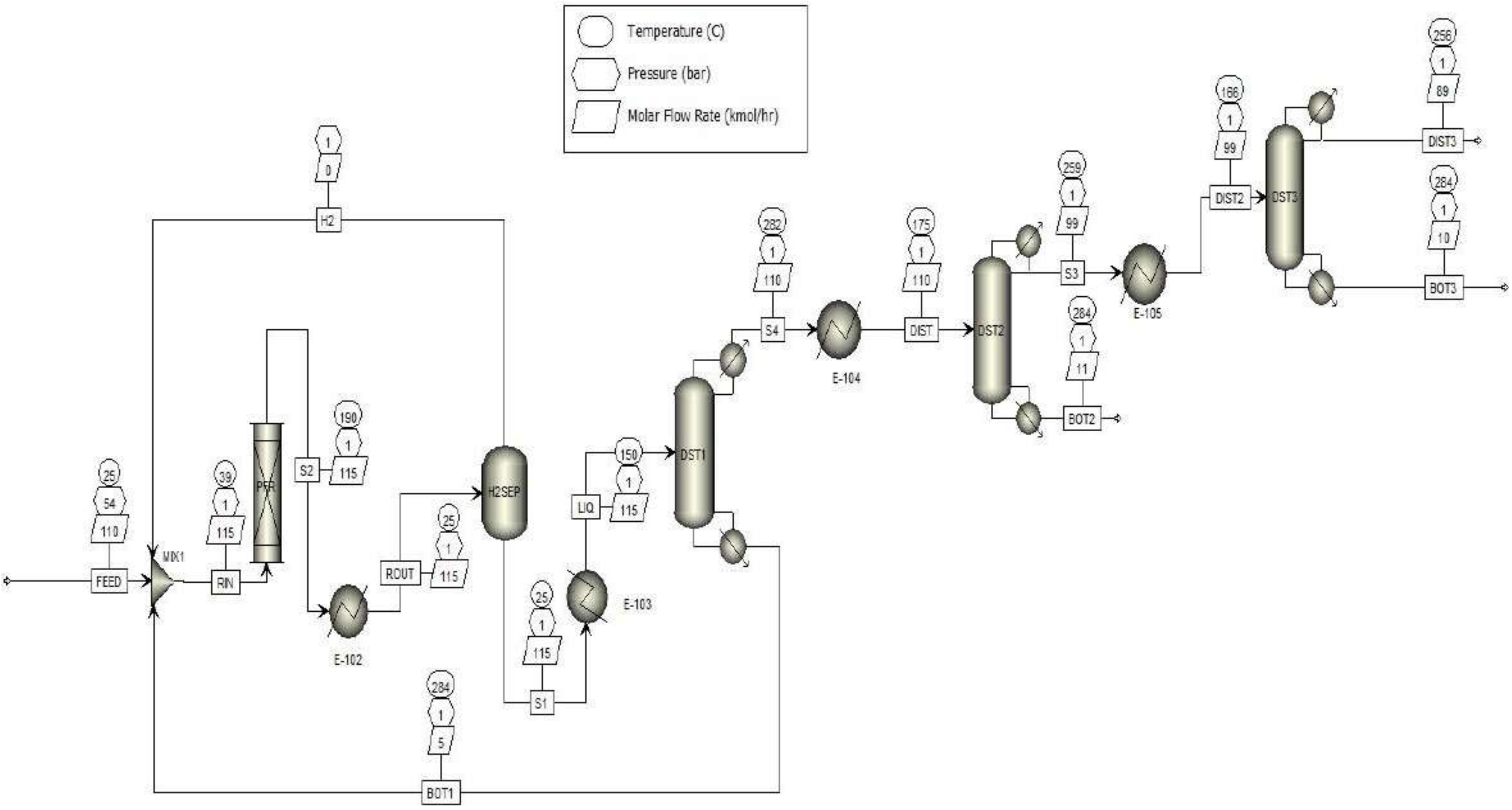


Figure 12-7 Simulation Flowsheet on Aspen Plus

```
                    + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
                    + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
     ++                                                                                            ++
     ++                                                                                            ++
     ++                           ASPEN PLUS CALCULATION REPORT                                    ++
     ++                                                                                            ++
     ++                                                                                            ++
                    + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
                    + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +

                      ASPEN PLUS IS A TRADEMARK OF          HOTLINE:
                     ASPEN TECHNOLOGY, INC.              U.S.A. 888/996-7100
                       781/221-6400                    EUROPE (44) 1189-226555
                     PLATFORM: WIN-X64                        MAY 6, 2023
                      VERSION: 37.0   Build 395               SATURDAY
                       INSTALLATION:                         4:57:15 P.M.
```

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```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0               05/06/2023  PAGE 1

                         RUN CONTROL SECTION

RUN CONTROL INFORMATION
-----------------------

THIS COPY OF ASPEN PLUS LICENSED TO
TYPE OF RUN: EDIT
INPUT FILE NAME: _0532lbk.inm
INPUT PROBLEM DATA FILE NAME : _0532lbk
OUTPUT PROBLEM DATA FILE NAME: _5650eib
LOCATED IN:
PDF SIZE USED FOR INPUT TRANSLATION:
  NUMBER OF FILE RECORDS (PSIZE) =     0
  NUMBER OF IN-CORE RECORDS      =   256
PSIZE NEEDED FOR SIMULATION    =     1
CALLING PROGRAM NAME:          apmain
LOCATED IN:                  f:\New folder (4)\Aspen Plus V11.0\Engine\\xeq
SIMULATION REQUESTED FOR ENTIRE FLOWSHEET
```

```
 ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 2

                          FLOWSHEET SECTION

 FLOWSHEET CONNECTIVITY BY STREAMS
 ---------------------------------
   STREAM     SOURCE     DEST          STREAM     SOURCE     DEST
   FEED       ----       MIX1          ROUT       E-102      H2SEP
   S1         H2SEP      E-103         LIQ        E-103      DST1
   DIST       E-104      DST2          BOT1       DST1       MIX1
   DIST2      E-105      DST3          BOT2       DST2       ----
   DIST3      DST3       ----          BOT3       DST3       ----
   RIN        MIX1       PFR           S2         PFR        E-102
   S3         DST2       E-105         H2         H2SEP      MIX1
   S4         DST1       E-104
 FLOWSHEET CONNECTIVITY BY BLOCKS
 --------------------------------
   BLOCK       INLETS                   OUTLETS
   PFR         RIN                      S2
   H2SEP       ROUT                     H2 S1
   E-103       S1                       LIQ
   DST1        LIQ                      S4 BOT1
   DST2        DIST                     S3 BOT2
   DST3        DIST2                    DIST3 BOT3
   MIX1        FEED BOT1 H2             RIN
   E-102       S2                       ROUT
   E-105       S3                       DIST2
   E-104       S4                       DIST
 CONVERGENCE STATUS SUMMARY
 --------------------------
   TEAR STREAM SUMMARY
   ===================
   STREAM    VARIABLE        MAXIMUM      MAX. ERR.    ABSOLUTE         CONV
ID       ID              ERR/TOL      RELATIVE     ERROR       STAT BLOCK
   ------    --------        --------     -------      ---------   ----
   ROUT      ACETOL MOLEFLOW    0.0000       0.0000       0.0000      #    $OLVER02
   #  = CONVERGED
   *  = NOT CONVERGED
 CONVERGENCE BLOCK:  $OLVER02
 ----------------------------
     Tear Stream  :  ROUT
     Tolerance used:  0.100D-03
     Trace molefrac:  0.100D-05
     MAXIT=   30 WAIT   1 ITERATIONS BEFORE ACCELERATING
     QMAX =   0.0     QMIN =  -5.0
```

```
 ASPEN PLUS   PLAT: WIN-X64   VER: 37.0              05/06/2023  PAGE 3

                        FLOWSHEET SECTION
 CONVERGENCE BLOCK:  $OLVER02 (CONTINUED)
    METHOD: WEGSTEIN      STATUS: CONVERGED
    TOTAL NUMBER OF ITERATIONS:     8
    NUMBER OF ITERATIONS ON LAST OUTER LOOP:     0
                   *** FINAL VALUES ***
    VAR#  TEAR STREAM VAR   STREAM    SUBSTREA COMPONEN UNIT        VALUE       PREV VALUE
ERR/TOL
    ----  ----------------  ------    -------- -------- ----        -----       ----------   -------
      1  TOTAL MOLEFLOW    ROUT      MIXED           KMOL/HR       114.8750     114.8750      0.0
      2  MOLE-FLOW        ROUT     MIXED   ACETOL   KMOL/HR         0.0         0.0         0.0
      3  MOLE-FLOW        ROUT     MIXED   WATER    KMOL/HR        0.1100      0.1100      0.0
      4  MOLE-FLOW        ROUT     MIXED   METHANOL KMOL/HR         0.0         0.0         0.0
      5  MOLE-FLOW        ROUT     MIXED   GLYCEROL KMOL/HR       108.5950     108.5950      0.0
      6  MOLE-FLOW        ROUT     MIXED   PROPA-01 KMOL/HR        6.0500      6.0500      0.0
      7  MOLE-FLOW        ROUT     MIXED   ETHYL-01 KMOL/HR        0.1200      0.1200      0.0
      8  MOLE-FLOW        ROUT     MIXED   HYDROGEN KMOL/HR         0.0         0.0         0.0
      9  PRESSURE        ROUT      MIXED           BAR            1.0000      1.0000      0.0
     10  MASS ENTHALPY     ROUT      MIXED           CAL/GM      -1699.7474   -1699.7474      0.0
                   *** ITERATION HISTORY ***
    TEAR STREAMS AND TEAR VARIABLES:

    ITERATION MAX-ERR/TOL  VAR# STREAM ID VAR DESCRIPTION  SUBSTREA COMPONEN ATTRIBUT
ELEMENT
    --------- -----------  ---- --------- ---------------  -------- -------- -------- -------
        1       0.000       2 ROUT     MOLE-FLO       MIXED    ACETOL
 COMPUTATIONAL SEQUENCE
 ----------------------
 SEQUENCE USED WAS:
   $OLVER02 H2SEP E-103 DST1 MIX1 PFR E-102
   (RETURN $OLVER02)
   E-104 DST2 E-105 DST3
 OVERALL FLOWSHEET BALANCE
 -------------------------




                 ***  MASS AND ENERGY BALANCE  ***

                      IN         OUT      GENERATION   RELATIVE DIFF.
  CONVENTIONAL COMPONENTS
       (KMOL/HR )
     ACETOL            0.00000       0.00000       0.00000       0.00000
     WATER           0.110000      0.110000       0.00000     -0.100619E-07
     METHANOL           0.00000       0.00000       0.00000       0.00000
     GLYCEROL           104.000       104.000       0.00000      0.607585E-09
     PROPA-01          6.05000       6.05000       0.00000     -0.100619E-07
     ETHYL-01          0.120000      0.120000       0.00000     -0.100619E-07
```

```
                                        FLOWSHEET SECTION

 OVERALL FLOWSHEET BALANCE (CONTINUED)

                ***  MASS AND ENERGY BALANCE  ***
                     IN         OUT      GENERATION   RELATIVE DIFF.
  CONVENTIONAL COMPONENTS
        (KMOL/HR )
    HYDROGEN           0.00000       0.00000       0.00000       0.00000
  TOTAL BALANCE
  MOLE(KMOL/HR )        110.280       110.280       0.00000      0.386585E-15
  MASS(KG/HR   )        10047.7       10047.7                    0.108703E-09
  ENTHALPY(CAL/SEC )   -0.474022E+07 -0.437211E+07               -0.776550E-01

                ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E          0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 5

                    PHYSICAL PROPERTIES SECTION

COMPONENTS
----------

 ID      TYPE  ALIAS         NAME
  ACETOL   C     C3H6O2-D1     ACETOL
  WATER    C     H2O           WATER
  METHANOL C     CH4O          METHANOL
  GLYCEROL C     C3H8O3        GLYCEROL
  PROPA-01 C     C3H8O2-2      PROPANEDIOL-1,2
  ETHYL-01 C     C2H6O2        ETHYLENE-GLYCOL
  HYDROGEN C     H2            HYDROGEN

                              REACTION SECTION

REACTION:   R-1       TYPE: POWERLAW
------------------------------------
    Unit operations referencing this reaction model:
    Reactor Name: PFR         Block Type: RPLUG
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 7

                         U-O-S BLOCK SECTION

BLOCK:  DST1     MODEL: RADFRAC
-------------------------------
   INLETS   - LIQ      STAGE  17
   OUTLETS  - S4       STAGE   1
           BOT1     STAGE  50
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                           IN              OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/HR )           114.875         114.875         0.00000
      MASS(KG/HR   )           10470.8         10470.8       0.235564E-12
      ENTHALPY(CAL/SEC )      -0.475134E+07   -0.407687E+07   -0.141955

                 ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E         0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR




                    ***********************
                    ****  INPUT DATA  ****
                    ***********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                               50
   ALGORITHM OPTION                              STANDARD
   ABSORBER OPTION                               NO
   INITIALIZATION OPTION                          STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                    NO
   INSIDE LOOP CONVERGENCE METHOD                    BROYDEN
   DESIGN SPECIFICATION METHOD                    NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                10
   MAXIMUM NUMBER OF FLASH ITERATIONS                   30
   FLASH TOLERANCE                               0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                 0.000100000
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 8

                         U-O-S BLOCK SECTION
BLOCK:  DST1     MODEL: RADFRAC (CONTINUED)
  ****   COL-SPECS   ****
   MOLAR VAPOR DIST / TOTAL DIST                          1.00000
   MOLAR REFLUX RATIO                                 1.30000
   DISTILLATE TO FEED RATIO                              0.96000
  ****    PROFILES   ****
   P-SPEC          STAGE   1  PRES, BAR                   1.00000

                      *******************
                      ****  RESULTS  ****
                      *******************
  ***   COMPONENT SPLIT FRACTIONS   ***
                        OUTLET STREAMS
                        --------------
               S4          BOT1
   COMPONENT:
   WATER       1.0000       0.0000
   GLYCEROL    .95769       .42313E-01
   PROPA-01    1.0000       0.0000
   ETHYL-01    1.0000       0.0000

  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE          C                     282.222
   BOTTOM STAGE TEMPERATURE       C                     284.481
   TOP STAGE LIQUID FLOW          KMOL/HR               143.364
   BOTTOM STAGE LIQUID FLOW       KMOL/HR                  4.59500
   TOP STAGE VAPOR FLOW           KMOL/HR               110.280
   BOILUP VAPOR FLOW              KMOL/HR               310.135
   MOLAR REFLUX RATIO                                 1.30000
   MOLAR BOILUP RATIO                                67.4940
   CONDENSER DUTY (W/O SUBCOOL)   CAL/SEC            -587,589.
   REBOILER DUTY                  CAL/SEC          1,262,060.

  ****   MAXIMUM FINAL RELATIVE ERRORS   ****

   DEW POINT                    0.10163E-08  STAGE=  1
   BUBBLE POINT                   0.93120E-09  STAGE=  1
   COMPONENT MASS BALANCE         0.46144E-08  STAGE= 17 COMP=WATER
   ENERGY BALANCE                 0.53042E-09  STAGE=  1
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0              05/06/2023  PAGE 9

                    U-O-S BLOCK SECTION

BLOCK:  DST1     MODEL: RADFRAC (CONTINUED)

  ****    PROFILES    ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
         FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                              ENTHALPY
STAGE TEMPERATURE   PRESSURE           CAL/MOL          HEAT DUTY
     C           BAR          LIQUID       VAPOR       CAL/SEC

  1   282.22       1.0000      -0.14364E+06 -0.12710E+06  -.58759+06
  2   283.41       1.0000      -0.14367E+06 -0.12811E+06
 16   283.47       1.0000      -0.14367E+06 -0.12816E+06
 17   283.47       1.0000      -0.14367E+06 -0.12816E+06
 18   284.40       1.0000      -0.14369E+06 -0.12897E+06
 31   284.48       1.0000      -0.14369E+06 -0.12904E+06
 32   284.48       1.0000      -0.14369E+06 -0.12904E+06
 33   284.48       1.0000      -0.14369E+06 -0.12904E+06
 34   284.48       1.0000      -0.14369E+06 -0.12904E+06
 49   284.48       1.0000      -0.14369E+06 -0.12904E+06
 50   284.48       1.0000      -0.14369E+06 -0.12904E+06   .12621+07

STAGE     FLOW RATE               FEED RATE             PRODUCT RATE
         KMOL/HR                 KMOL/HR                KMOL/HR
     LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1  143.4      110.3                                 110.2800
  2  143.9      253.6
 16   143.9      254.2
 17   313.7      254.2      114.8750
 18   314.6      309.1
 31   314.7      310.1
 32   314.7      310.1
 33   314.7      310.1
 34   314.7      310.1
 49   314.7      310.1
 50   4.595      310.1                            4.5950

   ****  MASS FLOW PROFILES  ****
STAGE     FLOW RATE               FEED RATE             PRODUCT RATE
         KG/HR                 KG/HR              KG/HR
     LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR

                                        ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE               FEED RATE             PRODUCT RATE
         KG/HR                 KG/HR              KG/HR
     LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID    VAPOR
```

```
 34 0.2898E+05 0.2856E+05
 49 0.2898E+05 0.2856E+05
 50  423.2     0.2856E+05                    423.1752

                 ****   MOLE-X-PROFILE     ****
 STAGE     WATER        GLYCEROL     PROPA-01     ETHYL-01
    1    0.18216E-04   0.99527      0.45624E-02   0.14788E-03
    2    0.80036E-05   0.99777      0.21513E-02   0.74022E-04
   16     0.78760E-05   0.99790      0.20284E-02   0.67797E-04
   17     0.78760E-05   0.99790      0.20284E-02   0.67797E-04
   18     0.14255E-06   0.99983      0.16457E-03   0.89838E-05
   31     0.31488E-29    1.0000      0.10652E-17   0.34192E-16
   32     0.56936E-31    1.0000      0.86292E-19   0.45237E-17
   33     0.10295E-32    1.0000      0.69905E-20   0.59850E-18
   34     0.18615E-34    1.0000      0.56630E-21   0.79184E-19
   49     0.13443E-60    1.0000      0.24049E-37   0.52729E-32
   50     0.24302E-62    1.0000      0.19459E-38   0.69628E-33

                 ****   MOLE-Y-PROFILE     ****
 STAGE     WATER        GLYCEROL     PROPA-01     ETHYL-01
    1    0.99746E-03   0.94305      0.54860E-01   0.10881E-02
    2    0.44397E-03   0.97257      0.26431E-01   0.55669E-03
   16     0.43718E-03   0.97410      0.24948E-01   0.51045E-03
   17     0.43718E-03   0.97410      0.24948E-01   0.51045E-03
   18     0.79931E-05   0.99786      0.20585E-02   0.68805E-04
   31     0.17672E-27    1.0000      0.13344E-16   0.26227E-15
   32     0.31955E-29    1.0000      0.10810E-17   0.34699E-16
   33     0.57780E-31    1.0000      0.87570E-19   0.45907E-17
   34     0.10448E-32    1.0000      0.70941E-20   0.60737E-18
   49     0.75449E-59    1.0000      0.30126E-36   0.40445E-31
   50     0.13639E-60    1.0000      0.24376E-37   0.53407E-32

                 ****   K-VALUES          ****
 STAGE     WATER        GLYCEROL     PROPA-01     ETHYL-01
    1    54.758       0.94753       12.024       7.3581
    2    55.472       0.97475       12.286       7.5206
   16     55.508       0.97616       12.300       7.5290
   17     55.508       0.97616       12.300       7.5290
   18     56.073       0.99804       12.508       7.6588
   31     56.124        1.0000       12.527       7.6704
   32     56.124        1.0000       12.527       7.6704
   33     56.124        1.0000       12.527       7.6704
   34     56.124        1.0000       12.527       7.6704
   49     56.124        1.0000       12.527       7.6704
   50     56.124        1.0000       12.527       7.6704
```

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                     U-O-S BLOCK SECTION

BLOCK:  DST1     MODEL: RADFRAC (CONTINUED)

                  ****   MASS-X-PROFILE     ****
 STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
    1    0.35663E-05   0.99612      0.37730E-02   0.99753E-04
    2    0.15663E-05   0.99817      0.17783E-02   0.49908E-04
   16    0.15413E-05   0.99828      0.16766E-02   0.45710E-04
   17    0.15413E-05   0.99828      0.16766E-02   0.45710E-04
   18    0.27885E-07   0.99986      0.13598E-03   0.60549E-05
   31    0.61596E-30    1.0000      0.88014E-18   0.23044E-16
   32    0.11138E-31    1.0000      0.71300E-19   0.30488E-17
   33    0.20139E-33    1.0000      0.57761E-20   0.40337E-18
   34    0.36415E-35    1.0000      0.46792E-21   0.53367E-19
   49    0.26298E-61    1.0000      0.19871E-37   0.35538E-32
   50    0.47538E-63    1.0000      0.16078E-38   0.46927E-33

                  ****   MASS-Y-PROFILE     ****
 STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
    1    0.19723E-03   0.95324      0.45819E-01   0.74129E-03
    2    0.87297E-04   0.97758      0.21952E-01   0.37712E-03
   16    0.85937E-04   0.97885      0.20715E-01   0.34570E-03
   17    0.85937E-04   0.97885      0.20715E-01   0.34570E-03
   18    0.15642E-05   0.99825      0.17016E-02   0.46390E-04
   31    0.34570E-28    1.0000      0.11026E-16   0.17676E-15
   32    0.62509E-30    1.0000      0.89318E-18   0.23386E-16
   33    0.11303E-31    1.0000      0.72357E-19   0.30940E-17
   34    0.20437E-33    1.0000      0.58616E-20   0.40934E-18
   49    0.14759E-59    1.0000      0.24892E-36   0.27259E-31
   50    0.26680E-61    1.0000      0.20142E-37   0.35995E-32

BLOCK:  DST2     MODEL: RADFRAC
-------------------------------
   INLETS   - DIST     STAGE   9
   OUTLETS  - S3       STAGE   1
              BOT2     STAGE  30
 PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                ***  MASS AND ENERGY BALANCE  ***
                         IN           OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(KMOL/HR )          110.280        110.280       0.128862E-15
     MASS(KG/HR   )          10047.7        10047.7       0.301242E-10
     ENTHALPY(CAL/SEC )   -0.451859E+07  -0.437312E+07  -0.321939E-01
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 12

                         U-O-S BLOCK SECTION

BLOCK:  DST2     MODEL: RADFRAC (CONTINUED)

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E         0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR




                    **********************
                    ****  INPUT DATA  ****
                    **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                  30
   ALGORITHM OPTION                                 STANDARD
   ABSORBER OPTION                                 NO
   INITIALIZATION OPTION                             STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                    NO
   INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
   DESIGN SPECIFICATION METHOD                        NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                10
   MAXIMUM NUMBER OF FLASH ITERATIONS                   30
   FLASH TOLERANCE                                   0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                    0.000100000

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                       0.0
   MOLAR REFLUX RATIO                               1.30000
   DISTILLATE TO FEED RATIO                           0.90000

  ****    PROFILES   ****

   P-SPEC         STAGE   1  PRES, BAR                1.00000
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 13

                         U-O-S BLOCK SECTION

BLOCK:  DST2     MODEL: RADFRAC (CONTINUED)

                      *******************
                      ****  RESULTS  ****
                      *******************


  ***   COMPONENT SPLIT FRACTIONS   ***

                        OUTLET STREAMS
                        --------------
              S3          BOT2
   COMPONENT:
   WATER       1.0000       0.0000
   GLYCEROL    .89396       .10604
   PROPA-01    1.0000       0.0000
   ETHYL-01    1.0000       0.0000


  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE          C                     258.579
   BOTTOM STAGE TEMPERATURE       C                     284.481
   TOP STAGE LIQUID FLOW          KMOL/HR               129.028
   BOTTOM STAGE LIQUID FLOW       KMOL/HR               11.0280
   TOP STAGE VAPOR FLOW           KMOL/HR               0.0
   BOILUP VAPOR FLOW              KMOL/HR               281.482
   MOLAR REFLUX RATIO                                   1.30000
   MOLAR BOILUP RATIO                                   25.5243
   CONDENSER DUTY (W/O SUBCOOL)   CAL/SEC              -999,993.
   REBOILER DUTY                  CAL/SEC           1,145,460.

  ****   MAXIMUM FINAL RELATIVE ERRORS   ****

   DEW POINT                    0.12432E-02  STAGE=  9
   BUBBLE POINT                 0.11941E-02  STAGE=  9
   COMPONENT MASS BALANCE       0.23813E-05  STAGE=  9 COMP=WATER
   ENERGY BALANCE               0.33032E-03  STAGE=  9
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 14

                        U-O-S BLOCK SECTION
BLOCK:  DST2     MODEL: RADFRAC (CONTINUED)
                                                    ****   PROFILES   ****
  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
         FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                                  ENTHALPY
STAGE TEMPERATURE   PRESSURE           CAL/MOL          HEAT DUTY
      C            BAR          LIQUID       VAPOR       CAL/SEC
  1   258.58        1.0000      -0.14265E+06 -0.11027E+06  -.99999+06
  2   281.96        1.0000      -0.14363E+06 -0.12688E+06
  8   283.39        1.0000      -0.14367E+06 -0.12810E+06
  9   283.45        1.0000      -0.14367E+06 -0.12809E+06
 10   284.39        1.0000      -0.14369E+06 -0.12897E+06
 28   284.48        1.0000      -0.14369E+06 -0.12904E+06
 29   284.48        1.0000      -0.14369E+06 -0.12904E+06
 30   284.48        1.0000      -0.14369E+06 -0.12904E+06   .11455+07
STAGE     FLOW RATE                FEED RATE             PRODUCT RATE
          KMOL/HR                  KMOL/HR               KMOL/HR
      LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID
11.0280

                                             ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                FEED RATE             PRODUCT
          KG/HR                 KG/HR                KG/HR
      LIQUID     VAPOR      LIQUID    VAPOR    MIXED      LIQUID
  1 0.2077E+05  0.000                          9032.0368
  2 0.1268E+05 0.2077E+05
  8 0.1274E+05 0.2177E+05
  9 0.2683E+05 0.2177E+05  .10048+05
 10 0.2693E+05 0.2582E+05
 28 0.2694E+05 0.2592E+05
 29 0.2694E+05 0.2592E+05
 30  1016.     0.2592E+05                      1015.6205


                        U-O-S BLOCK SECTION

BLOCK:  DST2     MODEL: RADFRAC (CONTINUED)

                    ****   MOLE-X-PROFILE     ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
     1    0.11083E-02   0.93673       0.60956E-01   0.12090E-02
     2    0.20297E-04   0.99472       0.50933E-02   0.16510E-03
     8    0.84334E-05   0.99774       0.21756E-02   0.72791E-04
     9    0.84104E-05   0.99775       0.21724E-02   0.72705E-04
    10     0.15586E-06   0.99981       0.18051E-03   0.98666E-05
    28     0.10200E-37    1.0000      0.62475E-23   0.23329E-20
    29     0.18886E-39    1.0000      0.51813E-24   0.31584E-21
```

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  30   0.34944E-41   1.0000      0.42847E-25  0.42572E-22

                 ****  MOLE-Y-PROFILE    ****
 STAGE    WATER       GLYCEROL     PROPA-01     ETHYL-01
   1   0.46095E-01  0.48740      0.46092      0.55854E-02
   2   0.11083E-02  0.93673      0.60956E-01  0.12090E-02
   8   0.46775E-03  0.97226      0.26723E-01  0.54731E-03
   9   0.46782E-03  0.97226      0.26727E-01  0.54738E-03
  10    0.87411E-05  0.99766      0.22578E-02  0.75564E-04
  28    0.57245E-36   1.0000      0.78263E-22  0.17894E-19
  29    0.10599E-37   1.0000      0.64906E-23  0.24226E-20
  30    0.19612E-39   1.0000      0.53675E-24  0.32655E-21

                 ****  K-VALUES         ****
 STAGE    WATER       GLYCEROL     PROPA-01     ETHYL-01
   1    41.591      0.52033      7.5615       4.6197
   2    54.604      0.94170      11.968       7.3231
   8    55.464      0.97446      12.283       7.5189
   9    55.496      0.97567      12.294       7.5260
  10     56.071      0.99796      12.508       7.6583
  28     56.124       1.0000      12.527       7.6704
  29     56.124       1.0000      12.527       7.6704
  30     56.124       1.0000      12.527       7.6704

                 ****  MASS-X-PROFILE    ****
 STAGE    WATER       GLYCEROL     PROPA-01     ETHYL-01
   1   0.21941E-03  0.94798      0.50972E-01  0.82464E-03
   2   0.39742E-05  0.99567      0.42124E-02  0.11138E-03
   8   0.16504E-05  0.99815      0.17983E-02  0.49078E-04
   9   0.16459E-05  0.99815      0.17957E-02  0.49020E-04
  10    0.30490E-07  0.99984      0.14915E-03  0.66500E-05
  28    0.19953E-38   1.0000      0.51622E-23  0.15723E-20
  29    0.36943E-40   1.0000      0.42812E-24  0.21286E-21
  30    0.68357E-42   1.0000      0.35404E-25  0.28692E-22

                 ****  MASS-Y-PROFILE    ****
 STAGE    WATER       GLYCEROL     PROPA-01     ETHYL-01
   1   0.10234E-01  0.55322      0.43227      0.42727E-02
   2   0.21941E-03  0.94798      0.50972E-01  0.82464E-03
   8   0.91978E-04  0.97734      0.22196E-01  0.37079E-03
   9   0.91991E-04  0.97734      0.22199E-01  0.37084E-03
  10    0.17106E-05  0.99808      0.18664E-02  0.50949E-04
  28    0.11198E-36   1.0000      0.64666E-22  0.12060E-19
  29    0.20734E-38   1.0000      0.53630E-23  0.16328E-20
  30    0.38364E-40   1.0000      0.44350E-24  0.22008E-21
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0               05/06/2023  PAGE 16

                      U-O-S BLOCK SECTION

BLOCK:  DST3     MODEL: RADFRAC
-------------------------------
   INLETS   - DIST2    STAGE  17
   OUTLETS  - DIST3    STAGE   1
              BOT3     STAGE  35
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                ***  MASS AND ENERGY BALANCE  ***
                           IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(KMOL/HR )         99.2520        99.2520       0.143180E-15
     MASS(KG/HR   )         9032.04        9032.04       0.871412E-10
     ENTHALPY(CAL/SEC )      -0.407271E+07   -0.393193E+07   -0.345673E-01

                ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E         0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR




                      **********************
                      ****  INPUT DATA  ****
                      **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                35
   ALGORITHM OPTION                                STANDARD
   ABSORBER OPTION                                 NO
   INITIALIZATION OPTION                           STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                NO
   INSIDE LOOP CONVERGENCE METHOD                  BROYDEN
   DESIGN SPECIFICATION METHOD                     NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS          25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS           10
   MAXIMUM NUMBER OF FLASH ITERATIONS              30
   FLASH TOLERANCE                                 0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE              0.000100000
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0               05/06/2023  PAGE 17

                        U-O-S BLOCK SECTION

BLOCK:  DST3     MODEL: RADFRAC (CONTINUED)
  ****   COL-SPECS   ****
   MOLAR VAPOR DIST / TOTAL DIST                          0.0
   MOLAR REFLUX RATIO                                 1.32000
   DISTILLATE TO FEED RATIO                              0.90000
                                                  ****    PROFILES   ****
   P-SPEC          STAGE   1  PRES, BAR                  1.00000
                   *******************
                   ****  RESULTS  ****
                   *******************
  ***   COMPONENT SPLIT FRACTIONS   ***

                        OUTLET STREAMS
                        --------------
              DIST3       BOT3
   COMPONENT:
   WATER       1.0000       0.0000
   GLYCEROL    .89325       .10675
   PROPA-01    1.0000       0.0000
   ETHYL-01    1.0000       0.0000
  ***    SUMMARY OF KEY RESULTS    ***
   TOP STAGE TEMPERATURE          C                     256.365
   BOTTOM STAGE TEMPERATURE       C                     284.481
   TOP STAGE LIQUID FLOW          KMOL/HR               117.911
   BOTTOM STAGE LIQUID FLOW       KMOL/HR                  9.92520
   TOP STAGE VAPOR FLOW           KMOL/HR                 0.0
   BOILUP VAPOR FLOW              KMOL/HR               258.864
   MOLAR REFLUX RATIO                                 1.32000
   MOLAR BOILUP RATIO                                 26.0815
   CONDENSER DUTY (W/O SUBCOOL)   CAL/SEC           -912,640.
   REBOILER DUTY                  CAL/SEC          1,053,420.
  ****   MAXIMUM FINAL RELATIVE ERRORS   ****
   DEW POINT                      0.73137E-06  STAGE=  4
   BUBBLE POINT                   0.69837E-06  STAGE=  4
   COMPONENT MASS BALANCE         0.22437E-05  STAGE= 17 COMP=WATER
   ENERGY BALANCE                 0.19135E-06  STAGE= 35

BLOCK:  DST3     MODEL: RADFRAC (CONTINUED)

  ****    PROFILES    ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
          FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                                 ENTHALPY
STAGE TEMPERATURE   PRESSURE          CAL/MOL          HEAT DUTY
      C            BAR          LIQUID      VAPOR       CAL/SEC
```

```
  1   256.37       1.0000      -0.14250E+06 -0.10909E+06  -.91264+06
  2   281.68       1.0000      -0.14362E+06 -0.12664E+06
 16   283.28       1.0000      -0.14367E+06 -0.12800E+06
 17   283.28       1.0000      -0.14367E+06 -0.12800E+06
 18   284.38       1.0000      -0.14369E+06 -0.12896E+06
 22   284.48       1.0000      -0.14369E+06 -0.12904E+06
 23   284.48       1.0000      -0.14369E+06 -0.12904E+06
 24   284.48       1.0000      -0.14369E+06 -0.12904E+06
 25   284.48       1.0000      -0.14369E+06 -0.12904E+06
 34   284.48       1.0000      -0.14369E+06 -0.12904E+06
 35   284.48       1.0000      -0.14369E+06 -0.12904E+06   .10534+07

STAGE     FLOW RATE                FEED RATE             PRODUCT RATE
          KMOL/HR                  KMOL/HR               KMOL/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1  207.2      0.000                          89.3268
  2  126.5      207.2
 16  127.1      216.4
 17  267.8      216.4       99.2520
 18  268.7      257.8
 22  268.8      258.9
 23  268.8      258.9
 24  268.8      258.9
 25  268.8      258.9
 34  268.8      258.9
 35  9.925      258.9                            9.9252

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                FEED RATE             PRODUCT RATE
          KG/HR                    KG/HR                 KG/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
  1 0.1883E+05  0.000                             8117.9783
  2 0.1164E+05 0.1883E+05
 16 0.1170E+05 0.1982E+05
 17 0.2465E+05 0.1982E+05  9032.0368
 18 0.2475E+05 0.2374E+05
 22 0.2475E+05 0.2384E+05
 23 0.2475E+05 0.2384E+05
 24 0.2475E+05 0.2384E+05

                          U-O-S BLOCK SECTION

BLOCK:  DST3     MODEL: RADFRAC (CONTINUED)

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                FEED RATE             PRODUCT RATE
          KG/HR                    KG/HR                 KG/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID    VAPOR
 25 0.2475E+05 0.2384E+05
 34 0.2475E+05 0.2384E+05
```

```
 35  914.1     0.2384E+05                          914.0585

                    ****   MOLE-X-PROFILE     ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
     1    0.12314E-02   0.92970       0.67729E-01   0.13434E-02
     2    0.22624E-04   0.99410       0.56891E-02   0.18443E-03
    16     0.92723E-05   0.99752       0.23948E-02   0.80159E-04
    17     0.92723E-05   0.99752       0.23948E-02   0.80159E-04
    18     0.17176E-06   0.99979       0.19889E-03   0.10873E-04
    22     0.20126E-13    1.0000       0.93899E-08   0.36518E-08
    23     0.37234E-15    1.0000       0.77831E-09   0.49434E-09
    24     0.68887E-17    1.0000       0.64513E-10   0.66919E-10
    25     0.12745E-18    1.0000       0.53474E-11   0.90588E-11
    34     0.32366E-34    1.0000       0.98730E-21   0.13818E-18
    35     0.59839E-36    1.0000       0.81586E-22   0.18612E-19

                    ****   MOLE-Y-PROFILE     ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
     1    0.49833E-01   0.45579       0.48846       0.59231E-02
     2    0.12314E-02   0.92970       0.67729E-01   0.13434E-02
    16     0.51367E-03   0.96953       0.29359E-01   0.60151E-03
    17     0.51367E-03   0.96953       0.29359E-01   0.60151E-03
    18     0.96292E-05   0.99742       0.24870E-02   0.83245E-04
    22     0.11295E-11    1.0000       0.11763E-06   0.28010E-07
    23     0.20897E-13    1.0000       0.97500E-08   0.37918E-08
    24     0.38662E-15    1.0000       0.80816E-09   0.51329E-09
    25     0.71529E-17    1.0000       0.66987E-10   0.69484E-10
    34     0.18165E-32    1.0000       0.12368E-19   0.10599E-17
    35     0.33584E-34    1.0000       0.10220E-20   0.14276E-18

                    ****   K-VALUES          ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
     1    40.468       0.49025       7.2120       4.4091
     2    54.432       0.93521       11.905       7.2841
    16     55.399       0.97194       12.259       7.5039
    17     55.399       0.97194       12.259       7.5039
    18     56.063       0.99763       12.504       7.6564
    22     56.124        1.0000       12.527       7.6704
    23     56.124        1.0000       12.527       7.6704
    24     56.124        1.0000       12.527       7.6704
    25     56.124        1.0000       12.527       7.6704
    34     56.124        1.0000       12.527       7.6704
    35     56.124        1.0000       12.527       7.6704
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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0               05/06/2023  PAGE 20

                         U-O-S BLOCK SECTION

BLOCK:  DST3     MODEL: RADFRAC (CONTINUED)

                    ****   MASS-X-PROFILE     ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
    1    0.24411E-03   0.94213       0.56711E-01   0.91750E-03
    2    0.44303E-05   0.99517       0.47057E-02   0.12443E-03
   16    0.18146E-05   0.99796       0.19797E-02   0.54049E-04
   17    0.18146E-05   0.99796       0.19797E-02   0.54049E-04
   18    0.33600E-07   0.99983       0.16434E-03   0.73280E-05
   22    0.39369E-14    1.0000       0.77586E-08   0.24611E-08
   23    0.72837E-16    1.0000       0.64310E-09   0.33317E-09
   24    0.13476E-17    1.0000       0.53305E-10   0.45101E-10
   25    0.24931E-19    1.0000       0.44184E-11   0.61053E-11
   34    0.63313E-35    1.0000       0.81578E-21   0.93125E-19
   35    0.11705E-36    1.0000       0.67412E-22   0.12544E-19
                    ****   MASS-Y-PROFILE     ****
  STAGE     WATER        GLYCEROL      PROPA-01      ETHYL-01
    1    0.11165E-01   0.52202       0.46225       0.45720E-02
    2    0.24411E-03   0.94213       0.56711E-01   0.91750E-03
   16    0.10106E-03   0.97509       0.24398E-01   0.40772E-03
   17    0.10106E-03   0.97509       0.24398E-01   0.40772E-03
   18    0.18845E-05   0.99789       0.20559E-02   0.56130E-04
   22    0.22095E-12    1.0000       0.97193E-07   0.18878E-07
   23    0.40878E-14    1.0000       0.80561E-08   0.25555E-08
   24    0.75629E-16    1.0000       0.66776E-09   0.34594E-09
   25    0.13992E-17    1.0000       0.55349E-10   0.46830E-10
   34    0.35533E-33    1.0000       0.10219E-19   0.71431E-18
   35    0.65695E-35    1.0000       0.84448E-21   0.96215E-19
BLOCK:  E-102    MODEL: HEATER
------------------------------
  INLET STREAM:          S2
  OUTLET STREAM:         ROUT
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                         IN            OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/HR )          114.875         114.875         0.00000
      MASS(KG/HR   )          10470.8         10470.8         0.00000
      ENTHALPY(CAL/SEC )    -0.417391E+07   -0.494383E+07    0.155732
                 ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000     KG/HR
   PRODUCT STREAMS CO2E         0.00000     KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000     KG/HR
   UTILITIES CO2E PRODUCTION    0.00000     KG/HR
   TOTAL CO2E PRODUCTION        0.00000     KG/HR
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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 21

                        U-O-S BLOCK SECTION

BLOCK:  E-102    MODEL: HEATER (CONTINUED)

                     ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE              C                      25.0000
  PRESSURE DROP                      BAR                   0.0
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                       0.000100000



                      ***  RESULTS  ***
  OUTLET TEMPERATURE    C                              25.000
  OUTLET PRESSURE       BAR                          1.0000
  HEAT DUTY             CAL/SEC                    -0.76991E+06
  OUTLET VAPOR FRACTION                                 0.0000



  V-L PHASE EQUILIBRIUM :

    COMP            F(I)          X(I)          Y(I)          K(I)
    WATER           0.95756E-03    0.95756E-03    0.74884       0.60726E-01
    GLYCEROL         0.94533        0.94533       0.15429E-01    0.12674E-05
    PROPA-01        0.52666E-01    0.52666E-01    0.23360       0.34442E-03
    ETHYL-01        0.10446E-02    0.10446E-02    0.21384E-02    0.15896E-03

BLOCK:  E-103    MODEL: HEATER
------------------------------
  INLET STREAM:          S1
  OUTLET STREAM:          LIQ
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                              IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/HR )           114.875         114.875         0.00000
      MASS(KG/HR   )          10470.8         10470.8         0.00000
      ENTHALPY(CAL/SEC )      -0.494382E+07   -0.475134E+07   -0.389341E-01
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                 05/06/2023  PAGE 22

                         U-O-S BLOCK SECTION

BLOCK:  E-103    MODEL: HEATER (CONTINUED)

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E         0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR

                    ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE               C                   150.000
  SPECIFIED PRESSURE                  BAR                 1.00000
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                   0.000100000



                     ***  RESULTS  ***
  OUTLET TEMPERATURE    C                            150.00
  OUTLET PRESSURE       BAR                          1.0000
  HEAT DUTY             CAL/SEC                      0.19248E+06
  OUTLET VAPOR FRACTION                              0.0000



  V-L PHASE EQUILIBRIUM :

    COMP             F(I)           X(I)           Y(I)           K(I)
    WATER           0.95756E-03    0.95756E-03    0.15457        6.1217
    GLYCEROL        0.94533        0.94533        0.26180        0.10503E-01
    PROPA-01        0.52666E-01    0.52666E-01    0.57754        0.41588
    ETHYL-01        0.10446E-02    0.10446E-02    0.60866E-02    0.22097

BLOCK:  E-104    MODEL: HEATER
------------------------------
  INLET STREAM:          S4
  OUTLET STREAM:         DIST
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                             IN            OUT       RELATIVE DIFF.
```

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ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 23

                          U-O-S BLOCK SECTION

BLOCK:  E-104    MODEL: HEATER (CONTINUED)
   TOTAL BALANCE
      MOLE(KMOL/HR )           110.280         110.280         0.00000
      MASS(KG/HR   )           10047.7         10047.7         0.00000
      ENTHALPY(CAL/SEC )      -0.389346E+07   -0.451859E+07    0.138347

                 ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E         0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR

                     ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE               C                     175.000
  PRESSURE DROP                      BAR                    0.0
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                      0.000100000



                      ***  RESULTS  ***
  OUTLET TEMPERATURE    C                             175.00
  OUTLET PRESSURE       BAR                          1.0000
  HEAT DUTY             CAL/SEC                     -0.62513E+06
  OUTLET VAPOR FRACTION                               0.0000



  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     WATER          0.99746E-03    0.99746E-03    0.11299        10.654
     GLYCEROL        0.94305        0.94305        0.31884        0.31796E-01
     PROPA-01        0.54860E-01    0.54860E-01    0.56205        0.96353
     ETHYL-01        0.10881E-02    0.10881E-02    0.61183E-02    0.52880

BLOCK:  E-105    MODEL: HEATER
-----------------------------
  INLET STREAM:          S3
  OUTLET STREAM:         DIST2
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 24

                          U-O-S BLOCK SECTION

BLOCK:  E-105    MODEL: HEATER (CONTINUED)

                  ***  MASS AND ENERGY BALANCE  ***
                             IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(KMOL/HR )           99.2520         99.2520         0.00000
     MASS(KG/HR   )          9032.04         9032.04       -0.201393E-15
     ENTHALPY(CAL/SEC )      -0.393294E+07   -0.407271E+07    0.343206E-01

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             0.00000      KG/HR
   PRODUCT STREAMS CO2E          0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR

                     ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE                C                     166.000
  PRESSURE DROP                        BAR                   0.0
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                      0.000100000



                      ***  RESULTS  ***
  OUTLET TEMPERATURE    C                          166.00
  OUTLET PRESSURE       BAR                        1.0000
  HEAT DUTY             CAL/SEC                   -0.13978E+06
  OUTLET VAPOR FRACTION                            0.0000



  V-L PHASE EQUILIBRIUM :

    COMP            F(I)          X(I)          Y(I)          K(I)
    WATER           0.11083E-02   0.11083E-02   0.13145       8.8290
    GLYCEROL        0.93673       0.93673       0.27337       0.21724E-01
    PROPA-01        0.60956E-01   0.60956E-01   0.58882       0.71907
    ETHYL-01        0.12090E-02   0.12090E-02   0.63610E-02   0.39164
```

```
 ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                 05/06/2023  PAGE 25

                          U-O-S BLOCK SECTION

 BLOCK:  H2SEP    MODEL: FLASH2
 ------------------------------
   INLET STREAM:          ROUT
   OUTLET VAPOR STREAM:   H2
   OUTLET LIQUID STREAM:  S1
   PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                               IN             OUT       RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(KMOL/HR )           114.875         114.875         0.00000
       MASS(KG/HR   )           10470.8         10470.8         0.00000
       ENTHALPY(CAL/SEC )      -0.494383E+07   -0.494382E+07   -0.119914E-06

                  ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            0.00000      KG/HR
    PRODUCT STREAMS CO2E         0.00000      KG/HR
    NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
    UTILITIES CO2E PRODUCTION     0.00000      KG/HR
    TOTAL CO2E PRODUCTION         0.00000      KG/HR

                      ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE C                          25.0000
   SPECIFIED PRESSURE    BAR                        1.01000
   MAXIMUM NO. ITERATIONS                            30
   CONVERGENCE TOLERANCE                              0.000100000

                       ***  RESULTS  ***
   OUTLET TEMPERATURE    C                          25.000
   OUTLET PRESSURE       BAR                       1.0100
   HEAT DUTY             CAL/SEC                  0.59284
   VAPOR FRACTION                                 0.0000



   V-L PHASE EQUILIBRIUM :

      COMP             F(I)          X(I)          Y(I)          K(I)
      WATER           0.95756E-03    0.95756E-03    0.74873        0.60134E-01
      GLYCEROL        0.94533        0.94533        0.15437E-01    0.12559E-05
      PROPA-01        0.52666E-01    0.52666E-01    0.23369        0.34125E-03
      ETHYL-01        0.10446E-02    0.10446E-02    0.21390E-02    0.15748E-03
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 26

                        U-O-S BLOCK SECTION

BLOCK:  MIX1     MODEL: MIXER
-----------------------------
  INLET STREAMS:         FEED        BOT1        H2
  OUTLET STREAM:         RIN
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                              IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/HR )            114.875          114.875         0.00000
      MASS(KG/HR   )          10470.8          10470.8         0.00000
      ENTHALPY(CAL/SEC )      -0.492362E+07   -0.492362E+07     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E          0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR

                      ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                30
  CONVERGENCE TOLERANCE                                   0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  PFR      MODEL: RPLUG
-----------------------------
  INLET STREAM:          RIN
  OUTLET STREAM:         S2
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                          IN          OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(KMOL/HR )         114.875       114.875       0.00000      0.247414E-15
  MASS(KG/HR   )        10470.8       10470.8                   0.00000
  ENTHALPY(CAL/SEC )   -0.492362E+07 -0.417391E+07              -0.152268

BLOCK:  PFR      MODEL: RPLUG (CONTINUED)

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      KG/HR
   PRODUCT STREAMS CO2E          0.00000      KG/HR
   NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
   UTILITIES CO2E PRODUCTION     0.00000      KG/HR
   TOTAL CO2E PRODUCTION         0.00000      KG/HR
```

```
                    ***  INPUT DATA  ***
   REACTOR TYPE:
     SPECIFIED TEMPERATURE
     VAPOR FLUID PHASE
   REACTOR TUBE LENGTH              METER             150.00
   REACTOR DIAMETER                 METER            0.52000
   REACTOR RISE                     METER            0.0000
   NUMBER OF REACTOR TUBES                               1
   REACTOR VOLUME                   L                31856.
   PRESSURE DROP OPTION:                             SPECIFIED
   HOLDUP OPTION:                                  NO-SLIP
   ERROR TOLERANCE                                   0.10000E-03
   INTEGRATION METHOD                                GEAR
   CORRECTOR METHOD                                  NEWTON
   INITIAL STEP SIZE FACTOR                          0.10000E-01
   CORRECTOR TOLERANCE FACTOR                              0.10000
   MAXIMUM NUMBER OF STEPS                               1000
   TEMPERATURE PROFILES:
     RELATIVE LOCATION        TEMPERATURE
          0.0000         190.00      C
    REACTION PARAGRAPH          ID:  R-1         TYPE:  POWERLAW
    GLOBAL BASES:
    KBASIS                                 MOLE-GAMMA
    CBASIS                                 MOLARITY
    SBASIS                                 GLOBAL
    STOICHIOMETRY:
    REACTION NUMBER:         1
      SUBSTREAM:  MIXED
ACETOL      1.0000     WATER      1.0000     GLYCEROL   -1.0000

    REACTION NUMBER:         2
      SUBSTREAM:  MIXED
ACETOL     -1.0000     PROPA-01    1.0000     HYDROGEN   -1.0000

    REACTION NUMBER:         3
      SUBSTREAM:  MIXED
METHANOL    1.0000     GLYCEROL   -1.0000     ETHYL-01    1.0000     HYDROGEN   -1.0000
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 28

                        U-O-S BLOCK SECTION

BLOCK:  PFR      MODEL: RPLUG (CONTINUED)

   REAC-DATA ENTRIES:

     REACTION NO    TYPE     PHASE       DELT           BASIS
                                          C

         1       KINETIC      L       0.0000         MOLARITY
         2       KINETIC      V       0.0000         MOLARITY
         3       KINETIC      V       0.0000         MOLARITY


   RATE PARAMETERS:

     REACTION NO   PREEXP. FACTOR   ACT. ENERGY   TEMP. EXPONENT   REF. TEMP
                                      CAL/MOL                  C

         1          0.38000E+13      48000.        0.0000
         2          0.48000E+27      64000.        0.0000
         3          0.33000E+08      26000.        0.0000

   POWERLAW EXPONENTS:

   REACTION NUMBER:         1
     SUBSTREAM:  MIXED
       GLYCEROL    1.0000

   REACTION NUMBER:         2
     SUBSTREAM:  MIXED
       ACETOL      1.0000      HYDROGEN    1.0000

   REACTION NUMBER:         3
     SUBSTREAM:  MIXED
       GLYCEROL    1.0000      HYDROGEN    1.0000

                      ***  RESULTS  ***

   REACTOR DUTY              CAL/SEC                   0.74971E+06
   RESIDENCE TIME            HR                    0.74383E-02
   REACTOR MINIMUM TEMPERATURE C                          190.00
   REACTOR MAXIMUM TEMPERATURE C                           190.00
```

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 ASPEN PLUS   PLAT: WIN-X64   VER: 37.0              05/06/2023  PAGE 29

                     U-O-S BLOCK SECTION

 BLOCK:  PFR      MODEL: RPLUG (CONTINUED)


        *** RESULTS PROFILE (PROCESS STREAM) ***

     LENGTH       PRESSURE     TEMPERATURE   VAPOR FRAC    RES-TIME
     METER        BAR          C                      HR

      0.0000       1.0000       190.00       1.0000       0.0000
      15.000       1.0000       190.00       1.0000      0.74383E-03
      30.000       1.0000       190.00       1.0000      0.14877E-02
      45.000       1.0000       190.00       1.0000      0.22315E-02
      60.000       1.0000       190.00       1.0000      0.29753E-02
      75.000       1.0000       190.00       1.0000      0.37192E-02
      90.000       1.0000       190.00       1.0000      0.44630E-02
      105.00       1.0000       190.00       1.0000      0.52068E-02
      120.00       1.0000       190.00       1.0000      0.59507E-02
      135.00       1.0000       190.00       1.0000      0.66945E-02
      150.00       1.0000       190.00       1.0000      0.74383E-02

     LENGTH       DUTY         LIQUID HOLDUP
     METER        CAL/SEC
      0.0000       0.0000       0.0000
      15.000       0.0000       0.0000
      30.000       0.0000       0.0000
      45.000       0.0000       0.0000
      60.000       0.0000       0.0000
      75.000       0.0000       0.0000
      90.000       0.0000       0.0000
      105.00       0.0000       0.0000
      120.00       0.0000       0.0000
      135.00       0.0000       0.0000
      150.00       0.0000       0.0000


        ***  TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

     LENGTH       WATER        GLYCEROL     PROPA-01     ETHYL-01
     METER

      0.0000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      15.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      30.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      45.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      60.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      75.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      90.000     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
      105.00     0.95756E-03  0.94533      0.52666E-01  0.10446E-02
```

120.00	0.95756E-03	0.94533	0.52666E-01	0.10446E-02
135.00	0.95756E-03	0.94533	0.52666E-01	0.10446E-02
150.00	0.95756E-03	0.94533	0.52666E-01	0.10446E-02

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0             05/06/2023  PAGE 30

                   U-O-S BLOCK SECTION

BLOCK:  PFR      MODEL: RPLUG (CONTINUED)


      ***  TOTAL  MASS FRACTION PROFILE (PROCESS STREAM) ***

    LENGTH       WATER        GLYCEROL     PROPA-01     ETHYL-01
    METER

     0.0000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     15.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     30.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     45.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     60.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     75.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     90.000     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     105.00     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     120.00     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     135.00     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
     150.00     0.18926E-03   0.95513      0.43968E-01   0.71133E-03
```

```
ASPEN PLUS   PLAT: WIN-X64   VER: 37.0                05/06/2023  PAGE 31

                         STREAM SECTION

BOT1 BOT2 BOT3 DIST DIST2
-------------------------


STREAM ID            BOT1      BOT2      BOT3      DIST      DIST2
FROM :               DST1      DST2      DST3      E-104     E-105
TO   :               MIX1      ----      ----      DST2      DST3

SUBSTREAM: MIXED
PHASE:               LIQUID    LIQUID    LIQUID    LIQUID    LIQUID
COMPONENTS: KMOL/HR
  ACETOL             0.0       0.0       0.0       0.0       0.0
  WATER              0.0       0.0       0.0       0.1100    0.1100
  METHANOL           0.0       0.0       0.0       0.0       0.0
  GLYCEROL           4.5950    11.0280   9.9252    104.0000  92.9720
  PROPA-01           0.0       4.7252-25 8.0976-22 6.0500    6.0500
  ETHYL-01           3.1994-33 4.6949-22 1.8473-19 0.1200    0.1200
  HYDROGEN           0.0       0.0       0.0       0.0       0.0
TOTAL FLOW:
  KMOL/HR            4.5950    11.0280   9.9252    110.2800  99.2520
  KG/HR              423.1752  1015.6206 914.0585  1.0048+04 9032.0369
  L/MIN              6.7663    16.2392   14.6153   148.4672  132.7586
STATE VARIABLES:
  TEMP   C           284.4812  284.4812  284.4813  175.0000  166.0000
  PRES   BAR         1.0000    1.0000    1.0000    1.0000    1.0000
  VFRAC              0.0       0.0       0.0       0.0       0.0
  LFRAC              1.0000    1.0000    1.0000    1.0000    1.0000
  SFRAC              0.0       0.0       0.0       0.0       0.0
ENTHALPY:
  CAL/MOL            -1.4369+05 -1.4369+05 -1.4369+05 -1.4751+05 -1.4772+05
  CAL/GM             -1560.2882 -1560.2882 -1560.2882 -1618.9765 -1623.3067
  CAL/SEC            -1.8341+05 -4.4018+05 -3.9617+05 -4.5186+06 -4.0727+06
ENTROPY:
  CAL/MOL-K          -109.7399  -109.7399  -109.7399  -121.5252  -122.5602
  CAL/GM-K           -1.1916    -1.1916    -1.1916    -1.3338    -1.3468
DENSITY:
  MOL/CC             1.1318-02  1.1318-02  1.1318-02  1.2380-02  1.2460-02
  GM/CC              1.0424     1.0424     1.0424     1.1279     1.1339
AVG MW               92.0947    92.0947    92.0947    91.1104    91.0011
                                                   STREAM SECTION

DIST3 FEED H2 LIQ RIN
---------------------
STREAM ID            DIST3     FEED      H2        LIQ       RIN
FROM :               DST3      ----      H2SEP     E-103     MIX1
TO   :               ----      MIX1      MIX1      DST1      PFR
CONV. MAX. REL. ERR:     0.0       0.0       0.0       0.0   -5.6253-06
SUBSTREAM: MIXED
PHASE:               LIQUID    LIQUID    MISSING   LIQUID    LIQUID
```

```
COMPONENTS: KMOL/HR
  ACETOL              0.0       0.0       0.0       0.0       0.0
  WATER              0.1100    0.1100    0.0       0.1100    0.1100
  METHANOL            0.0       0.0       0.0       0.0       0.0
  GLYCEROL           83.0468   104.0000    0.0     108.5950   108.5950
  PROPA-01            6.0500    6.0500    0.0       6.0500    6.0500
  ETHYL-01            0.1200    0.1200    0.0       0.1200    0.1200
  HYDROGEN            0.0       0.0       0.0       0.0       0.0
TOTAL FLOW:
  KMOL/HR            89.3268   110.2800    0.0     114.8750   114.8750
  KG/HR            8117.9784  1.0048+04    0.0     1.0471+04  1.0471+04
  L/MIN             129.2535   133.5170    0.0     151.6329   140.2913
STATE VARIABLES:
  TEMP   C          256.3655    25.0000   MISSING   150.0000    38.8438
  PRES   BAR          1.0000    54.0000    1.0100     1.0000     1.0000
  VFRAC               0.0       0.0      MISSING     0.0        0.0
  LFRAC               1.0000    1.0000   MISSING     1.0000     1.0000
  SFRAC               0.0       0.0      MISSING     0.0        0.0
ENTHALPY:
  CAL/MOL          -1.4250+05 -1.5474+05   MISSING -1.4890+05 -1.5430+05
  CAL/GM           -1567.9709 -1698.3834   MISSING -1633.5691 -1692.8023
  CAL/SEC          -3.5358+06 -4.7402+06   MISSING -4.7513+06 -4.9236+06
ENTROPY:
  CAL/MOL-K          -112.3087  -141.3875   MISSING  -124.5252  -139.2851
  CAL/GM-K             -1.2358    -1.5518   MISSING    -1.3662    -1.5281
DENSITY:
  MOL/CC           1.1518-02  1.3766-02   MISSING  1.2626-02  1.3647-02
  GM/CC              1.0468     1.2542    MISSING    1.1509     1.2439
AVG MW               90.8795    91.1104   MISSING    91.1498    91.1498


ROUT S1 S2 S3 S4
----------------

STREAM ID            ROUT       S1        S2        S3        S4
FROM :              E-102     H2SEP      PFR      DST2      DST1
TO   :             H2SEP      E-103     E-102     E-105     E-104

SUBSTREAM: MIXED
PHASE:              LIQUID    LIQUID    VAPOR     LIQUID    VAPOR
COMPONENTS: KMOL/HR
  ACETOL              0.0       0.0       0.0       0.0       0.0
  WATER              0.1100    0.1100    0.1100    0.1100    0.1100
  METHANOL            0.0       0.0       0.0       0.0       0.0
  GLYCEROL          108.5950  108.5950  108.5950   92.9720  104.0000
  PROPA-01            6.0500    6.0500    6.0500    6.0500    6.0500
  ETHYL-01            0.1200    0.1200    0.1200    0.1200    0.1200
  HYDROGEN            0.0       0.0       0.0       0.0       0.0
TOTAL FLOW:
  KMOL/HR           114.8750  114.8750  114.8750   99.2520  110.2800
  KG/HR            1.0471+04 1.0471+04 1.0471+04 9032.0369 1.0048+04
  L/MIN             139.0571  139.0571 7.1377+04  143.7821 8.3297+04
```

```
 STATE VARIABLES:
   TEMP   C            25.0000    25.0000   190.0000   258.5787   282.2216
   PRES   BAR           1.0000     1.0100     1.0000     1.0000     1.0000
   VFRAC                0.0        0.0        1.0000     0.0        1.0000
   LFRAC                1.0000     1.0000     0.0        1.0000     0.0
   SFRAC                0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   CAL/MOL          -1.5493+05 -1.5493+05 -1.3080+05 -1.4265+05 -1.2710+05
   CAL/GM           -1699.7474 -1699.7472 -1435.0420 -1567.5939 -1394.9962
   CAL/SEC          -4.9438+06 -4.9438+06 -4.1739+06 -3.9329+06 -3.8935+06
 ENTROPY:
   CAL/MOL-K          -141.3604  -141.3604   -90.5553  -112.0998   -83.4287
   CAL/GM-K             -1.5509    -1.5509    -0.9935    -1.2319    -0.9157
 DENSITY:
   MOL/CC            1.3768-02  1.3768-02  2.6823-05  1.1505-02  2.2066-05
   GM/CC                1.2550     1.2550  2.4449-03     1.0470  2.0104-03
 AVG MW                91.1498    91.1498    91.1498    91.0011    91.1104
```

PROBLEM STATUS SECTION

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                                   BLOCK STATUS
                                   ------------
****************************************************************************************************

***                    Calculations were completed normally                                    ***
***                    All Unit Operation blocks were completed normally                       ***
***                    All streams were flashed normally                                       ***
***                    All Convergence blocks were completed normally                          ***
***                                                                                            ***
****************************************************************************************************
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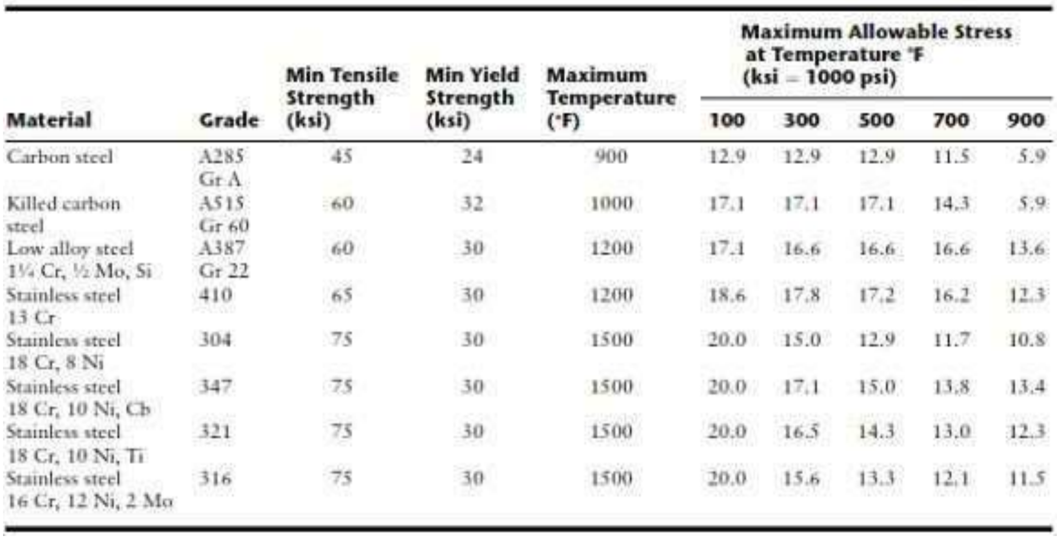
APPENDICES

Appendix-A

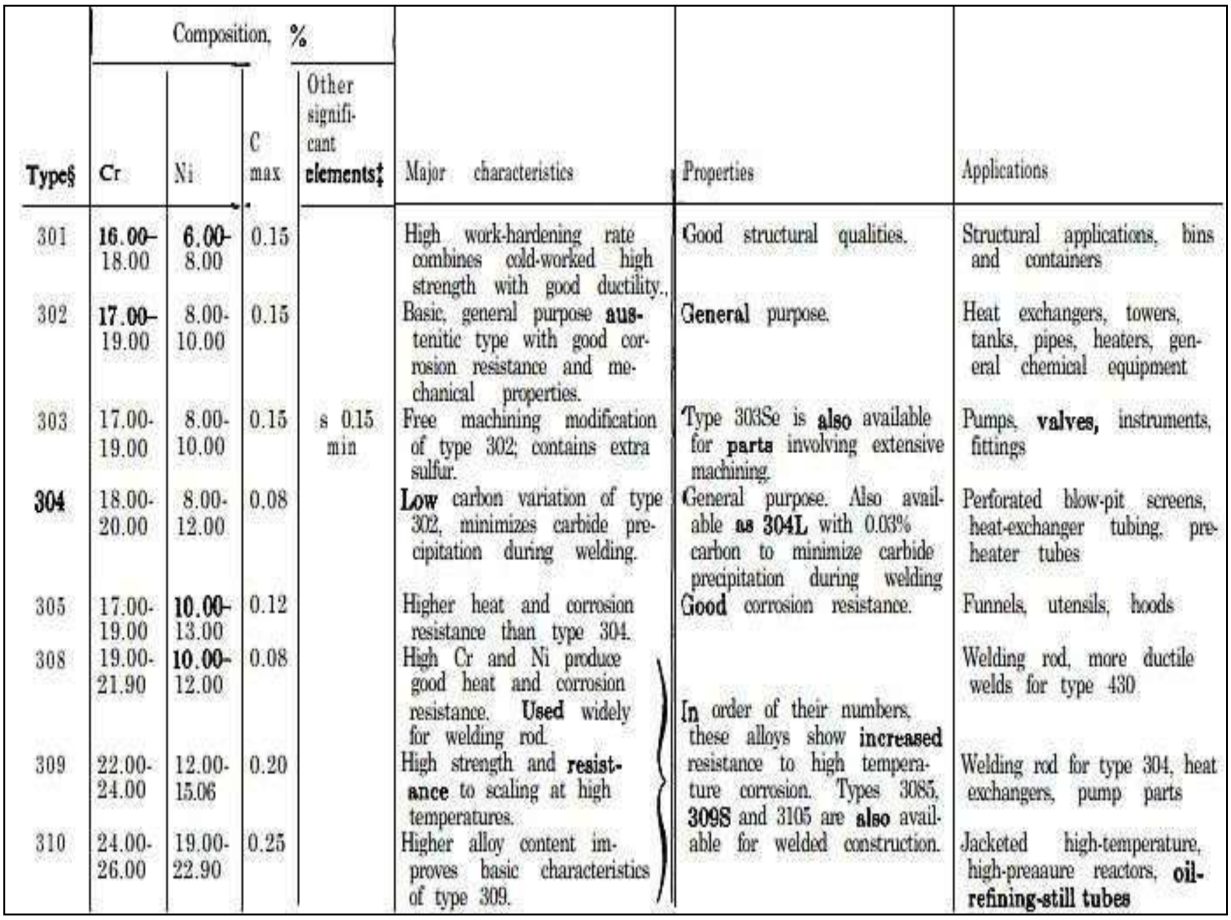
List of Tables

Table A-4: Maximum Allowable Stress



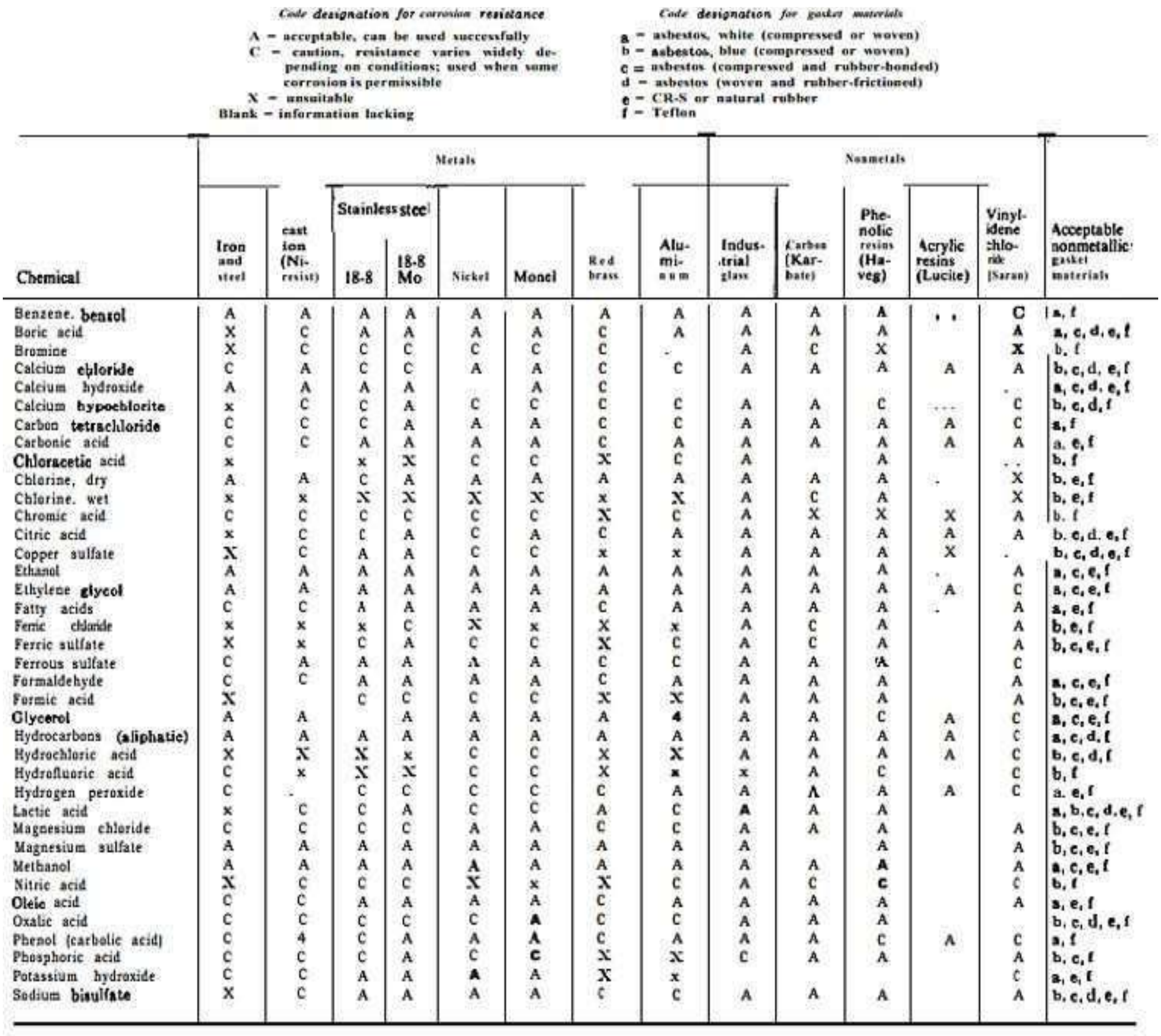
Material	Grade	Min Tensile Strength (ksi)	Min Yield Strength (ksi)	Maximum Temperature (°F)	Maximum Allowable Stress at Temperature °F (ksi = 1000 psi)				
					100	300	500	700	900
Carbon steel	A285 Gr A	45	24	900	12.9	12.9	12.9	11.5	5.9
Killed carbon steel	A515 Gr 60	60	32	1000	17.1	17.1	17.1	14.3	5.9
Low alloy steel 1¼ Cr, ½ Mo, Si	A387 Gr 22	60	30	1200	17.1	16.6	16.6	16.6	13.6
Stainless steel 13 Cr	410	65	30	1200	18.6	17.8	17.2	16.2	12.3
Stainless steel 18 Cr, 8 Ni	304	75	30	1500	20.0	15.0	12.9	11.7	10.8
Stainless steel 18 Cr, 10 Ni, Cb	347	75	30	1500	20.0	17.1	15.0	13.8	13.4
Stainless steel 18 Cr, 10 Ni, Ti	321	75	30	1500	20.0	16.5	14.3	13.0	12.3
Stainless steel 16 Cr, 12 Ni, 2 Mo	316	75	30	1500	20.0	15.6	13.3	12.1	11.5

Table A-7: Stainless Steels most commonly used in the Chemical Process Industries



	Composition, %						
Type§	Cr	Ni	C max	Other significant elements‡	Major characteristics	Properties	Applications
301	16.00–18.00	6.00-8.00	0.15		High work-hardening rate combines cold-worked high strength with good ductility.,	Good structural qualities.	Structural applications, bins and containers
302	17.00–19.00	8.00-10.00	0.15		Basic, general purpose **austenitic** type with good corrosion resistance and mechanical properties.	**General** purpose.	Heat exchangers, towers, tanks, pipes, heaters, general chemical equipment
303	17.00-19.00	8.00-10.00	0.15	s 0.15 min	Free machining modification of type 302; contains extra sulfur.	Type 303Se is **also** available for **parts** involving extensive machining.	Pumps, **valves,** instruments, fittings
304	18.00-20.00	8.00-12.00	0.08		**Low** carbon variation of type 302, minimizes carbide precipitation during welding.	General purpose. Also available **as 304L** with 0.03% carbon to minimize carbide precipitation during welding	Perforated blow-pit screens, heat-exchanger tubing, preheater tubes
305	17.00-19.00	**10.00-**13.00	0.12		Higher heat and corrosion resistance than type 304.	**Good** corrosion resistance.	Funnels, utensils, hoods
308	19.00-21.90	**10.00-**12.00	0.08		High Cr and Ni produce good heat and corrosion resistance. **Used** widely for welding rod.	In order of their numbers, these alloys show **increased** resistance to high temperature corrosion. Types 3085, **309S** and 3105 are **also** available for welded construction.	Welding rod, more ductile welds for type 430
309	22.00-24.00	12.00-15.06	0.20		High strength and **resistance** to scaling at high temperatures.		Welding rod for type 304, heat exchangers, pump parts
310	24.00-26.00	19.00-22.90	0.25		Higher alloy content improves basic characteristics of type 309.		Jacketed high-temperature, high-preaaure reactors, **oil-refining-still tubes**

Table A-13: Corrosion Resistance of Constructional Materials



Code designation for corrosion resistance

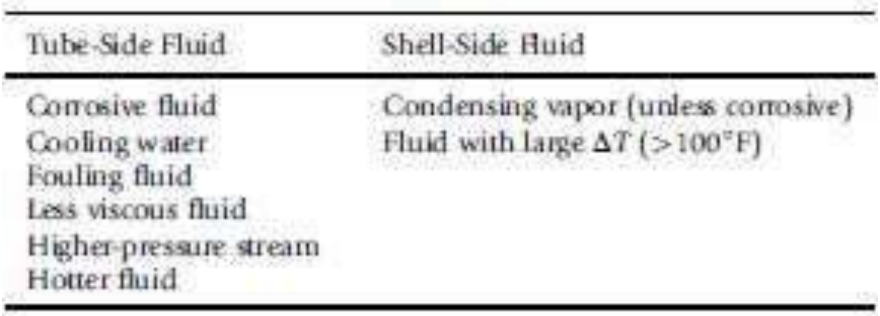
A = acceptable, can be used successfully
C = caution, resistance varies widely depending on conditions; used when some corrosion is permissible
X = unsuitable
Blank = information lacking

Code designation for gasket materials

a = asbestos, white (compressed or woven)
b = asbestos, blue (compressed or woven)
c = asbestos (compressed and rubber-bonded)
d = asbestos (woven and rubber-frictioned)
e = CR-S or natural rubber
f = Teflon

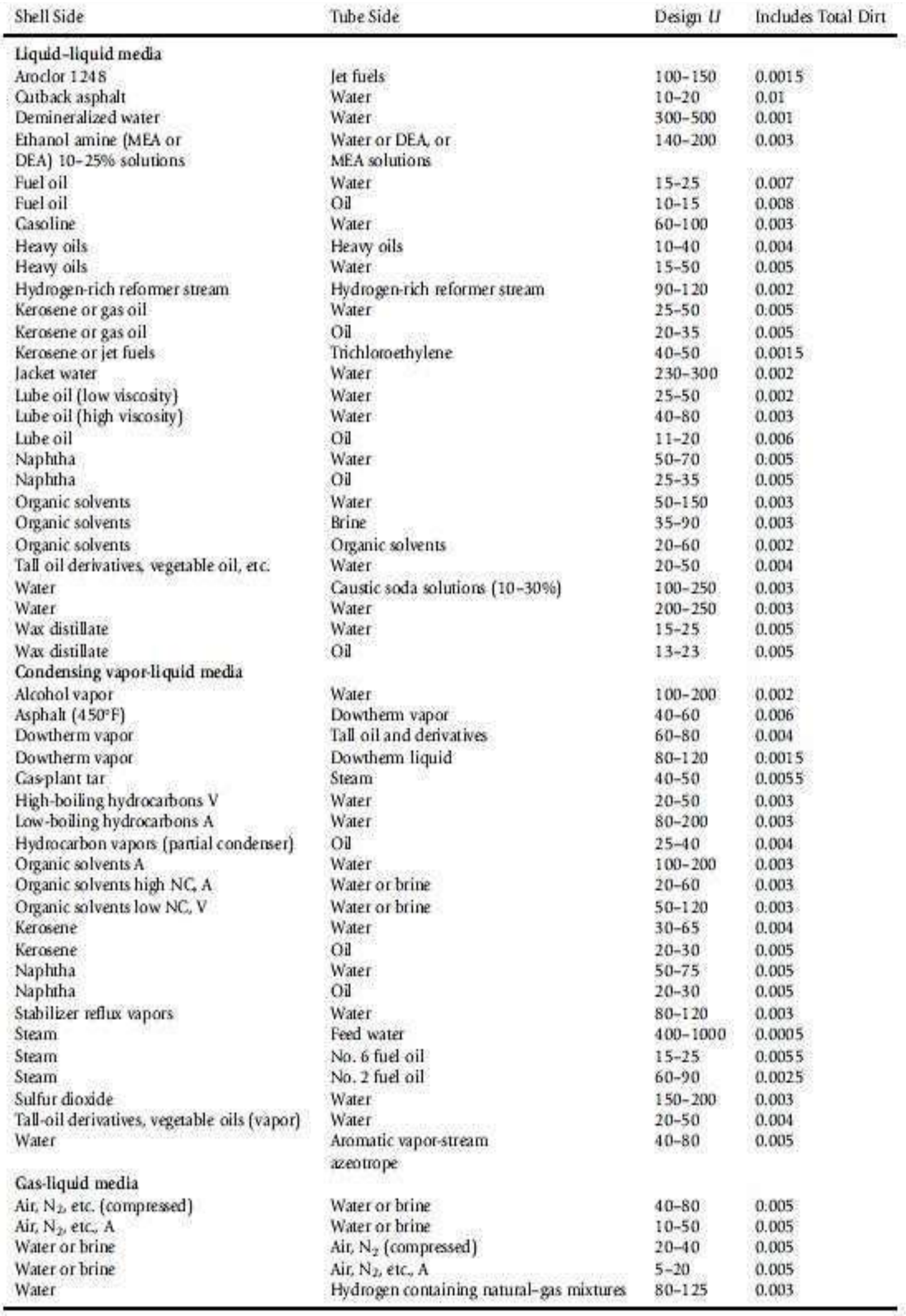
Chemical	Metals								Nonmetals					Acceptable nonmetallic gasket materials
			Stainless steel											
	Iron and steel	cast iron (Ni-resist)	18-8	18-8 Mo	Nickel	Monel	Red brass	Alu-mi-num	Indus-trial glass	Carbon (Kar-bate)	Phe-nolic resins (Ha-veg)	Acrylic resins (Lucite)	Vinyl-idene chlo-ride (Saran)	
Benzene, benzol	A	A	A	A	A	A	A	A	A	A	A	. .	C	a, f
Boric acid	X	C	A	A	A	A	C	A	A	A	A		A	a, c, d, e, f
Bromine	X	C	C	C	C	C	C	.	A	C	X		X	b, f
Calcium chloride	C	A	C	C	A	A	C	C	A	A	A	A	A	b, c, d, e, f
Calcium hydroxide	A	A	A	A		A	C						.	a, c, d, e, f
Calcium hypochlorite	x	C	C	A	C	C	C	C	A	A	C	. . .	C	b, c, d, f
Carbon tetrachloride	C	C	C	A	A	A	C	C	A	A	A	A	C	a, f
Carbonic acid	C	C	A	A	A	A	C	A	A	A	A	A	A	a, e, f
Chloracetic acid	x		x	X	C	C	X	C	A		A		. .	b, f
Chlorine, dry	A	A	C	A	A	A	A	A	A	A	A	.	X	b, e, f
Chlorine, wet	x	x	X	X	X	X	x	X	A	C	A		X	b, e, f
Chromic acid	C	C	C	C	C	C	X	C	A	X	X	X	A	b, f
Citric acid	x	C	C	A	C	A	C	A	A	A	A	A	A	b, c, d, e, f
Copper sulfate	X	C	A	A	C	C	x	x	A	A	A	X	.	b, c, d, e, f
Ethanol	A	A	A	A	A	A	A	A	A	A	A	.	A	a, c, e, f
Ethylene glycol	A	A	A	A	A	A	A	A	A	A	A	A	C	a, c, e, f
Fatty acids	C	C	A	A	A	A	C	A	A	A	A	.	A	a, e, f
Ferric chloride	x	x	x	C	X	x	X	x	A	C	A		A	b, e, f
Ferric sulfate	X	x	C	A	C	C	X	C	A	C	A		A	b, c, e, f
Ferrous sulfate	C	A	A	A	A	A	C	C	A	A	A		C	
Formaldehyde	C	C	A	A	A	A	C	A	A	A	A		A	a, c, e, f
Formic acid	X		C	C	C	C	X	X	A	A	A		A	b, c, e, f
Glycerol	A	A		A	A	A	A	4	A	A	C	A	C	a, c, e, f
Hydrocarbons (aliphatic)	A	A	A	A	A	A	A	A	A	A	A	A	C	a, c, d, f
Hydrochloric acid	X	X	X	x	C	C	X	X	A	A	A	A	C	b, c, d, f
Hydrofluoric acid	C	x	X	X	C	C	X	x	x	A	C		C	b, f
Hydrogen peroxide	C	.	C	C	C	C	C	A	A	A	A	A	C	a, e, f
Lactic acid	x	C	C	A	C	C	A	C	A	A	A			a, b, c, d, e, f
Magnesium chloride	C	C	C	C	A	A	C	C	A	A	A		A	b, c, e, f
Magnesium sulfate	A	A	A	A	A	A	A	A	A		A		A	b, c, e, f
Methanol	A	A	A	A	A	A	A	A	A	A	A		A	a, c, e, f
Nitric acid	X	C	C	C	X	x	X	C	A	C	C		C	b, f
Oleic acid	C	C	A	A	A	A	C	A	A	A	A		A	a, e, f
Oxalic acid	C	C	C	C	C	A	C	C	A	A	A			b, c, d, e, f
Phenol (carbolic acid)	C	4	C	A	A	A	C	A	A	A	C	A	C	a, f
Phosphoric acid	C	C	C	A	C	C	X	X	C	A	A		A	b, c, f
Potassium hydroxide	C	C	A	A	A	A	X	x					C	a, e, f
Sodium bisulfate	X	C	A	A	A	A	C	C	A	A	A		A	b, c, d, e, f

Table A-10: Criteria for Fluid Placement, in order of Priority



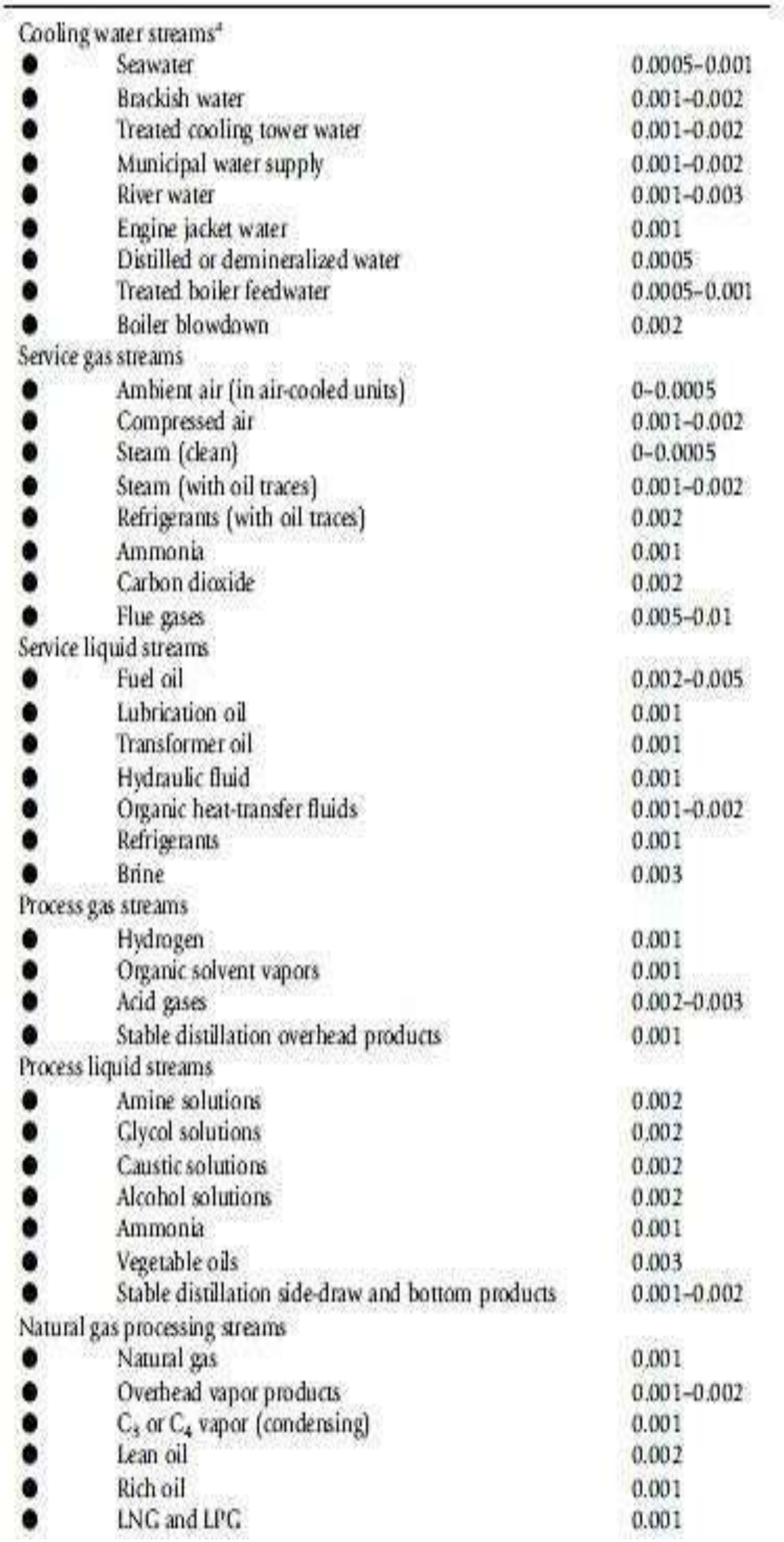
Tube-Side Fluid	Shell-Side Fluid
Corrosive fluid	Condensing vapor (unless corrosive)
Cooling water	Fluid with large ΔT (>100°F)
Fouling fluid	
Less viscous fluid	
Higher-pressure stream	
Hotter fluid	

Table A-16: Typical Values of Overall Heat-Transfer Coefficients in Tubular Heat Exchangers



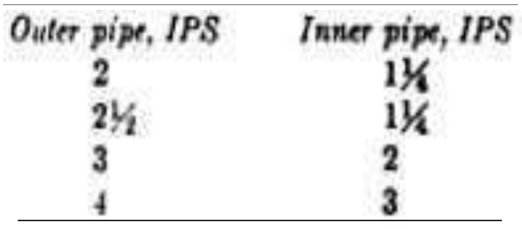
Shell Side	Tube Side	Design *U*	Includes Total Dirt
Liquid–liquid media			
Aroclor 1248	Jet fuels	100–150	0.0015
Cutback asphalt	Water	10–20	0.01
Demineralized water	Water	300–500	0.001
Ethanol amine (MEA or DEA) 10–25% solutions	Water or DEA, or MEA solutions	140–200	0.003
Fuel oil	Water	15–25	0.007
Fuel oil	Oil	10–15	0.008
Gasoline	Water	60–100	0.003
Heavy oils	Heavy oils	10–40	0.004
Heavy oils	Water	15–50	0.005
Hydrogen-rich reformer stream	Hydrogen-rich reformer stream	90–120	0.002
Kerosene or gas oil	Water	25–50	0.005
Kerosene or gas oil	Oil	20–35	0.005
Kerosene or jet fuels	Trichloroethylene	40–50	0.0015
Jacket water	Water	230–300	0.002
Lube oil (low viscosity)	Water	25–50	0.002
Lube oil (high viscosity)	Water	40–80	0.003
Lube oil	Oil	11–20	0.006
Naphtha	Water	50–70	0.005
Naphtha	Oil	25–35	0.005
Organic solvents	Water	50–150	0.003
Organic solvents	Brine	35–90	0.003
Organic solvents	Organic solvents	20–60	0.002
Tall oil derivatives, vegetable oil, etc.	Water	20–50	0.004
Water	Caustic soda solutions (10–30%)	100–250	0.003
Water	Water	200–250	0.003
Wax distillate	Water	15–25	0.005
Wax distillate	Oil	13–23	0.005
Condensing vapor-liquid media			
Alcohol vapor	Water	100–200	0.002
Asphalt (450°F)	Dowtherm vapor	40–60	0.006
Dowtherm vapor	Tall oil and derivatives	60–80	0.004
Dowtherm vapor	Dowtherm liquid	80–120	0.0015
Gas-plant tar	Steam	40–50	0.0055
High-boiling hydrocarbons V	Water	20–50	0.003
Low-boiling hydrocarbons A	Water	80–200	0.003
Hydrocarbon vapors (partial condenser)	Oil	25–40	0.004
Organic solvents A	Water	100–200	0.003
Organic solvents high NC, A	Water or brine	20–60	0.003
Organic solvents low NC, V	Water or brine	50–120	0.003
Kerosene	Water	30–65	0.004
Kerosene	Oil	20–30	0.005
Naphtha	Water	50–75	0.005
Naphtha	Oil	20–30	0.005
Stabilizer reflux vapors	Water	80–120	0.003
Steam	Feed water	400–1000	0.0005
Steam	No. 6 fuel oil	15–25	0.0055
Steam	No. 2 fuel oil	60–90	0.0025
Sulfur dioxide	Water	150–200	0.003
Tall-oil derivatives, vegetable oils (vapor)	Water	20–50	0.004
Water	Aromatic vapor-stream azeotrope	40–80	0.005
Gas-liquid media			
Air, N_2, etc. (compressed)	Water or brine	40–80	0.005
Air, N_2, etc., A	Water or brine	10–50	0.005
Water or brine	Air, N_2 (compressed)	20–40	0.005
Water or brine	Air, N_2, etc., A	5–20	0.005
Water	Hydrogen containing natural–gas mixtures	80–125	0.003

Table A-19: Typical Values of Fouling Factors (H. Ft2.˚f/Btu



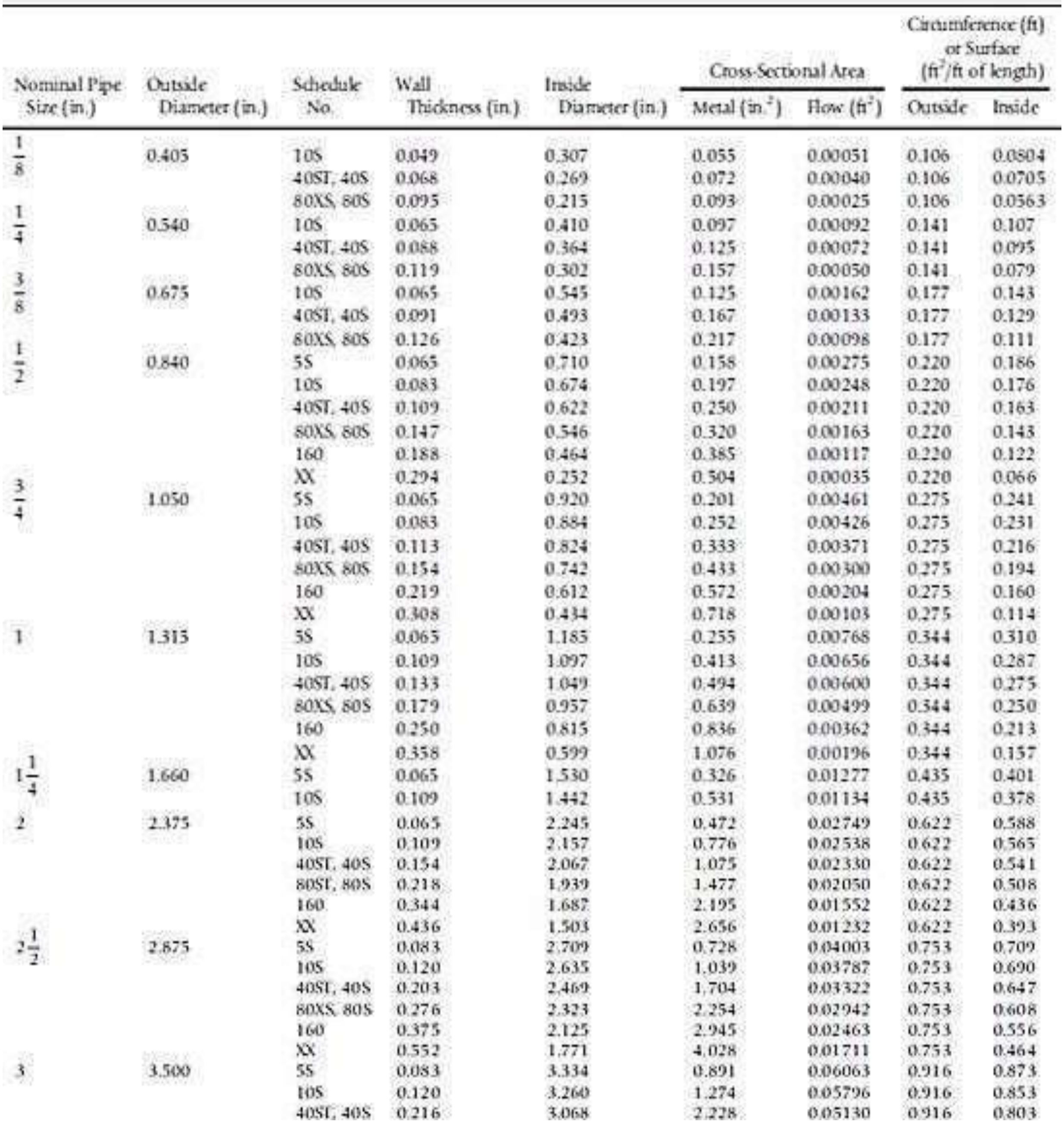
Cooling water streams[a]	
● Seawater	0.0005–0.001
● Brackish water	0.001–0.002
● Treated cooling tower water	0.001–0.002
● Municipal water supply	0.001–0.002
● River water	0.001–0.003
● Engine jacket water	0.001
● Distilled or demineralized water	0.0005
● Treated boiler feedwater	0.0005–0.001
● Boiler blowdown	0.002
Service gas streams	
● Ambient air (in air-cooled units)	0–0.0005
● Compressed air	0.001–0.002
● Steam (clean)	0–0.0005
● Steam (with oil traces)	0.001–0.002
● Refrigerants (with oil traces)	0.002
● Ammonia	0.001
● Carbon dioxide	0.002
● Flue gases	0.005–0.01
Service liquid streams	
● Fuel oil	0.002–0.005
● Lubrication oil	0.001
● Transformer oil	0.001
● Hydraulic fluid	0.001
● Organic heat-transfer fluids	0.001–0.002
● Refrigerants	0.001
● Brine	0.003
Process gas streams	
● Hydrogen	0.001
● Organic solvent vapors	0.001
● Acid gases	0.002–0.003
● Stable distillation overhead products	0.001
Process liquid streams	
● Amine solutions	0.002
● Glycol solutions	0.002
● Caustic solutions	0.002
● Alcohol solutions	0.002
● Ammonia	0.001
● Vegetable oils	0.003
● Stable distillation side-draw and bottom products	0.001–0.002
Natural gas processing streams	
● Natural gas	0.001
● Overhead vapor products	0.001–0.002
● C_3 or C_4 vapor (condensing)	0.001
● Lean oil	0.002
● Rich oil	0.001
● LNG and LPG	0.001

Table A-25: Double Pipe Exchanger Fittings



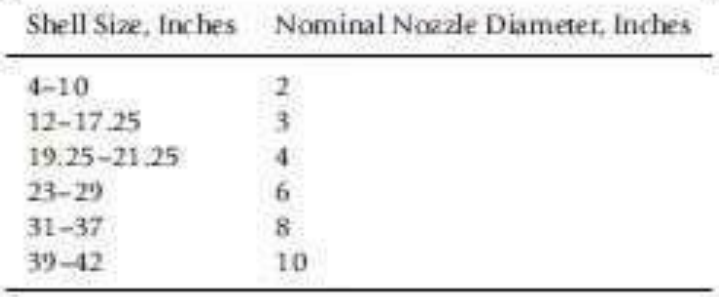
Outer pipe, IPS	*Inner pipe, IPS*
2	1¼
2½	1¼
3	2
4	3

Table A-22: Properties of Steel Pipe



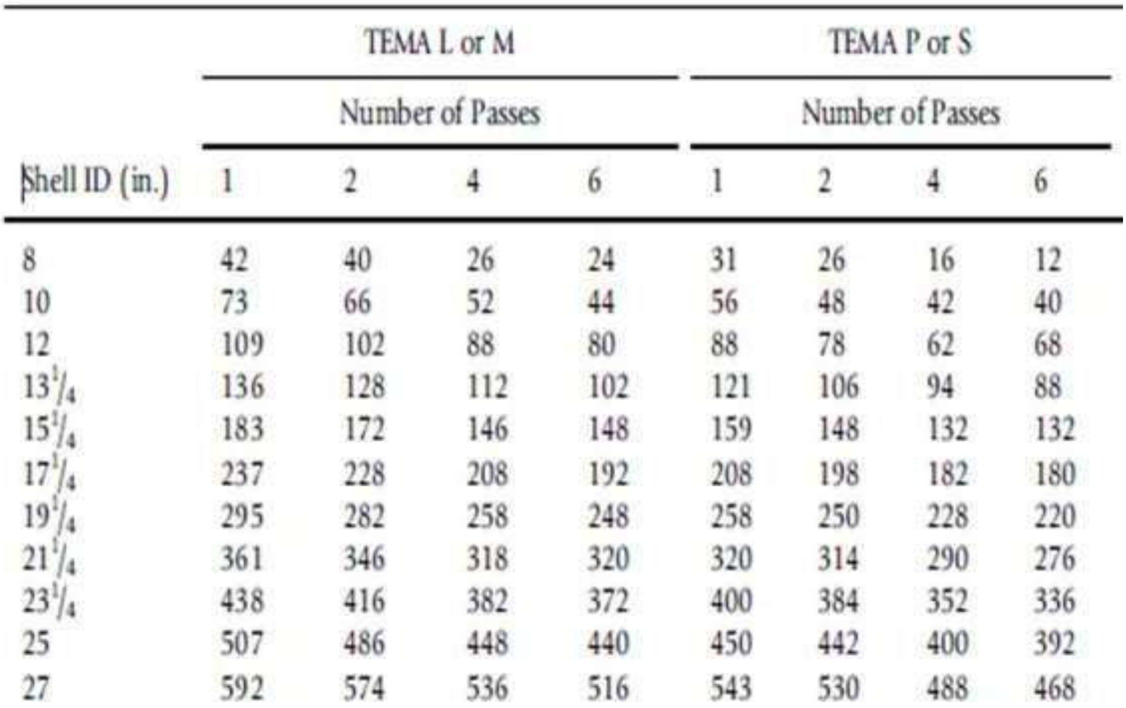
Nominal Pipe Size (in.)	Outside Diameter (in.)	Schedule No.	Wall Thickness (in.)	Inside Diameter (in.)	Cross-Sectional Area		Circumference (ft) or Surface (ft²/ft of length)	
					Metal (in.²)	Flow (ft²)	Outside	Inside
$\frac{1}{8}$	0.405	10S	0.049	0.307	0.055	0.00051	0.106	0.0804
		40ST, 40S	0.068	0.269	0.072	0.00040	0.106	0.0705
		80XS, 80S	0.095	0.215	0.093	0.00025	0.106	0.0563
$\frac{1}{4}$	0.540	10S	0.065	0.410	0.097	0.00092	0.141	0.107
		40ST, 40S	0.088	0.364	0.125	0.00072	0.141	0.095
		80XS, 80S	0.119	0.302	0.157	0.00050	0.141	0.079
$\frac{3}{8}$	0.675	10S	0.065	0.545	0.125	0.00162	0.177	0.143
		40ST, 40S	0.091	0.493	0.167	0.00133	0.177	0.129
		80XS, 80S	0.126	0.423	0.217	0.00098	0.177	0.111
$\frac{1}{2}$	0.840	5S	0.065	0.710	0.158	0.00275	0.220	0.186
		10S	0.083	0.674	0.197	0.00248	0.220	0.176
		40ST, 40S	0.109	0.622	0.250	0.00211	0.220	0.163
		80XS, 80S	0.147	0.546	0.320	0.00163	0.220	0.143
		160	0.188	0.464	0.385	0.00117	0.220	0.122
		XX	0.294	0.252	0.504	0.00035	0.220	0.066
$\frac{3}{4}$	1.050	5S	0.065	0.920	0.201	0.00461	0.275	0.241
		10S	0.083	0.884	0.252	0.00426	0.275	0.231
		40ST, 40S	0.113	0.824	0.333	0.00371	0.275	0.216
		80XS, 80S	0.154	0.742	0.433	0.00300	0.275	0.194
		160	0.219	0.612	0.572	0.00204	0.275	0.160
		XX	0.308	0.434	0.718	0.00103	0.275	0.114
1	1.315	5S	0.065	1.185	0.255	0.00768	0.344	0.310
		10S	0.109	1.097	0.413	0.00656	0.344	0.287
		40ST, 40S	0.133	1.049	0.494	0.00600	0.344	0.275
		80XS, 80S	0.179	0.957	0.639	0.00499	0.344	0.250
		160	0.250	0.815	0.836	0.00362	0.344	0.213
		XX	0.358	0.599	1.076	0.00196	0.344	0.157
$1\frac{1}{4}$	1.660	5S	0.065	1.530	0.326	0.01277	0.435	0.401
		10S	0.109	1.442	0.531	0.01134	0.435	0.378
2	2.375	5S	0.065	2.245	0.472	0.02749	0.622	0.588
		10S	0.109	2.157	0.776	0.02538	0.622	0.565
		40ST, 40S	0.154	2.067	1.075	0.02330	0.622	0.541
		80ST, 80S	0.218	1.939	1.477	0.02050	0.622	0.508
		160	0.344	1.687	2.195	0.01552	0.622	0.436
		XX	0.436	1.503	2.656	0.01232	0.622	0.393
$2\frac{1}{2}$	2.875	5S	0.083	2.709	0.728	0.04003	0.753	0.709
		10S	0.120	2.635	1.039	0.03787	0.753	0.690
		40ST, 40S	0.203	2.469	1.704	0.03322	0.753	0.647
		80XS, 80S	0.276	2.323	2.254	0.02942	0.753	0.608
		160	0.375	2.125	2.945	0.02463	0.753	0.556
		XX	0.552	1.771	4.028	0.01711	0.753	0.464
3	3.500	5S	0.083	3.334	0.891	0.06063	0.916	0.873
		10S	0.120	3.260	1.274	0.05796	0.916	0.853
		40ST, 40S	0.216	3.068	2.228	0.05130	0.916	0.803

Table A-30: Guidelines for Sizing Nozzles



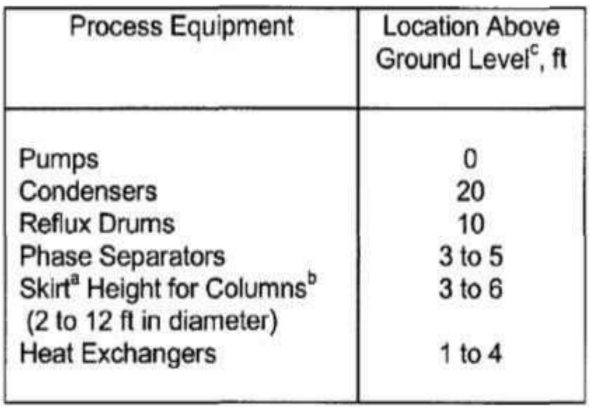
Shell Size, Inches	Nominal Nozzle Diameter, Inches
4–10	2
12–17.25	3
19.25–21.25	4
23–29	6
31–37	8
39–42	10

Table A-28: Tube Counts for 3/4-In. Od Tubes On 1-In. Triangular Pitch



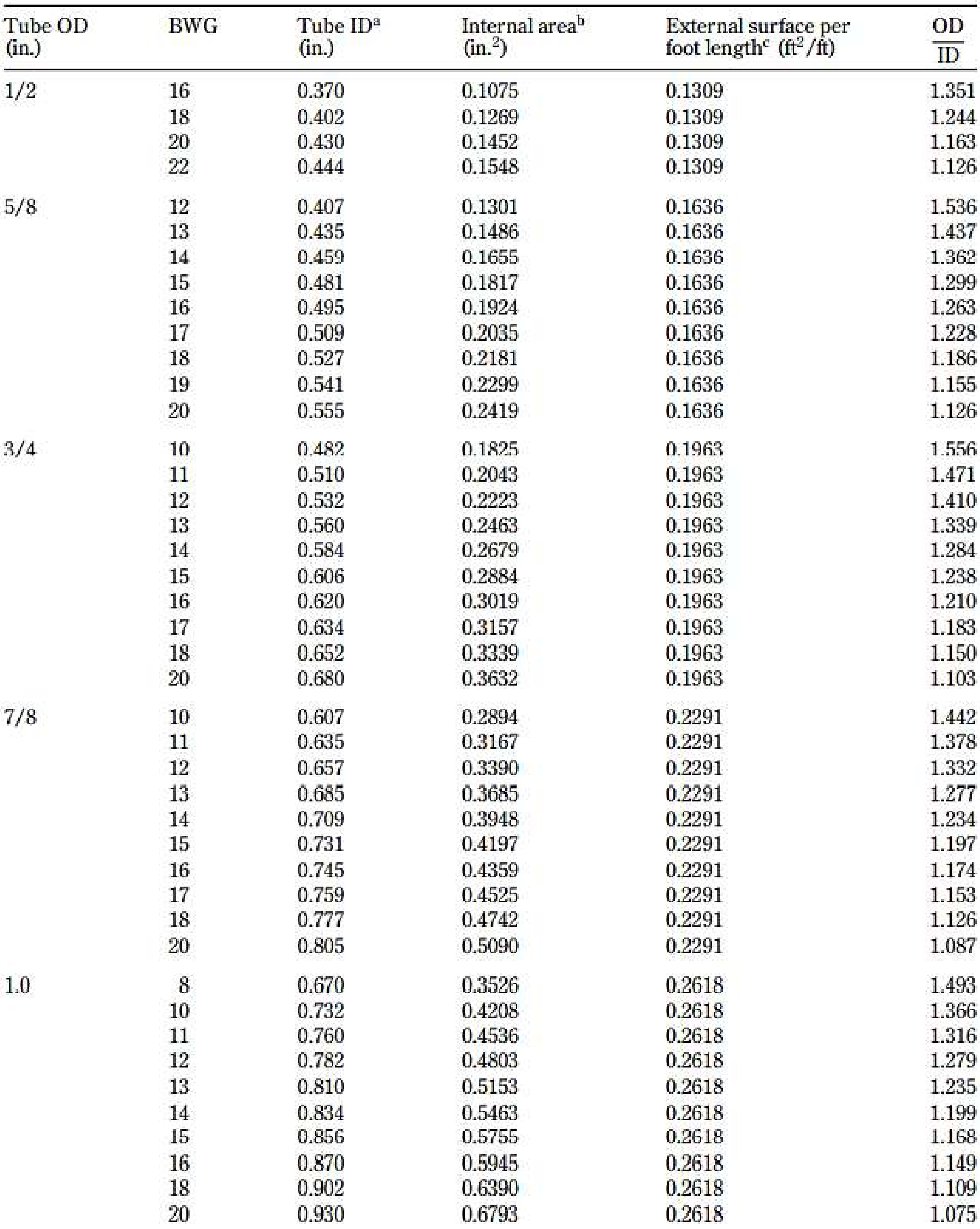
	TEMA L or M				TEMA P or S			
	Number of Passes				Number of Passes			
Shell ID (in.)	1	2	4	6	1	2	4	6
8	42	40	26	24	31	26	16	12
10	73	66	52	44	56	48	42	40
12	109	102	88	80	88	78	62	68
$13\frac{1}{4}$	136	128	112	102	121	106	94	88
$15\frac{1}{4}$	183	172	146	148	159	148	132	132
$17\frac{1}{4}$	237	228	208	192	208	198	182	180
$19\frac{1}{4}$	295	282	258	248	258	250	228	220
$21\frac{1}{4}$	361	346	318	320	320	314	290	276
$23\frac{1}{4}$	438	416	382	372	400	384	352	336
25	507	486	448	440	450	442	400	392
27	592	574	536	516	543	530	488	468

Table A-33: Selection of Pump Head



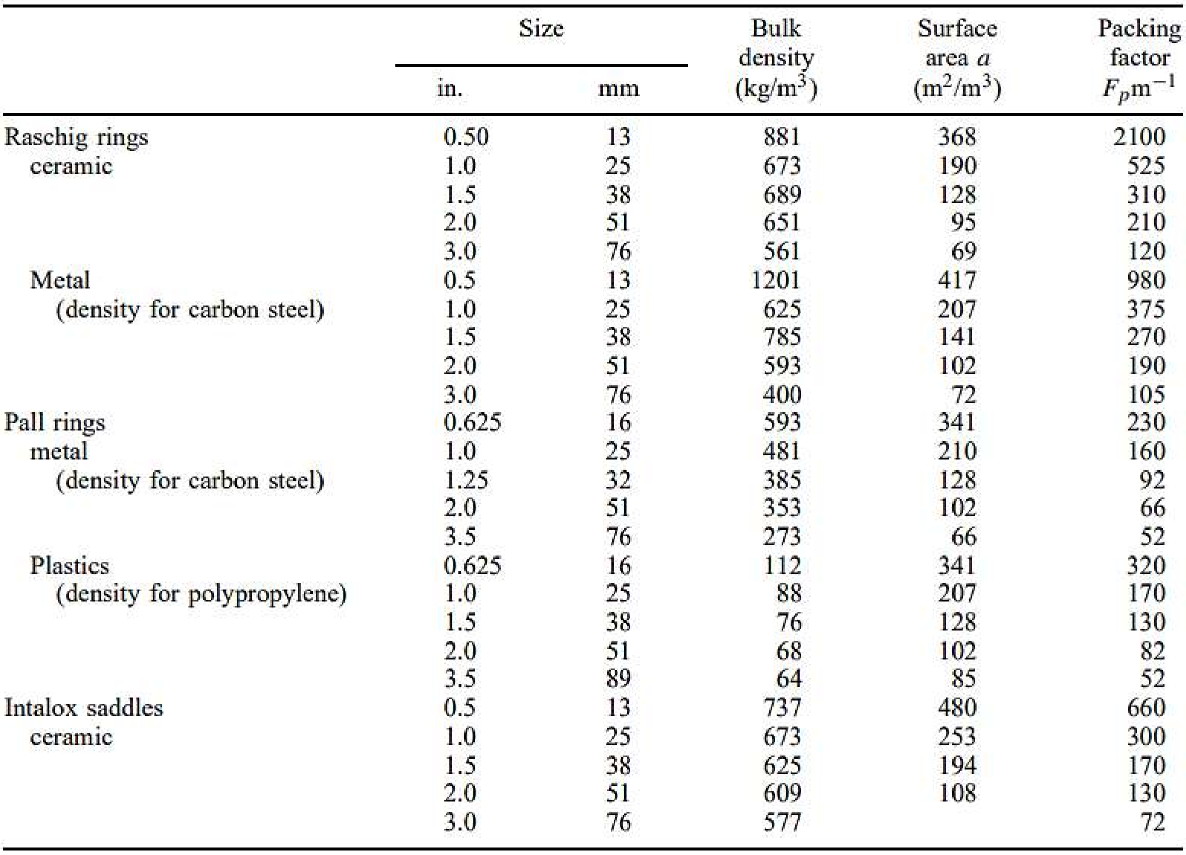
Process Equipment	Location Above Ground Level[c], ft
Pumps	0
Condensers	20
Reflux Drums	10
Phase Separators	3 to 5
Skirt[a] Height for Columns[b] (2 to 12 ft in diameter)	3 to 6
Heat Exchangers	1 to 4

Table A-36: Dimensions of Heat Exchanger, Tubing Dimensions**.**



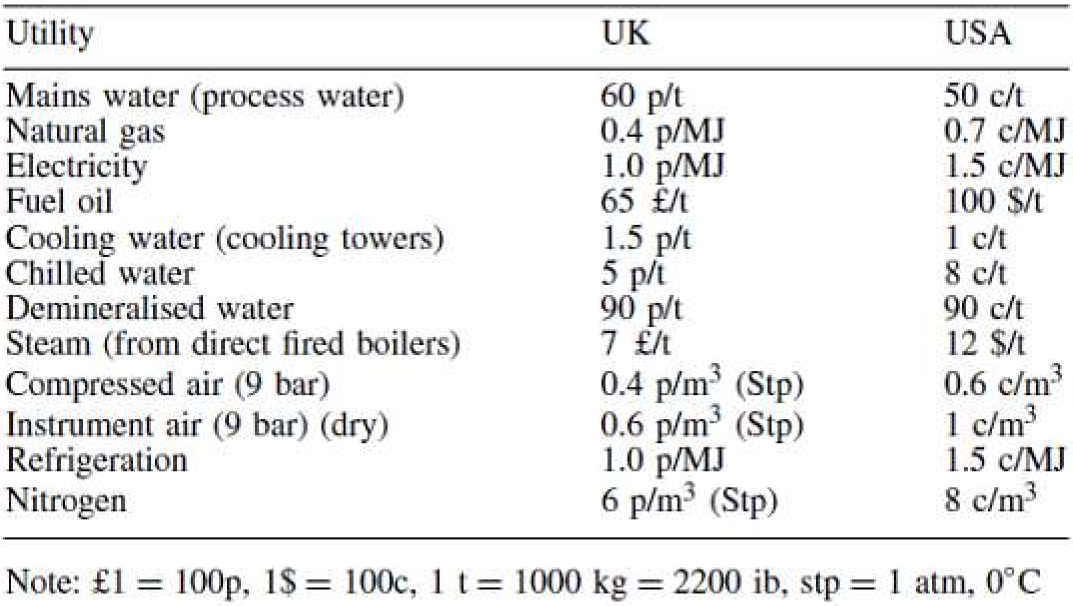
Tube OD (in.)	BWG	Tube ID[a] (in.)	Internal area[b] (in.^{2})	External surface per foot length[c] (ft^2/ft)	$\frac{OD}{ID}$
1/2	16	0.370	0.1075	0.1309	1.351
	18	0.402	0.1269	0.1309	1.244
	20	0.430	0.1452	0.1309	1.163
	22	0.444	0.1548	0.1309	1.126
5/8	12	0.407	0.1301	0.1636	1.536
	13	0.435	0.1486	0.1636	1.437
	14	0.459	0.1655	0.1636	1.362
	15	0.481	0.1817	0.1636	1.299
	16	0.495	0.1924	0.1636	1.263
	17	0.509	0.2035	0.1636	1.228
	18	0.527	0.2181	0.1636	1.186
	19	0.541	0.2299	0.1636	1.155
	20	0.555	0.2419	0.1636	1.126
3/4	10	0.482	0.1825	0.1963	1.556
	11	0.510	0.2043	0.1963	1.471
	12	0.532	0.2223	0.1963	1.410
	13	0.560	0.2463	0.1963	1.339
	14	0.584	0.2679	0.1963	1.284
	15	0.606	0.2884	0.1963	1.238
	16	0.620	0.3019	0.1963	1.210
	17	0.634	0.3157	0.1963	1.183
	18	0.652	0.3339	0.1963	1.150
	20	0.680	0.3632	0.1963	1.103
7/8	10	0.607	0.2894	0.2291	1.442
	11	0.635	0.3167	0.2291	1.378
	12	0.657	0.3390	0.2291	1.332
	13	0.685	0.3685	0.2291	1.277
	14	0.709	0.3948	0.2291	1.234
	15	0.731	0.4197	0.2291	1.197
	16	0.745	0.4359	0.2291	1.174
	17	0.759	0.4525	0.2291	1.153
	18	0.777	0.4742	0.2291	1.126
	20	0.805	0.5090	0.2291	1.087
1.0	8	0.670	0.3526	0.2618	1.493
	10	0.732	0.4208	0.2618	1.366
	11	0.760	0.4536	0.2618	1.316
	12	0.782	0.4803	0.2618	1.279
	13	0.810	0.5153	0.2618	1.235
	14	0.834	0.5463	0.2618	1.199
	15	0.856	0.5755	0.2618	1.168
	16	0.870	0.5945	0.2618	1.149
	18	0.902	0.6390	0.2618	1.109
	20	0.930	0.6793	0.2618	1.075

Table A-37: Design data for various packing



	Size		Bulk density (kg/m^3)	Surface area a (m^2/m^3)	Packing factor F_pm^{-1}
	in.	mm			
Raschig rings ceramic	0.50	13	881	368	2100
	1.0	25	673	190	525
	1.5	38	689	128	310
	2.0	51	651	95	210
	3.0	76	561	69	120
Metal (density for carbon steel)	0.5	13	1201	417	980
	1.0	25	625	207	375
	1.5	38	785	141	270
	2.0	51	593	102	190
	3.0	76	400	72	105
Pall rings metal (density for carbon steel)	0.625	16	593	341	230
	1.0	25	481	210	160
	1.25	32	385	128	92
	2.0	51	353	102	66
	3.5	76	273	66	52
Plastics (density for polypropylene)	0.625	16	112	341	320
	1.0	25	88	207	170
	1.5	38	76	128	130
	2.0	51	68	102	82
	3.5	89	64	85	52
Intalox saddles ceramic	0.5	13	737	480	660
	1.0	25	673	253	300
	1.5	38	625	194	170
	2.0	51	609	108	130
	3.0	76	577		72

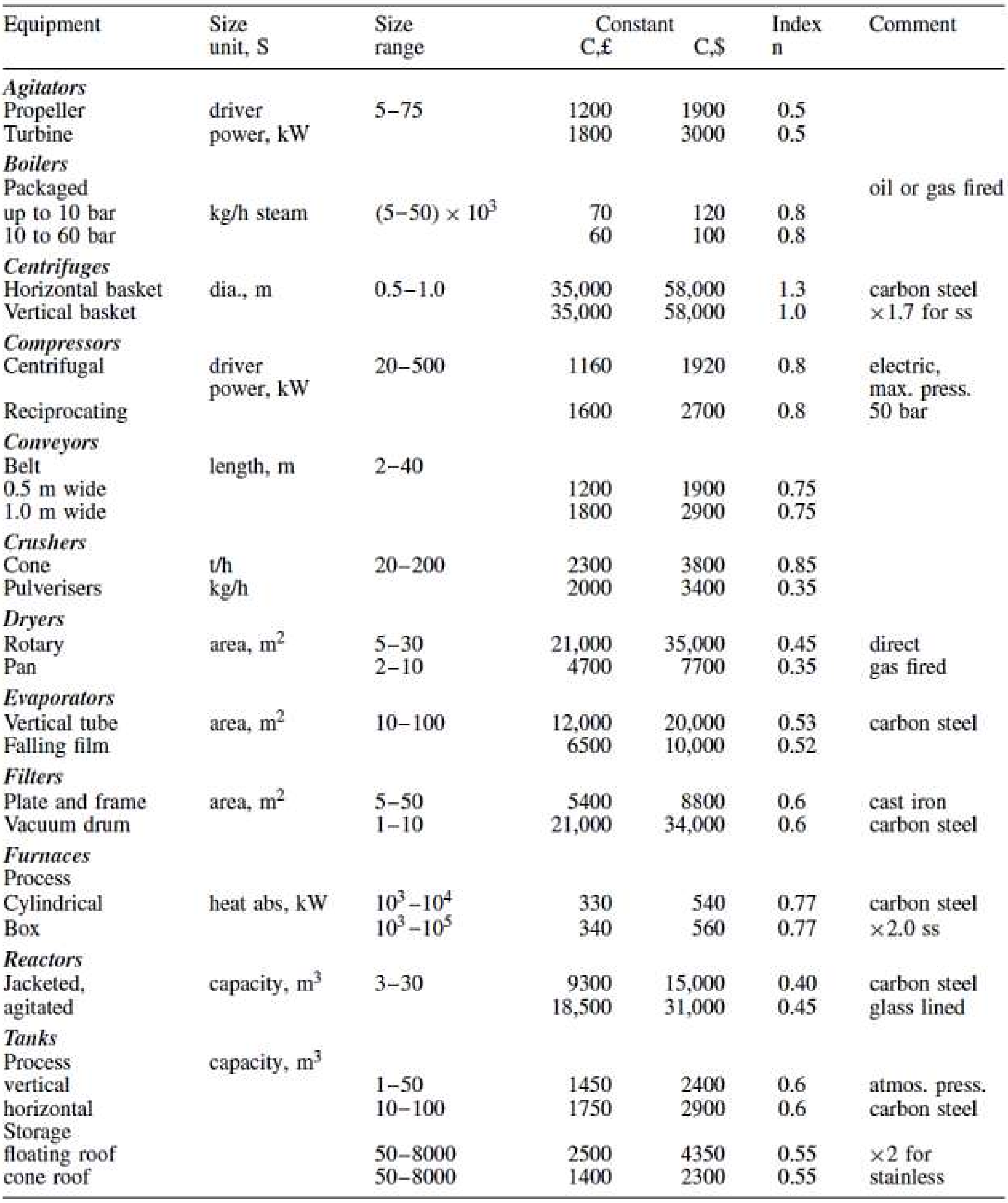
Table A-38: Cost of Utilities



Utility	UK	USA
Mains water (process water)	60 p/t	50 c/t
Natural gas	0.4 p/MJ	0.7 c/MJ
Electricity	1.0 p/MJ	1.5 c/MJ
Fuel oil	65 £/t	100 $/t
Cooling water (cooling towers)	1.5 p/t	1 c/t
Chilled water	5 p/t	8 c/t
Demineralised water	90 p/t	90 c/t
Steam (from direct fired boilers)	7 £/t	12 $/t
Compressed air (9 bar)	0.4 p/m^3 (Stp)	0.6 c/m^3
Instrument air (9 bar) (dry)	0.6 p/m^3 (Stp)	1 c/m^3
Refrigeration	1.0 p/MJ	1.5 c/MJ
Nitrogen	6 p/m^3 (Stp)	8 c/m^3

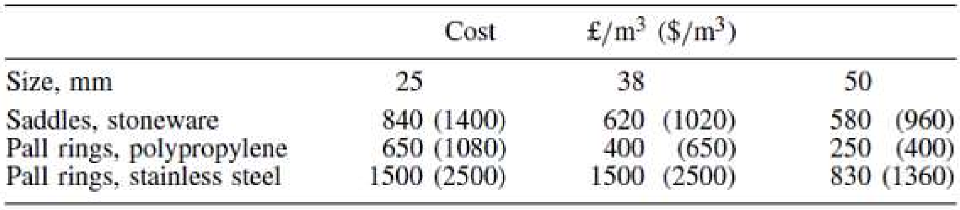
Note: £1 = 100p, 1$ = 100c, 1 t = 1000 kg = 2200 ib, stp = 1 atm, 0°C

Table A-39: Cost of Equipment, Basis mid 2004



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

Table A-40: Cost of Column Packing.



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

Appendix B

List of Figures:

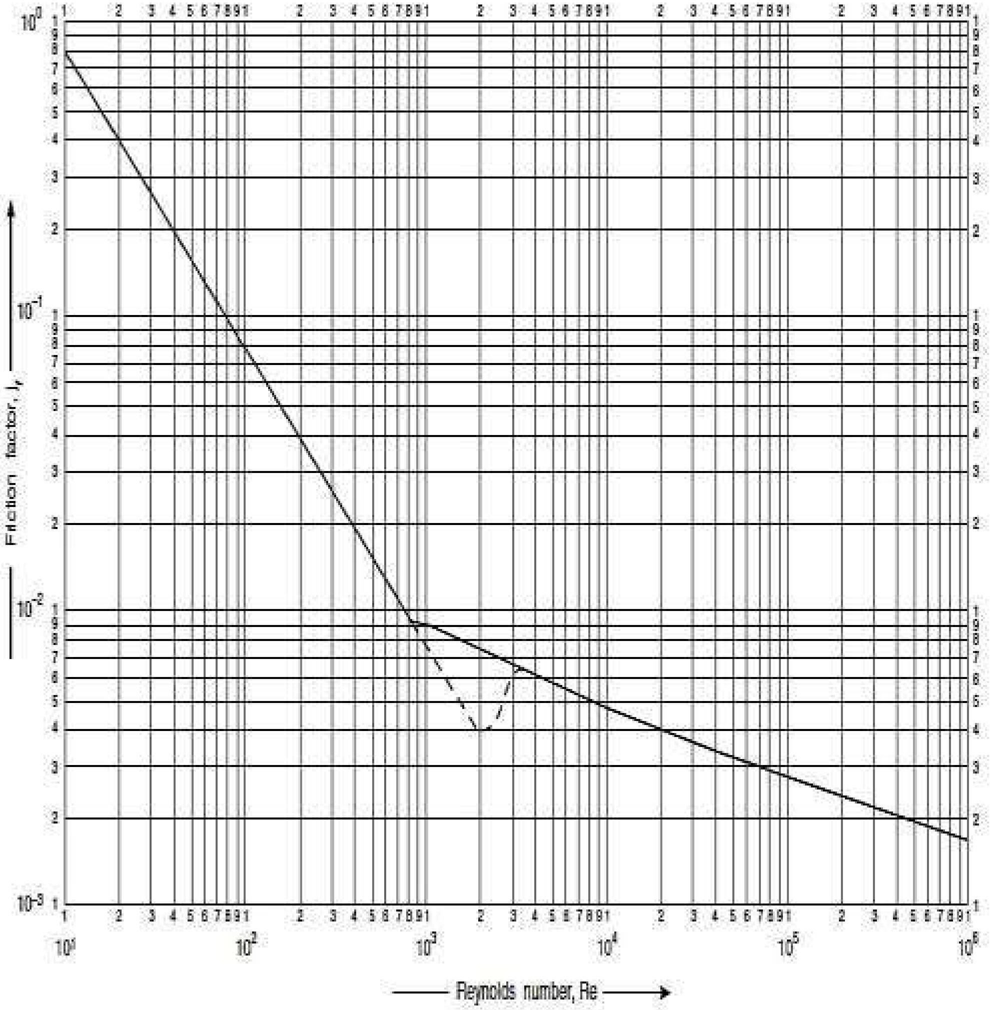


Figure B-1: Tube-Side Friction Factors

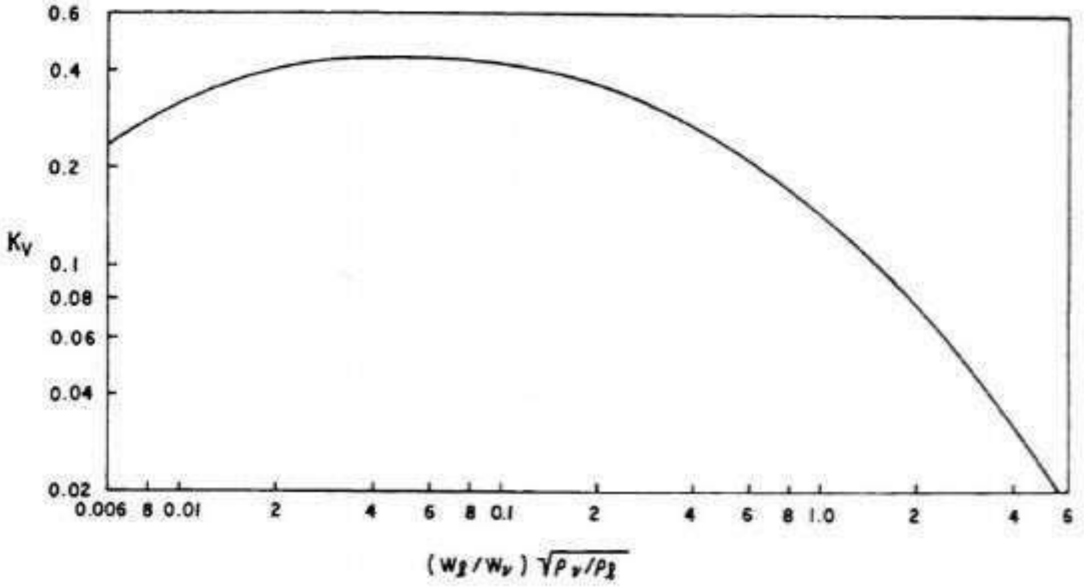


Figure B-2: Design Vapor Velocity Factor for Vertical-Liquid Separators At 85% Of Flooding

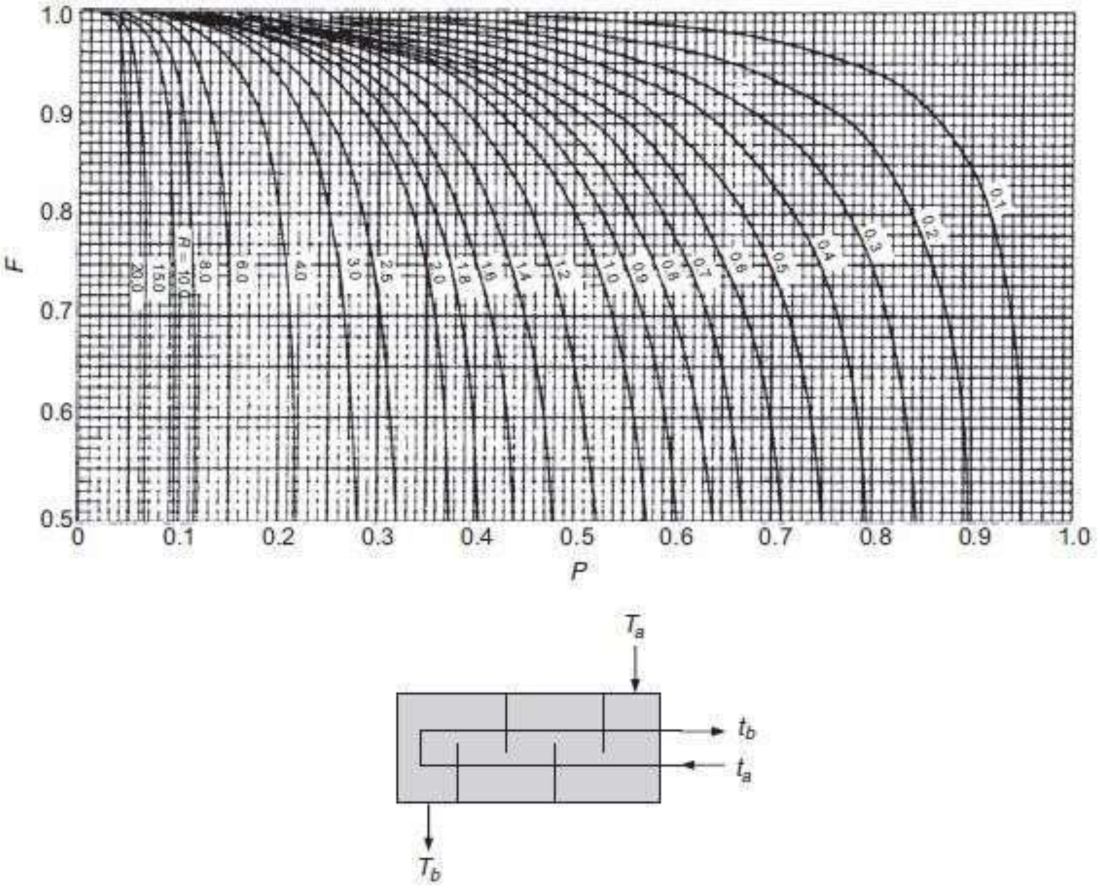
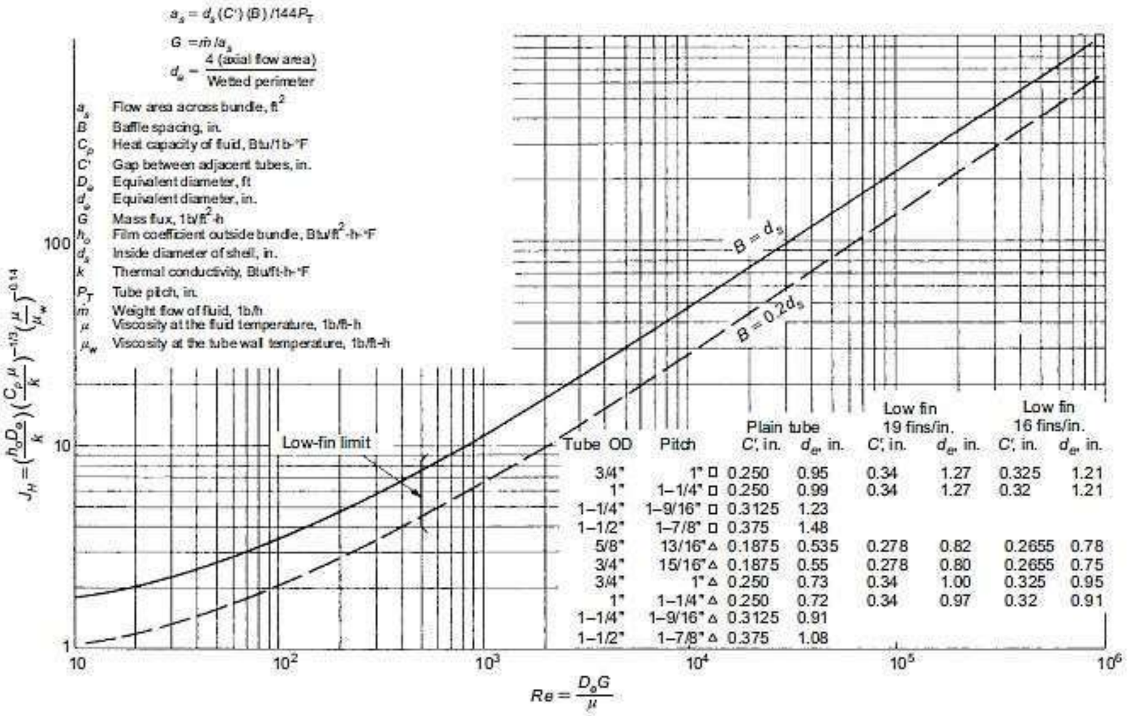


Figure B-3: LMTD Correction Factor for 1–2 Exchangers



$a_s = d_s(C')(B)/144P_T$

$G = \dot{m}/a_s$

$d_e = \frac{4\ (\text{axial flow area})}{\text{Wetted perimeter}}$

a_s	Flow area across bundle, ft^2
B	Baffle spacing, in.
C_p	Heat capacity of fluid, Btu/1b·°F
C'	Gap between adjacent tubes, in.
D_e	Equivalent diameter, ft
d_e	Equivalent diameter, in.
G	Mass flux, 1b/ft^2·h
h_o	Film coefficient outside bundle, Btu/ft^2·h·°F
d_s	Inside diameter of shell, in.
k	Thermal conductivity, Btu/ft·h·°F
P_T	Tube pitch, in.
$\dot{m}$	Weight flow of fluid, 1b/h
μ	Viscosity at the fluid temperature, 1b/ft·h
μ_w	Viscosity at the tube wall temperature, 1b/ft·h

		Plain tube		Low fin 19 fins/in.		Low fin 16 fins/in.	
Tube OD	Pitch	C', in.	d_e, in.	C', in.	d_e, in.	C', in.	d_e, in.
3/4"	1" □	0.250	0.95	0.34	1.27	0.325	1.21
1"	1–1/4" □	0.250	0.99	0.34	1.27	0.32	1.21
1–1/4"	1–9/16" □	0.3125	1.23				
1–1/2"	1–7/8" □	0.375	1.48				
5/8"	13/16" △	0.1875	0.535	0.278	0.82	0.2655	0.78
3/4"	15/16" △	0.1875	0.55	0.278	0.80	0.2655	0.75
3/4"	1" △	0.250	0.73	0.34	1.00	0.325	0.95
1"	1–1/4" △	0.250	0.72	0.34	0.97	0.32	0.91
1–1/4"	1–9/16" △	0.3125	0.91				
1–1/2"	1–7/8" △	0.375	1.08				

Figure B-4: Correlation for Shell-Side Heat-Transfer Coefficient

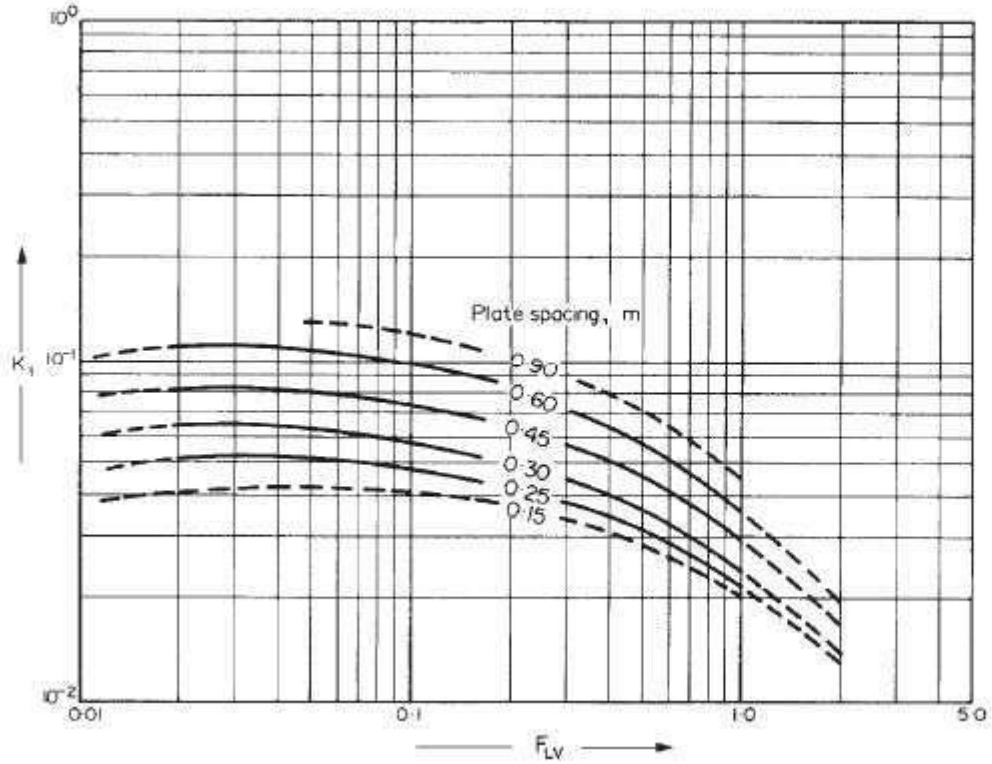


Figure B-5: Flooding Velocity, Sieve Plates

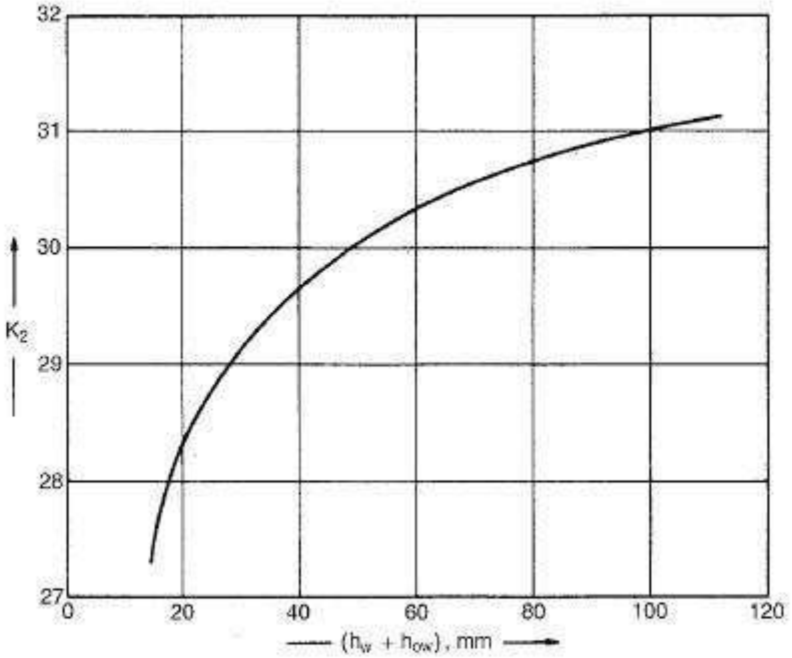


Figure B-6: Weep-Point Correlation

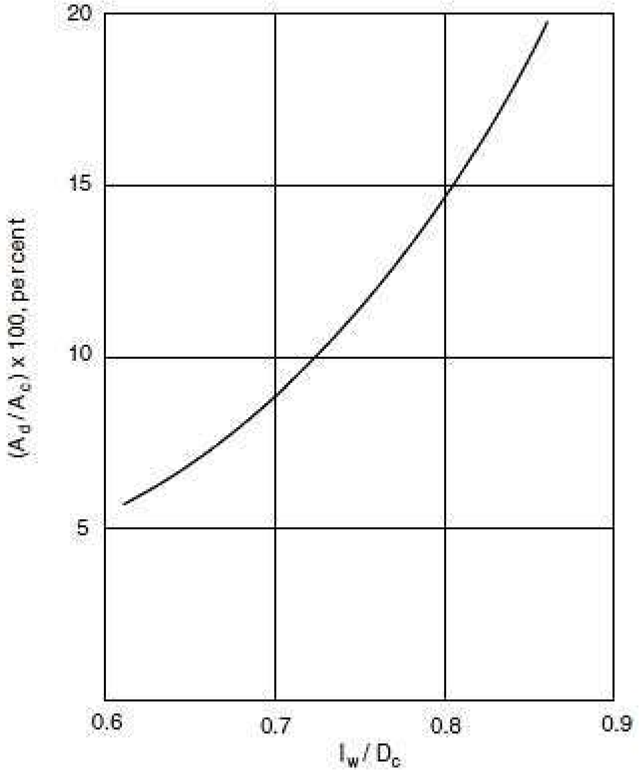


Figure B-7: Relation between down comer area and Weir Length

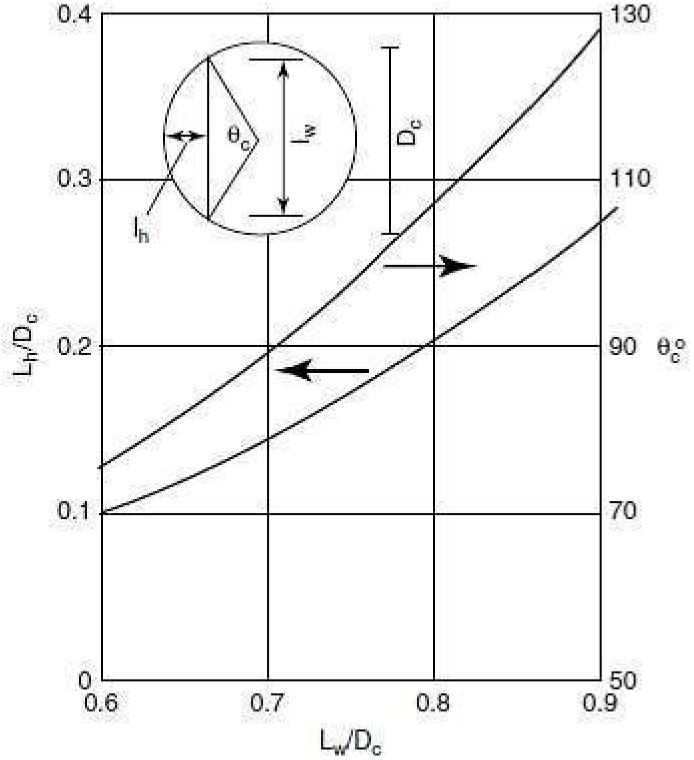


Figure B-8: Relation between angle Subtended By Chord, Chord Height and Chord Length

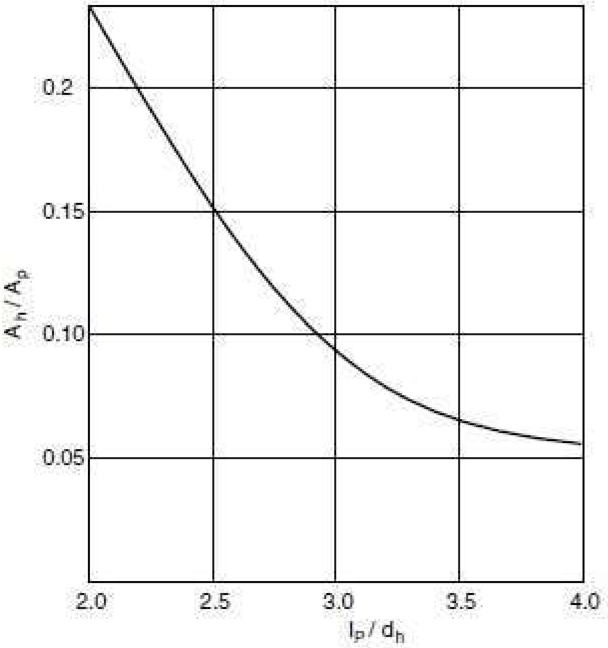


Figure B-9: Relation between Hole Area and Pitch

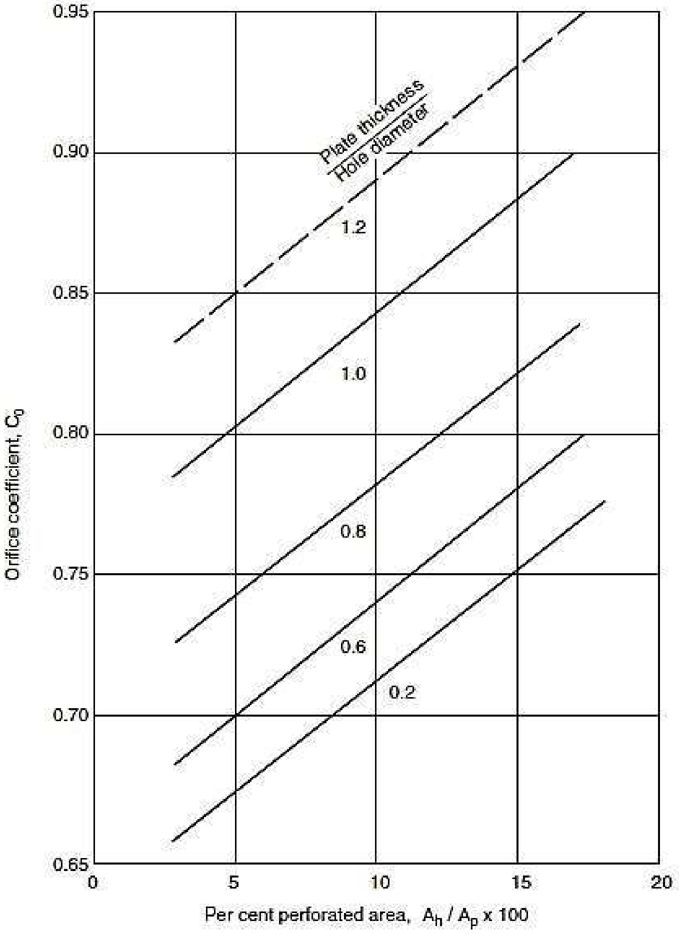


Figure B-10: Discharge Coefficient, Sieve Plates

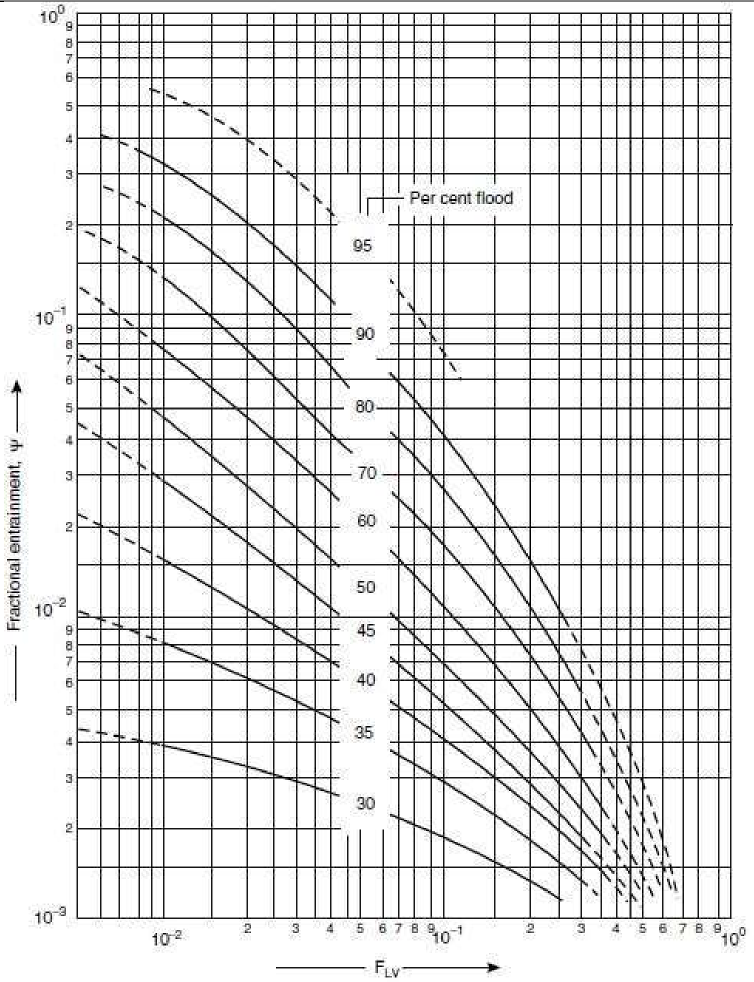


Figure B-11: Entrainment Correlation for Sieve Plates

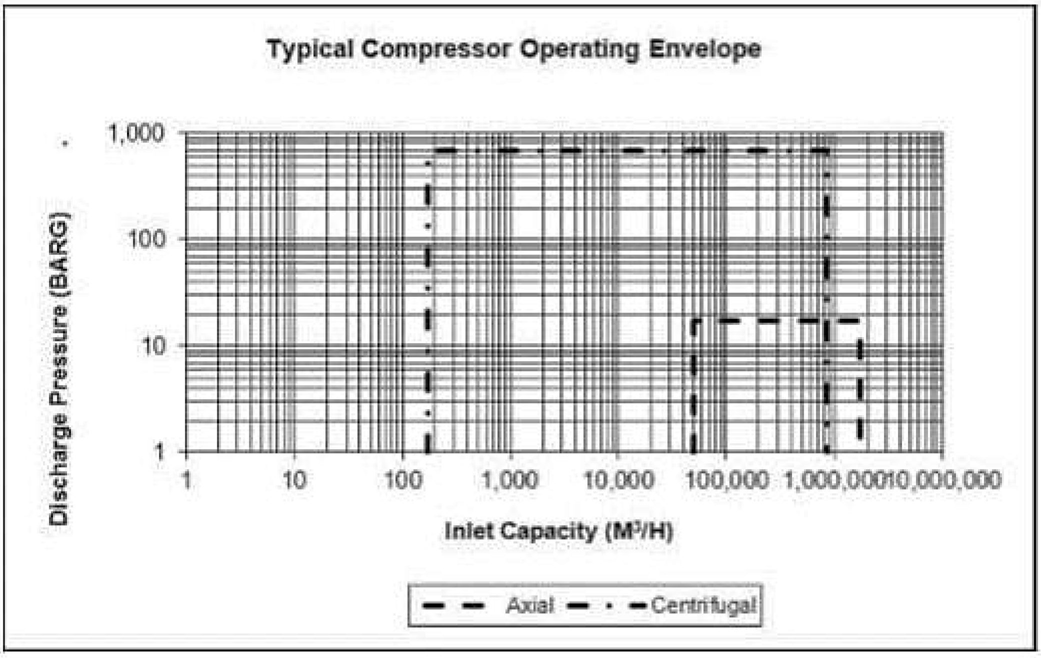


Figure B-12: Compressor Selection Chart

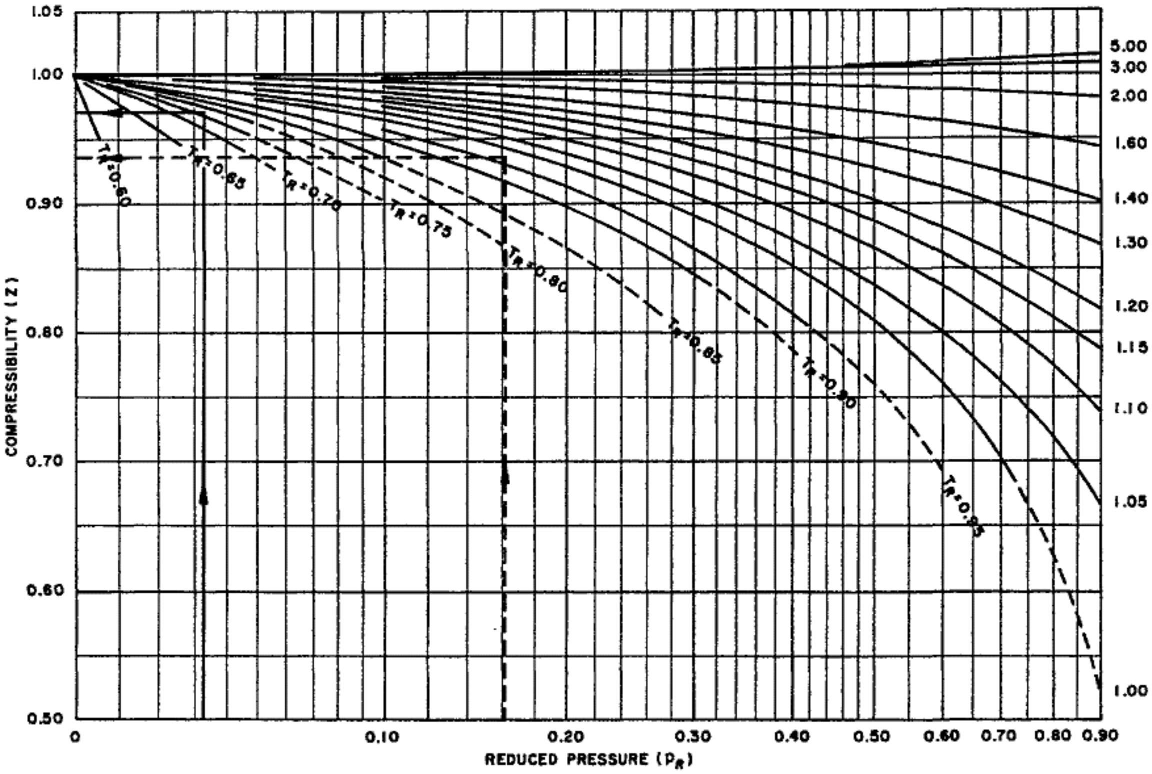


Figure B-13: Compressibility factor chart

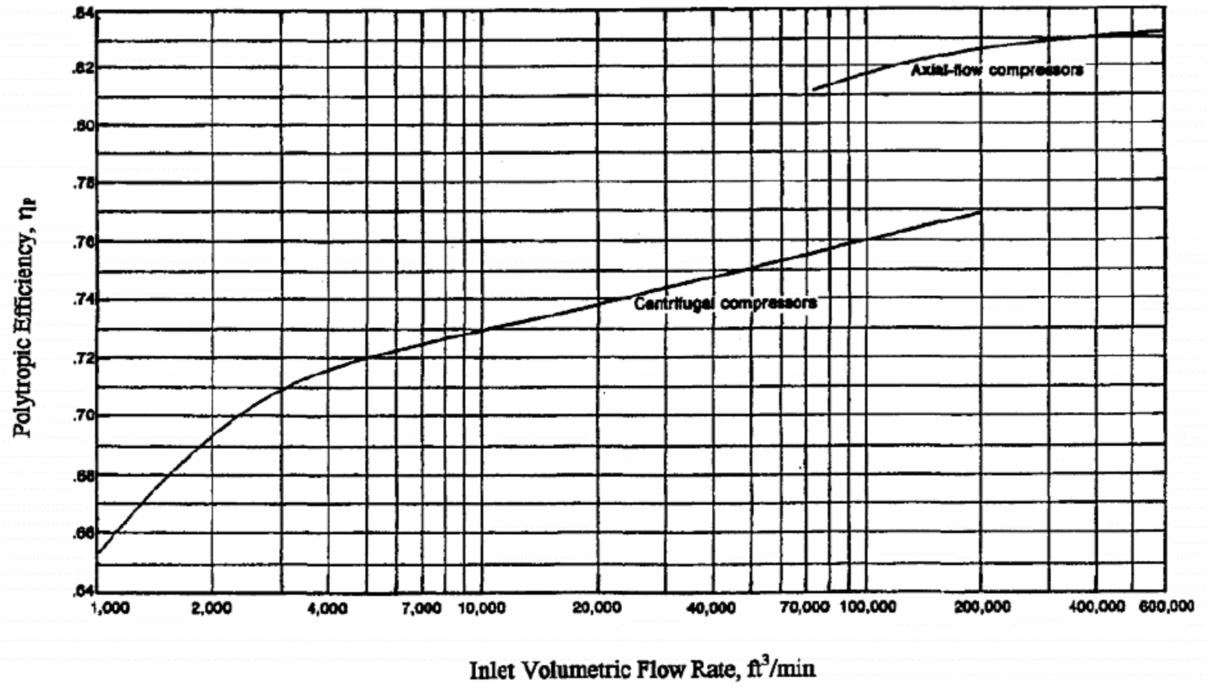


Figure B-14: Polytropic efficiency for Axial and Centrifugal Compressors.

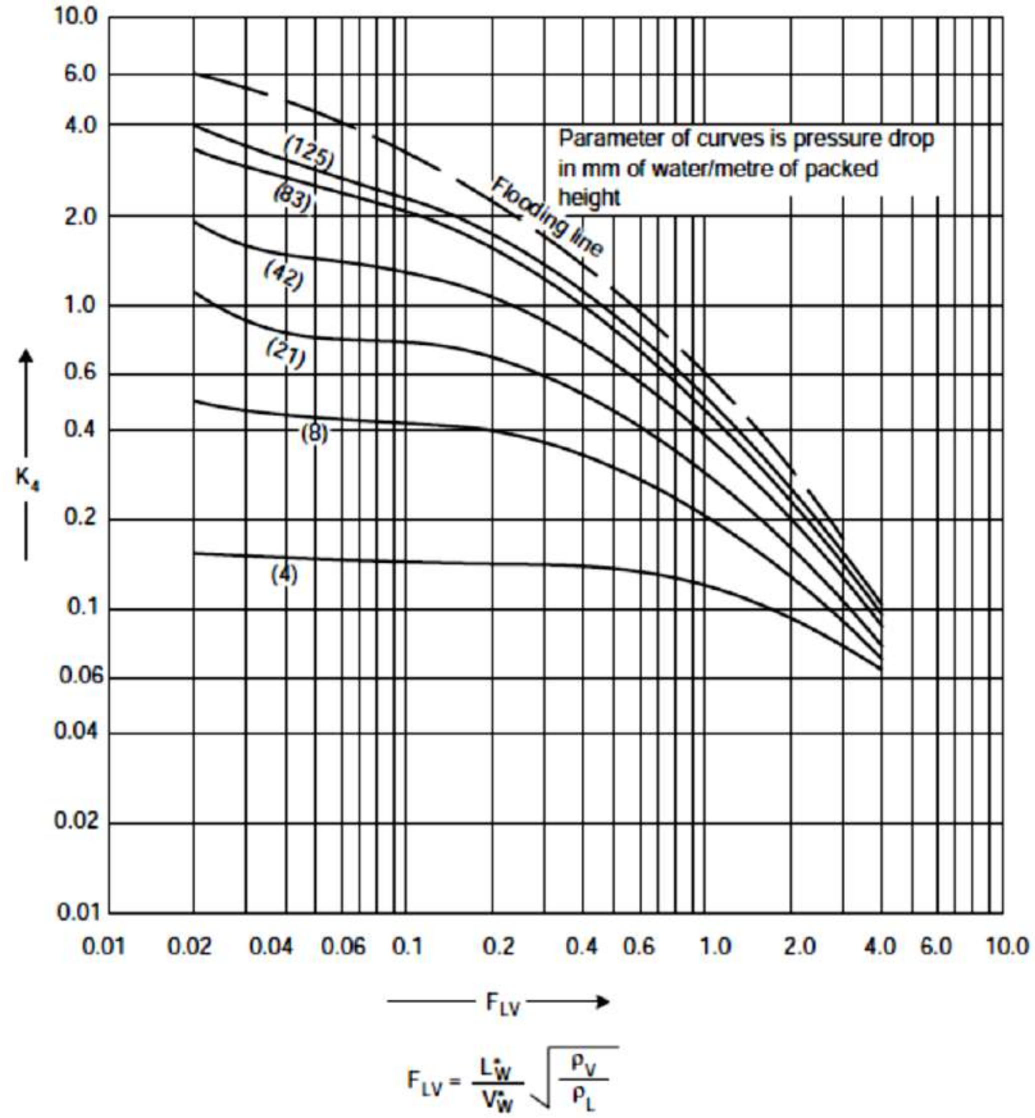


Figure B-15: Generalized pressure drop correlation.

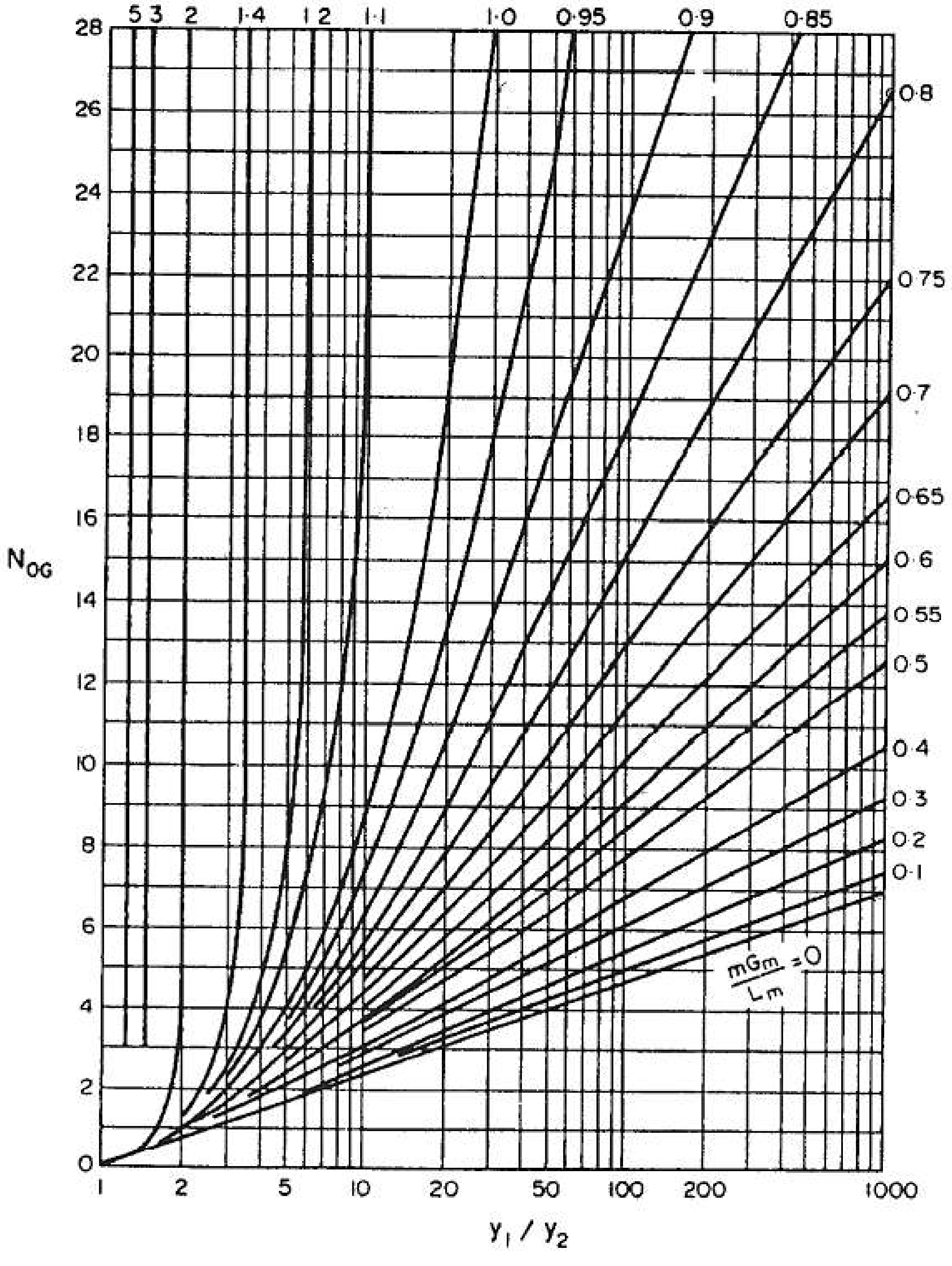


Figure B-16: Number of transfer units NOG as a function of y1/y2 with mGm/Lm as parameter

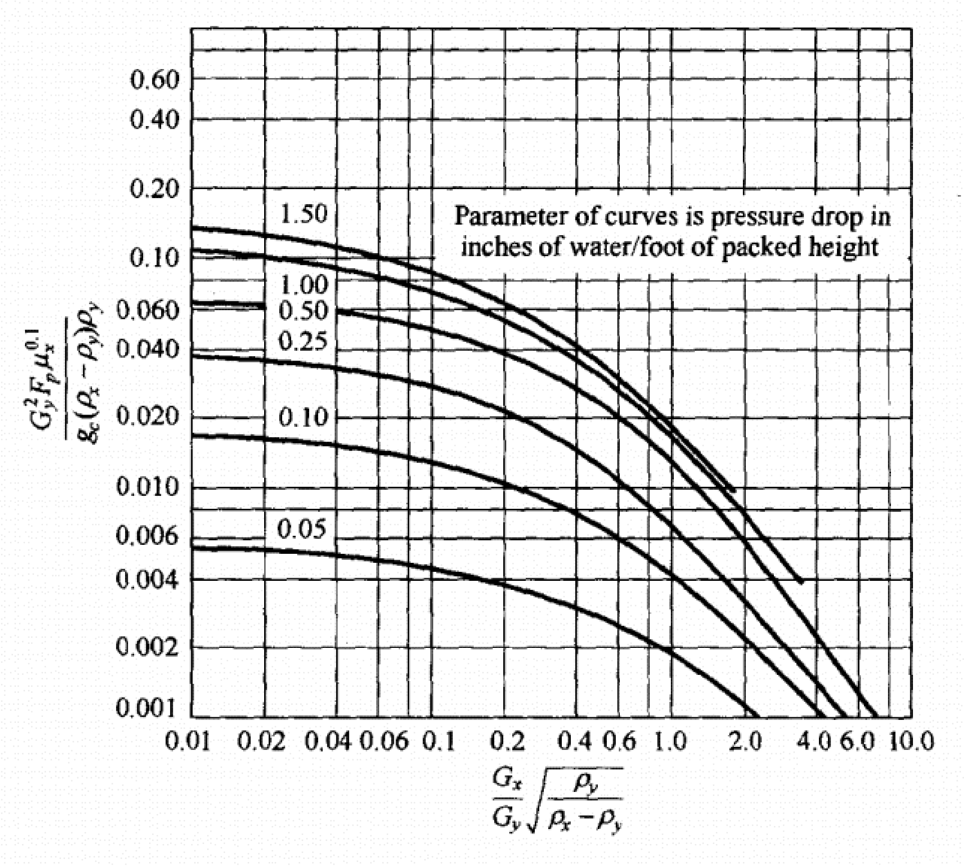
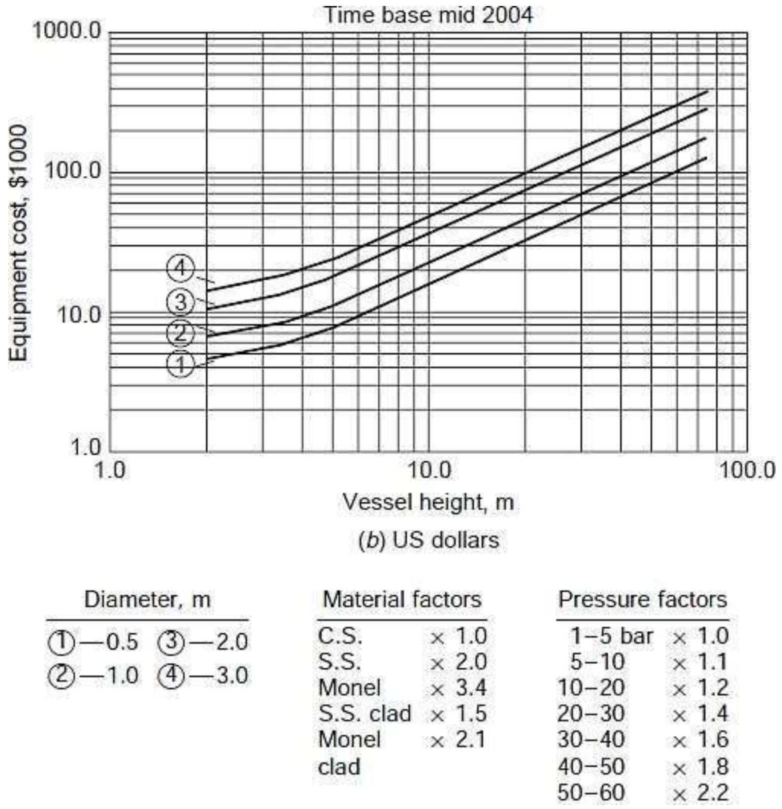


Figure B-17: Generalized correlation for pressure drop in packed columns. (1 in H2O/ft = 817 Pa/m)



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 B-18: Cost of Reactor

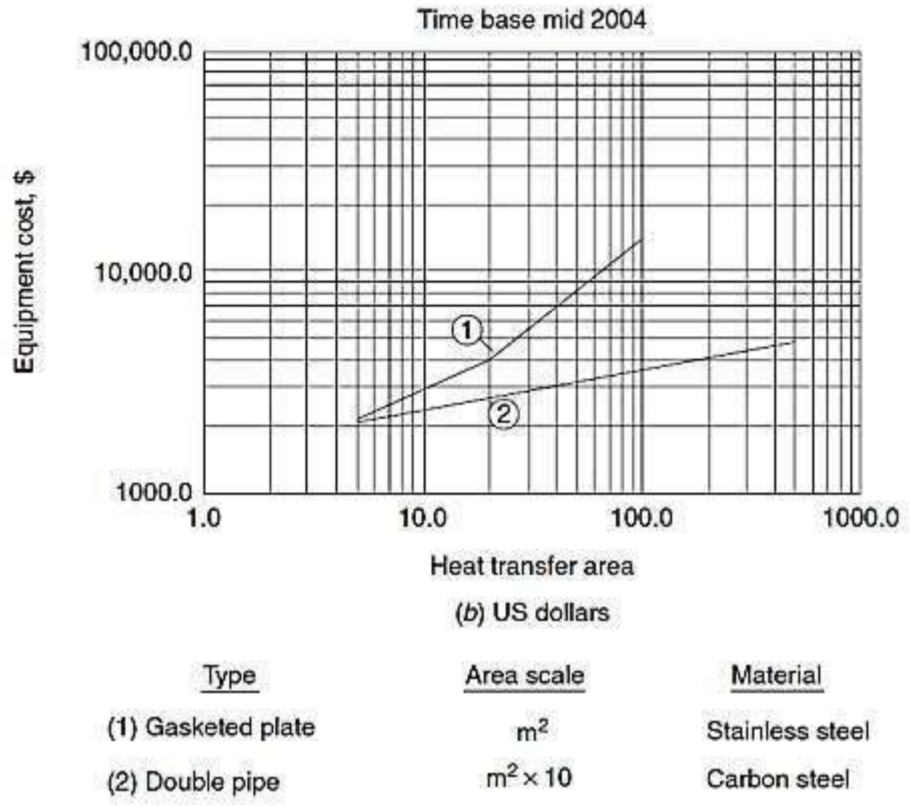


Figure B-19: Cost of Double Pipe Heat Exchanger

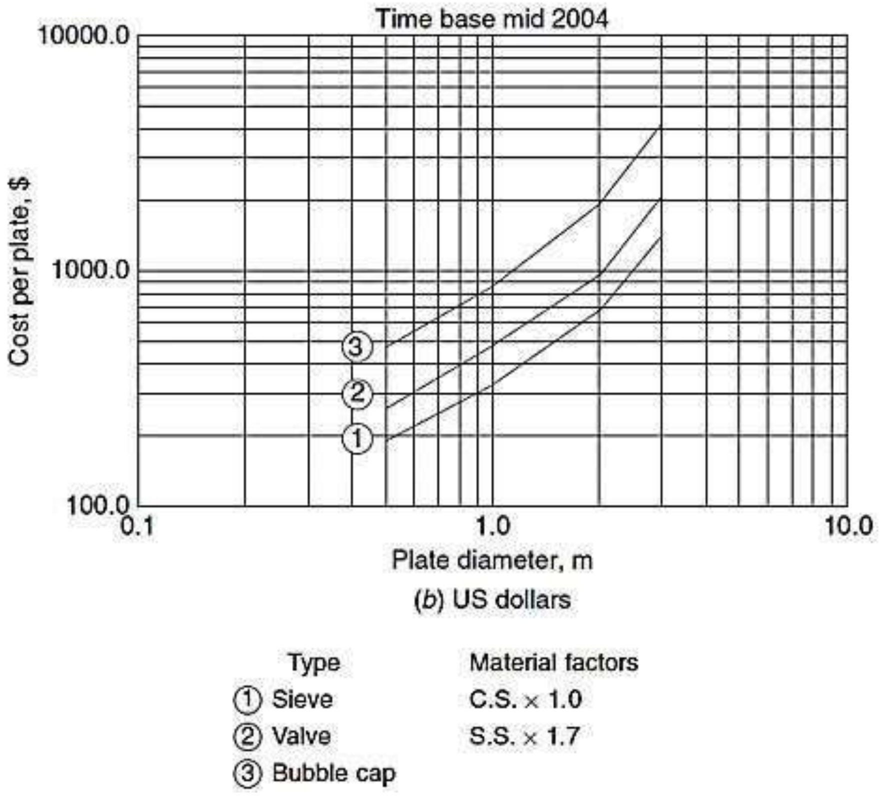
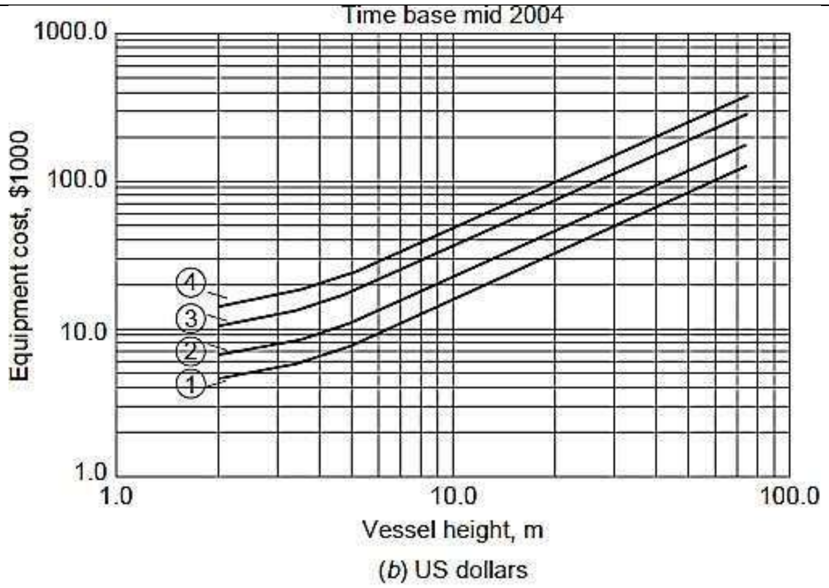


Figure B-20: Cost per Plate

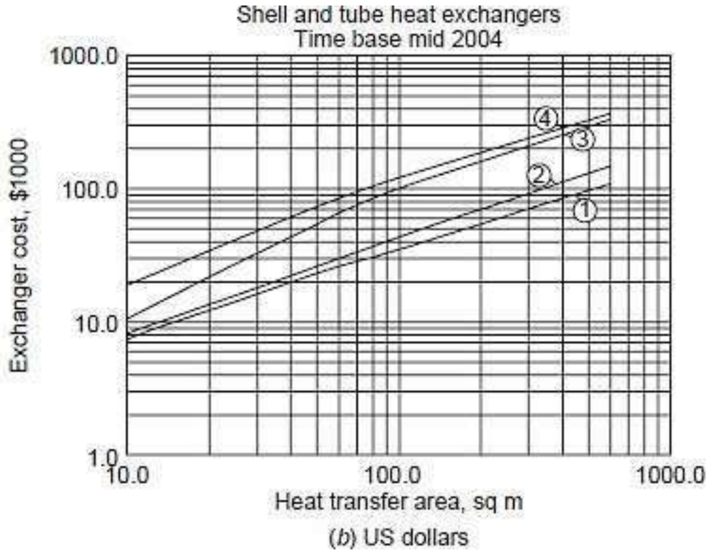


Diameter, m	
①—0.5	③—2.0
②—1.0	④—3.0

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 B-21: Cost of Tower



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 B-22: Cost of Shell and Tube Heat Exchange