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CHEMICAL ENGINEERING PROGRAM

SEMESTER II 2020/2021

PRODUCTION OF PROPYLENE GLYCOL

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TITLE : PRODUCTION OF PROPYLENE GLYCOL

SUBMISSION DATE : 8TH JULY 2021

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DECLARATION

We hereby declare the work in this project is our own except for quotations and summaries which have been duly acknowledged.

8 JULY 2021

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CORRECTION PART

Commented by	Correction	Page num
Prof. Madya Dr. Masli Irwan Rosli	1. Summarize properties for all chemical involved	17
	2. Report plant capacity in tonnes/year	8
	3. Compare plant capacity with other manufacturer	8
	4. PFD: Temperature unit	14
	5. Discuss why there is big error between SuperPro and manual calculation	40
	6. KKKR2422: Put codes to appendix	90
	7. Add error handling in the algorithm	8
Dr Manal Ismail	1. PFD: Add pumps add the distillation columns	14
	2. Edit waste management: explain about the purity and the price for the byproducts	21
	3. KKKR2463 : Add all the parameter for the heat and mass calculation and put the calculation in the report	44
	4. Edit mass balance for distillation column. Cannot have 100% purity	29
Prof. Dr. Jamaliah Jahim & Ts. Dr. Abdullah Amru Indera Luthfi	KKKR2473: Add a new subtopic for volume calculation part and subtopic 7.4 was edited	53

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EXECUTIVE SUMMARY

Propylene glycol also known as 1,2-propanediol is a small molecule with two hydroxyl groups (-OH). It is a colourless, odourless, and fully water-soluble liquid. Propylene glycol is a synthetic chemical made from the hydration of propylene oxide, a petroleum-derived product. Propylene glycol is used in a variety of drugs, including oral, topical, and intravenous. It's been used as a solvent and a drug stabiliser. Because of its water miscibility, it can be used to dissolve insoluble pharmaceutical formulations. The demand for this propylene glycol increases rapidly in the past few years due to the pandemic Covid-19. The plant capacity of our plant is 1060 kg/hr which contribute about 0.5% to the global demand. The main objective of this project is to produce our main product which is propylene glycol from the reaction of glycerol dehydration, which produces acetol and water, preceded by acetol hydrogenation to produce propylene glycol. Mass balance is performed for all the unit operation involve and energy balance is performed for our main reactor. The overall mass balance is 1729.25 kg/h for both inlet and outlet stream. The values of flowrates are compared with the values obtained using SuperPro. For energy balance at the reactor, we obtained +15651.073 kJ/hr. The positive sign of Q indicates that the reaction is an endothermic reaction. Heat is absorbed. The Reynold number is 55.5628 indicates the laminar flow. By using Stokes-Einstein formula, D_{AB} is 88.74×10^{-5} m^2/s therefore N_A is 6.645×10^{-4} kg mol / $s.m^2$. The designated reactor is made of stainless steel 316. The rate law for the reaction at the reactor has been derived. Mass balance for the reactor unit has been calculated using GNU Octave. An algorithm was created to programmed and to show the flowrate is balanced by inserting the required input.

TABLE OF CONTENT

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

BACKGROUND OF STUDY

1.1 INTRODUCTION

Propylene glycol also known as 1,2-propanediol is a small molecule with two hydroxyl groups (-OH). It is a colourless, odourless, and fully water-soluble liquid. Propylene glycol is a synthetic chemical made from the hydration of propylene oxide, a petroleum-derived product (Tonya M. B., 2018). Propylene glycol is a synthetic liquid material that absorbs water with a chemical formula of $C_3H_8O_2$ (Rebekah E.,2018). The molecular structure of propylene glycol is shown in Figure 1.1.

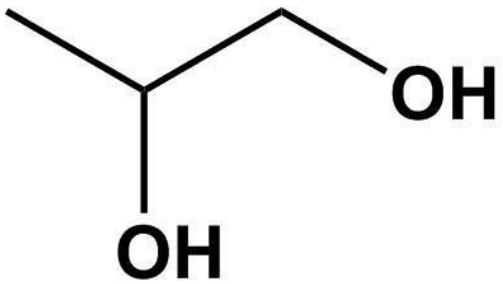

Figure 1.1 Molecular structure of propylene glycol

Source: (InKemia, 2021)

Propylene Glycol is commonly used as a raw material and as an auxiliary material in a variety of industries. Food preservative in the food industry, softener, and moisturizer in the cosmetics industry, one of the formulations in the pharmacy industry, and additives in the paint products industry are only a couple of the uses (Kirk and Othmer 1992).

In the production of propylene glycol, glycerol and hydrogen are used as the raw material. It involves two-step mechanism in which the first stage reaction is the glycerol dehydration followed by acetol hydrogenation that produces propylene glycol. The glycerol used is the refined glycerol which obtained from the pre-treatment of the crude glycerol. As for the secondary reaction, it is a direct reaction between glycerol and hydrogen which produces ethylene glycol and methanol. The chemical and physical properties of propylene glycol is shown in Table 1.1 below.

Table 1.1: Chemical and physical properties of propylene glycol

Property	Propylene Glycol
Physical state	liquid
Appearance	Clear & Colourless
Odor	Odorless
Boiling point	187°C/368.6°F
Melting point	-60°C/-76°F
Water solubility	Soluble
Specific gravity	1.036
Molecular weight	76.1 g/mole
Molecular formula	$C_3H_8O_2$

Source: (MSDS of Propylene glycol, Thermo Fisher Scientific, 2009)

1.2 USAGE OF PROPYLENE GLYCOL

Propylene glycol has only recently been used in a modern antifreeze formulation that replaces ethylene glycol-based formulations because it was less harmful. Pets have been known to eat any ethylene glycol-based antifreeze that has dripped or spilled in the driveway, which has also resulted in death. On the other hand, propylene glycol antifreeze is a non-toxic substitute. This is due to the fact that when it is ingested, it is broken down into two chemicals: acetic acid (also known as vinegar) and pyruvic acid (a natural byproduct of the glucose metabolism process). Propylene glycol, like ethylene glycol, is used in antifreeze because it decreases the freezing point of water by interfering with the formation of ice crystals (Bell-Young 2018). Propylene glycol is a major component of aircraft de-icers and is also used to break up ice on airport runways (Ajiboye 2020).

On the other hand, propylene glycol is also used in a variety of foods because it does not react on its own, allowing it to function without interacting with other ingredients (Bell-Young 2018). It is safe for consumption and the FDA approves its use

in food at certain concentrations. It may form up to 97% of the contents of seasonings and flavorings, 24% of confections and frosting, and 5% of alcoholic beverages and nuts/nut products (Ajiboye 2020). Propylene glycol may provide homogeneous distribution in a mixture by attracting and retaining water-based and oil-based substances. This implies, for example, that it will uniformly spread food colouring. Because of its hygroscopicity and miscibility, PG is an outstanding humectant, keeping foods like baked goods moist. This also aids in their preservation (Bell-Young 2018).

Furthermore, propylene glycol is used in a variety of drugs, including oral, topical, and intravenous. It's been used as a solvent and a drug stabiliser. Because of its water miscibility, it can be used to dissolve insoluble pharmaceutical formulations. Propylene glycol is used in a similar way to help the body absorb chemicals more effectively during intravenous medications. Although there have been questions about propylene glycol's toxicity, it's important to note that it breaks down in the body in 48 hours and doesn't shape any dangerous crystals. Since it does not settle in our bodies, it is referred to as non-bio-accumulative (Bell-Young 2018).

Not only that, propylene glycol is used as a humectant in both the food and cosmetic industries. It works well in moisturisers and hair-care items by attracting water from the air and locking it in. Plant-based PG is gaining popularity in cosmetics, including at Lush, due to its natural production. To ensure optimum protection and performance, many cosmetic grade propylene glycols have been obtained from plants rather than being converted from propene, a by-product of fossil fuels (Bell-Young 2018).

E-cigarettes contain a number of chemicals whose safety has been questioned on several occasions. One of these chemicals is propylene glycol. Vegetable glycerin and propylene glycol are commonly found in the liquid used in e-cigarette cartridges. These are also flavoured and contain nicotine. Glycerin is a viscous material, and its inclusion in e liquid aids in the formation of thicker vapour clouds. However, due to its viscosity as a liquid, it may be difficult to transport the e-liquid to the atomiser. Propylene glycol is added as a thinner as a result. Propylene glycol allows the e-liquid

to be absorbed more readily by the cotton in the atomiser, and its low density prevents residue from forming within (Bell-Young 2018).

CHAPTER II

ECONOMIC ISSUES

2.1 THE DEMAND AND SUPPLY OF PROPYLENE GLYCOL

Economic issue is one of the important aspects that need to be discuss. The demand for the propylene glycol increases drastically among Malaysians and also people all around the world from 2020 up until now. The major reason for these drastic changes due to the pandemic Covid-19. The fragrance industry's demand for propylene glycol remained high, while the pharmaceutical industry saw a significant increase in demand to combat the spread of the Covid-19 virus. This causes the demand towards propylene glycol product increase in recent years and expected to grow in more upcoming years.

In 2017 the demand for the propylene glycol product in the world market is 2.63 million tonnes. From the year 2018 to 2026 the demand for the propylene glycol product increase with Compound Annual Growth Rate (CAGR) of 4.4% and expected to reach 3.27 million tonnes in 2022. That means we estimated in the year 2018 the demand will be 2.75 million tonnes, 2.87 million tonnes in the year 2019, 2.99 million tonnes in 2020 and 3.13 million tonnes in 2021. Thus, it is proven that the demand towards propylene glycol product is increasing highly every year and expected to increase more in future (Anon. 2019).

On the other hand, the supply for propylene glycol product in the world market is 2.55 million tonnes in the year 2017 and increase with Compound Annual Growth Rate (CAGR) 3.9% and expected to reach 3.08 million tonnes in the year 2022. In 2018, the supply is 2.65 million tonnes, 2.75 million tonnes in 2019, 2.86 million tonnes in 2020 and 2.97 million tonnes in 2021 (Anon. 2020).

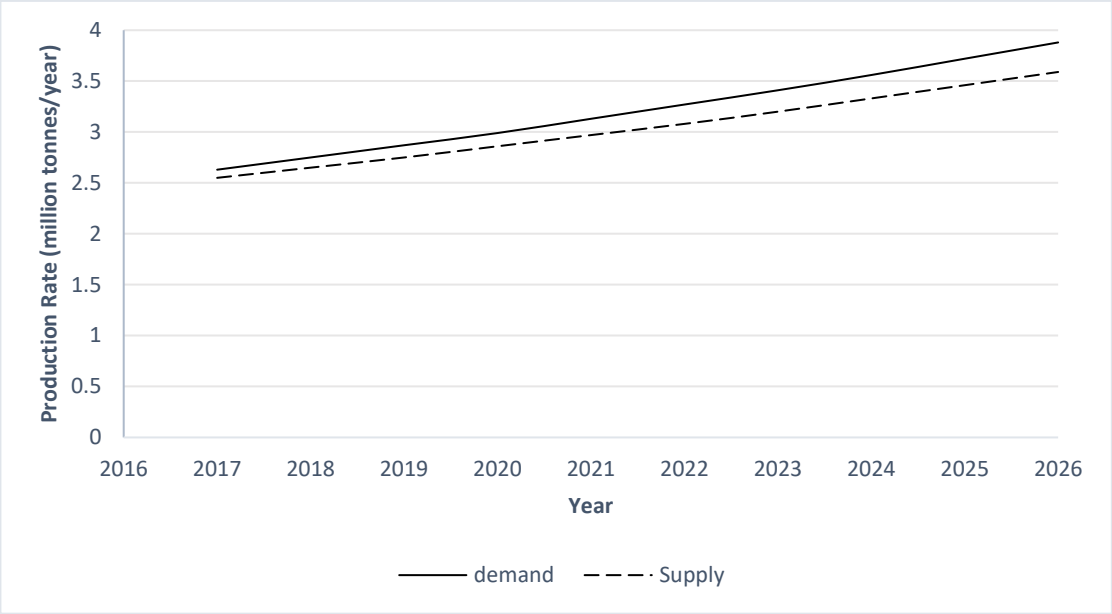

Figure 2.1 Supply and Demand for propylene glycol from year 2017 to 2026

Source: (Metadata and Definitions, 2020)

2.2 THE PRICE OF THE PROPYLENE GYLCOL

Propylene glycol has been affected by recent logistical challenges, which have limited supply and as a result, driven up prices. Despite the fact that production and distribution had remained constant through early 2020, according to recent market pricing. Then, the market price for 99.5% and 99.9% propylene glycol is $1015 to $1400 per metric ton and $1.0 to $3.0 per kilogram (Statista 2021). We make an assumption that the market price for the propylene glycol will be same all around the world which is match to the industrial standards. Graph below shows the price of propylene glycol in year 2017 until 2021.

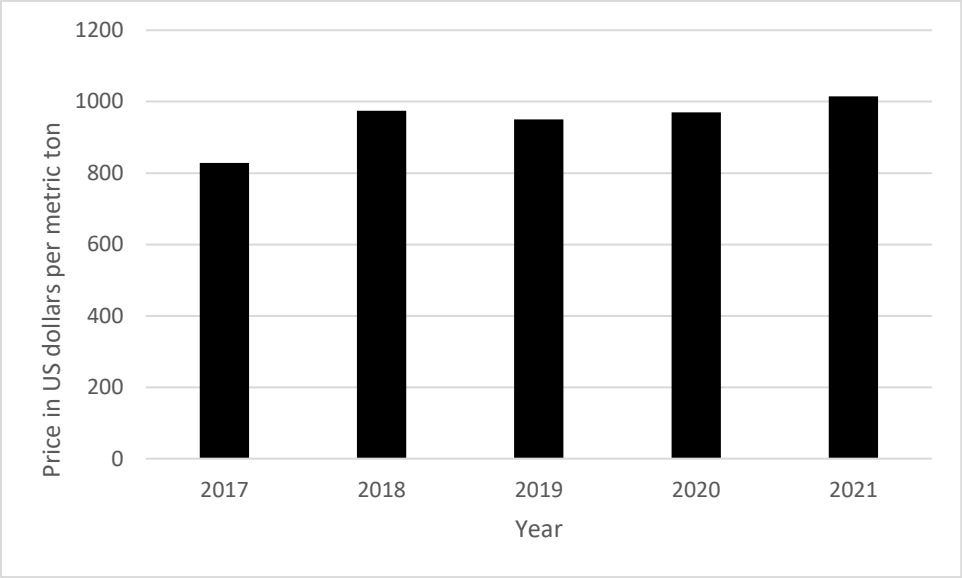

Figure 2.2 Price of Propylene Glycol in 2017 to 2021

Source: (Statista, 2021)

Currency rate: 1 US dollar = 4.11529 Malaysia Ringgit (April 20, 2021)

2.3 LIST OF COMPANIES PRODUCING PROPYLENE GLYCOL

Transportation, building and renovation, food and drinks, pharmaceuticals, cosmetics and personal care, and others are all parts of the global propylene glycol market. The Dow Chemical Company, LyondellBasell Industries, BASF, Shell Chemicals, Arch Chemicals, SKC Chemicals Group, Global Bio-chem Technology Group Co. Ltd., and others are some of the key players in the global Propylene Glycol industry. The global Propylene Glycol market is led by Dow Chemical Company and LyondellBasell Industries, with a combined market share of over 40%. Table 2.1 shows the list of companies that involve in the production of propylene glycol.

Table 2.1: List of Propylene Glycol Producing Companies

No.	Company	Location	Plant Capacity (tonne per year)
1.	Global Bio-chemical Technology Group	China	200 000
2.	ARCO Chemical Company	Texas, United States	163 000
3.	The Dow Chemical Co	USA	150 000
4.	Bharat Petroleum Corporation Limited (BPCL)	India	100 000
5.	Archer Daniels Midland	Decatur,Illinois	100 000
6.	Zhenhai Refining and Chemical	China	100,000
7.	Texaco Chemical Company	Beaumon, Texas United States	68 000
8.	Ashland Chemical Cargill	Europe	65 000
9.	Eastmen Chemical Company	West Virginia, USA	36 000

Source: (ChemAnalyst, 2020)

2.4 PLANT CAPACITY

Propylene Glycol (PG) is a colorless and odorless plastic substance with many applications in the dairy, pharmaceutical and chemical industries. Because of its widespread used, PG demand is expected to rise steadily. Although the production and delivery have been consistent through early 2020, PG has fallen victim to recent logistical difficulties that have restricted supply and consequently pushed up prices due to COVID-19, inclimate and volatile weather that affects available supply and current PG price. Demand is expected to rise more during the forecast period of 2021 to 2026 at CAGR of 4.4 percent. As the demand increases, the supply also will rise at CAGR of 3.9%.

The global demand for propylene glycol is forecast to rise from 2,634,900 tonnes (2017) to 3,882,119 tonnes by 2026 while the supply of PG is estimated to rise from 2,545,840 tonnes (2017) to 3,592,287 tonnes (2026). Thus, this coming year of 2022, the production rate of plant is estimated as below:

Deficiency = Demand – Supply

= 3,267,885 tonnes/year – 3,082,541 tonnes/year

= 185,344 tonnes/year

In order to achieve the highest quality and quantity propylene glycol, the processing cycle will be 24 hours in one day, and maintenance will be performed once a year. The 0.05 in calculation below represents the 5% of world shortfall and demand that had to be met in order to produce a good amount of propylene glycol.

Plant Capacity = (0.05 × deficient) ÷ Production time a year

= (0.05 × 185,344,000 kg/year) ÷ (364 days × 24 hours)

= 1060 kg/hours

= 92672 tonne per year

According to the calculations, the plant's annual production is 1060 kg, which is sufficient to meet 5% of global shortage and demand. For 8736 hours a year, the unit can deliver 1060 kg of propylene glycol in continuous production. The purity of the manufactured propylene glycol is 99.5% and it will be in liquid form.

The plant capacity had to be compared to ensure that the production rate of propylene glycol would be comparable to the other firm. In the list of company, The lowest plant capacity of propylene glycol is 36000 tonne per year while the highest plant capacity of propylene glycol is 200000 tonne per year. This being stated, our plant capacity of

92672 tonne per year meets the criteria because it is within the range of other firms plant capacities

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CHAPTER III

PRODUCTION OF PROPYLENE GLYCOL

3.1 INTRODUCTION FOR PROCESS DESCRIPTION

Propylene Glycol can be produced in four different forms. Non-isothermal hydrogenolysis at atmospheric pressure and additional hydrogen is the most effective process. This method has three steps and uses glycerol as a basis. To begin, crude glycerol will be pre-treated to produce refined glycerol, The refined glycerol would then react in the reactor, producing propylene glycol and a byproduct. The primary reaction in the reactor will occur simultaneously by following a sequence that begins with glycerol dehydration and ends with acetol hydrogenation. To summarize the process, acetol and water will be produced as a result of glycerol dehydration in the presence of a catalyst. The acetol will next react with water to form the primary product, propylene glycol. Finally, the reactor mixture would be purified to extract pure propylene. We decided to show the process only after the glycerol was pre-treated and we used refined glycerol as our raw material. The sequence for the entire procedure is depicted in Figure 3.1 below.

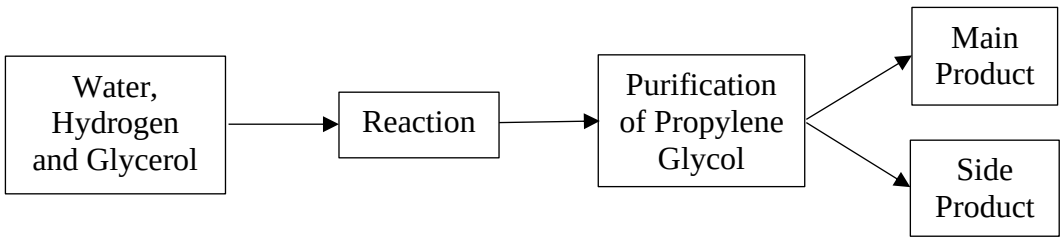


Figure 3.1 Simplified process description in block diagram

3.2 PROCESS DESCRIPTION OF PROPYLENE GLYCOL

3.2.1 Reaction of Acetol, Glycerol and Hydrogen

The two-step mechanism is used in this production of propylene glycol (PG) (Pudi et al. 2015). The first stage reaction is glycerol dehydration, which produces acetol and water, preceded by acetol hydrogenation to produce PG. A secondary reaction is a direct reaction between glycerol and hydrogen that results in the formation of ethylene glycol (EG) and methanol.

Dehydration of Glycerol

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$$

Acetol Hydrogenation

$$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

Glycerol and Hydrogen

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

The most appropriate reactor for this process is a packed bed reactor, which is commonly used for heterogeneous system and accurately predicts tubular flow. This reactor allows for a vigorous heat exchange in the reaction zone which assures that all particles in the flow have a uniform residence time, this reactor will also accelerate mass transfer between phases and reduce the difference in reactant particle residence time, The reactor can run in either a continuous gas or distributed liquid phase (Raweewan Klaewkla et al. 2011).

a. Reactor (R-101)

In this reactor, the reactions of glycerol, acetol and hydrogen will happen simultaneously and Cu/Al_2O_3 will be the catalyst solid in the reactor. The recorded glycerol conversion is 88.7%, with a 94.3% selectivity to propylene glycol and 35.48% selectivity to ethylene glycol. The molar ratio hydrogen/glycerol is 5:1. The significant amount of hydrogen required is owing to the inherent exothermic reaction that will occur during the procedure. As a result, hydrogen will be utilized to cool down the reaction, allowing it to return to its original form. The reactor would contain unreacted

glycerol, propylene glycol, water, methanol, acetol, hydrogen gas, and ethylene glycol after the reactions occur. The operating temperature will be 180 ˚C and the pressure will be 20 bar.

We decide that 205 ˚C, 20 bar will be the optimal condition at the entrance (stream 7 & 9) since the process's typical working conditions range from 20 to 50 bar and 200 to 350 ˚C. Akiyama et al. suggest a gradient temperature reactor with an entry temperature varying from 170 to 230 ˚C and a second reaction stage temperature ranging from 135 to 190 ˚C. We assume temperatures of 200 (stream 10) and 120 ˚C (stream 12) at the reactor's top and bottom, since complete conversion of glycerol to propylene glycol is achieved with the maximum yield at these temperatures (i.e., 96.9%). Since the optimum yield is 96.9%, the expectation is that 7.6 % unreacted glycerol would come out of the bottom (stream 12). The top of the reactor would produce hydrogen gas, methanol, water and acetol while the bottom would produce propylene glycol, ethylene glycol and unreacted glycerol.

b. Flash (F-101)

The gas phase gases from the reactor are cooled to 30 ˚C (stream 10) and sent to a flash unit, where the hydrogen gas from the reactor is returned and the remainder liquid is sent to the distillation unit. The operating unit of flash is 25 ˚C and 5 bar.

3.2.2 Purification of Propylene Glycol

Propylene glycol (PG) purification is needed to extract the PG while preserving the purity of the PG while extracting the other unwanted substance. The distillation method is the most effective way to separate it. The bottom of each distillation column will have a boiler and the top column will have a condenser and reflux, ensuring that the purities of the split substance can be controlled.

a. Distillation Column (D-101)

The liquid phased (stream 16) from the flash unit would enter the first distillation to separate the unwanted product, making waste management simpler. Methanol is

separated from water and acetol in the first column. Since the boiling point of methanol is 64.7 ˚C, the operating temperature for this unit is 70 ˚C. The bottom of each distillation column will have a boiler and the top column will have a condenser and reflux, ensuring that the purities of the split substance can be controlled. Methanol will has a 99.97% purity.

b. Distillation Column (D-102)

The reactor's bottom product (R-101) will be transferred to D-102 for separation. Since the boiling points of PG and EG are 188.2 ˚C and 197 ˚C, respectively the acceptable working temperature for this column is 192 ˚C. The PG will be collected at the top of the column with purity of 99.5% while the EG and unreacted glycerol will be transferred to the last column.

c. Distillation Column (D-103)

The D-101 separated water and acetol would be transferred to the third distillation column to be separated. Since the boiling point of water is 100 ˚C, the working temperature of this unit at atmospheric pressure would be 130 ˚C. Water will accumulate at the top of the column, while acetol accumulates at the bottoms with purity of 95%

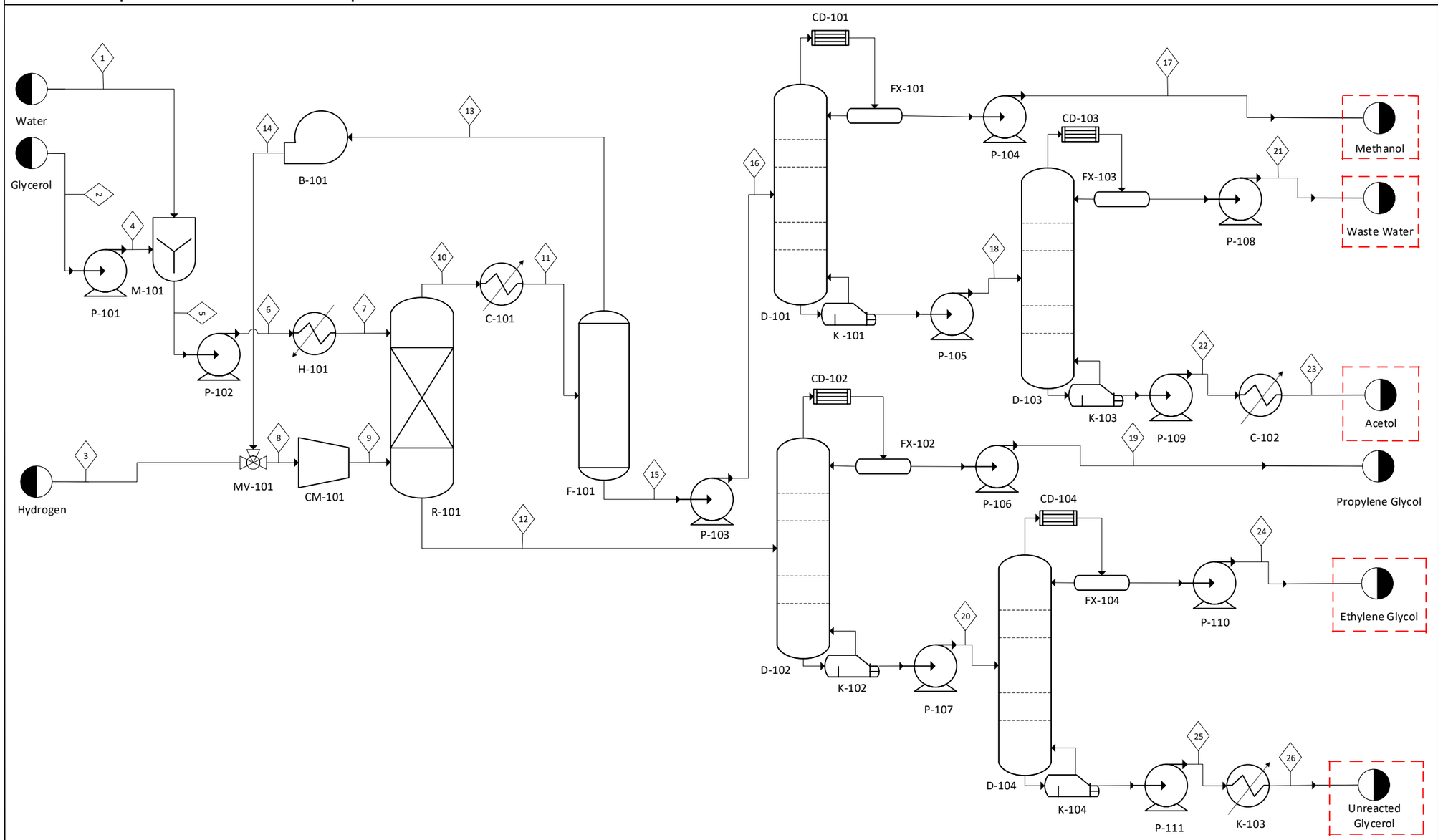
d. Distillation Column (D-104)

This column's working temperature is 230 ˚C, where it can separate the EG and unreacted glycerol. EG with purity of 99.5% will accumulate at the top of the column, while unreacted glycerol accumulates at the bottoms.

3.3 PROCESS FLOW DIAGRAM

Figure 3.2 Process Flow Diagram

M-101 Mixer	C-101 Cooler	R-101 Reactor	D-101 Distillation column	CD-101 Condenser	FX-101 Reflux	K-101 Kettle Reboiler
H-101 Heater	C-102 Cooler	F-101 Flash	D-102 Distillation column	CD-102 Condenser	FX-102 Reflux	K-102 Kettle Reboiler
MV-101 Mixer Valve	C-103 Cooler	P-101 Pump	D-103 Distillation column	CD-103 Condenser	FX-103 Reflux	K-103 Kettle Reboiler
CM-101 Compressor	B-101 Blower	P-102 Pump	D-104 Distillation column	CD-104 Condenser	FX-104 Reflux	K-104 Kettle Reboiler
P-103 Pump	P-104 Pump	P-105 Pump	P-106 Pump	P-107 Pump	P-108 Pump	P-109 Pump
P-110 Pump	P-111 Pump					



Title: Production of Propylene Glycol

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Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
Temperature (°C)	25	25	25	25	25	25	205	27	27	200	30	120	30	27	30	30	0	70	50	192	50	130	50	50	230	50
Pressure (bar)	1	1	1	3	1	3	3	5	20	5	1	5	1	5	1	1	1	1	1	1	1	1	1	1	1	1
Phase	l	l	g	l	l	l	l	g	g	g	l + g	l	g	g	l	l	l	l	l	l	l	l	l	l	l	l
Water (kg/h)	200	0	0	0	200	200	200	0	0	459.02	25.5	0	0	0	459.02	459.02	0.01	459.01	0	0	457.37	1.64	1.64	0	0	0
Glycerol (kg/h)	0	1500	0	1500	1500	1500	1500	0	0	0	0	113.62	0	0	0	0	0	0	0	113.62	0	0	0	0	113.62	113.62
Hydrogen (kg/h)	0	0	29.25	0	0	0	0	7500	7500	7470.75	7470.75	0	7470.75	7470.75	0	0	0	0	0	0	0	0	0	0	0	0
Methanol (kg/h)	0	0	0	0	0	0	0	0	0	21.73	21.73	0	0	0	21.73	21.73	21.72	0.01	0	0	0	0	0	0	0	0
Acetol (kg/h)	0	0	0	0	0	0	0	0	0	32.78	32.78	0	0	0	32.78	32.78	0	32.78	0	0	1.64	31.14	31.14	0	0	0
Proplyene Glycol (kg/h)	0	0	0	0	0	0	0	0	0	0	0	1060	0	0	0	0	0	0	1054.7	5.3	0	0	0	0.18	5.12	5.12
Ethylene Glycol (kg/h)	0	0	0	0	0	0	0	0	0	0	0	42.1	0	0	0	0	0	0	5.3	36.8	0	0	0	36.62	0.18	0.18
Total flow rate (kg/h)	200	1500	29.25	1500	1700	1700	1700	7500	7500	7984.28	7984.28	1215.72	7470.75	7470.75	513.53	513.53	21.73	491.8	1060	155.72	459.02	32.78	32.78	36.8	118.92	118.92

Input

Output

Stream number

Date : 24 Jun 2021

CHAPTER IV

SAFETY ISSUES AND ENVIRONMENTAL

4.1 INTRODUCTION

Environmental concerns are the adverse effects on the biophysical environment of human activity. Environmental conservation, for the benefit of both the environment and humans, is a method of protecting the natural environment at individual, organisational or governmental levels (Cabaniss 2014). All industrial processes produce waste of some form that must be carefully treated and disposed of at varying levels in compliance with regulations set by governments. Emissions to air, water and soil, smell, noise and visual effects, and waste management are key areas for consideration. It is necessary to note that for every engineer or industry, emission considerations are both a moral and legal duty (Sinnott 2013).

There are a few effects on the environment due to the waste produced from the industrial production of propylene glycol. The production of this product may cause water and air pollution due to the release of waste water and purge.

4.2 SAFETY ISSUES OF THE RAW MATERIALS AND THE METHOD OF HANDLING AND STORAGE

Industrial facilities have particular safety issues because more than just the workers on the factory floor are affected by risks and accidents. A workplace fire, lost days due to injury, or chemical hazards can impact your production quality, which can delay delivery times, distribution, relationships with sellers, and satisfaction with customers. Industrial safety works hard to prevent risks to the workplace, including chemical exposures, poor ergonomics, and physical hazards, so that without interruption to production, business can continue as normal (Resources 2018). Due to the safety issues,

the handling and storage of materials is vital. These operations provide a continuous flow of parts and assemblies through the workplace in addition to raw materials, and ensure that materials are available when needed

4.2.1 Properties and Safety Issues of Raw Materials

Raw Material and Product	Properties	First Aid Action
Hydrogen	Sources of ignition if exposed to air. Lightest element and will explode at concentrations ranging from 4-75 percent by volume in the presence of sunlight, a flame or a spark.	• Remove the affected person from the gas source or contaminated area. • If the affected person not breathing spontaneously, administer rescue breathing. • Summon an emergency ambulance, if not available contact a physician.
Glycerol	Stable under normal temperatures and pressures. Hygroscopic: absorbs moisture or water from the air. So, its incompatible materials when expose to moist air or water.	• Rinse immediately with plenty of water also under eyelids, for at least 15 minutes. Get medical attention. • If inhaled, remove to fresh air.
Methanol	Highly flammable liquid and vapor. Toxic if swallowed, in contact with skin or if inhaled.	Rinse with water immediately if get contact with skin and eye. Do not apply (chemical) neutralizing agents. Remove clothing before washing. Consult a doctor and medical service.

Water	Not classified as a hazardous chemical.	Adverse effects not expected from water in case of skin contact. Only take off contaminated clothing. If still unwell, seek medical advice.
Acetol	Strong oxidizing agents, alkali metals, nitric acid, sulfuric acid and stable under normal temperatures and pressures.	Rinse immediately with plenty of water under eyelids and skin, for at least 15 minutes. Get medical attention.
Propylene Glycol	Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of inhalation.	Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.
Ethylene Glycol	Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant, permeator), of eye contact, of inhalation. Severe over-exposure can result in death.	If get contact directly with eye, check for and remove any contact lenses. In case of contact, immediately flush eyes with of plenty of water for at least 15 minutes. Get medical attention if irritation occurs.

Table 4.1 Properties of Raw Materials and Products

Source: (Safety Data Sheet, 2019)

From table 4.1, all the chemical that involve in the plant is not dangerous at room temperature except methanol. For propylene glycol and ethylene glycol is hazardous in case of ingestion. Hydrogen also dangerous if expose at certain condition.

4.2.2 Method of Handling and Storing

Raw Material and Product	Handling Procedures	Storage Requirements
Hydrogen	• Handle this material only in sealed, purged systems. • Handle sealed gas cylinders in accordance with CGA P-1, Safe Handling of Compressed Gases in Containers.	• Protect the cylinders from direct sunlight, precipitation, mechanical damage, and temperatures above 55°C (130°F). • Store cylinders in accordance with CGA P-1, Safe Handling of Compressed Gases in Containers, local building and fire codes and other relevant regulations. Materials should be segregated by the hazards they comprise for storage.
Glycerol	Wash thoroughly after handling. Wash thoroughly after handling. Avoid contact with eyes, skin, and clothing. Keep container tightly closed. Avoid ingestion and inhalation. Wash clothing before reuse	Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances
Methanol	• Use spark-/explosion proof appliances and lighting system. • Take precautions against electrostatic charges.	Store in a cool area. Store in a dry area. Keep container in a well-ventilated place. Fireproof storeroom. Keep locked up.
Water	Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work	• Keep container closed when not in use. • Keep away from metallic sodium. • Keep far from sources of ignition and direct sunlight.
Acetol	• Use proper personal protective equipment and use adequate ventilation.	• Keep away from heat, sparks and flame. • Store in a tightly closed container,

	• Avoid contact with eyes, skin, clothing, heat, sparks and flames.	cool, dry and well-ventilated area away from incompatible substances.
Propylene Glycol	Avoid contact with skin and eyes.	Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 23°C (73.4°F).
Ethylene Glycol	Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label.	Keep container tightly closed. Keep container in a cool, well-ventilated area.

Table 4.2 Method of Handling and Storaging

Source: (Safety Data Sheet, 2019)

4.3 ENVIRONMENTAL ISSUES

The red dotted boxes in the process flow diagram in Figure 4.1 indicate the waste that had been produced. The wastes are wastewater, methanol, ethylene glycol and unreacted glycerol. In reactor (R-101), the reactions of glycerol, acetol and hydrogen will happen simultaneously and Cu/Al_2O_3 will be the catalyst solid in the reactor. The recorded glycerol conversion is 88.7%, with a 94.3% selectivity to propylene glycol. The reactor would contain unreacted glycerol, propylene glycol, ethylene glycol at upper outlet and water, methanol, acetol, hydrogen gas at down outlet after the reactions occur. After flash process, methanol, water and acetol have been successfully change phase to liquid will go through distillation to be separated while hydrogen will be recycled back for acetol hydrogenation reaction. At downstream of reactor, the unreacted glycerol, propylene glycol, ethylene glycol will go through distillation process for them to be separated as well.

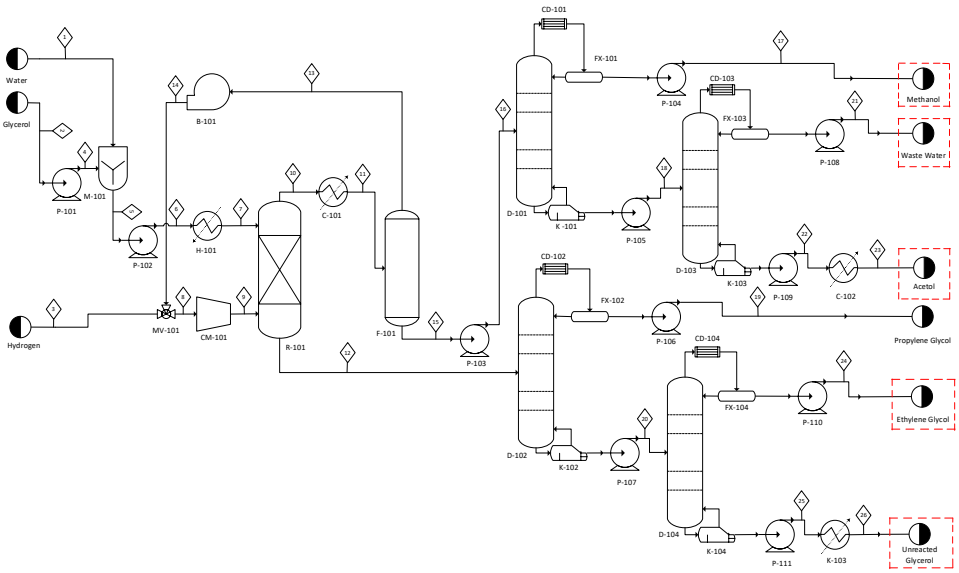

Figure 4.1 Process Flow Diagram

4.3.1 Waste Generation

A few waste products will be generated during the manufacturing of chemical products. The waste product that is generated can be harmful to humans and the environment, so it is best to handle it before releasing it into the environment to avoid negative consequences in the future. In the production of propylene glycol, the wastes formed are wastewater and unreacted glycerol.

a. Wastewater

Wastewater produced after going through the distillation column needs to be treated until it is safe before being released into the environment. The primary goal of wastewater treatment is to eliminate as many dissolved solids as possible before returning the residual water, known as effluent, to the environment. The dissolved and suspended substance in the wastewater in the production of propylene glycol are methanol and acetol. If wastewater is not well regulated, it may have a negative effect on the environment and human health. Fish and wildlife habitats may be harmed, oxygen levels may be depleted, beach closures and other bans on public water usage, restrictions on fish and shellfish fishing, and drinking water pollution may occur (Anon. 2018).

b. Unreacted Glycerol

Unreacted glycerol accumulated at the bottom in the distillation column should be treated before disposing it. Since waste glycerol cannot be disposed of in the environment, it can pollute water and cause environmental problems (Yazdani and Gonzalz 2007). It has been recommended that certain approaches to reduce water contamination be used to reduce the costs associated with disposing of untreated waste glycerol.

4.3.2 Waste Management

There are several methods for managing waste products, including waste treatment, waste recovery. Water is the sole byproduct that requires waste treatment. Following treatment, water can be reused as an intake in the process. As a initial supply, water and unreacted glycerol can be used in the process. Methanol with a purity of 99.97% can be sold for RM 4160 per tonne . Acetol with a purity of 95% can be sold for RM 933 per kg. Ethylene glycol with a purity of 99.5% can be sold as antifreeze. Antifreeze is used to prevent freezing and as a heat transfer medium in automobiles, heavy machinery and homes. The price of ethylene glycol is RM 2290 per tonne.

a. Wastewater

The key steps for preventing and controlling chemical wastewater leakage are as follows: first, the manufacturing process and facilities should be reformed, emissions should be minimized, wastewater should not be discharged and systematic utilization and recycling should be carried out: the wastewater to be discharged should be chosen based on water quality and specifications.

The primary purpose of the primary treatment procedure is to remove suspended solids, colloids, oil slicks and heavy oil from water. Natural sedimentation, floating and oil separation processes, as well as water temperature and volume correction can be used. Secondary treatment mostly eliminates biodegradable organic solutes and certain colloids, decreases biochemical oxygen demand and a portion of chemical oxygen

demand in wastewater and is typically performed using biological approaches. The aim of tertiary treatment is to eliminate organic contaminants and dissolved inorganic pollutants in wastewater that are difficult to biodegrade. Activated carbon adsorption and ozone oxidation are two commonly used processes, but ion exchange and membrane isolation approaches can also be used. Approximately 50% of the incoming biochemical oxygen demand (BOD) and 92% of the incoming chemical oxygen demand (COD) are removed (Anon. 2018).

4.3.3 Environmental Act

The compilation of rules, legislation, agreements, and common law that regulates how humans communicate with their environment is known as environmental law. Environmental law's goal is to protect the environment while also establishing guidelines for how citizens should use natural resources. Environmental regulations not only seek to protect the environment from destruction, but also to define who is allowed to use natural resources and under what conditions. Pollution, the use of natural resources, forest conservation, mineral harvesting, and animal and fish populations can all be controlled by laws (Path 2020).

The volume of wastewater discharged from processing plants must be treated before it is released to the sewers. The quality of effluent from treatment plants and ambient air quality standards and emission standards is regulated by the Environmental Quality Act 1974 (No.127 of 1974) states that, an act concerning to the prevention, abatement, control of pollution and enhancement of the environment. Its regulation such as the Environmental Quality (Industrial Effluent) Regulations 2009. All industries and factories in Malaysia must obey the national law of environmental acts and regulation. Any projects or production plants needs to get the authorization of Ministry of Environmental Malaysia before opening it. This can be related to our production because one of our waste is wastewater. The wastewater was produced after going through the distillation column and it will be treated just like what have been mentioned in the waste management part.

CHAPTER V

MASS AND ENERGY BALANCE

5.1 INTRODUCTION

One of physics' fundamental rules asserts that mass cannot be created or destroyed. As a result, the concept of mass conservation is applied. The accounting of all mass in a chemical or pharmaceutical process is known as mass balance. The principle of mass balance may be applied to any process, although with varying degrees of success. In the case of many reaction processes, mass balancing entails determining the amount of reactions for all single reactions in a process.

5.2 STOICHIOMETRY

Understanding the connection between reactants and products in a reaction is critical in chemistry. Stoichiometry is precisely what it sounds like. It is the quantitative relationship that exists between the number of moles (and hence mass) if different products and reactants in a chemical reaction. Chemical reaction must be balanced, which means that the product must have same number of different atoms as the reactants. By putting coefficients in front of the reactant and products, we can balance them. These are called stoichiometric coefficients (Washington University,2021).

Reactions:

Main Reaction:

$C_3H_8O_3\ (l) \rightarrow C_3H_6O_2\ (l) + H_2O\ (g)$…….. **(1)**

$C_3H_6O_2(l)\ +\ H_2(g) \rightarrow C_3H_8O_2(l)$ ……. **(2)**

Side Reaction:

$C_3H_8O_3(l) + H_2(g) \rightarrow C_2H_6O_2(g) + CH_3OH(l)$…….. **(3)**

5.3 MASS BALANCE OF EACH UNIT OPERATION

Based on the chapter where demand and supply are discussed, out propylene glycol production rate is 1060 kg/h. The unit operation required to create the highest grade of propylene glycol would be a packed bed reactor with a catalyst (R-101), a flash column (F-101) and 4 distilled columns.

Table 5.1 Summarized stream table of PBR (R-101)

Component	**Formula**	**Inlet stream**	**Outlet stream**
		Mass flow rate(kg/h)	**Mass flow rate (kg/h)**
Water	H_2O	200	459.02
Glycerol	$C_3H_8O_3$	1500	113.62
Hydrogen	H_2	7500	7470.75
Acetol	$C_3H_6O_2$	0	32.78
Methanol	CH_3OH	0	21.73
Ethylene Glycol	$C_2H_6O_2$	0	42.1
Propylene Glycol	$C_3H_8O_2$	0	1060
Total		9200	9200

5.3.1 M-101 Mixer

Since the glycerol texture is a little sticky, water is added to the glycerol stream to dilute it.

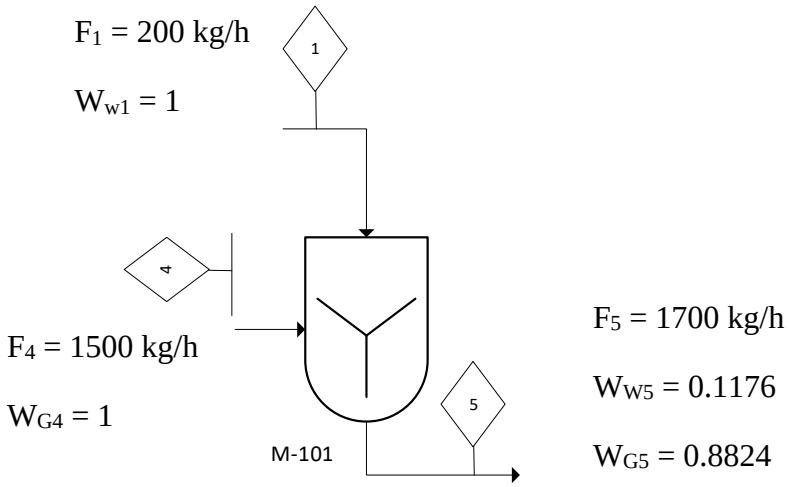

Figure 5.1: Mixer, M-101

Table 5.2 Mass and Molar Flow Rate of Each Component in Mixer M-101

		Inlet stream 1		Inlet stream 4		Outlet stream 5	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Glycerol	92.1	0	0	16.28	1500	16.28	1500
Water	18	11.11	200	0	0	11.11	200
Total		11.11	200	16.28	1500	27.39	1700

Inlet flow rate = Outlet flow rate

200 kg/h + 1500 kg/h = 1700 kg/h

1700 kg/h = 1700 kg/h

5.3.2 MX-101 Mixer Valve

The recycling hydrogen from stream 11 will be mixed with the newly input hydrogen gas at the mixer valve.

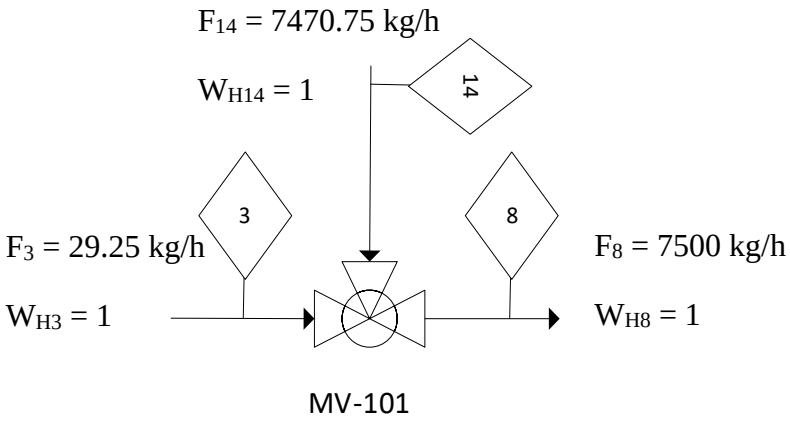

Figure 5.2: Mixer Valve, MV-101

Table 5.3 Mass and Molar Flow Rate of Each Component in Mixer Valve MV-101

		Inlet stream 3		Inlet stream 14		Outlet stream 8	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Hydrogen	2	14.63	29.25	3735.38	7470.75	3750	7500
Total		14.63	29.25	3735.38	7470.75	3750	7500

Inlet flow rate = Outlet flow rate

29.25 kg/h +7470.75 kg/h = 7500 kg/h

7500 kg/h = 7500 kg/h

5.3.3 R-101 Reactor

This reactor undergoes three reactions. Glycerol dehydration consumes 88.22% of the glycerol to produce acetol. Then 96.86% of the acetol will react with hydrogen to form propylene glycol.

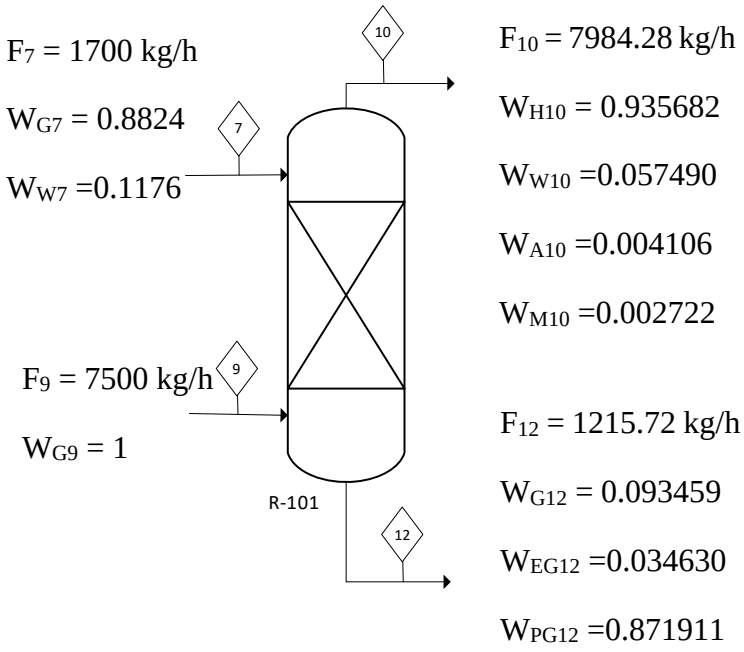

Figure 5.3: Reactor, R-101

Table 5.4 Mass and Molar Flow Rate of Each Component in Reactor R-101

		Inlet stream 7		Inlet stream 9		Outlet stream 10		Outlet stream 12	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component									
Glycerol	92	16.30	1500	0	0	0	0	1.24	113.62
Hydrogen	2	0	0	3750	7500	3735.37	7470.75	0	0
Water	18	11.11	200	0	0	25.5	459.02	0	0
Acetol	74	0	0	0	0	0.44	32.78	0	0
Methanol	32	0	0	0	0	0.68	21.73	0	0
EG	62	0	0	0	0	0	0	0.68	42.1

PG	76	0	0	0	0	0	0	13.95	1060
Total		27.41	1700	3750	7500	3761.99	7984.28	15.87	1215.72

Inlet flow rate = Outlet flow rate

1700 kg/h + 7500 kg/h = 7984.28 kg/h + 1215.72 kg/h

9200 kg/h = 9200 kg/h

5.3.4 F-101 Flash

In flash unit operation, the hydrogen gas from the reactor is returned and the remainder liquid is sent to the distillation unit

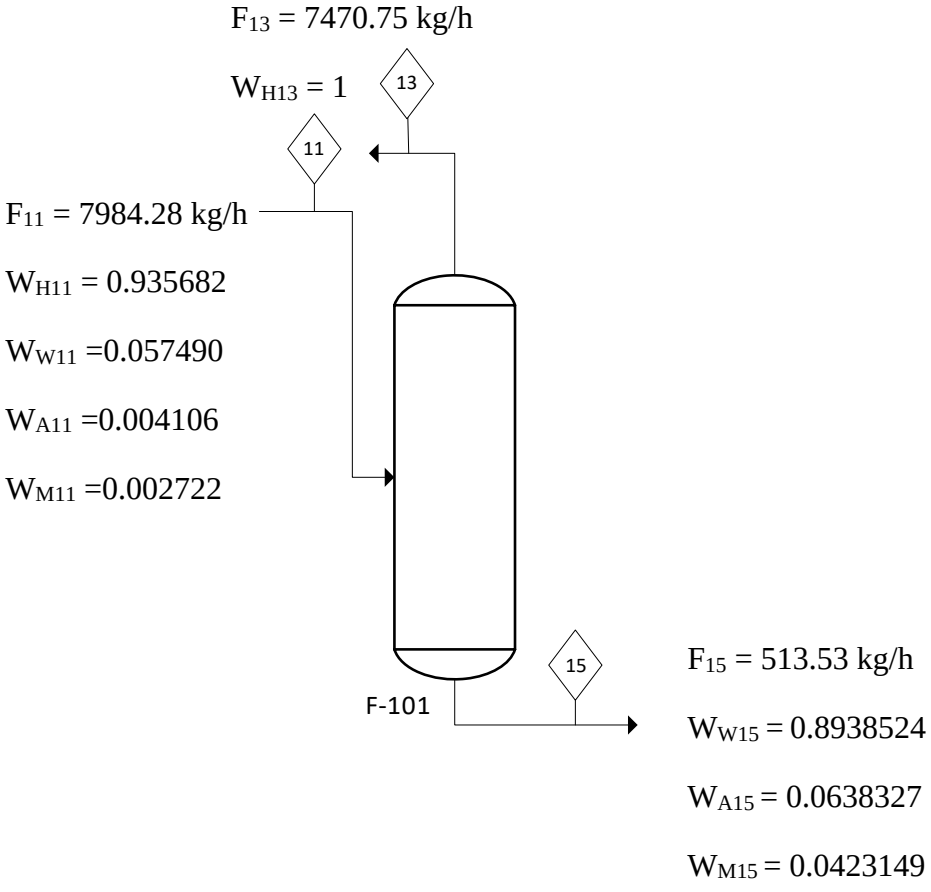

Figure 5.4: Flash, F-101

Table 5.5 Mass and Molar Flow Rate of Each Component in Flash F-101

		Inlet stream 11		Outlet stream 13		Outlet stream 15	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Hydrogen	2	3735.37	7470.75	3735.37	7470.75	0	0
Water	18	25.5	459.02	0	0	25.5	459.02
Acetol	74	0.44	32.78	0	0	0.44	32.78
Methanol	32	0.68	21.73	0	0	0.68	21.73
Total		3761.99	7984.28	3735.37	7470.75	26.62	513.53

Inlet flow rate = Outlet flow rate

7984.28 kg/h = 7470.75 kg/h + 513.53 kg/h

7984.28 kg/h = 7984.28 kg/h

5.3.5 D-101 Distillation Column

The liquid phased (stream 13) from the flash unit would enter the first distillation to separate the unwanted product, making waste management simpler. Methanol is separated from water and acetol in the first column. The purity of methanol that will be produced in stream 17 is 99.97%

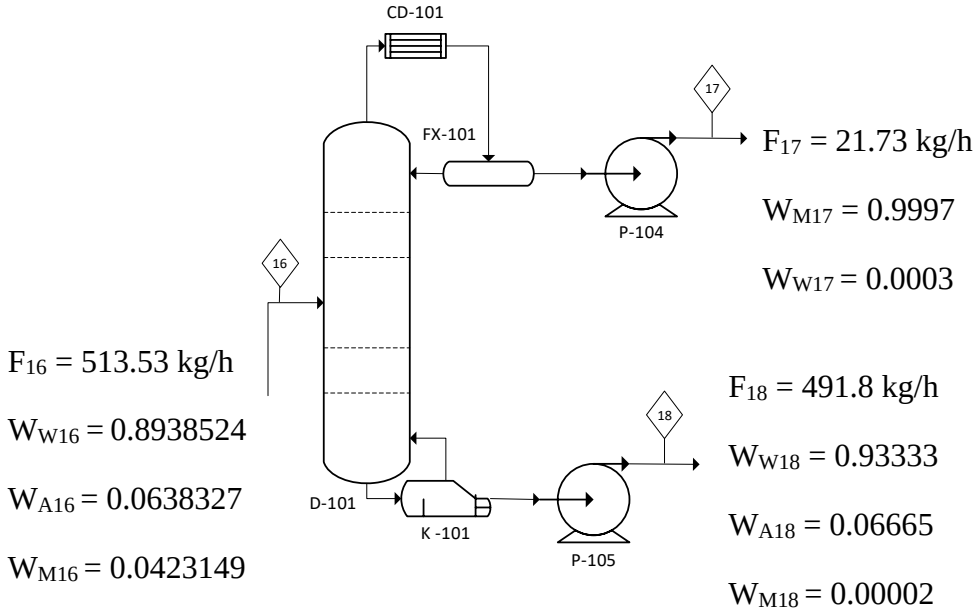

Figure 5.5: Distillation Column, D-101

Table 5.6 Mass and Molar Flow Rate of Each Component in Distillation Column D-101

		Inlet stream 16		Outlet stream 17		Outlet stream 18	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Water	18	25.501	459.02	0.001	0.01	25.5	459.01
Acetol	74	0.44	32.78	0	0	0.44	32.78
Methanol	32	0.6791	21.73	0.6788	21.72	0.0003	0.01
Total		26.62	513.53	0.68	21.73	25.94	491.8

Inlet flow rate = Outlet flow rate

513.53 kg/h = 21.73 kg/h + 491.8 kg/h

513.53 kg/h = 513.53 kg/h

5.3.6 D-103 Distillation Column

The D-101 separated water and acetol would be transferred to the second distillation column to be separated. Water will accumulate at the top of the column, while acetol accumulates at the bottoms. At stream 22, acetol will be produced at 95% of purity.

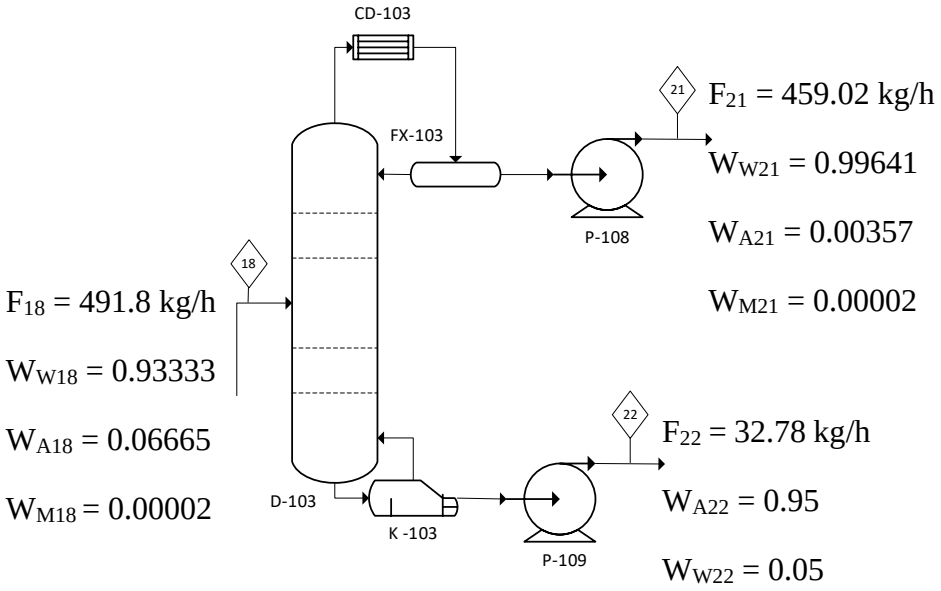

Figure 5.6: Distillation Column, D-103

Table 5.7 Mass and Molar Flow Rate of Each Component in Distillation Column D-103

		Inlet stream 18		Outlet stream 21		Outlet stream 22	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Water	18	25.5	459.01	25.41	457.37	0.09	1.64
Acetol	74	0.44	32.78	0.02	1.64	0.42	31.14
Methanol	32	0.0003	0.01	0.0003	0.01	0	0
Total		25.94	491.8	25.43	459.02	0.51	32.78

Inlet flow rate = Outlet flow rate

491.8 kg/h = 459.02 kg/h + 32.78 kg/h

491.8 kg/h = 491.8 kg/h

5.3.7 D-102 Distillation Column

The reactor's bottom product (R-101) will be transferred to D-103 for separation. The PG will be collected at the top of the column while the EG and unreacted glycerol will be transferred to the last column. Our main product, propylene glycol will be produced at 99.5% purity.

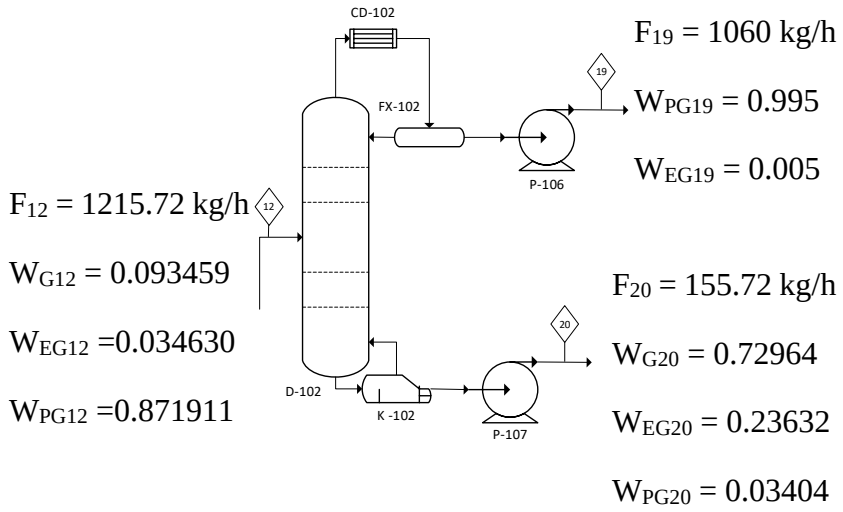

Figure 5.7: Distillation Column, D-102

Table 5.8 Mass and Molar Flow Rate of Each Component in Distillation Column D-102

		Inlet stream 12		Outlet stream 19		Outlet stream 20	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							
Glycerol	92	1.24	113.62	0	0	1.24	113.62
EG	62	0.68	42.1	0.09	5.3	0.593	36.8
PG	76	13.95	1060	13.88	1054.7	0.07	5.3
Total		15.87	1215.72	13.97	1060	1.9	155.72

Inlet flow rate = Outlet flow rate

1215.72 kg/h = 1060 kg/h + 155.72 kg/h

1215.72 kg/h = 1215.72 kg/h

5.3.8 D-104 Distillation Column

This distillation column separates the EG and unreacted glycerol. EG will accumulate at the top of the column, while unreacted glycerol accumulates at the bottoms. At stream 24, ethylene glycol will has purity of 99.5%

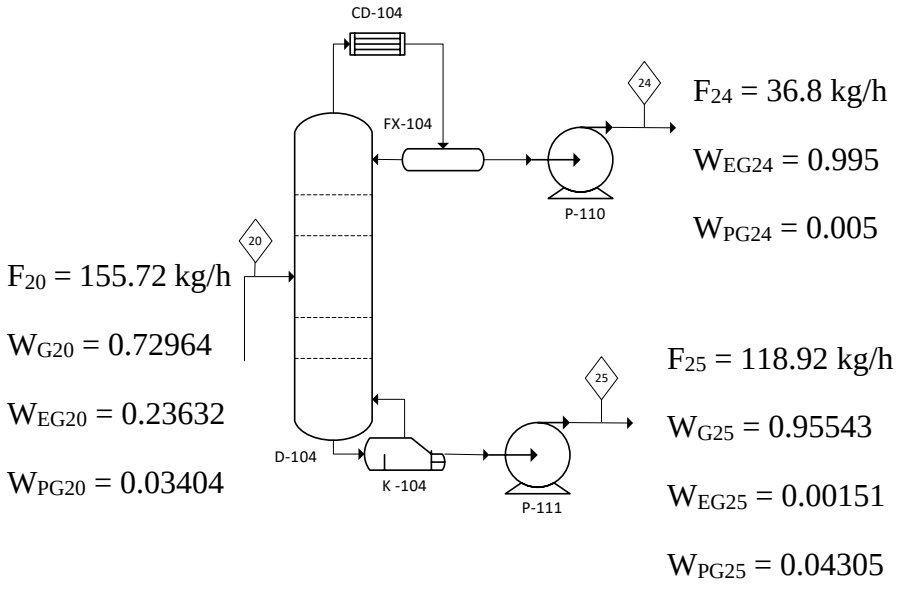

Figure 5.8: Distillation Column, D-104

Table 5.9 Mass and Molar Flow Rate of Each Component in Distillation Column D-104

		Inlet stream 20		Outlet stream 24		Outlet stream 25	
	Molecular weight	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate	Molar flow rate	Mass flow rate
	(g/mol)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)	(kmol/h)	(kg/h)
Component							

Glycerol	92.1	1.24	113.62	0	0	1.24	113.62
EG	62	0.593	36.8	0.591	36.62	0.003	0.18
PG	76	0.07	5.3	0.002	0.18	0.067	5.12
Total		1.9	155.72	0.59	36.8	1.31	118.92

Inlet flow rate = Outlet flow rate

155.72 kg/h = 36.8 kg/h + 118.92 kg/h

155.72 kg/h = 155.72 kg/h

5.3.9 Overall Mass Balance

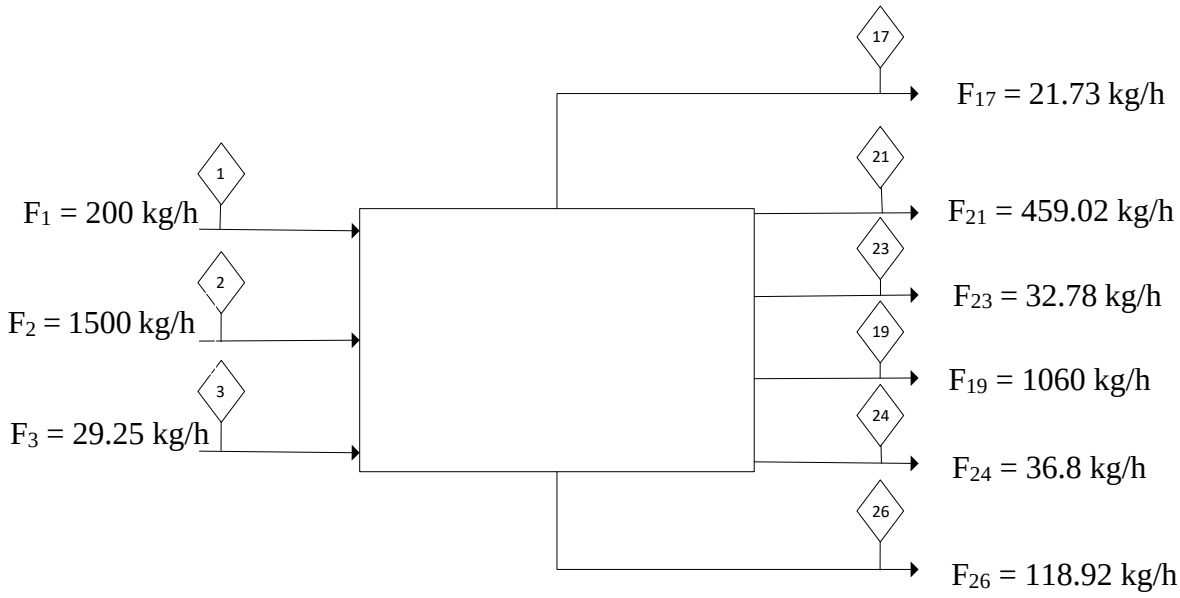

Figure 5.9 Overall Mass Balance

Total Inlet Mass flowrate = Total Outlet Mass flowrate

$F_1 + F_2 + F_3 = F_{17} + F_{21} + F_{23} + F_{19} + F_{24} + F_{26}$

200 kg/h + 1500 kg/h +29.25 kg/h = 21.73 kg/h + 459.02 kg/h +32.78 kg/h +1060 kg/h + 36.8 kg/h + 118.92 kg/h

1729.25 kg/h = 1729.25 kg/h

5.4 ENERGY BALANCE

The energy balance of a system is used to determine the amount of energy that flows into or out of each process unit. It calculates how much heat is absorbed or released during a reaction. The reaction is considered exothermic if heat is released and endothermic when the heat is absorbed during the reaction.

The assumptions used in the calculations are as follows:

1. The flow in the unit processes are in steady state.

2. The reference temperature is fixed at 25℃ or 298 K

3. There is no potential energy, kinetic energy and work done by the system.

The enthalpy change of components is calculated using the formula below:

$$\Delta H = \int_{T_{ref}}^{T} Cp\ dT$$

where the Cp is $A + BT + CT^2 + DT^3$

Rate of heat transfer can be calculated by using the formula below:

$$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r\Delta H_{rxn}$$

5.4.1 Fixed Bed Reactor (R-101)

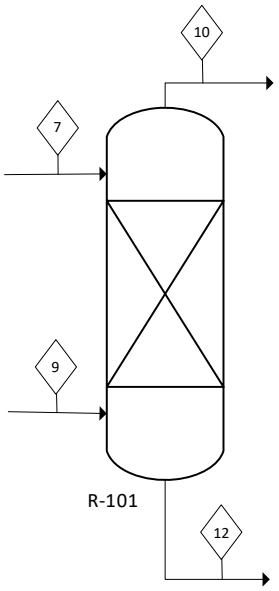

Figure 5.10 Packed Bed Reactor, R-101

The equations with each rate of reaction that occurs in the packed bed reactor are shown as below.

$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$ r_1 =14.39 kmol/hr

$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$ r_2 =13.947 kmol/hr

$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + C_3H_8O_2$ r_3 =0.679 kmol/hr

ΔH_{rxn} *can be calculated by using the formula* $\Delta H_{rxn} = \Delta H_{product} - \Delta H_{reactant}$

Table 5.10 Heat of formation for each component in the system.

Component	Enthalpy of Formation, ΔH_f (kJ/kmol)
Glycerol	-577.9
Acetol	-370.06
Water	-285.8
Hydrogen	0
Propylene glycol	-501
Ethylene glycol	-389.43

Methanol	-238.42

Source: (NIST, 2018)

Table 5.11 Coefficient values for heat capacity of each component

Component	A	B	C	D
Glycerol	132.145	8.6007×10^{-1}	-1.9745×10^{-3}	1.8068×10^{-6}
Water	92.053	-3.9953×10^{-2}	-2.1103×10^{-4}	5.3469×10^{-7}
Hydrogen	27.13	9.27×10^{-3}	-1.38×10^{-5}	7.46×10^{-9}
Ethylene glycol	75.878	6.4182×10^{-1}	-1.6493×10^{-3}	1.6937×10^{-6}
Methanol	40.152	3.1046×10^{-1}	-1.0291×10^{-3}	1.4598×10^{-6}

Source: (Chemical Properties Handbook)

Table 5.12 Heat capacity of each component

Component	Cp (J/mol.K)
Acetol	86.03
Propylene glycol	180.3

Source: (NIST,2018)

Reference temperature=298.15K

$$\Delta H = \int_{T_{ref}}^{T} Cp\, dT$$

Heat of reaction 1, $\Delta H_{rxn,\ 1} = \left(\Delta H_{f\ acetol} + \Delta H_{f\ water}\right) - \Delta H_{f\ glycerol}$

$$= (-370.06 - 285.8) - (-577.9)$$

$$= -77.96\ kJ/kmol$$

Heat of reaction 2, $\Delta H_{rxn,\ 2} = \Delta H_{f\ propylene\ glycol} - (\Delta H_{f\ acetol} + \Delta H_{f\ hydrogen})$

$$= -501 - (-370.06 + 0)$$

$$= -130.94\ kJ/kmol$$

Heat of reaction 3, $\Delta H_{rxn,\ 3} = \left(\Delta H_{f\ ethylene\ glycol} + \Delta H_{f\ methanol}\right) - \left(\Delta H_{f\ propylene\ glycol} + \Delta H_{f\ hydrogen}\right)$

$$= (-389.43 - 238.42) - (-501 + 0)$$

$$= -126.85\ kJ/kmol$$

$$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r\Delta H_{rxn}$$

Q = 19644.442 – 959.173 + [14.39(-77.96) + 13.947(-130.94) + 0.679(-126.85)]

Q = +15651.073 kJ/hr

Hence total reaction in Packed Bed Reactor (R-101) is endothermic reaction because of positive value of Q. Thus, the heat is absorbed.

5.5 COMPARISON MASS BALANCE WITH SUPERPRO

The output flowrate obtained from the mass balance calculations are compared to the output flowrate obtained from SuperPro calculations. Figure 5.11 shows the input flowrate for each component in R-101 calculated using SuperPro while figure 5.12 shows the output flowrate for each component in R-101 calculated using SuperPro.

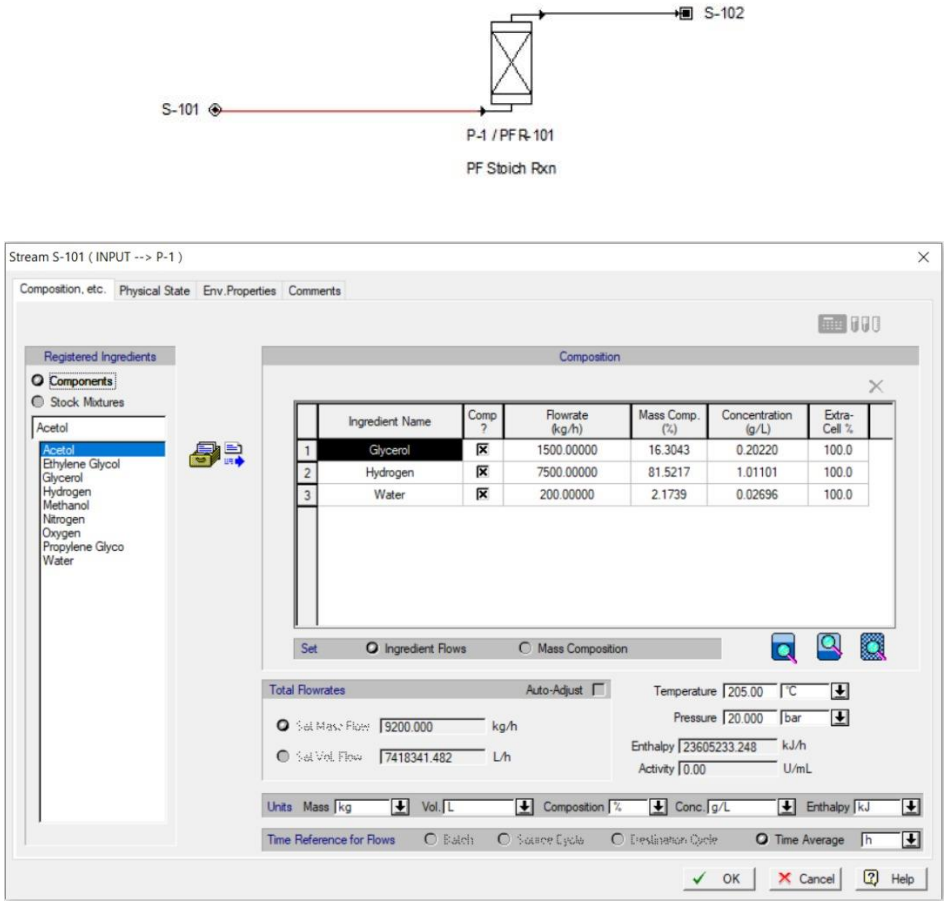

Figure 5.11 Inlet flowrate of each component in R-101 by using SuperPro

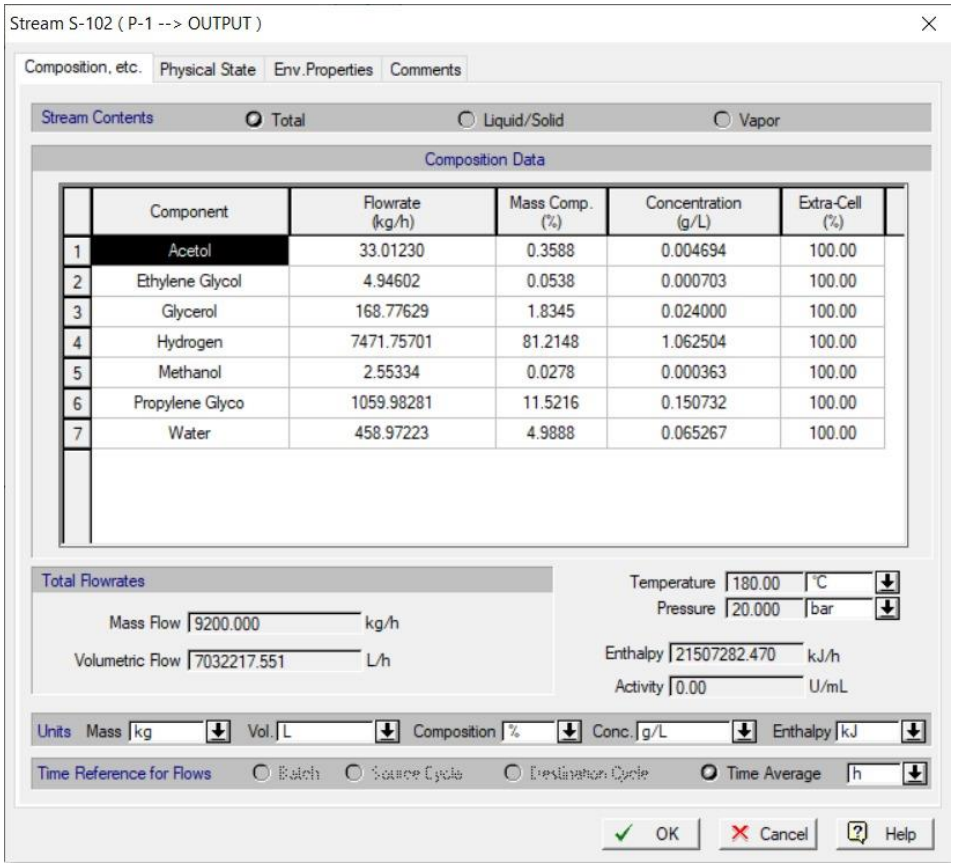

Figure 5.12 The output flowrate of each component in R-101 by using SuperPro

Table 5.13 Mass balance comparison in R-101

Component	Manual Mass Balance	SuperPro	Percentage Error (%)
Glycerol	114	168.77629	48.05
Hydrogen	7470.75	7471.75701	0.0135
Water	459.02	458.97223	0.0104
Acetol	32.78	33.01230	0.7087
Methanol	21.73	2.55334	88.25
Ethylene glycol	42.1	4.94602	88.25
Propylene glycol	1060	1059.98281	0.000016

Table 5.13 shows the comparison of output mass flowrate for each component from the manual mass balance calculation with the SuperPro calculation in R-101. The

percentage error of manual mass balance calculation with SuperPro is between 0.000016% to 88.25%. The percentage error between SuperPro are due to SuperPro does not have the unit PBR in the program. Thus, leading it to large difference in the percentage error.

5.6 COMPARISON ENERGY BALANCE WITH SUPERPRO

The inlet and outlet enthalpy calculated using energy balance calculations are compared to the inlet and outlet enthalpy calculated using SuperPro.

Table 5.14 Energy balance comparison in R-101

	Manual Mass Balance	SuperPro	Percentage Error (%)
Total Inlet Enthalpy (kJ/h)	959.173	23605233.248	100
Total Outlet Enthalpy (kJ/h)	19644.442	21507282.470	99.91

Based on Table 5.13, the percentage error of the total inlet enthalpy between the manual mass balance calculation with the SuperPro calculation in R-101 is 100% while the percentage error of the total outlet enthalpy between mass balance calculation with the SuperPro calculation in R-101 is 99.91%.

CHAPTER VI

HEAT AND MASS TRANSFER

6.1 INTRODUCTION TO HEAT AND MASS TRANSFER

Momentum transfer, heat transfer, and mass transfer are the three main transport processes that can be classed as unit operations. Many chemical and other processes involve the transfer of energy in the form of heat. A temperature difference acts as a driving force for heat transfer, and heat moves from a high to a low temperature region. Heat transmission can take place by one or more of the three primary heat transfer mechanisms: conduction, convection, or radiation. Because of a concentration difference between two sites, mass transfer occurs when a component in a mixture migrates in the same phase or from phase to phase. Distillation, absorption, drying, liquid-liquid extraction, adsorption, and membrane processes all include mass transfer. The essential mechanisms for mass transfer from one phase to another or across a single phase are the same whether the phase is a gas, liquid, or solid.

6.2 HEAT TRANSFER

The heat and mass transfer will be focused on R-101, packed bed reactor. In this reactor, the reactions of glycerol, acetol and hydrogen will happen simultaneously and Cu/Al_2O_3 will be the catalyst solid in the reactor to produce our main product which is propylene glycol. The transfer of heat conduction follows the basic equation and is written as Fourier's Law:

$$\frac{qx}{A} = -k\frac{dt}{dx}$$

Where,

qx = transfer rate in the x direction (Watts)

A= cross sectional area normal to the direction of flow of heat in m^2

T = temperature in K

X = distance in m

k = thermal conductivity in W/m.K in SI unit

In natural convection, the rate of heat transfer from solid to fluid or vice versa is calculated using the following equation:

$$q=hoA(Tw-Tf)$$

Where,

q = heat transfer rate in W

A = area in m^2

Tw = temperature of solid surface in K,

Tf = average or bulk temperature of fluid flowing past in K

hc = convective heat transfer coefficient in $W/m^2.K$

6.2.1 Heat transfer in Packed Bed Reactor (PBR)

Consider the PBR is in cylindrical shape and shows the direction of heat flow by both conduction and convection from inner side of the reactor, through the walls and to the atmosphere. We use steam jacket as our process is an endothermic reaction.

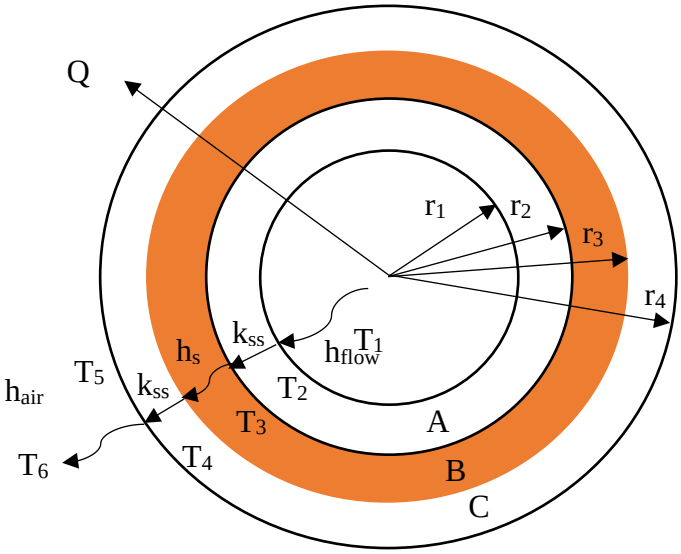

Figure 6.1 Schematic diagram of radial heat flow through multilayer cylinder

The overall equation of combine heat transfer of conduction and convection of a multilayer cylindrical wall is as follow:

$$q = \frac{T_1 - T_6}{\frac{1}{h_{flow}A_1} + \frac{(r_2 - r_1)}{k_{ss}A_{lm}} + \frac{1}{h_s A_3} + \frac{(r_4 - r_3)}{k_{ss}A_{Clm}} + \frac{1}{h_{air}A_4}}$$

$$q = \frac{T_1 - T_6}{\Sigma R}$$

$\Sigma R = 0.015831$

$$q = \frac{T_1 - T_6}{\Sigma R} = \frac{473.15 - 298.15}{0.015831} = 11054.2606 \text{ W}$$

The parameter for calculating the heat transfer:

Bulk density, $\rho_m = \frac{Total\ mass\ flowrate}{Total\ volumetric\ flowrate} = \frac{9200}{7783.6986} = 1.182$ kg/m^3

Velocity, $v = \frac{\Sigma F}{\rho \times A_1} = \frac{9200}{1.182(12.9553)} = 600.79$ m/h = 0.1669 m/s

Reynold's number, $N_{Re} = \frac{\rho VD}{\mu b} = \frac{1.182(0.1669)(1.4358)}{0.005107} = 55.5628$

Since the Reynold's number is less than 2100, thus this is a laminar flow

Bulk heat capacity, C_p = (0.01234)(2.4) + (0.81204)(14.5046) + (0.04989)(4.184) + (0.00356)(110.78) + (0.00236)(2.53) + (0.00458)(2.36) + (0.11522)(2.5) = 12.7159 kJ/kg.K = C_{pm}

Prandtl Number, $N_{pr} = \frac{\mu_b C_{pm}}{k} = \frac{0.005107(12.7159)}{13}$ = 0.004995

Nusselt Number, $Nu = \frac{hD}{k} = 1.86\left(RePr\frac{D}{L}\right)^{\frac{1}{3}}\left(\frac{\mu_b}{\mu_w}\right)^{0.14}$

$Nu = 1.86\left(55.5628\ x\ 0.004995\ x\ \frac{1.4358}{2.8716}\right)^{\frac{1}{3}}(1)^{0.14}$ = 0.963

$h = \frac{Nu(k)}{D}$ = $\frac{0.963(13)}{1.4358}$ = 8.719 W/m^2.K

Thermal conductivity and convective heat transfer coefficient show below:

k_{ss} = 13 W/m. K

h_{flow} = 8.719 W/m^2. K

h_{air} = 10 W/m^2. K

h_s = 4000 W/m^2. K

Resistance inside reactor, $R_1 = \frac{1}{h_{flow}A_1} = \frac{1}{(8.719)(12.9553)} = 0.008853$

Resistance of inner wall, $R_2 = \frac{r_2 - r_1}{k_{ss}A_{Alm}} = \frac{0.7679-0.7179}{13(13.4002)}$ = 0.000287

Resistance of steam, $R_4 = \frac{1}{h_s A_3} = \frac{1}{4000(14.7587)} = 0.000017$

Resistance of outer cover, $R_6 = \frac{r_4 - r_3}{k_{ss} A_{Clm}} = \frac{0.8679 - 0.8179}{13(14.3021)} = 0.000289$

Resistance of outside reactor, $R_7 = \frac{1}{h_{air} A_4} = \frac{1}{(10)(15.6610)} = 0.006385$

$\Sigma R = 0.015831$

6.2.2 Factor influencing heat transfer rate

From Fourier's law of conduction and Newton's law of cooling, the heat transfer rate, q, is affected by following factors:

· Surface area (A ↑, q ↑)

· Thermal conductivity (k ↑, q ↑)

· Temperature difference (ΔT ↑, q ↑)

· Distance of heat transfer (Δx ↑, q ↓)

· Convective heat transfer coefficients (h_c ↑, q ↑)

The coefficient h is a function of the system geometry, fluid properties, flow velocity and temperature difference. Therefore, the system geometry, fluid properties and flow velocity may also affect the heat transfer rate in the R-101.

6.3 MASS TRANSFER

Mass transfer or mass transport occurs when a component in a mixture migrates in the same phase or phase to phase because of difference in concentration between two points. There are two types of mass transport mechanisms which are molecular diffusion

dan convective mass transfer. Mass transfer by molecular diffusion is a movement of molecules through a fluid due to gradient concentration. Mass transfer by convection involves the transport of material between a boundary surface and a moving fluid.

6.3.1 Mass Transfer in Packed Bed Reactor (R-101)

The rate of mass transfer in the reactor (R-101), Packed Bed Reactor is calculated. The diffusivity, D_{AB} is determined by using Stokes-Einstein equation. The major component at point 1 and point 2 are glycerol and propylene glycol. Hence, species A is glycerol and species B is propylene glycol. The pressure, P is at 2000 kPa or 20 bar or 19.738 atm and the temperature, T is at 180 ˚C or 453.15 K.

From Table 6.3-2 (Geankoplis 1993), solute molar volume at its normal boiling point:

V_A of A = 96.20 x10^3 m^3/kgmol (Glycerol)

μ = 0.0111 Pa.s (Glycerol)

Diffusivity using Stokes-Einstein formula:

$$D_{AB} = \frac{9.96x10^{-7}T}{\mu\, V_A^{\frac{1}{3}}}$$

$$D_{AB} = \frac{9.96x10^{-7}(453.15)}{(0.0111)(96.20x10^{3})^{\frac{1}{3}}}$$

D_{AB} =88.74x10^{-5} m^2/s

The equation for molecular diffusion of mass law (Fick's Law) are shown below:

Parameter:

D_{AB} =88.74x10^{-5} m^2/s ,

Average concentration, C_{AV} = 14.24 kmol/m^3

Mole fraction of A, $(x_{A1} - x_{A2}) = 0.151$ (glycerol),

Height of the reactor, $\Delta z = 2.8716$ m,

$$N_A = \frac{D_{AB} C_{AV}}{(z_2 - z_1)} (x_{A1} - x_{A2})$$

$$N_A = \frac{(88.74x10^{-5})(14.24)}{(2.8716)} (0.163 - 0.012)$$

$= 6.645x10^{-4}$ kg mol / $s.m^2$

where, N_A is the mass flux (kg mol / m^2), D_{AB} is the diffusivity coefficient in m^2/s, Cav is the average total concentration, xA1 and xA2 is the mole fraction of A at point 1 and point 2 respectively.

6.3.2 Mass Transfer and Supporting Parameter

Diffusivity, mass flux, and Reynold number between glycerol and propylene glycol are calculated. The calculation is shown in Appendix D.

Table 6.1 Mass Transfer and Parameter

Parameter	Value
Diffusivity, D_{AB}	$2.28412x10^{-6}$ cm^2/s
Mass flux, N_A	$3.841x10^{-7}$ kg mol / $s.m^2$
Reynold number, N_{Re}	55.5628

Factors Influence Mass Transfer Rate

From the Fick's law equation, factors affecting the mass transfer rate are listed below:

- Concentration gradient, Δc (Δc ↑, J^*_{AZ} ↑)

- Molecular diffusivity, D_{AB} ($D_{AB}\uparrow$, $J^*_{AZ}\uparrow$)
- Distance of diffusion, Δz ($\Delta z\uparrow$, $J^*_{AZ}\downarrow$)
- Convective mass transfer coefficient, k_c ($k_c\uparrow$, $J^*_{AZ}\uparrow$)

Symbol:

J^*_{AZ} = rate of mass transfer

↑ = increase

↓ = decrease

The mass transfer coefficient is a function of the system geometry, fluid properties, flow velocity and temperature difference. Therefore, the system geometry, fluid properties and flow velocity may also affect the mass transfer rate in the PBR.

CHAPTER VII

CHEMICAL REACTION ENGINEERING I

7.1 INTRODUCTION

A chemical reactor is a sealed compartment in which a chemical reaction occurs. It is often known in chemical engineering to be a process vessel used to carry out a chemical reaction, which is one of the standard unit operations in chemical process analysis. Many aspects influence reactor design, but the thermodynamics and kinetics of the chemical processes being carried out are very important. Batch and continuous reactors are the two basic types of reactors. The batch reactor, continuous stirred-tank reactor (CSTR) and plug flow tubular reactor are the three main general chemical reactors (PFR). Each of these reactor types has its own set of traits, benefits and drawbacks.

7.2 REACTOR SELECTION

A proper reactor is chosen in order to accomplish the most optimal reaction process possible. A packed bed reactor has been adopted for the manufacturing of propylene glycol. PBR is a tubular solid catalyst particle filled catalyst that is commonly used to catalyze gas processes. The chemical reaction occurs on the catalyst's surface. We employed PBR since our reaction is heterogeneous and the procedure requires a catalyst to speed up the reaction.

The main reaction that are occur in the reactor are shown below:

$$\underset{\text{(Glycerol)}}{C_3H_8O_3} \rightarrow \underset{\text{(Acetol)}}{C_3H_6O_2} + \underset{\text{(Water)}}{H_2O} \qquad (7.1)$$

$$\underset{\text{(Acetol)}}{C_3H_6O_2} + \underset{\text{(Hydrogen)}}{H_2} \rightarrow \underset{\text{(Propylene Glycol)}}{C_3H_8O_2} \qquad (7.2)$$

The entering optimal condition at the entrance of the reactor is 205 ˚C, and 20 bar while the exiting condition is 200 ˚C at 20 bar for the top and 120 ˚C at 20 bar for the bottom. The catalyst used in this reactor is Cu/Al_2O_3 to encourage glycerol conversion and acetol hydrogenation. The benefit of employing a packed bed reactor over other catalytic reactors is the greater conversion per weight of catalyst. The catalyst used determines the conversion rather than capacity of the reactor. Another advantage of PBR is that it is simple to manufacture, has minimal operating and maintenance costs and is effective at high temperatures and pressures. The PBR is constructed of stainless steel. Stainless steel is extremely corrosion resistant and has a high endurance and hardness. Stainless steel is a totally recyclable and eco-friendly material.

7.3 GENERAL MASS BALANCE EQUATION AND KINETIC RATE EXPRESSION

The general mole equation is:

IN - OUT + GENERATION = ACCUMULATION

$$\begin{pmatrix} Rate\ of \\ flow \\ of\ A\ into \\ the \\ system \end{pmatrix} - \begin{pmatrix} Rate\ of \\ flow\ of \\ A\ out \\ of \\ the\ system \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of \\ A\ by\ chemical \\ reaction \\ within\ the \\ system \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation \\ of\ A \\ within\ the \\ system \end{pmatrix}$$

$$F_{A|w} - F_{A|W\,+\,\Delta w} + \int_0^W r\,dW = \frac{dN_A}{dt}$$

After further derivation (Appendix C), we get the weight of catalyst,

$$W = F_{AO} \int_0^x \frac{dX}{-r}$$

7.4 KINETIC RATE EXPRESSION

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O \quad \ldots\ldots\ldots\ldots\ldots (1)$$

$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$…… (2)

The kinetic rate expression for the two main reactions had been derived. Appendix C contains the calculating method. Tables 7.1 and 7.2 provide the kinetic reaction expressions of each component for the first and second reactions respectively. The kinetic rate reaction for the second reaction differs from the first reaction due to the representation of hydrogen gas in chemical equations above where a substantial amount of hydrogen gas is required to generate the product.

Table 7.1 Kinetic reaction expression of each component for 1st reaction

Species	Symbol	Initially	Change	Remaining	Concentration
$C_3H_8O_3$	A	F_{Ao}	$-F_{Ao}X$	$F_A = F_{Ao}(1-X)$	$C_A = C_{Ao}(1-X)$
$C_3H_6O_2$	B	$F_{Bo} = \Theta_{\boldsymbol{B}} F_{Ao}$	$F_{Ao}X$	$F_B = F_{Ao}(\Theta_{\boldsymbol{B}} + X)$	$C_B = C_{Ao}(\Theta_{\boldsymbol{B}} + X)$
H_2O	C	$F_{Co} = \Theta_{\boldsymbol{C}} F_{Ao}$	$F_{Ao}X$	$F_C = F_{Ao}(\Theta_{\boldsymbol{C}} + X)$	$C_C = C_{Ao}(\Theta_{\boldsymbol{C}} + X)$

Table 7.2 Kinetic reaction expression of each component for 2nd reaction

Species	Symbol	Initially	Change	Remaining	Concentration
$C_3H_6O_2$	A	F_{Ao}	$-F_{Ao}X$	$F_A = F_{Ao}(1-X)$	$C_A = \frac{C_A(1-X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$
H_2	B	$F_{Bo} = \Theta_{\boldsymbol{B}} F_{Ao}$	$-F_{Ao}X$	$F_B = F_{Ao}(\Theta_{\boldsymbol{B}} - X)$	$C_B = C_{Ao}\frac{(\Theta_B - X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$
$C_3H_8O_2$	C	$F_{Co} = \Theta_{\boldsymbol{C}} F_{Ao}$	$F_{Ao}X$	$F_C = F_{Ao}(\Theta_{\boldsymbol{C}} + X)$	$C_C = C_{Ao}\frac{(\Theta_C - X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$

7.5 GRAPH LEVENSPIEL PLOT (VOLUME)

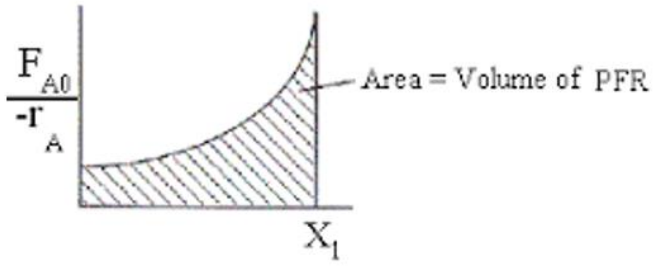

Figure 7.1 Graph Levenspiel Plot of PBR

The graph above may be plotted using the equation below and the volume of the reactor required can be calculated using the equation below. The length of the reactor may also be determined using the volume derived from the graph. The area under the curve of the graph in figure 7.1 represent the volume value for the reactor.

$$\frac{V}{F_{Ao}} = \int_0^X \frac{dX}{-r_A}$$

$$V = \int_0^X \left(\frac{F_{Ao}}{-r_A}\right) dX$$

7.6 CATALYST

Baron J. J. Berzelius invented the word “catalysis” in 1835 to characterize the quality of compounds that assist chemical processes without being consumed in them. Catalysis, in a wide sense also includes elements that slow the pace of a process. While catalysts can have a significant impact on the pace of a reaction, the equilibrium composition of reactants and products is still governed purely by thermodynamics. In the production of Propylene Glycol, Cu/Al_2O_3 has been used to act as a heterogenous catalyst.

The fundamental advantage of utilizing a heterogeneous catalyst is the simplicity with which the catalyst can be separated from the product stream, which

benefits in the development of continuous chemical processes. Furthermore, heterogeneous catalysts are often more resistant to hard working condition than their homogeneous counterparts. Adsorption of reactants from a fluid phase onto a solid surface, surface reaction of adsorbed species and desorption of products into the fluid phase are all part of a heterogeneous catalytic reaction.

7.7 REACTION AND BY-PRODUCTS

The reactor undergoes three reactions which are glycerol dehydration, acetol hydrogenation and glycerol hydrogenation. The first two reactions, dehydration of glycerol and hydrogenation of acetol are the most important in this process. These two reactions will result in the primary product. The first reaction produces acetol, which may then be employed in the second reaction. Finally, the second reaction will provide the major component, propylene glycol. The third reaction is a side reaction that results in the formation of byproducts such as methanol and ethylene glycol. The catalyst is used to improve the selectivity of the primary product. This method generates methanol, acetol, water, ethylene glycol and unreacted glycerol as byproducts. All of the byproducts will not be deemed trash and the purity of the byproducts will be monitored because they may still be sold at a profit.

7.8 SEPARATION METHOD OF THE PRODUCT

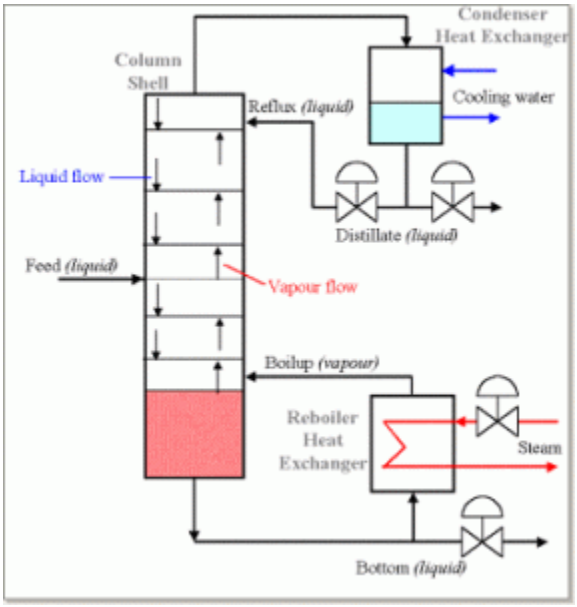

Figure 7.2 Process in distillation column.

Source: (SRS Engineering Corporation, 2018)

We chose the distillation process as our product separation method due to its high purity and ease of management. The distillation process is used to separate the product as a separation procedure. Distillation, also known as classical distillation is the process of separating the constituents or substances of a liquid mixture by selective boiling and condensation.

The distillation column is depicted in Figure 7.1 as a series of stacked plates. At one or more places, a liquid feed comprising a combination of two or more liquids enters the column. The liquid runs over the plates while vapor bubbles up through the perforations in the plates. The vapor comes into touch with the liquid multiple times as it moves down the column. The liquid and vapor phases are brought into contact due to one of a high molecule of higher boiling material releases energy to convert from the vapor to the liquid phase, whereas another molecule of a lower boiling material uses free energy to convert from the liquid to the vapor phase (Anon. 2018).

7.9 PRODUCT STABILIZING

The average period for propylene glycol to become unstable is two years. There are various precautions that must be taken to ensure that the product lasts that long. To begin, all reactor and column materials utilized in this process must be highly grade stainless steel, all stainless steels have a strong corrosion resistance. Low alloyed grades are resistant to corrosion in air, highly alloyed grades are resistance to corrosion in most acids, alkaline solutions and chloride carrying environment even at high temperature and pressure, Stainless steel also have a good temperature resistance.

Second, the product’s packaging must be flawlessly controlled. Propylene Glycol has a two-year shelf life when stored at room temperature in closed containers away from sunlight and other UV light sources. This shelf life is confirmed by a continuous stability resting procedure. The shelf life of a product refers to the amount of time it may be stored under proper circumstances and still meets it sales specifications. Where product heating is used (for example, in bulk storage and/or

transport containers), the temperature of the product should be managed to avoid unintended overheating over lengthy periods, which might lead to rapid oxidative deterioration of the product. Dow advise heating up to no more than 40 ˚C as a general guideline. Metal drums are the most commonly recommended product container for industrial use.

CHAPTER VIII

CHEMICAL ENGINEERING COMPUTATION

8.1 INTRODUCTION

GNU Octave is a proprietary programming language and multi-paradigm numerical computing environment. The mass balance for the propylene glycol generation process in the reactor was computed using this GNU Octave programme. To compute the mass balance, the user must enter the desired input amount of molar flowrate and output amount of molar flowrate at the reactor. The reactor R-101 is used in the GNU Octave coding for the manufacture of propylene glycol.

8.2 ALGORITHM

An algorithm is a set of instructions for completing a task or producing a certain outcome. There should be no ambiguity in the steps. The mass balance algorithm for the reactor in the propylene glycol manufacturing process is illustrated below.

1. Start
2. Fix the stoichiometry coefficient for glycerol, hydrogen, water, acetol, methanol, ethylene glycol and propylene glycol based on the process that occur at the reactor.
3. Input the molar flowrate of glycerol, hydrogen, water, acetol, methanol, ethylene glycol and propylene glycol.
4. If the inlet molar flowrate is less than 0, ‘Error! Enter positive value only’ will appear in the program and the program will ask the user to re-enter the value of the inlet molar flowrate.
5. Input the rate of reaction, r for each process in the reactor R-101.

6. Compute the output molar flowrate for glycerol, hydrogen, water, acetol, methanol, ethylene glycol and propylene glycol by addition of input molar flowrate with a variable in which the variable is the multiplication of the stoichiometric coefficient with the reaction rate, r of the corresponding components.
7. Set the molecular weight or molar mass of for glycerol, hydrogen, water, acetol, methanol, ethylene glycol and propylene glycol equal to 92.1, 2, 18, 74, 32, 62, 76 respectively.
8. Change the input and output molar flowrate of all the components in the reactor to mass flowrate by multiplying it with their respective molecular weight.
9. Compute the total input and output mass flowrate of the reactor by adding the input mass flowrate of all components and output mass flowrate of all components.
10. Display the input and output flowrate of each component and the total flowrate to check whether it is balance or not.
11. End

8.3 FLOWCHART

Algorithm is represented visually or graphically in a flowchart. Each part is represented by a standard symbol. The flowchart for calculating the mass balance is shown in Figure 8.1.

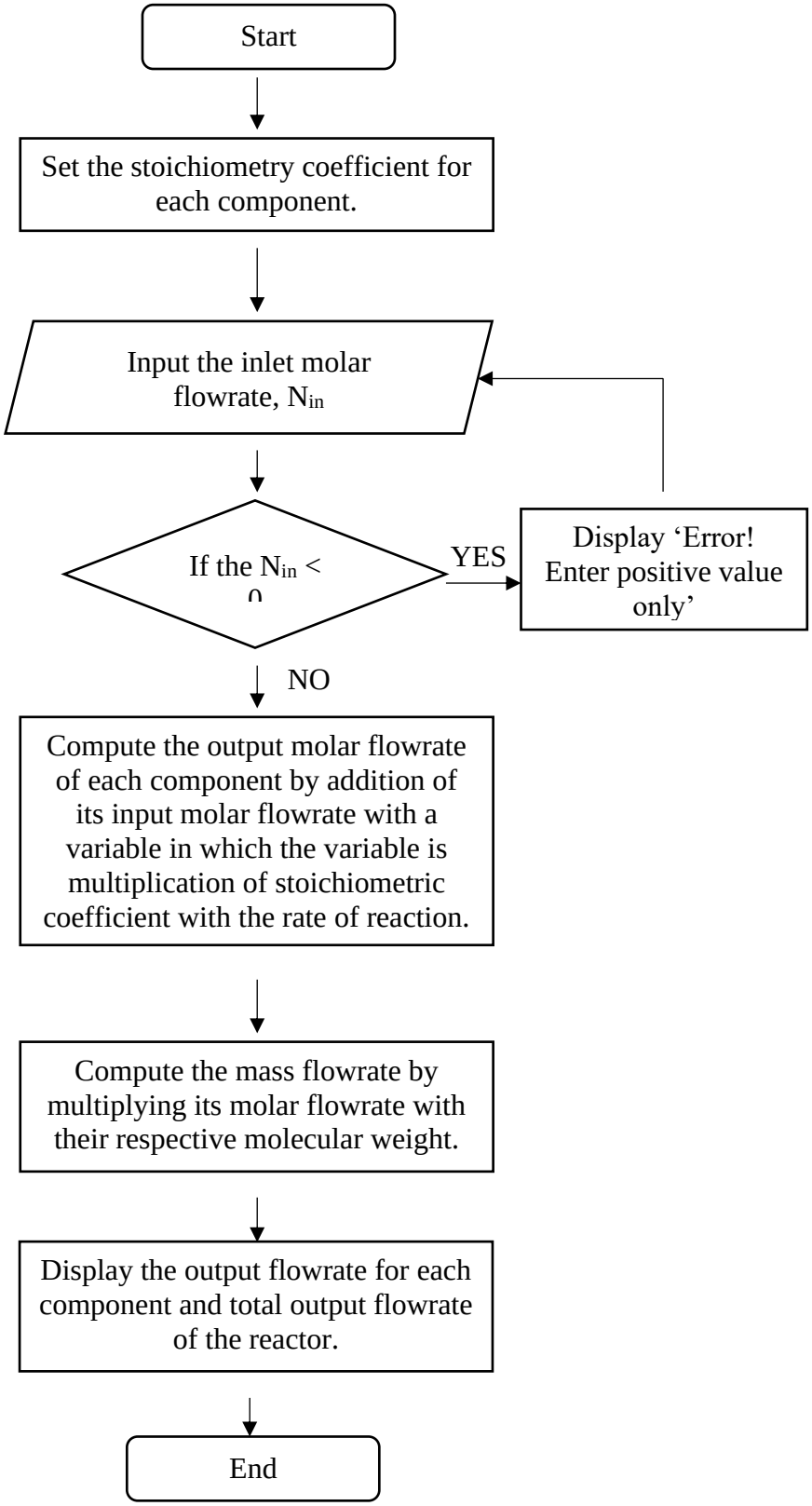

Figure 8.1 Flowchart for mass balance calculation

8.4 GNU OCTAVE PROGRAMMING

The coding of GNU Octave for production of propylene glycol involves in reactor R-101 is shown in Appendix D.

8.4.1 Result of GNU Octave Programming

```
Enter the input molar flowrate of glycerol= 16.3
Enter the input molar flowrate of hydrogen= 3750
Enter the input molar flowrate of water= 11.11
Enter the input molar flowrate of acetol= 0
Enter the input molar flowrate of methanol= 0
Enter the input molar flowrate of ethylene  glycol= 0
Enter the input molar flowrate of propylene glycol= 0
```

Table of mass balance in reactor R-101

Component	Inlet Mass Flowrate (kg/h)	Outlet Mass Flowrate (kg/h)
Glycerol	1499.60	113.25
Hydrogen	7500.00	7470.75
Water	199.98	459.00
Acetol	0.00	32.78
Methanol	0.00	21.73
Ethylene glycol	0.00	42.10
Propylene glycol	0.00	1059.97
Total	9199.58	9199.58

Mass balance in = Mass balance out

9199.58kg/h = 9199.58kg/h (Balanced!)

Figure 8.2 Result of the GNU Octave program

Figure 8.2 shows the result of the GNU Octave program of the input and output mass flowrate of each component and the total input and output mass flowrate.

8.5 COMPARISON WITH MANUAL CALCULATION AND SUPERPRO

Table 8.1 shows the comparison of output mass flowrate from the programming with the manual mass balance and SuperPro in R-101.

Table 8.1 Mass balance comparison by component in R-101

Component	Programming Flowrate (kg/h)	Mass Balance Flowrate (kg/h)	SuperPro (kg/h)	Percentage Error 1 (%)	Percentage Error 2 (%)
Glycerol	113.25	114	168.77629	0.6623	49.03
Hydrogen	7470.75	7470.75	7471.75701	0	0.0134
Water	459	459.02	458.97223	0.00436	0.00605

Acetol	32.78	32.78	33.01230	0	0.7087
Methanol	21.73	21.73	2.55334	0	88.25
Ethylene glycol	42.10	42.1	4.94602	0	88.25
Propylene glycol	1059.97	1060	1059.98281	0.00283	0.00121

Based on table 8.1, the percentage error 1 is the percentage error betwen programming and manual mass balance calculation for outlet mass flowrate of each component in reactor R-101 which is in between 0% to 0.6623%. The percentage error 2 is the percentage error between programming and SuperPro mass balance calculation. The percentage error 2 is between 0.00121% to 88.25%. The difference in the percentage error 1 are due to decimal point taken when calculating the manual calculation. The difference in percentage error 2 are due to SuperPro does not have the unit PBR in the program. Thus, leading to large difference in the percentage error.

CONCLUSION

Propylene Glycol is a small molecule with two hydroxyl groups (-OH) which is known by other name such as 1,2-propanediol with molecular formular of $C_3H_8O_2$. Propylene Glycol is a substance that has a lot of benefits and usage. It is commonly used as a solvent and a drug stabiliser. The main objective of this project which is to produce propylene glycol in large scale is achieved.

For the economic aspect of production of propylene glycol, the world consumption od propylene glycol is increasing year to year. The market growth of propylene glycol is expected to grow with CAGR of 4.4% over 2017 to 2026. The plant capacity of propylene glycol in our process is 1060 kg/hours which contribute about 5% of global demand.

Later, in the following chapter is discussion about the safety issue on material and method to handle our propylene glycol. It was discussed about environmental issue where we discuss about the waste generated in our process which are wastewater and unreacted glycerol and techniques on how the waste is managed in our process.

Based on the project, mass balance for entire plant and energy balance for reactor have been performed. From referring to overall mass balance inlet mass flow rate is equal to outlet mass flowrate which is 1729.25 kg/hours. The energy balance performed in the packed bed reactor show that the reaction is +15651.073 kJ/hour, thus the reaction is endothermic. Heat is released to the surrounding. Calculation of mass balance is also done by using SuperPro simulation and there is a difference in value between both manual and SuperPro simulation.

There are two types of heat transfer mechanism involved in the packed bed reactor which is conduction and convection. The calculated overall heat transfer of a reactor is 11054.2606W. The diffusivity, D_{AB} was calculated by using Stokes-Einstein equation which is 88.74×10^{-5} m/s and the molecular diffusion of mass transfer that has been calculated is 6.645×10^{-4} kgmol/m^2s. There are also some of the factors that is influencing the heat transfer rate and mass transfer rate. The general mole balance equation is the starting point to determine the various input and output chemical species in the reaction process at certain operating conditions. The general mole balance equation of the packed bed reactor is similar to packed bed reactor derived. For the

chemical engineering computation, algorithm and flowchart to compute the mass balance in the packed bed reactor is constructed. The GNU Octave program is also constructed with the percentage error between 0% to 0.6623% compared to the manual calculation of mass balance in the packed bed reactor.

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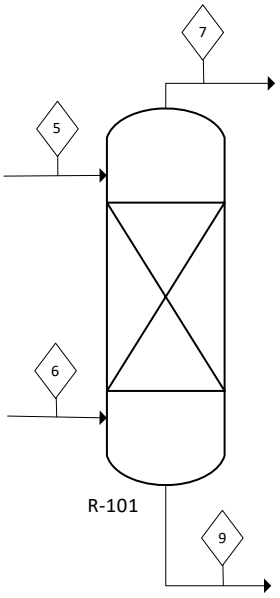
APPENDIX A

MASS BALANCE

Reactor, R-101



	5	6	7	9
Glycerol	0.8824	0	0	0.0937
Hydrogen	0	1	0.3454	0
Water	0.1176	0	0.5852	0
Acetol	0	0	0.0416	0
Methanol	0	0	0.0278	0
EG	0	0	0	0.0347
PG	0	0	0	0.8746
Total	1700	300	783.8	1216.2

$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$ - ①

$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$ - ②

$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH$ - ③

REQUIRE REACTANT

$$C_3H_6O_2 + H_2 \rightarrow C_3H_8O_2$$

$$N_{2PG} = 1060kg/h \div 76 = 13.947kmol/h$$

Since $\alpha = 1\ or - 1$, so

$$N_{2Acetol} = N_{2PG} = N_{2H} = 13.947\text{kmol/h}$$

$$r_2 = 13.947kmol/h$$

$$F_{2H} = 27.894kg/h$$

EXCESS REACTANT

$$Y = \frac{N_{2PG}}{N_{1Acetol}} = 0.969$$

$$\frac{13.947}{N_{1Acetol}} = 0.969$$

$$N_{1Water} = N_{1Acetol} = N_{1Glycerol} = 14.393kmol/h$$

$$r_1 = 14.39kmol/h$$

$$F_{1Water} = 14.39(18) = 259.02kg/h$$

$$N_{excess\ Acetol} = 14.39 - 13.947 = 0.443kmol/h$$

$$F_{excess\ Acetol} = 0.443(74) = 32.78kg/h$$

$$F_{Glycerol} = 14.39(92) = 1323.88kg/h$$

REACTION 3

<u>Ratio overall reactor</u>

Glycerol:Hydrogen

1:5

$$F_{G(3)} + 1323.88 : F_{H(3)} + 27.894$$

Assume Total glycerol= 1500kg/h and total hydrogen 7500kg/h

$$F_{G(3)} = 1500 - 1323.88 = 176.12kg/h$$

$$F_{H(3)} = 7500 - 27.894 = 7472.106kg/h$$

REQUIRE REACTANT

$$C_3H_8O_3 + H_2 \rightarrow C_2H_6O_2 + CH_3OH \text{ - } ③$$

$$N_{G(3)} = \frac{176.12}{92} = 1.914kmol/h$$

$$N_{H(3)} = \frac{7472.106}{2} = 3736.053kmol/h$$

$$S_{EG} = \frac{r_3}{N_{G(3)}}$$

$$0.3548 = \frac{r_3}{1.914}$$

$$r_3 = 0.679kmol/h$$

$N_{G(3i)} = N_{G(3o)} - \alpha r_3$

$N_{G(3i)} = 0 - (-1)0.678 = 0.679kmol/h$

$N_{G(3)} = N_{H(3)} = N_{EG(3)} = N_{M(3)}$

$N_{M(3)} = 0.679(32) = 21.73kg/h$

$N_{EG(3)} = 0.679(62) = 42.1kg/h$

EXCESS REACTANT

$$N_{G(excess)} = 1.914 - 0.679 = 1.235kmol/h = 113.62kg/h$$

$$N_{H(excess)} = 3736.053 - 0.678 = 3735.375kmol/h = 7470.75kg/h$$

INPUT AND OUTPUT

Consider total recycle of H_2

$Total_{H_2} = 7500kg/h$

$Recycle_{H_2} = 7470.75kg/h$

$Input = 7500 - 7470.75 = 29.25kg/h$

Assuming 200kg/h of water added in stream glycerol to dilute the 1500kg/h glycerol.

$$Total\ water = 200 + 259.02 = 459.02kg/h$$

	IN (kg/h)	OUT (kg/h)
Glycerol	1500	113.62
Hydrogen	7500	7470.75
Water	200	459.02
Acetol	0	32.78
Methanol	0	21.73
EG	0	42.1
PG	0	1060
Total	9200	9200

ENERGY BALANCE

Inlet Enthalpy

Stream 7

$\Delta H_{glycerol} = \int_{298.15}^{478.15} 132.145 + 8.6007 \times 10^{-1}T + -1.9745 \times 10^{-3}T^2 + 1.8068 \times 10^{-6}T^3 dT$

$= 49412$ J/mol

$= 49.412\ kJ/kmol$

$\Delta H_{water} = \int_{298.15}^{478.15} 92.053 + -3.9953 \times 10^{-2}T + -2.1103 \times 10^{-4}T^2 + 5.3469 \times 10^{-7}T^3\ dT$

$= 13884$ J/mol

$= 13.884\ kJ/kmol$

Stream 9

$\Delta H_{hydrogen} = \int_{298.15}^{298.15} 27.13 + 9.27 \times 10^{-3}T + -1.38 \times 10^{-5}T^2 + 7.46 \times 10^{-9}T^3\ dT$

$= 0$ kJ/kmol

Outlet Enthalpy

Stream 10

$\Delta H_{methanol} = \int_{298.15}^{473.15} 40.152 + 3.1046 \times 10^{-1}T + -1.0291 \times 10^{-3}T^2 + 1.4598 \times 10^{-6}T^3\ \ dT$

$= 16142$ J/mol

$= 16.142\ kJ/kmol$

$\Delta H_{water} = \int_{298.15}^{473.15} 92.053 + -3.9953 \times 10^{-2}T + -2.1103 \times 10^{-4}T^2 + 5.3469 \times 10^{-7}T^3\ dT$

$= 13469$ J/mol

$= 13.469\ kJ/kmol$

$\Delta H_{hydrogen} = \int_{298.15}^{473.15} 27.13 + 9.27 \times 10^{-3}T + -1.38 \times 10^{-5}T^2 + 7.46 \times 10^{-9}T^3\ dT$

$=$ 5087 J/mol

$= 5.087\ kJ/kmol$

$\Delta H_{acetol} = \int_{298.15}^{473.15} 86.03\ \mathrm{dT}$

$= 15055$ J/mol

$= 15.055\ kJ/kmol$

Stream 12

$\Delta H_{propylene\ glycol} = \int_{298.15}^{393.15} 180.3\ \mathrm{dT}$

$= 17128.5$ J/mol

$= 17.129\ kJ/kmol$

$\Delta H_{ethylene\ glycol} = \int_{298.15}^{393.15} 75.878 + 6.4182 \times 10^{-1}T + -1.6493 \times 10^{-3}T^2 + 1.6937 \times 10^{-6}T^3\ dT$

$= 16216$ J/mol

$= 16.216\ kJ/kmol$

$\Delta H_{unreacted\ glycerol} = \int_{298.15}^{393.15} 132.145 + 8.6007 \times 10^{-1}T + -1.9745 \times 10^{-3}T^2 + 1.8068\ \times 10^{-6}T^3 dT$

$= 25466$ J/mol

$= 25.466\ kJ/kmol$

$\Delta H_{outlet} = \sum N\Delta H$

$\Delta H_{outlet} =$ 3735.37(5.087) + 25.5(13.469) + 0.44(15.055) + 0.68(16.142) + 1.24(25.466) + 0.68(16.216) + 13.95(17.129)

$\Delta H_{outlet} = 19644.442\ kJ$/hr

$\Delta H_{inlet} = \sum N\Delta H$

$\Delta H_{inlet} =$ 16.29(49.412) + 11.11(13.884) + 150(0)

$\Delta H_{inlet} = 959.173\ kJ$/hr

APPENDIX B

HEAT TRANSFER CALCULATION

a. Calculating the bulk density

Table 6.2 Mass Flowrates, density and volumetric flowrates

Component	Mass flowrate (kg/h)	ρ (kg/m^3)	V (m^3/h)
Glycerol	113.62	1260	0.0902
Hydrogen	7470.75	0.96	7782.0313
Water	459.02	997	0.4604
Acetol	32.78	1019	0.0322
Methanol	21.73	792	0.0274
Ethylene glycol	42.1	1110	0.0379
Propylene glycol	1060	1040	1.0192
Total	9200	-	7783.6986

Bulk density, $\rho_m = \frac{Total\ mass\ flowrate}{Total\ volumetric\ flowrate} = \frac{9200}{7783.6986} = 1.182\ kg/m^3$

b. Calculating the volume

Total volumetric flowrate, $V_{total} = \frac{7783.6986\ m^3}{h}\left(\frac{1\ h}{3600\ s}\right) = 2.1621\ m^3/s$

We set the residence time to be = 2.15 seconds

Hence, $V_{total} = 2.1621\ (2.15) = 4.6485\ m^3$

c. Calculating the height of the reactor

$V = \pi r^2 L$, $D = 2r$, $L = 2D = 2(2r)$

$$\frac{Internal\ diameter\ of\ reactor, D}{Height\ of\ reactor, L} = \frac{1}{2}$$

$4.6485 = 4\pi r^3$, $r^3 = 0.3699$ so r= 0.7179

Radius of inner reactor, $r_1 = 0.7179$ m

Radius of outer reactor, $r_2 = 0.7679$ m

Radius of cooling jacket, $r_3 = 0.8179$ m

Radius of outer cover, $r_4 = 0.8679$ m

Hence, height of reactor, L = 2D = 2(2r) = 4r = 4(0.7179) = 2.8716 m

d. Calculating the area and the log mean area inside the reactor

Based on the radiuses and the height of the reactor, the area are as follows:

$A_1 = 2\pi L r_1 = 2\pi$ (2.8716) (0.7179) =12.9553 m^3

$A_2 = 2\pi L r_2 = 2\pi$ (2.8716) (0.7679) = 13.8551 m^3

$A_3 = 2\pi L r_3 = 2\pi$ (2.8719) (0.8179) = 14.7587 m^3

$A_4 = 2\pi L r_4 = 2\pi$ (2.8719) (0.8679) = 15.6610 m^3

Log Mean Areas are calculated as follows:

$$A_{Alm} = \frac{A_2 - A_1}{\ln \frac{A_2}{A_1}} = \frac{13.8551 - 12.9553}{\ln \frac{13.8551}{12.9553}} = 13.4002$$

$$A_{Blm} = \frac{A_3 - A_2}{\ln \frac{A_3}{A_2}} = \frac{14.7587 - 13.8551}{\ln \frac{14.7587}{13.8551}} = 14.3021$$

$$A_{Clm} = \frac{A_4 - A_3}{\ln \frac{A_4}{A_3}} = \frac{15.6610 - 14.7587}{\ln \frac{15.6610}{14.7587}} = 15.2054$$

e. Calculating the Reynold's number

Table 6.3 Dynamic viscosity of components

Component	Dynamic viscosity μ (Pa.s)	Mass fraction, w
Glycerol	0.0111	0.01234
Hydrogen	8.8×10^{-6}	0.81204
Water	8.9×10^{-4}	0.04989
Acetol	1.593×10^{-3}	0.00356
Methanol	1.51×10^{-5}	0.00236
Ethylene glycol	0.0161	0.00458
Propylene glycol	0.042	0.11522

Bulk viscosity,

$\mu b = \Sigma(w.\mu)$

$\mu b = (0.01234)(0.0111) + (0.81204)(8.8 \times 10^{-6}) + (0.04989)(8.9 \times 10^{-4}) + (0.00356)(1.593 \times 10^{-3}) + (0.00236)(1.51 \times 10^{-5}) + (0.00458)(0.0161) + (0.11522)(0.042) = 0.005107$ Pa.s

Velocity in the reactor,

$$v = \frac{\Sigma F}{\rho \times A_1} = \frac{9200}{1.182(12.9553)} = 600.79 \text{ m/h} = 0.1669 \text{ m/s}$$

Reynold's number,

$$N_{Re} = \frac{\rho VD}{\mu b} = \frac{1.182(0.1669)(1.4358)}{0.005107} = 55.5628$$

Since the Reynold's number is less than 2100, thus this is a laminar flow

f. Calculating dimensionless number

Table 6.4 Specific heat capacity of components

Component	C_p (kJ/kg.K)	Mass fraction, w
Glycerol	2.4	0.01234
Hydrogen	14.5046	0.81204
Water	4.184	0.04989
Acetol	110.78	0.00356
Methanol	2.53	0.00236
Ethylene glycol	2.36	0.00458
Propylene glycol	2.5	0.11522

Bulk heat capacity,

$C_p = \Sigma(wC_p)$

C_p = (0.01234)(2.4) + (0.81204)(14.5046) + (0.04989)(4.184) + (0.00356)(110.78) + (0.00236)(2.53) + (0.00458)(2.36) + (0.11522)(2.5) = 12.7159 kJ/kg.K = C_{pm}

Since the reactor is made of stainless steel 316, then

k = 13 W/m.K

Prandtl Number,

$N_{pr} = \frac{\mu_b C_{pm}}{k} = \frac{0.005107(12.7159)}{13} = 0.004995$

Sieder - Tate correlation of Nusselt number is used to calculate the laminar flow heat transfer coefficient

Since $\mu_b = \mu_w$ since the temperature is the same for the bulk and wall of the reactor

$$Nu = \frac{hD}{k} = 1.86\left(RePr\frac{D}{L}\right)^{\frac{1}{3}}\left(\frac{\mu_b}{\mu_w}\right)^{0.14}$$

$Nu = 1.86\left(55.5628\ x\ 0.004995\ x\ \frac{1.4358}{2.8716}\right)^{\frac{1}{3}}(1)^{0.14} = 0.963$

$h = \frac{Nu(k)}{D} = \frac{0.963(13)}{1.4358} = 8.719$ W/m^2.K

g. Calculating for resistance

Thermal conductivity and convective heat transfer coefficient show below:

$k_{ss} = 13$ W/m. K

$h_{flow} = 8.719$ W/m^2. K

$h_{air} = 10$ W/m^2. K

$h_s = 4000$ W/m^2. K

Resistance inside reactor, $R_1 = \frac{1}{h_{flow}A_1} = \frac{1}{(8.719)(12.9553)} = 0.008853$

Resistance of inner wall, $R_2 = \frac{r_2 - r_1}{k_{ss}A_{Alm}} = \frac{0.7679-0.7179}{13(13.4002)} = 0.000287$

Resistance of steam, $R_4 = \frac{1}{h_s A_3} = \frac{1}{4000(14.7587)} = 0.000017$

Resistance of outer cover, $R_6 = \frac{r_4 - r_3}{k_{ss} A_{Clm}} = \frac{0.8679 - 0.8179}{13(14.3021)} = 0.000289$

Resistance of outside reactor, $R_7 = \frac{1}{h_{air} A_4} = \frac{1}{(10)(15.6610)} = 0.006385$

MASS TRANSFER CALCULATION

CALCULATION OF MOLECULAR WEIGHT

a. Molecular weight at point 1

Table 6.5 Mass Flow Rate, Molecular Weight, and Mole Fraction of Component at Point 1 of Reactor (R-101)

Component / Input	Mass flow rate, F(kg/hr)	Molecular weight, M(g/mol)	Mole fraction, x
Hydrogen	7500	2	0.815
Water	200	18	0.022
Glycerol	1500	92	0.163
Acetol	0	74	0
Methanol	0	32	0
Ethylene Glycol (EG)	0	62	0
Propylene Glycol (PG)	0	76	0

Molecular weight at point 1, $M_A = 2(0.815) + 18(0.022) + 92(0.163)$

$= 17.022$ g/mol

b. Molecular weight at point 2

Table 6.6 Mass Flow Rate, Molecular Weight, and Mole Fraction of Component at Point 2 of Reactor (R-101)

Component / Output	Mass flow rate, F(kg/hr)	Molecular weight, M(g/mol)	Mole fraction, x
Hydrogen	7470.75	2	0.812
Water	459.02	18	0.050
Glycerol	113.62	92	0.012
Acetol	32.78	74	0.004
Methanol	21.73	32	0.002
Ethylene Glycol (EG)	42.1	62	0.005
Propylene Glycol (PG)	1060	76	0.115

Molecular weight at point 2, $M_B = 2(0.812) + 18(0.050) + 92(0.012) + 74(0.004) + 32(0.002) + 62(0.005) + 76(0.115)$

$= 13.038$ g/mol

CALCULATION OF CONCENTRATION

c. Concentration at point 1

Table 6.7 Mass Flow Rate, Density, and Mole Fraction of Component at Point 1 of Reactor (R-101)

Component / Input	Mass flow rate, F(kg/hr)	Density, ρ(kg/m^3)	Mole fraction, x
Hydrogen	7500	0.96	0.815
Water	200	997	0.022
Glycerol	1500	1260	0.163
Acetol	0	1019	0
Methanol	0	792	0
Ethylene Glycol (EG)	0	1110	0
Propylene Glycol (PG)	0	1040	0

Density at point 1, $\rho_A = 0.96(0.815) + 997(0.022) + 1260(0.163)$

$= 228.10 \text{ kg/m}^3$

Concentration at point 1, $C_A = \frac{\rho A}{MA}$

$= \frac{228.10}{17.022}$

$= 13.40 \text{ kmol/m}^3$

d. Concentration at point 2

Table 6.8 Mass Flow Rate, Density, and Mole Fraction of Component at Point 2 of Reactor (R-101)

Component / Output	Mass flow rate, F(kg/hr)	Density, ρ(kg/m^3)	Mole fraction, x
Hydrogen	7470.75	0.96	0.812
Water	459.02	997	0.050
Glycerol	113.62	1260	0.012
Acetol	32.78	1019	0.004
Methanol	21.73	792	0.002
Ethylene Glycol (EG)	42.1	1110	0.005
Propylene Glycol (PG)	1060	1040	0.115

Density at point 2, $\rho_B = 0.96(0.812) + 997(0.050) + 1260(0.012) + 1019(0.004) + 792(0.002) + 1110(0.005) + 1040(0.115)$

$= 196.56 \text{ kg/m}^3$

Concentration at point 2, $C_B = \frac{\rho B}{MB}$

$= \frac{196.56}{13.038}$

$= 15.08 \text{ kmol/m}^3$

Average concentration, $C_{AV} = \frac{CA + CB}{2}$

$$= \frac{13.40 + 15.08}{2}$$

$$= 14.24 \text{ kmol/m}^3$$

CALCULATION OF DIFFUSIVITY, D_{AB} AND MASS FLUX, N_A

e. Calculation Diffusivity, D_{AB}

The diffusivity, D_{AB} is determined by using Fuller et al. method. The major component at point 1 and point 2 are glycerol and propylene glycol. Hence, species A is glycerol and species B is propylene glycol. The pressure, P is at 2000 kPa or 20 bar or 19.738 atm and the temperature, T is at 180 ˚C or 453.15 K.

From Table 6.3-2 (Geankoplis 1993), solute molar volume at its normal boiling point:

$V_A = 14.8(3) + 3.7(8) + 7.4(3)$

$=96.20 \text{ x}10^3 \text{ m}^3/\text{kgmol}$

$\mu = 0.0111$ Pa.s (Glycerol)

Diffusivity using Stokes-Einstein formula:

$$D_{AB} = \frac{9.96x10^{-7}T}{\mu V_A^{\frac{1}{3}}}$$

$$D_{AB} = \frac{9.96x10^{-7}(453.15)}{(0.0111)(96.20x10^3)^{\frac{1}{3}}}$$

$D_{AB} = 88.74\text{x}10^{-5} \text{ cm}^2/\text{s}$

f. Calculation of Fick's Law, N_A

$$N_A = \frac{D_{AB}C_{AV}}{(z_2 - z_1)}(x_{A1} - x_{A2})$$

$$N_A = \frac{(88.74x10^{-5})(14.24\ )}{(2.8716)}(0.163 - 0.012)$$

$= 6.645x10^{-4}$ kg mol / s.m^2

CALCULATION OF DIMENSIONLESS NUMBER

g. Reynold Number

$N_{Re} = 55.5628$

From calculation in (heat transfer), the Reynolds number is less than 2100 is a laminar flow

APPENDIX C

CHEMICAL REACTION ENGINEERING I

REACTOR SELECTION

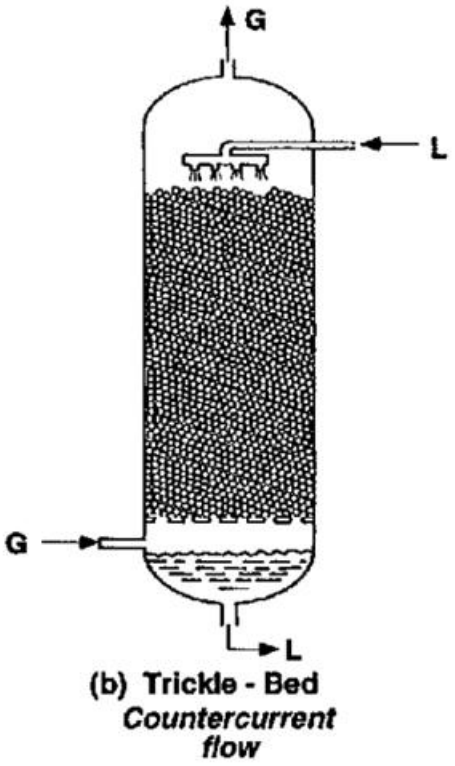


Figure 7.3 Packed Bed Reactor

Source:Research Gate

The reactor that we use is Trickle-bed Countercurrent flow. The diagram above depicts how our reactor operates at the plant. The liquid will enter the reactor from the top while the gas will enter from the bottom. The reaction will take place in the reactor's center, where all of the solid catalyst is situated.

GENERAL MASS BALANCE EQUATION AND KINETIC RATE EXPRESSION

The general mole equation is:

IN - OUT + GENERATION = ACCUMULATION

$$\begin{pmatrix} Rate\ of \\ flow \\ of\ A\ into \\ the \\ system \end{pmatrix} - \begin{pmatrix} Rate\ of \\ flow\ of \\ A\ out \\ of \\ the\ system \end{pmatrix} + \begin{pmatrix} Rate\ of \\ generation\ of \\ A\ by\ chemical \\ reaction \\ within\ the \\ system \end{pmatrix} = \begin{pmatrix} Rate\ of \\ accumulation \\ of\ A \\ within\ the \\ system \end{pmatrix}$$

$$F_{A|w} \quad - \quad F_{A|W\,+\,\Delta w} \quad + \quad \int_0^W r\,dW \quad = \quad \frac{dN_A}{dt}$$

After further derivation (Appendix C), we get the weight of catalyst,

$$W = F_{AO} \int_0^x \frac{dX}{-r}$$

Since the PBR will be operated in steady state, hence, The accumulation will be zero. PBR is assumed to have no radial gradients in concentration, temperature or reaction rate

$$\frac{dN_A}{dt} = 0\ ; \int_0^W r\,dW \quad = r\,dW$$

$$F_{A|w} - F_{A|W\,+\,\Delta w} + r\,dW = 0$$

We get the differential form of the mole balance for packed bed reactor by dividing by W and taking the limit as W=0. When pressure loss across the reactor and catalyst decay are taken into account, the integral version of the packed catalyst bed design equation (1) mat be utilized to compute catalyst weight.

$$\frac{F_{A|w} - F_{A|W\,+\,\Delta w}}{\Delta W} + \frac{r\Delta W}{\Delta W} = 0$$

$$\frac{F_{A|w} - F_{A|W\,+\,\Delta w}}{\Delta W} = r$$

$$\frac{dF_A}{dW} = r \text{ ---- (1)}$$

$$w = \int_{F_A}^{F_{AO}} \frac{dF_A}{r} \quad \text{------(2)}$$

In term of conversion,

$$F_A = F_{Ao} - F_{Ao}X$$

$$F_A - F_{Ao} = -F_{Ao}X$$

By differentiating,

$$dF_A = -F_{Ao}dX \text{ -------(3)}$$

The differential form of the PBR design equation by putting equation (3) into equation (1). In the absence of pressure drop, we may integrate (4) with X=0 and W=0 limits to get:

$$-F_{Ao}\frac{dX}{dW} = r \text{ ------(4)}$$

$$W = F_{Ao}\int_0^x \frac{dX}{-r}$$

KINETIC RATE EXPRESSION

$$\Theta_{\boldsymbol{B}} = \frac{F_{Bo}}{F_{Ao}}$$

$$\Theta_{\boldsymbol{B}} = \frac{C_{Bo}V_o}{C_{Ao}V_{Bo}}$$

$$\Theta_{\boldsymbol{B}} = \frac{Y_{Bo}}{Y_{Ao}}$$

$$\Theta_{\boldsymbol{C}} = \frac{F_{Co}}{F_{Ao}}$$

$$\Theta_{\boldsymbol{C}} = \frac{C_{Co}V_o}{C_{Ao}V_{Bo}}$$

$$\Theta_{\boldsymbol{C}} = \frac{Y_{Co}}{Y_{Ao}}$$

1st Reaction

Let A = $C_3H_8O_3$

B = $C_3H_6O_2$

C = H_2O

Reaction stoicheometry:

$-r_A = r_B = r_c$

Rate law:

$-r_A = kC_A$

$= k\,C_{AO}(1-X)$

Table 7.3 Kinetic reaction expression of each component for 1st reaction

Species	Symbol	Initially	Change	Remaining	Concentration
$C_3H_8O_3$	A	F_{Ao}	$-F_{Ao}X$	$F_A = F_{Ao} - F_{Ao}X$ $= F_{Ao}(1-X)$	$C_A = C_{Ao} - C_{Ao}X$ $= C_{Ao}(1-X)$
$C_3H_6O_2$	B	$F_{Bo} = \Theta_B F_{Ao}$	$F_{Ao}X$	$F_B = F_{Bo} + F_{Ao}X$ $= \Theta_B F_{Ao} + F_{Ao}X$ $= F_{Ao}(\Theta_B + X)$	$C_B = C_{Bo} + C_{Ao}X$ $= \Theta_B F_{Ao} + C_{Ao}X$ $= C_{Ao}(\Theta_B + X)$
$C_3H_6O_2$	C	$F_{Co} = \Theta_C F_{Ao}$	$F_{Ao}X$	$F_C = F_{Co} + F_{Ao}X$ $= \Theta_C F_{Ao} + F_{Ao}X$ $= F_{Ao}(\Theta_C + X)$	$C_C = C_{Co} + C_{Ao}X$ $= \Theta_C F_{Ao} + C_{Ao}X$ $= C_{Ao}(\Theta_C + X)$

2nd Reaction

$-r_A = kC_AC_B$

$$= k\left[\left(C_{Ao}\frac{(1-X)}{(1+\varepsilon X)}\frac{P}{P_o}\frac{T_o}{T}\right)\left(C_{Ao}\frac{(\Theta_B-X)}{(1+\varepsilon X)}\frac{P}{P_o}\frac{T_o}{T}\right)\right]$$

$$= k\left[\frac{C_{A0}}{(1+\varepsilon X)}\frac{P}{P_o}\frac{T_o}{T}\right]^2(1-X)(\Theta_B - X)$$

Since $\varepsilon = 0$

$$-r_A = k\left[C_{Ao}\frac{P}{P_o}\frac{T_o}{T}\right]^2(1-X)(\Theta_B - X)$$

Table 7.4 Kinetic reaction expression of each component for 2nd reaction

Species	Symbol	Initially	Change	Remaining	Concentration
$C_3H_6O_2$	A	F_{Ao}	$-F_{Ao}X$	$F_A = F_{Ao}(1-X)$	$C_A = \frac{C_A(1-X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$

H_2	B	$F_{Bo} = \Theta_{\boldsymbol{B}} F_{Ao}$	$-F_{Ao}X$	$F_B = F_{Ao}(\Theta_{\boldsymbol{B}} - X)$	$C_B = C_{Ao}\frac{(\Theta_B - X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$
$C_3H_8O_2$	C	$F_{Co} = \Theta_{\boldsymbol{C}} F_{Ao}$	$F_{Ao}X$	$F_C = F_{Ao}(\Theta_{\boldsymbol{C}} + X)$	$C_C = C_{Ao}\frac{(\Theta_C - X)}{(1+\varepsilon X)}(\frac{P}{P_o})(\frac{T_o}{T})$

APPENDIX D

CHEMICAL ENGINEERING COMPUTATION

GNU OCTAVE PROGRAMMING

```
clear,clc
%INTEGRATED PROJECT YEAR 2 2020/2021
%KK8
%PRODUCTION OF PROPYLENE GLYCOL
%GROUP MEMBERS:
% 1. AZRUL ZULHILMI BIN AHMAD ROSLI          (A173752)
% 2. NURIN FARAWANI BINTI MUHAMAD YUSRI      (A173797)
% 3. NUR HAFIZAH BINTI KHAIRUDDIN           (A173831)
% 4. AIMAN ARIF BIN ABDUL RAMLI             (A173840)

%GNU OCTAVE CODING FOR MASS BALANCE IN REACTOR (R-101)
%DEFINE EACH COMPONENT
%A = Glycerol
%B = Hydrogen
%C = Water
%D = Acetol
%E = Methanol
%F = Ethylene glycol
%G = Propylene glycol

%Stoichiometry coefficient of components:
%a = Glycerol
```

```
%b = Hydrogen

%c = Water

%d = Acetol

%e = Methanol

%f = Ethylene glycol

%g = Propylene glycol


%For reaction 1, r1

a1 = -1;

c1 = 1;

d1 = 1;


%For reaction 2, r2

d2 = -1;

b2 = -1;

g2 = 1;


%For reaction 3, r3

a3 = -1;

b3 = -1;

f3 = 1;

e3 = 1;


%Ni = Input molar flowrate

NiA = input('Enter the input molar flowrate of glycerol= ');

while NiA <= 0;

  disp('Error! Enter positive value only');
```

```
  NiA = input('Enter the input molar flowrate of glycerol= ');
endwhile
NiB = input('Enter the input molar flowrate of hydrogen= ');
while NiB <= 0;
  disp('Error! Enter positive value only');
  NiB = input('Enter the input molar flowrate of hydrogen= ');
endwhile
NiC = input('Enter the input molar flowrate of water= ');
while NiC <= 0;
  disp('Error! Enter positive value only');
  NiC = input('Enter the input molar flowrate of water= ');
endwhile
NiD = input('Enter the input molar flowrate of acetol= ');
while NiD < 0;
  disp('Error! Enter positive value only');
  NiD = input('Enter the input molar flowrate of acetol= ');
endwhile
NiE = input('Enter the input molar flowrate of methanol= ');
while NiE < 0;
  disp('Error! Enter positive value only');
  NiE = input('Enter the input molar flowrate of methanol= ');
endwhile
NiF = input('Enter the input molar flowrate of ethylene  glycol= ');
while NiF < 0;
  disp('Error! Enter positive value only');
  NiF = input('Enter the input molar flowrate of ethylene  glycol= ');
endwhile
```

```
NiG = input('Enter the input molar flowrate of propylene glycol= ');
while NiG < 0;
  disp('Error! Enter positive value only');
  NiG = input('Enter the input molar flowrate of propylene glycol= ');
endwhile

%Rate of reaction in kmol/h
r1 = 14.39;
r2 = 13.947;
r3 = 0.679;

%No = Output molar flowrate
%Output molar flowrate of each component
NoA = NiA+(a1*r1)+(a3*r3);
NoB = NiB+(b2*r2)+(b3*r3);
NoC = NiC+(c1*r1);
NoD = NiD+(d1*r1)+(d2*r2);
NoE = NiE+(e3*r3);
NoF = NiF+(f3*r3);
NoG = NiG+(g2*r2);

%Molecular weight of each component in g/mol
MA = 92;
MB = 2;
MC = 18;
MD = 74;
ME = 32;
```

```
MF = 62;

MG = 76;


%Fi = Input mass flowrate

FiA = NiA*MA;

FiB = NiB*MB;

FiC = NiC*MC;

FiD = NiD*MD;

FiE = NiE*ME;

FiF = NiF*MF;

FiG = NiG*MG;


%Fo = Output mass flowrate

FoA = NoA*MA;

FoB = NoB*MB;

FoC = NoC*MC;

FoD = NoD*MD;

FoE = NoE*ME;

FoF = NoF*MF;

FoG = NoG*MG;


%Total mass flowrate

FiT = FiA+FiB+FiC+FiD+FiE+FiF+FiG;

FoT = FoA+FoB+FoC+FoD+FoE+FoF+FoG;


%Component inlet and outlet mass flowrate

A = [FiA;FoA]';
```

```
B = [FiB;FoB]';

C = [FiC;FoC]';

D = [FiD;FoD]';

E = [FiE;FoE]';

F = [FiF;FoF]';

G = [FiG;FoG]';

T = [FiT;FoT]';

R = [A;B;C;D;E;F;G;T];


%The result in table

fprintf('\n \t\t\t\t\tTable of mass balance in reactor R-101\n');

fprintf('\t-------------------------------------------------------------------------------------------------\n')

fprintf('\t Component\t\t\tInlet Mass Flowrate (kg/h) \t\tOutlet Mass Flowrate (kg/h)\n')

fprintf('\t-------------------------------------------------------------------------------------------------\n')

fprintf('\t Glycerol                \t\t%.2f \t\t\t\t %.2f\n',A)

fprintf('\t Hydrogen                \t\t%.2f \t\t\t\t %.2f\n',B)

fprintf('\t Water                   \t\t%.2f \t\t\t\t\t %.2f\n',C)

fprintf('\t Acetol                   \t\t%.2f \t\t\t\t\t %.2f\n',D)

fprintf('\t Methanol                \t\t%.2f \t\t\t\t\t %.2f\n',E)

fprintf('\t Ethylene glycol          \t\t%.2f \t\t\t\t\t %.2f\n',F)

fprintf('\t Propylene glycol         \t\t%.2f \t\t\t\t\t %.2f\n',G)

fprintf('\t Total                   \t\t%.2f \t\t\t\t %.2f\n',T)

fprintf('\t-------------------------------------------------------------------------------------------------\n')


fprintf('\n\n \t\t\t\t\t\tMass balance in = Mass balance out')
```

```
fprintf('\n\n  \t\t\t\t\t  9199.58kg/h = 9199.58kg/h\t(Balanced!)\n')
```

SAFETY DATA SHEET

Creation Date 19-Nov-2009 **Revision Date** 19-Mar-2019 **Revision Number** 7

1. Identification

Product Name **Propylene Glycol**

Cat No. : **P355-1; P355-4; P355-20; P355-200; S801501; XXBA147**

CAS-No 57-55-6
Synonyms 1,2-Propanediol; 1,2-Dihydroxypropane; Methyl Glycol (USP/FCC)

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Emergency Telephone Number
CHEMTREC®, Inside the USA: 800-424-9300
CHEMTREC®, Outside the USA: 001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is not considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

This chemical is not considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Label Elements
None required

Hazards not otherwise classified (HNOC)
None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
1,2-Propylene glycol	57-55-6	>95

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. If symptoms persist, call a physician.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Get medical attention if symptoms occur.

Inhalation Remove to fresh air. Get medical attention immediately if symptoms occur. If not breathing, give artificial respiration.

Ingestion Do NOT induce vomiting. Get medical attention immediately if symptoms occur.

Most important symptoms and effects No information available.

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.

Unsuitable Extinguishing Media No information available

Flash Point 99 °C / 210.2 °F

Method - No information available

Autoignition Temperature 400 °C / 752 °F

Explosion Limits

Upper 12.6 vol %

Lower 2.6 vol %

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition. Thermal decomposition can lead to release of irritating gases and vapors.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO_2).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	1	N/A

6. Accidental release measures

Personal Precautions	Use personal protective equipment as required. Ensure adequate ventilation.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling	Ensure adequate ventilation. Wear personal protective equipment/face protection.
Storage	Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

8. Exposure controls / personal protection

Exposure Guidelines

Engineering Measures	Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Viscous liquid Liquid
Appearance	Clear Colourless
Odor	Odorless
Odor Threshold	No information available
pH	6.5-7.5 100g/l aq. sol
Melting Point/Range	-60 °C / -76 °F
Boiling Point/Range	187 °C / 368.6 °F
Flash Point	99 °C / 210.2 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	12.6 vol %
Lower	2.6 vol %
Vapor Pressure	0.13 mbar @ 20 °C
Vapor Density	2.62 (Air = 1.0)
Specific Gravity	1.03 - 1.04
Solubility	Soluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	400 °C / 752 °F
Decomposition Temperature	No information available
Viscosity	45 mPa.s at 20 °C
Molecular Formula	C3 H8 O2

Molecular Weight 76.10

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Hygroscopic.

Conditions to Avoid Incompatible products. Excess heat. Exposure to moist air or water.

Incompatible Materials Strong oxidizing agents, Acids

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information
Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1,2-Propylene glycol	LD50 = 20 g/kg (Rat)	LD50 = 20800 mg/kg (Rabbit)	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
1,2-Propylene glycol	57-55-6	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

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Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
1,2-Propylene glycol	EC50: = 19000 mg/L, 96h (Pseudokirchneriella subcapitata)	LC50: = 51600 mg/L, 96h static (Oncorhynchus mykiss) LC50: 41 - 47 mL/L, 96h static (Oncorhynchus mykiss) LC50: = 710 mg/L, 96h (Pimephales promelas) LC50: = 51400 mg/L, 96h static (Pimephales promelas)	= 710 mg/L EC50 Photobacterium phosphoreum 30 min	EC50: > 10000 mg/L, 24h (Daphnia magna) EC50: > 1000 mg/L, 48h Static (Daphnia magna)

Persistence and Degradability Miscible with water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

Component	log Pow
1,2-Propylene glycol	-0.9

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated
TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
1,2-Propylene glycol	57-55-6	X	ACTIVE	-

Legend:
TSCA - Toxic Substances Control Act, (40 CFR Part 710)
X - Listed
'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories
Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Australia (AICS), China (IECSC), Korea (ECL).

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
1,2-Propylene glycol	57-55-6	X	-	200-338-0	X	X	X	X	KE-29267

U.S. Federal Regulations

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
1,2-Propylene glycol	-	X	X	-	X

U.S. Department of Transportation
Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Slight risk, Grade 1

16. Other information

Prepared By
Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

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Print Date 19-Mar-2019
Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer
The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS

MATERIAL SAFETY DATA SHEET

Methanol

Section 1 - Chemical Product and Company Identification

MSDS Name:	**Methanol**
Synonyms:	Methyl alcohol

Company Identification: (INDIA)	Veritas House, 70 Mint Road, Fort, Mumbai - 400 001. INDIA
For information in the INDIA, call:	Tel: +91 - 22 - 2275 5555 / 6184 0000, Fax: +91 - 22 - 2275 5556 / 6184 0001

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name:	%	EINECS#
67-56-1	Methanol	99.8%	200-659-6

Hazard Symbols:	T F
	
Risk Phrases:	11 23/24/25 39/23/24/25

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Highly flammable. Toxic by inhalation, in contact with skin and if swallowed. Toxic : danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.

Potential Health Effects

Eye:	Produces irritation, characterized by a burning sensation, redness, tearing, inflammation, and possible corneal injury. May cause painful sensitization to light.
Skin:	Causes moderate skin irritation. May be absorbed through the skin in harmful amounts. Prolonged and/or repeated contact may cause defatting of the skin and dermatitis.
Ingestion:	May be fatal or cause blindness if swallowed. Cannot be made non-poisonous. May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May cause systemic toxicity with acidosis. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma and possible death due to respiratory failure. May cause cardiopulmonary system effects.
Inhalation:	May cause adverse central nervous system effects including headache, convulsions, and possible death. May cause visual impairment and possible permanent blindness. Causes irritation of mucous membrane.
Chronic:	Prolonged or repeated skin contact may cause dermatitis. Chronic inhalation and ingestion may cause effects similar to those of acute inhalation and ingestion. Chronic exposure may cause reproductive disorders and teratogenic effects. Laboratory experiments have resulted in mutagenic effects.

Section 4 - First Aid Measures

Eyes:	Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.
Skin:	Get medical aid immediately. Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes.
Ingestion:	If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately. Wash mouth out with water.
Inhalation:	Get medical aid immediately. Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.
Notes to Physician:	Effects may be delayed. Ethanol may inhibit methanol metabolism. Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information:	Containers can build up pressure if exposed to heat and/or fire. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Water runoff can cause environmental damage. Dike and collect water used to fight fire. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Flammable Liquid. Can release vapors that form explosive mixtures at temperatures above the flashpoint. Water may be ineffective. Material is lighter than water and a fire may be spread by the use of water. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.
Extinguishing Media:	Use water spray to cool fire-exposed containers. Use foam, dry chemical, or carbon dioxide. Use flooding quantities of water as spray.

Section 6 - Accidental Release Measures

General Information:	Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks:	Use water spray to disperse the gas/vapor. Remove all sources of ignition. Absorb spill using an absorbent, non-combustible material such as earth, sand, or vermiculite. Do not use combustible materials such as sawdust. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors. Water spray may reduce vapor but may not prevent ignition in closed spaces.

Section 7 - Handling and Storage

Handling:	Wash thoroughly after handling. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Do not breathe dust, vapor, mist, or gas. Do not get in eyes, on skin, or on clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep away from heat, sparks and flame. Do not ingest or inhale. Use only in a chemical fume hood. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
Storage:	Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a cool, dry place. Store in a tightly closed container. Flammables-area.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls:	
	Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local explosion-proof ventilation to keep airborne levels to acceptable levels.
Exposure Limits	**CAS# 67-56-1:**
	United Kingdom, WEL - TWA: 200 ppm TWA; 266 mg/m3 TWA United Kingdom, WEL - **STEL:** 250 ppm STEL; 333 mg/m3 STEL
	United States OSHA: 200 ppm TWA; 260 mg/m3 TWA
	Belgium-TWA: 200ppm VLE; 266mg/m3 VLE Belgium-STEL: 250ppm VLE; 333 mg/m3 VLE
	France-VME: 200ppm VME; 260mg/m3 VME France-VLE: 1000ppm VLE; 1300mg/m3 VLE
	Germany: 200 ppm TWA; 270 mg/m3 TWA Germany: skin notation
	Japan: 200 ppm OEL; 260 mg/m3 OEL
	Malaysia: 200 ppm TWA; 262 mg/m3 TWA
	Netherlands: 200 ppm MAC; 260 mg/m3 MAC
	Russia: 5 mg/m3 TWA (vapour)
	Spain: 200ppm VLA-ED; 266mg/m3 VLA-ED Spain: 250ppm VLA-EC; 333mg/m3 VLA-EC

Personal Protective Equipment	
Eyes:	Wear chemical splash goggles.
Skin:	Wear appropriate protective gloves to prevent skin exposure.
Clothing:	Wear appropriate protective clothing to prevent skin exposure.
Respirators:	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State:	Clear liquid
Color:	APHA: 10 max
Odor:	alcohol-like
pH:	Not available
Vapor Pressure:	128hPa @20 deg C
Viscosity:	0.55 cP @20 deg C
Boiling Point:	64.7 deg C @760mmHg (148.46°F)
Freezing/Melting Point:	-98 deg C (-144.40°F)
Autoignition Temperature:	455 deg C (851.00 deg F)
Flash Point:	12 deg C (53.60 deg F)
Explosion Limits: Lower:	6 Vol %
Explosion Limits: Upper:	31 Vol %
Decomposition Temperature:	Not available
Solubility in water:	Miscible
Specific Gravity/Density:	0.792 g/cc
Molecular Formula:	CH4O
Molecular Weight:	32.04

Section 10 - Stability and Reactivity

Chemical Stability:	Stable under normal temperatures and pressures.
Conditions to Avoid:	Incompatible materials, ignition sources, exposure to moist air or water.
Incompatibilities with Other Materials	Oxidizing agents, reducing agents, acids, acid chlorides, alkali metals, magnesium, potassium, sodium, metals as powders (e.g. hafnium, raney nickel), and acid anhydrides.
Hazardous Decomposition Products	Carbon monoxide, carbon dioxide, formaldehyde.
Hazardous Polymerization	Will not occur.

Section 11 - Toxicological Information

RTECS#:	CAS# 67-56-1: PC1400000
LD50/LC50:	RTECS: **CAS# 67-56-1:** Draize test, rabbit, eye: 40 mg Moderate; Draize test, rabbit, eye: 100 mg/24H Moderate; Draize test, rabbit, skin: 20 mg/24H Moderate; Inhalation, rabbit: LC50 = 81000 mg/m3/14H; Inhalation, rat: LC50 = 64000 ppm/4H; Oral, mouse: LD50 = 7300 mg/kg; Oral, rabbit: LD50 = 14200 mg/kg; Oral, rat: LD50 = 5600 mg/kg; Skin, rabbit: LD50 = 15800 mg/kg;
Carcinogenicity:	Methanol - Not listed as a carcinogen by ACGIH, IARC, NTP, or CA Prop 65.
Other:	See actual entry in RTECS for complete information.

Section 12 - Ecological Information

Other:	Avoid entering into waters or underground water. Do not empty into drains.

Section 13 - Disposal Considerations

Dispose of in a manner consistent with federal, state, and local regulations.

Section 14 - Transport Information

	IATA	**IMO**	**RID/ADR**
Shipping Name:	METHANOL	METHANOL	METHANOL
Hazard Class:	3 (6.1)	3 (6.1)	3 (6.1)
UN Number:	1230	1230	1230
Packing Group:	II	II	II

USA RQ: CAS# 67-56-1: 5000 lb final RQ; 2270 kg final RQ

Section 15 - Regulatory Information

European/International Regulations
European Labeling in Accordance with EC Directives
Hazard Symbols: T F
Risk Phrases:
➢ R 11 Highly flammable.
➢ R 23/24/25 Toxic by inhalation, in contact with skin and if swallowed.
➢ R 39/23/24/25 Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.
Safety Phrases:
➢ S 7 Keep container tightly closed.
➢ S 16 Keep away from sources of ignition - No smoking.
➢ S 36/37 Wear suitable protective clothing and gloves.
➢ S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).
WGK (Water Danger/Protection)
➢ CAS# 67-56-1: 1
Canada
➢ CAS# 67-56-1 is listed on Canada's DSL List
US Federal
➢ TSCA
➢ CAS# 67-56-1 is listed on the TSCA Inventory.

Section 16 - Other Information

MSDS Creation Date:	July 22, 2015
Revision #0 Date	

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall the company be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential, or exemplary damages howsoever arising, even if the company has been advised of the possibility of such damages.

Danger

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Trade name : Hydrogen
SDS no : SDS-067A-CLP
Chemical description : Hydrogen
CAS No : 1333-74-0
EC no : 215-605-7
EC index no : 001-001-00-9
Registration-No. : Listed in Annex IV / V REACH, exempted from registration.
Chemical formula : H_2

1.2. Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : Industrial and professional. Perform risk assessment prior to use.
Test gas/Calibration gas.
Laboratory use.
Chemical reaction / Synthesis.
Use as a fuel.
Shield gas for welding processes.
Use for manufacture of electronic/photovoltaic components.
Laser gas.
Contact supplier for more information on uses.
Uses advised against : Do not inflate in party balloons because of the risk of explosion.

1.3. Details of the supplier of the safety data sheet

Company identification : Air Liquide UK Ltd.
Station Road, Coleshill
B46 1JY Birmingham United Kingdom
01675 462424
genenq.aluk@airliquide.com

1.4. Emergency telephone number

Emergency telephone number : 01675 462695

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Physical hazards	Flammable gases, Category 1	H220
	Gases under pressure : Compressed gas	H280

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :

GHS02 GHS04

Signal word (CLP) : Danger

Hazard statements (CLP) : H220 - Extremely flammable gas.
H280 - Contains gas under pressure; may explode if heated.

Precautionary statements (CLP)

- Prevention : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
- Response : P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely.
P381 - In case of leakage, eliminate all ignition sources.
- Storage : P403 - Store in a well-ventilated place.
P410+P403 - Protect from sunlight. Store in a well-ventilated place.

2.3. Other hazards

: None.

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Hydrogen	(CAS No) 1333-74-0 (EC no) 215-605-7 (EC index no) 001-001-00-9 (Registration-No.) *1	100	Flam. Gas 1, H220 Press. Gas (Comp.), H280

Contains no other components or impurities which will influence the classification of the product.

**1: Listed in Annex IV / V REACH, exempted from registration.*

**2: Registration deadline not expired.*

**3: Registration not required: Substance manufactured or imported < 1t/y.*

3.2. Mixture : Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

- Inhalation : Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
- Skin contact : Adverse effects not expected from this product.
- Eye contact : Adverse effects not expected from this product.
- Ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

: In high concentrations may cause asphyxiation. Symptoms may include loss of mobility/consciousness. Victim may not be aware of asphyxiation.

4.3. Indication of any immediate medical attention and special treatment needed

: None.

SECTION 5: Firefighting measures

5.1. Extinguishing media

- Suitable extinguishing media : Water spray or fog.
  Dry powder.
- Unsuitable extinguishing media : Do not use water jet to extinguish.
  Carbon dioxide.

5.2. Special hazards arising from the substance or mixture

Specific hazards : Exposure to fire may cause containers to rupture/explode.

Hazardous combustion products : None.

5.3. Advice for firefighters

Specific methods : Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas receptacles to rupture. Cool endangered receptacles with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.

If possible, stop flow of product.

Use water spray or fog to knock down fire fumes if possible.

Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.

Move containers away from the fire area if this can be done without risk.

Special protective equipment for fire fighters : In confined space use self-contained breathing apparatus.

Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.

Standard EN 137 - Self-contained open-circuit compressed air breathing apparatus with full face mask.

Standard EN 469 - Protective clothing for firefighters. Standard - EN 659: Protective gloves for firefighters.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

: Evacuate area.

Consider the risk of potentially explosive atmospheres.

Wear self-contained breathing apparatus when entering area unless atmosphere is proved to be safe.

Eliminate ignition sources.

Ensure adequate air ventilation.

Act in accordance with local emergency plan.

Stay upwind.

6.2. Environmental precautions

: Try to stop release.

6.3. Methods and material for containment and cleaning up

: Ventilate area.

6.4. Reference to other sections

: See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Safe use of the product : Do not breathe gas.

Avoid release of product into atmosphere.

The substance must be handled in accordance with good industrial hygiene and safety procedures.

Only experienced and properly instructed persons should handle gases under pressure.

Consider pressure relief device(s) in gas installations.

Ensure the complete gas system was (or is regularily) checked for leaks before use.

Do not smoke while handling product.

Use only properly specified equipment which is suitable for this product, its supply pressure and temperature. Contact your gas supplier if in doubt.

Assess the risk of potentially explosive atmospheres and the need for explosion-proof equipment.

Purge air from system before introducing gas.

Take precautionary measures against static discharge.

Keep away from ignition sources (including static discharges).

Consider the use of only non-sparking tools.

Safe handling of the gas receptacle : Refer to supplier's container handling instructions.

Do not allow backfeed into the container.

Protect cylinders from physical damage; do not drag, roll, slide or drop.

When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders.

Leave valve protection caps in place until the container has been secured against either a wall or bench or placed in a container stand and is ready for use.

If user experiences any difficulty operating cylinder valve discontinue use and contact supplier.

Never attempt to repair or modify container valves or safety relief devices.

Damaged valves should be reported immediately to the supplier.

Keep container valve outlets clean and free from contaminants particularly oil and water.

Replace valve outlet caps or plugs and container caps where supplied as soon as container is disconnected from equipment.

Close container valve after each use and when empty, even if still connected to equipment.

Never attempt to transfer gases from one cylinder/container to another.

Never use direct flame or electrical heating devices to raise the pressure of a container.

Do not remove or deface labels provided by the supplier for the identification of the cylinder contents.

Suck back of water into the container must be prevented.

7.2. Conditions for safe storage, including any incompatibilities

: Observe all regulations and local requirements regarding storage of containers.
Containers should not be stored in conditions likely to encourage corrosion.
Container valve guards or caps should be in place.
Containers should be stored in the vertical position and properly secured to prevent them from falling over.
Stored containers should be periodically checked for general condition and leakage.
Keep container below 50°C in a well ventilated place.
Store containers in location free from fire risk and away from sources of heat and ignition.
Keep away from combustible materials.
Segregate from oxidant gases and other oxidants in store.
All electrical equipment in the storage areas should be compatible with the risk of a potentially explosive atmosphere.

7.3. Specific end use(s)

: None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls

8.2.1. Appropriate engineering controls

: Provide adequate general and local exhaust ventilation.
Systems under pressure should be regularly checked for leakages.
Gas detectors should be used when flammable gases/vapours may be released.
Consider work permit system e.g. for maintenance activities.

8.2.2. Individual protection measures, e.g. personal protective equipment

: A risk assessment should be conducted and documented in each work area to assess the risks related to the use of the product and to select the PPE that matches the relevant risk. The following recommendations should be considered:
PPE compliant to the recommended EN/ISO standards should be selected.

• Eye/face protection : Wear safety glasses with side shields.
Standard EN 166 - Personal eye-protection.

• Skin protection

- Hand protection : Wear working gloves when handling gas containers.
Standard EN 388 - Protective gloves against mechanical risk.

- Other : Consider the use of flame resistant anti-static safety clothing.
Standard EN ISO 14116 - Limited flame spread materials.
Standard EN ISO 1149-5 - Protective clothing: Electrostatic properties.
Wear safety shoes while handling containers.
Standard EN ISO 20345 - Personal protective equipment - Safety footwear.

• Respiratory protection : None necessary.

• Thermal hazards : None necessary.

8.2.3. Environmental exposure controls

: Specific risk management measures are not required beyond good industrial hygiene and safety procedures.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance

• Physical state at 20°C / 101.3kPa	:	Gas
• Colour	:	Colourless.
Odour	:	Odourless.
Odour threshold	:	Odour threshold is subjective and inadequate to warn of overexposure.
pH	:	Not applicable.
Melting point / Freezing point	:	-259 °C
Boiling point	:	-253 °C
Flash point	:	Not applicable for gases and gas mixtures.
Evaporation rate	:	Not applicable for gases and gas mixtures.
Flammability (solid, gas)	:	
Explosive limits	:	4 - 77 vol %
Vapour pressure [20°C]	:	Not applicable.
Vapour pressure [50°C]	:	Not applicable.
Relative density, liquid (water=1)	:	0.07
Relative density, gas (air=1)	:	0.07
Water solubility	:	1.6 mg/l
Partition coefficient n-octanol/water (Log Kow)	:	Not applicable for inorganic gases.
Auto-ignition temperature	:	560 °C
Viscosity	:	Not applicable.
Explosive properties	:	Not applicable.
Oxidising properties	:	None.

9.2. Other information

Molar mass	:	2 g/mol
Critical temperature [°C]	:	-240 °C
Other data	:	Burns with an invisible flame.

SECTION 10: Stability and reactivity

10.1. Reactivity

: No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

: Stable under normal conditions.

10.3. Possibility of hazardous reactions

: May react violently with oxidants.
Can form explosive mixture with air.

10.4. Conditions to avoid

: Keep away from heat/sparks/open flames/hot surfaces. – No smoking.

10.5. Incompatible materials

: Air, Oxidiser.
For additional information on compatibility refer to ISO 11114.

10.6. Hazardous decomposition products

: Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : No known toxicological effects from this product.

Skin corrosion/irritation : No known effects from this product.

Serious eye damage/irritation : No known effects from this product.

Respiratory or skin sensitisation : No known effects from this product.

Germ cell mutagenicity : No known effects from this product.

Carcinogenicity : No known effects from this product.

Toxic for reproduction : Fertility : No known effects from this product.

Toxic for reproduction : unborn child : No known effects from this product.

STOT-single exposure : No known effects from this product.

STOT-repeated exposure : No known effects from this product.

Aspiration hazard : Not applicable for gases and gas mixtures.

SECTION 12: Ecological information

12.1. Toxicity

Assessment : No ecological damage caused by this product.

EC50 48h - Daphnia magna [mg/l] : No data available.

EC50 72h - Algae [mg/l] : No data available.

LC50 96 h - Fish [mg/l] : No data available.

12.2. Persistence and degradability

Assessment : No ecological damage caused by this product.

12.3. Bioaccumulative potential

Assessment : No ecological damage caused by this product.

12.4. Mobility in soil

Assessment : No ecological damage caused by this product.

12.5. Results of PBT and vPvB assessment

Assessment : Not classified as PBT or vPvB.

12.6. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Do not discharge into areas where there is a risk of forming an explosive mixture with air. Waste gas should be flared through a suitable burner with flash back arrestor.

Do not discharge into any place where its accumulation could be dangerous.

Ensure that the emission levels from local regulations or operating permits are not exceeded.

List of hazardous waste codes (from Commission Decision 2001/118/EC) : 16 05 04: Gases in pressure containers (including halons) containing dangerous substances.

13.2. Additional information

: None.

SECTION 14: Transport information

14.1. UN number

UN-No. : 1049

14.2. UN proper shipping name

Transport by road/rail (ADR/RID) : HYDROGEN, COMPRESSED

Transport by air (ICAO-TI / IATA-DGR) : HYDROGEN, COMPRESSED

Transport by sea (IMDG) : HYDROGEN, COMPRESSED

14.3. Transport hazard class(es)

Labelling :

2.1 : Flammable gases.

Transport by road/rail (ADR/RID)

Class : 2

Classification code : 1F

Hazard identification number : 23

Tunnel Restriction : B/D - Tank carriage : Passage forbidden through tunnels of category B, C, D and E. Other carriage : Passage forbidden through tunnels of category D and E

Transport by air (ICAO-TI / IATA-DGR)

Class / Div. (Sub. risk(s)) : 2.1

Transport by sea (IMDG)

Class / Div. (Sub. risk(s)) : 2.1

Emergency Schedule (EmS) - Fire : F-D

Emergency Schedule (EmS) - Spillage : S-U

14.4. Packing group

Transport by road/rail (ADR/RID) : Not applicable

Transport by air (ICAO-TI / IATA-DGR) : Not applicable

Transport by sea (IMDG) : Not applicable

14.5. Environmental hazards

Transport by road/rail (ADR/RID) : None.

Transport by air (ICAO-TI / IATA-DGR) : None.

Transport by sea (IMDG) : None.

14.6. Special precautions for user

Packing Instruction(s)

Transport by road/rail (ADR/RID)	:	P200
Transport by air (ICAO-TI / IATA-DGR)		
Passenger and Cargo Aircraft	:	Forbidden.
Cargo Aircraft only	:	200.
Transport by sea (IMDG)	:	P200

Special transport precautions : Avoid transport on vehicles where the load space is not separated from the driver's compartment.

Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency.

Before transporting product containers:

- Ensure there is adequate ventilation.
- Ensure that containers are firmly secured.
- Ensure cylinder valve is closed and not leaking.
- Ensure valve outlet cap nut or plug (where provided) is correctly fitted.
- Ensure valve protection device (where provided) is correctly fitted.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

: Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

EU-Regulations

Restrictions on use	:	None.
Seveso directive 96/82/EC	:	Listed.

National regulations

National legislation	:	Ensure all national/local regulations are observed.
Kenn-Nr.	:	741

15.2. Chemical safety assessment

: A CSA does not need to be carried out for this product.

SECTION 16: Other information

Indication of changes	:	Revised safety data sheet in accordance with commission regulation (EU) No 453/2010.
Training advice	:	Ensure operators understand the flammability hazard. The hazard of asphyxiation is often overlooked and must be stressed during operator training.
Further information	:	This Safety Data Sheet has been established in accordance with the applicable European Union legislation.
DISCLAIMER OF LIABILITY	:	Before using this product in any new process or experiment, a thorough material compatibility and safety study should be carried out. Details given in this document are believed to be correct at the time of going to press. Whilst proper care has been taken in the preparation of this document, no liability for injury or damage resulting from its use can be accepted.

End of document

MATERIAL SAFETY DATA SHEET

Glycerol

Section 1 - Chemical Product and Company Identification

MSDS Name: Glycerol

Catalog Numbers: 15892-0000, 15892-0010, 15892-0025, 15892-0250, 18469-0000, 18469-5000, 32725-0000, 32725-5000, 33203-0000, 33203-0010, 33203-0025, 33203-1000, 41098-0000, 41098-5000

Synonyms: Glycerine

Company Identification:
Acros Organics BVBA
Janssen Pharmaceuticalaan 3a
2440 Geel, Belgium

Company Identification: (USA)
Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

For information in the US, call: 800-ACROS-01

For information in Europe, call: +32 14 57 52 11

Emergency Number, Europe: +32 14 57 52 99

Emergency Number US: 201-796-7100

CHEMTREC Phone Number, US: 800-424-9300

CHEMTREC Phone Number, Europe: 703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name:	%	EINECS#
56-81-5	Glycerol	>99%	200-289-5

Hazard Symbols: None listed

Risk Phrases: None listed

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Not available

Potential Health Effects

Eye: May cause mild eye irritation.

Skin: May cause mild skin irritation. Low hazard for usual industrial handling.

Ingestion: May cause irritation of the digestive tract. May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May cause headache. Expected to be a low ingestion hazard.

Inhalation: May cause respiratory tract irritation. Low hazard for usual industrial handling.

Chronic: May cause kidney injury.

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid.

Skin: Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Get medical aid if irritation develops or persists.

Ingestion: Get medical aid. Wash mouth out with water.

Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear.

Extinguishing Media: Use water spray, dry chemical, carbon dioxide, or chemical foam.

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Do not let this chemical enter the environment.

Section 7 - Handling and Storage

Handling: Avoid breathing dust, vapor, mist, or gas. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

Storage: Store in a cool, dry place. Store in a tightly closed container.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls:

Use adequate ventilation to keep airborne concentrations low.

Exposure Limits

CAS# 56-81-5:

United Kingdom, WEL - TWA: 10 mg/m3 TWA (mist) United Kingdom, WEL - STEL: 30 mg/m3 STEL (mist)

United States OSHA: 15 mg/m3 TWA (total dust); 5 mg/m3 TWA (respirable fraction)

Belgium - TWA: 10 mg/m3 VLE (mist)

France - VME: 10 mg/m3 VME

Malaysia: 10 mg/m3 TWA (mist)

Netherlands: 10 mg/m3 MAC (mist)

Spain: 10 mg/m3 VLA-ED

Personal Protective Equipment

Eyes: Wear chemical splash goggles.

Skin: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Viscous liquid

Color: clear, colorless

Odor:	odorless
pH:	5 (100 g/l aq.sol.)
Vapor Pressure:	0.003mbar @50 deg C
Viscosity:	1069 mPa s @20 deg C
Boiling Point:	290 deg C @760mmHg (554.00°F)
Freezing/Melting Point:	18 deg C (64.40°F)
Autoignition Temperature:	400 deg C (752.00 deg F)
Flash Point:	160 deg C (320.00 deg F)
Explosion Limits: Lower:	0.9 Vol %
Explosion Limits: Upper:	Not available
Decomposition Temperature:	
Solubility in water:	>500 g/l (20°C)
Specific Gravity/Density:	1.261
Molecular Formula:	C3H8O3
Molecular Weight:	92.09

Section 10 - Stability and Reactivity

Chemical Stability:	Stable under normal temperatures and pressures. Hygroscopic: absorbs moisture or water from the air.
Conditions to Avoid:	Incompatible materials, exposure to moist air or water, temperatures above 140°C.
Incompatibilities with Other Materials	Strong oxidizing agents, lead oxide, nitric acid, sulfuric acid, hydrogen peroxide, potassium permanganate, calcium hypochlorite, perchloric acid.
Hazardous Decomposition Products	Carbon monoxide, carbon dioxide.
Hazardous Polymerization	Will not occur.

Section 11 - Toxicological Information

RTECS#: CAS# 56-81-5: MA8050000

LD50/LC50: RTECS:
CAS# 56-81-5: Draize test, rabbit, eye: 126 mg Mild;
Draize test, rabbit, eye: 500 mg/24H Mild;
Draize test, rabbit, skin: 500 mg/24H Mild;
Inhalation, rat: LC50 = >570 mg/m3/1H;
Oral, mouse: LD50 = 4090 mg/kg;
Oral, rabbit: LD50 = 27 gm/kg;
Oral, rat: LD50 = 12600 mg/kg;
Skin, rabbit: LD50 = >10 gm/kg;
.
Other:

Carcinogenicity: Glycerol - Not listed as a carcinogen by ACGIH, IARC, NTP, or CA Prop 65.

Other: The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

Section 12 - Ecological Information

Ecotoxicity: Daphnia: Daphnia: EC50: >10000 mg/l; 24h; .
Fish: Leuciscus idus: LC50: > 10000 mg/l; 24h; .

Other: Do not empty into drains. Readily biodegradable.
Log POW: -2.66 (calc.)

Section 13 - Disposal Considerations

Dispose of in a manner consistent with federal, state, and local regulations.

Section 14 - Transport Information

	IATA	IMO	RID/ADR
Shipping Name:	Not regulated as a hazardous material	Not regulated as a hazardous material	Not regulated as a hazardous material
Hazard Class:			
UN Number:			
Packing Group:			

Section 15 - Regulatory Information

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:Not available

Risk Phrases:

Safety Phrases:

S 24/25 Avoid contact with skin and eyes.

WGK (Water Danger/Protection)

CAS# 56-81-5: 0

Canada

CAS# 56-81-5 is listed on Canada's DSL List

US Federal

TSCA

CAS# 56-81-5 is listed on the TSCA Inventory.

Section 16 - Other Information

MSDS Creation Date: 7/16/1996

Revision #1 Date 8/08/2005

Revisions were made in Sections: General revision.

SAFETY DATA SHEET

Creation Date 02-Feb-2010 **Revision Date** 17-Jan-2018 **Revision Number** 4

1. Identification

Product Name **Ethylene glycol**

Cat No. : **E177-4; E177-20**

CAS-No 107-21-1
Synonyms Monoethylene glycol; 1,2-Ethanediol

Recommended Use Laboratory chemicals.
Uses advised against Not for food, drug, pesticide or biocidal product use

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Emergency Telephone Number
CHEMTREC®, Inside the USA: 800-424-9300
CHEMTREC®, Outside the USA: 001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity	Category 4
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Central nervous system (CNS).	
Specific target organ toxicity - (repeated exposure)	Category 2
Target Organs - Kidney, Liver.	

Label Elements

Signal Word
Warning

Hazard Statements
Harmful if swallowed
May cause drowsiness or dizziness
May cause damage to organs through prolonged or repeated exposure

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Response
Get medical attention/advice if you feel unwell
Inhalation
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician if you feel unwell
Ingestion
IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth
Storage
Store in a well-ventilated place. Keep container tightly closed
Store locked up
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)

WARNING. Reproductive Harm - https://www.p65warnings.ca.gov/.

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Ethylene glycol	107-21-1	>95

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.

Inhalation Move to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Get medical attention immediately if symptoms occur. If not breathing, give artificial respiration.

Ingestion Do not induce vomiting. Call a physician or Poison Control Center immediately.

Most important symptoms and effects Breathing difficulties.

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable Extinguishing Media No information available

Flash Point 111 °C / 231.8 °F

Method - DIN 51758

Autoignition Temperature 413 °C / 775.4 °F

Explosion Limits
Upper 15.30 vol %
Lower 3.20 vol %
Sensitivity to Mechanical Impact No information available
Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical
Thermal decomposition can lead to release of irritating gases and vapors. Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products
Carbon monoxide (CO) Carbon dioxide (CO_2)
Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	1	N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment.
Environmental Precautions Should not be released into the environment. See Section 12 for additional ecological information.

Methods for Containment and Clean Up Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling Wear personal protective equipment. Ensure adequate ventilation. Do not breathe vapors or spray mist. Avoid contact with skin, eyes and clothing.

Storage Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat and sources of ignition.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Ethylene glycol	TWA: 25 ppm STEL: 50 ppm STEL: 10 mg/m³	(Vacated) Ceiling: 50 ppm (Vacated) Ceiling: 125 mg/m³		Ceiling: 100 mg/m³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists
OSHA - Occupational Safety and Health Administration

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Viscous liquid Liquid
Appearance	Colorless
Odor	Odorless
Odor Threshold	No information available
pH	5.5-7.5 50% aq. sol
Melting Point/Range	-13 °C / 8.6 °F
Boiling Point/Range	196 - 198 °C / 384.8 - 388.4 °F @ 760 mmHg
Flash Point	111 °C / 231.8 °F
Method -	DIN 51758
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	15.30 vol %
Lower	3.20 vol %
Vapor Pressure	0.12 mmHg @ 20 °C
Vapor Density	2.14 (Air = 1.0)
Specific Gravity	1.113
Solubility	miscible
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	413 °C / 775.4 °F
Decomposition Temperature	> 500°C
Viscosity	21 cP (20°C)
Molecular Formula	C2 H6 O2
Molecular Weight	62.06

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Hygroscopic.
Conditions to Avoid	Incompatible products. Excess heat. Exposure to moist air or water.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases, Aldehydes
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO_2)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Ethylene glycol	7712 mg/kg (Rat)	9530 µL/kg (Rabbit) 10600 mg/kg (Rat)	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation May cause eye, skin, and respiratory tract irritation

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Ethylene glycol	107-21-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Central nervous system (CNS)

STOT - repeated exposure Kidney Liver

Aspiration hazard No information available

Symptoms / effects,both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains. .

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Ethylene glycol	EC50: 6500 - 13000 mg/L, 96h (Pseudokirchneriella subcapitata)	LC50: = 16000 mg/L, 96h static (Poecilia reticulata) LC50: 40000 - 60000 mg/L, 96h static (Pimephales promelas) LC50: = 40761 mg/L, 96h static (Oncorhynchus mykiss) LC50: = 41000 mg/L, 96h (Oncorhynchus mykiss) LC50: 14 - 18 mL/L, 96h static (Oncorhynchus mykiss) LC50: = 27540 mg/L, 96h static (Lepomis macrochirus)	Not listed	EC50: = 46300 mg/L, 48h (Daphnia magna)

Persistence and Degradability Persistence is unlikely

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Ethylene glycol	-1.93

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated
TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

All of the components in the product are on the following Inventory lists: X = listed

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Ethylene glycol	X	X	-	203-473-3	-		X	X	X	X	X

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b) Not applicable

SARA 313

Component	CAS-No	Weight %	SARA 313 - Threshold Values %
Ethylene glycol	107-21-1	>95	1.0

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Ethylene glycol	X		-

OSHA Occupational Safety and Health Administration
Not applicable

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Ethylene glycol	5000 lb	-

California Proposition 65 This product does not contain any Proposition 65 chemicals

Component	CAS-No	California Prop. 65	Prop 65 NSRL	Category
Ethylene glycol	107-21-1	Developmental	-	Developmental

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Ethylene glycol	X	X	X	X	-

U.S. Department of Transportation

Reportable Quantity (RQ): Y
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Slight risk, Grade 1

16. Other information

Prepared By
Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date 02-Feb-2010
Revision Date 17-Jan-2018
Print Date 17-Jan-2018
Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer
The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS

Water

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Issue date: 11/15/2013 Revision date: 06/26/2020 Supersedes: 06/12/2018 Version: 1.4

SECTION 1: Identification

1.1. Identification

Product form : Substance

Substance name : Water

CAS-No. : 7732-18-5

Product code : LC26750

Formula : H2O

1.2. Recommended use and restrictions on use

Use of the substance/mixture : For laboratory and manufacturing use only.

Recommended use : Laboratory chemicals

Restrictions on use : Not for food, drug or household use

1.3. Supplier

LabChem, Inc.

1010 Jackson's Pointe Ct.

Zelienople, PA 16063 - USA

T 412-826-5230 - F 724-473-0647

info@labchem.com - www.labchem.com

1.4. Emergency telephone number

Emergency number : CHEMTREC: 1-800-424-9300 or +1-703-741-5970

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Not classified

2.2. GHS Label elements, including precautionary statements

Not classified as a hazardous chemical.

Other hazards not contributing to the classification : None.

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
Water (Main constituent)	(CAS-No.) 7732-18-5	100	Not classified

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general : If you feel unwell, seek medical advice (show the label where possible).

First-aid measures after inhalation : Allow affected person to breathe fresh air. Allow the victim to rest. Adverse effects not expected from this product.

First-aid measures after skin contact : Adverse effects not expected from this product. Take off contaminated clothing.

First-aid measures after eye contact : Adverse effects not expected from this product.

First-aid measures after ingestion : Do NOT induce vomiting. Adverse effects not expected from this product.

4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms : Based on available data, the classification criteria are not met.

Symptoms/effects : Not expected to present a significant hazard under anticipated conditions of normal use.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Foam. Dry powder. Carbon dioxide. Water spray. Sand.

5.2. Specific hazards arising from the chemical

Fire hazard : Not flammable.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions : Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection.

Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep container closed when not in use.

Incompatible products : Metallic sodium.

Incompatible materials : Sources of ignition. Direct sunlight.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Water (7732-18-5)
No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls : Provide adequate general and local exhaust ventilation.

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Safety glasses.

Eye protection:

Chemical goggles or safety glasses

Respiratory protection:

None necessary.

Personal protective equipment symbol(s):

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Liquid
Color	:	Colorless
Odor	:	None.
Odor threshold	:	No data available
pH	:	7
Melting point	:	0 °C
Freezing point	:	No data available
Boiling point	:	100 °C
Critical temperature	:	374.1 °C
Critical pressure	:	218.3 atm
Flash point	:	No data available
Relative evaporation rate (butyl acetate=1)	:	No data available
Flammability (solid, gas)	:	Non flammable.
Vapor pressure	:	17.535 mm Hg
Vapor pressure at 50 °C	:	92.51 mm Hg
Relative vapor density at 20 °C	:	No data available
Relative density	:	1
Specific gravity / density	:	0.99823 g/ml
Molecular mass	:	18 g/mol
Solubility	:	Soluble in acetic acid. Soluble in acetone. Soluble in ammonia. Soluble in ammonium chloride. Soluble in ethanol. Soluble in glycerol. Soluble in hydrochloric acid. Soluble in methanol. Soluble in nitric acid. Soluble in sulfuric acid. Soluble in sodium hydroxide solution. Soluble in propylene glycol.
Log Pow	:	No data available
Auto-ignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, kinematic	:	1.004 mm²/s
Viscosity, dynamic	:	1.002 cP
Explosion limits	:	No data available
Explosive properties	:	Not applicable.
Oxidizing properties	:	None.

9.2. Other information

VOC content : 0 %

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Not established.

10.4. Conditions to avoid

Extremely high or low temperatures.

10.5. Incompatible materials

Metallic sodium.

10.6. Hazardous decomposition products

Hydrogen. oxygen.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

Water (7732-18-5)	
LD50 oral rat	≥ 90000 mg/kg
ATE US (oral)	90000 mg/kg body weight

Skin corrosion/irritation : Not classified
pH: 7
Serious eye damage/irritation : Not classified
pH: 7
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified (Based on available data, the classification criteria are not met)
Reproductive toxicity : Not classified
STOT-single exposure : Not classified
STOT-repeated exposure : Not classified
Aspiration hazard : Not classified
Viscosity, kinematic : 1.004 mm²/s
Likely routes of exposure : Skin and eye contact.
Potential Adverse human health effects and symptoms : Based on available data, the classification criteria are not met.
Symptoms/effects : Not expected to present a significant hazard under anticipated conditions of normal use.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

Water (7732-18-5)	
Persistence and degradability	Not established.

12.3. Bioaccumulative potential

Water (7732-18-5)	
Bioaccumulative potential	Not established.

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Other information : No other effects known.

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Not regulated

Transport by sea

Not regulated

Air transport

Not regulated

SECTION 15: Regulatory information

15.1. US Federal regulations

Water (7732-18-5)
Listed on the United States TSCA (Toxic Substances Control Act) inventory

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

15.2. International regulations

CANADA

Water (7732-18-5)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

No additional information available

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

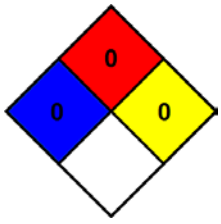
Revision date : 06/26/2020

Other information : None.

NFPA health hazard : 0 - Materials that, under emergency conditions, would offer no hazard beyond that of ordinary combustible materials.

NFPA fire hazard : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating		
Health	:	0 Minimal Hazard - No significant risk to health
Flammability	:	0 Minimal Hazard - Materials that will not burn
Physical	:	0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.
Personal protection	:	A A - Safety glasses

SDS US LabChem

Material Safety Data Sheet
Acetone-alcohol, 1:1

Section 1 - Chemical Product and Company Identification

MSDS Name:
Acetone-alcohol, 1:1
Catalog Numbers:
LC10440
Synonyms:
None
Company Identification:
LabChem Inc
200 William Pitt Way
Pittsburgh, PA 15238
Company Phone Number:
(412) 826-5230
Emergency Phone Number:
(800) 424-9300
CHEMTREC Phone Number:
(800) 424-9300 or
011-703-527-3887

Section 2 – Composition, Information on Ingredients

CAS#	Chemical Name:	Percent
67-64-1	Acetone	50
67-56-1	Methyl alcohol	2.5
67-63-0	Isopropyl alcohol	2.5
64-17-5	Ethyl alcohol	40

Section 3 - Hazards Identification

Emergency Overview

Appearance: *Clear, colorless solution.*

Danger! *Flammable liquid. May be fatal or cause blindness if swallowed. Causes severe eye irritation. May cause irritation to skin, respiratory and digestive tracts. May cause central nervous system depression. May cause liver and kidney damage. May cause reproductive and fetal effects.*

Target Organs: *Kidneys, central nervous system, liver.*

Potential Health Effects

Eye:

Contact with liquid or vapor causes irritation, characterized by a burning sensation, redness, tearing, inflammation, and possible corneal injury. May cause painful sensitization to light.

Skin:

May cause skin irritation. Prolonged or repeated contact may cause irritation or dermatitis. Exposure may cause irritation characterized by redness, dryness, and inflammation.

Ingestion:

May cause irritation of the digestive tract. Symptoms may include: headache, excitement, fatigue, nausea, vomiting, stupor, and coma. May cause systemic toxicity with acidosis. May cause liver and kidney damage. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma and possible death due to respiratory failure.

Inhalation:

May cause irritation of the respiratory tract. Inhalation of high concentrations may cause central nervous system effects characterized by headache, dizziness, unconsciousness and coma.

Chronic:

Prolonged or repeated skin contact may cause defatting and dermatitis. Denatured ethanol is associated with respiratory irritation, central nervous system depression, visual impairment, dermatitis, conjunctivitis, sensory and motor impairment.

Section 4 - First Aid Measures

Eyes:

Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower lids until no evidence of chemical remains. Get medical aid at once.

Skin:

Immediately flush skin with plenty of water for at least 15 minutes, occasionally lifting the upper and lower lids until no evidence of chemical remains. Remove contaminated clothing to reduce further exposure. Get medical aid.

Ingestion:

Do not induce vomiting. If vomiting occurs naturally, keep head lower than hips to prevent aspiration into lungs. Give conscious victim 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid at once.

Inhalation:

Move victim to fresh air immediately. If breathing is difficult, give oxygen. Give artificial respiration if necessary. Get medical aid at once.

Notes to Physician:

Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information:

As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Flammable Liquid. Vapor-air mixtures are explosive at temperatures above the flash point. Vapors can travel to a source of ignition and flash back. Use water spray to keep fire-exposed containers cool. Containers can build up pressure if exposed to heat and/or fire.

Extinguishing Media:

For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam.

Autoignition Temperature:

869°F (465°C)

Flash Point:
57°F (14°C)
NFPA Rating:
CAS# 67-64-1: Health-1; Flammability-3; Instability-0
CAS# 67-56-1: Health-1; Flammability-3; Instability-0
CAS# 67-63-0: Health-1; Flammability-3; Instability-0
CAS# 64-17-5: Health-0; Flammability-3; Instability-0
Explosion Limits:
Lower: 2.6 Upper: 19

Section 6 - Accidental Release Measures

General Information:
Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks:
Remove all sources of ignition. Absorb spill using an absorbent, non-combustible material such as earth, sand, diatomaceous earth, vermiculite, or other suitable absorbent, and transfer to a suitable container labeled for disposal. Label reclaimed spill material as flammable.

Section 7 - Handling and Storage

Handling:
Wash thoroughly after handling. Use with adequate ventilation. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, liquid and vapor, and can be dangerous. Avoid contact with heat, sparks and flame. Avoid ingestion and inhalation. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
Storage:
Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls:
Facilities using or storing this material should be equipped with an eyewash and safety shower. Use adequate general and local exhaust ventilation to keep airborne levels below the permissible exposure limits. Ventilation equipment must be explosion-proof.
Exposure Limits:

Chemical Name:	ACGIH	NIOSH	OSHA
Acetone	250 ppm TWA; 590 mg/m3 TWA	1000 ppm TWA; 2400 mg/m3 TWA	500 ppm TWA;750 ppm STEL
Methyl alcohol	200 ppm TWA; 260 mg/m3 TWA	200 ppm TWA; 260 mg/m3 TWA	200 ppm TWA;250 ppm STEL; skin - potential for cutaneous absorption
Isopropyl alcohol	400 ppm TWA; 980 mg/m3 TWA	400 ppm TWA; 980 mg/m3 TWA	(400 ppm) TWA;(500ppm) STEL
Ethyl alcohol	1000 ppm TWA; 1900 mg/m3 TWA	1000 ppm TWA; 1900 mg/m3 TWA	1000 ppm TWA

OSHA Vacated PELs:

Acetone: 750 ppm TWA; 1800 mg/m3 TWA
Methyl alcohol: 200 ppm TWA; 260 mg/m3 TWA
Isopropyl alcohol: 400 ppm TWA; 980 mg/m3 TWA
Ethyl alcohol: 1000 ppm TWA; 1900 mg/m3 TWA

Personal Protective Equipment

Eyes:

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133.

Skin:

Wear appropriate protective gloves to prevent skin exposure.

Clothing:

Wear appropriate protective clothing to prevent skin exposure.

Respirators:

A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

Section 9 - Physical and Chemical Properties

Physical State:	Liquid
Color:	Colorless
Odor:	Solvent odor
pH:	Not available
Vapor Pressure:	Not available
Vapor Density:	Not available
Evaporation Rate:	Not available
Viscosity:	Not available
Boiling Point:	Not available
Freezing/Melting Point:	Not available
Decomposition Temperature:	Not available
Solubility in water:	Soluble
Specific Gravity/Density:	0.79
Molecular Formula:	Not applicable
Molecular Weight:	Not applicable

Section 10 - Stability and Reactivity

Chemical Stability:

Stable under normal temperatures and pressures.

Conditions to Avoid:

High temperatures, incompatible materials, ignition sources, excess heat.

Incompatibilities with Other Materials:

Strong oxidizing agents, alkali metals, nitric acid, sulfuric acid.

Hazardous Decomposition Products:

Carbon monoxide, carbon dioxide, formaldehyde.

Hazardous Polymerization:

Has not been reported.

Material Safety Data Sheet
Acetone-alcohol, 1:1

Section 11 - Toxicological Information

RTECS:

CAS# 67-64-1: AL3150000.
CAS# 67-56-1: PC1400000.
CAS# 67-63-0: NT8050000.
CAS# 64-17-5: KQ6300000.

LD50/LC50:

CAS# 67-64-1:
Inhalation, rat: LC50 =50100 mg/m3/8H
Oral, mouse: LD50 = 3 gm/kg
Oral, rat: LD50 = 5800 mg/kg
Skin, rabbit: LD50 = 20 gm/kg.

CAS# 67-56-1:
Inhalation, rat: LC50 =64000 ppm/4H
Oral, rat: LD50 = 5600 mg/kg
Skin, rabbit: LD50 = 15800 mg/kg.

CAS# 67-63-0:
Inhalation, rat: LC50 =72600 mg/m3
Oral, rat: LD50 = 5000 mg/kg
Skin, rabbit: LD50 = 12800 mg/kg.

CAS# 64-17-5:
Inhalation, rat: LC50 = 20000 ppm/10H
Oral, mouse: LD50 = 3450 mg/kg
Oral, rat: LD50 = 7060 mg/kg

Carcinogenicity:

CAS# 67-64-1: Not listed as a carcinogen by ACGIH, IARC, NIOSH, NTP, OSHA, or CA Prop 65.
CAS# 67-56-1: Not listed as a carcinogen by ACGIH, IARC, NIOSH, NTP, OSHA, or CA Prop 65.
CAS# 67-63-0: Not listed as a carcinogen by ACGIH, IARC, NIOSH, NTP, OSHA, or CA Prop 65.
CAS# 64-17-5: Not listed as a carcinogen by ACGIH, IARC, NIOSH, NTP, OSHA, or CA Prop 65.

Epidemiology:

Prenatal exposure to ethanol is associated with a distinct pattern of congenital malformations that have collectively been termed the "fetal alcohol syndrome". Among the characteristics of this syndrome are intrauterine and postnatal growth deficiency, a distinctive pattern of physical malformation, and behavioral/cognitive impairment such as fine motor dysfunction and mental retardation. Not all affected children have all of the features of the syndrome. Central Nervous System depressant.

Teratogenicity:

CAS# 64-17-5: Oral, Human - woman: TDLo = 41 gm/kg (female 41 week(s) after conception) Effects on Newborn - Apgar score (human only) and Effects on Newborn - other neonatal measures or effects and Effects on Newborn - drug dependence.

Reproductive:

CAS# 64-17-5: Intrauterine, Human - woman: TDLo = 200 mg/kg (female 5 day(s) pre-mating) Fertility - female fertility index (e.g. # females pregnant per # sperm positive females; # females pregnant per # females mated).

Mutagenicity:

CAS# 64-17-5: DNA Inhibition: Human, Lymphocyte = 220 mmol/L.; Cytogenetic Analysis: Human, Lymphocyte = 1160 gm/L.; Cytogenetic Analysis: Human, Fibroblast = 12000 ppm.;

Cytogenetic Analysis: Human, Leukocyte = 1 pph/72H (Continuous).; Sister Chromatid Exchange: Human, Lymphocyte = 500 ppm/72H (Continuous).

Neurotoxicity:

No information found

Section 12 - Ecological Information

No information found

Section 13 - Disposal Considerations

Dispose of in accordance with Federal, State, and local regulations.

Section 14 - Transport Information

US DOT

Shipping Name: Flammable liquid, n.o.s. (Acetone, ethanol)
Hazard Class: 3
UN Number: UN1993
Packing Group: PG II

Section 15 - Regulatory Information

US Federal

TSCA:

CAS# 67-64-1 is listed on the TSCA Inventory.
CAS# 67-56-1 is listed on the TSCA Inventory.
CAS# 67-63-0 is listed on the TSCA Inventory.
CAS# 64-17-5 is listed on the TSCA Inventory.

SARA Reportable Quantities (RQ):

CAS# 67-64-1: final RQ = 5000 pounds (2270 kg)
CAS# 67-56-1: final RQ = 5000 pounds (2270 kg)

CERCLA/SARA Section 313:

This material contains Methyl alcohol (CAS# 67-56-1, 2.5%), and Isopropyl alcohol (CAS# 67-63-0, 2.5%), which are subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.

OSHA - Highly Hazardous:

None of the components are on this list.

US State

State Right to Know:

Acetone can be found on the following state Right-to-Know lists: California, New Jersey, Florida, Pennsylvania, Minnesota, Massachusetts.
Methyl alcohol can be found on the following state Right-to-Know lists: California, New Jersey, Florida, Pennsylvania, Minnesota, Massachusetts.

Isopropyl alcohol can be found on the following state Right-to-Know lists: California, New Jersey, Florida, Pennsylvania, Minnesota, Massachusetts.
Ethyl alcohol can be found on the following state Right-to-Know lists: California, New Jersey, Florida, Pennsylvania, Minnesota, Massachusetts.

California Regulations:

WARNING: This product contains Ethyl alcohol, a chemical known to the state of California to cause birth defects or other reproductive harm.

European/International Regulations

Canadian DSL/NDSL:

CAS# 67-64-1 is listed on Canada's DSL List.
CAS# 67-56-1 is listed on Canada's DSL List.
CAS# 67-63-0 is listed on Canada's DSL List.
CAS# 64-17-5 is listed on Canada's DSL List.

Canada Ingredient Disclosure List:

CAS# 67-64-1 is listed on Canada's Ingredient Disclosure List.
CAS# 67-56-1 is listed on Canada's Ingredient Disclosure List.
CAS# 67-63-0 is listed on Canada's Ingredient Disclosure List.
CAS# 64-17-5 is listed on Canada's Ingredient Disclosure List.

Section 16 - Other Information

MSDS Creation Date: November 23, 1997
Revision Date: March 24, 2010

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