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PRODUCTION OF POLYURETHANE FROM POLYETHYLENE TEREPHTHALATE

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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.

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EXECUTIVE SUMMARY

Polyurethanes are plastic polymers made by combining diisocyanates with polyols with chemical formula $C_3H_8N_2O$. It also known as polyfoam plastic sponge. Polyurethane demand is estimated to be 25.29 million tonnes in 2025 compound annual growth rate (CAGR) of 5.22% from 2017 to 2025. So, our plant is designed to generate around 39,500 tonnes per year, or 4,770.5 kg per hour, and it will run every day except for roughly 20 days for maintenance needs. For the purity for the Polyurethane, we manage to get 98% of purity. In the production line, it go through 3 reaction process and 3 separator included. The first step is the aminolysis process, which involves reacting waste PET with ethanolamine to produce BHETA with 85% conversion of PET. After that, BHETA reacts with caprolactone to form Polyol with 90% conversion of BHETA, which is then combined with two hydroxyl groups in Polyester Hexamethylene Diisocyanate (HDI) to form Polyurethane with 90% conversion of Polyol. The waste or side product generated during production will be handled first before being released. The mass balance is balanced, and the energy balance is calculated. Superpro, Matlab and Symmetry software been used to obtain and compare the mass balance and energy balance values with the manual calculation. The percentage error also included. Numerical method that been used in finding the roots based on the equation in the reactor also been discussed. Other than that, the stages, diameter and height of the separator unit which is distillation column were calculated which is 22 stages, 2.62 ft and 50.6 ft. one of the reactor used in the plant is continuous stirred tank reactor (CSTR) and the general mle balance equation for CSTR and kinetic rate expression are also equated.

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CHAPTER I

BACKGROUND OF STUDY

1.1 INTRODUCTION

Polyurethanes are plastic polymers made by combining diisocyanates with polyols with chemical formula $C_3H_8N_2O$. It also known as polyfoam plastic sponge. It was produced by the exothermic reaction between those chemicals which is polyol and diisocyanates.

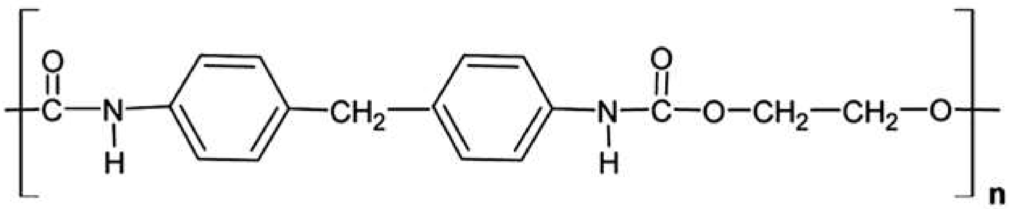

Figure 1.1 Polyurethane structure

Source: Rahman et al, 2018

Polyurethanes were invented by Professor Dr. Otto Bayer in 1930s (Hood, 2019). It was used in many industries which is aviation, railway, architecture, and sports. It also used in manufacture of plastic products, synthesis rubber product, synthetic fibre, hard and soft foam plastics, adhesives, and coating. The usage of polyurethanes extensive during World War II, when it was utilized as a replacement for rubber because at that time rubber was expensive and hardly to obtain. During the war, the applications were developed, largely involving coatings of different kinds, from aeroplane finishes to resistant clothing. In 1950, polyurethanes were used in many industries like adhesives, elastomers, rigid foams, in the latter part of the same decade and flexible cushioning foams similar to those used today (Allan Clements, 2020).

In this project, Polyethylene Terephthalate (PET) waste has been chosen as the raw material for synthesis of Polyurethanes. PET is a semicrystalline thermoplastic polymer, which is used in the preparation of a variety of products. PET began to be used popularly for production of disposable soft drink in 1987, more than 700 million pounds of PET were consumed in their production. As the result, because of high application, large amount of PET waste is also generated. As the production increase the PET waste also increase that also causes effect to environment (Das & Mahanwar, 2020).

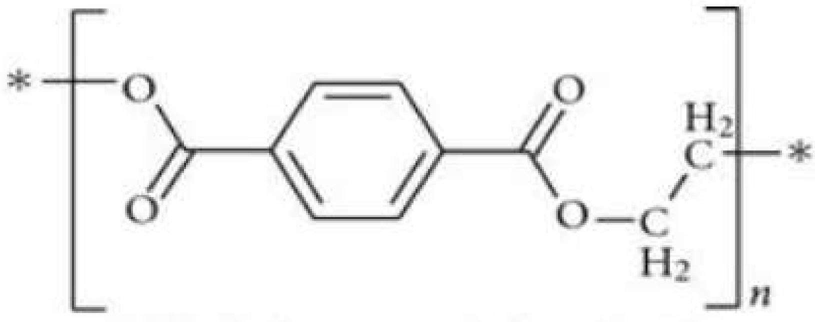

Figure 1.2 Polyethylene terephthalate structure

Source: Prasad et al., 2011

1.2 PHYSICAL AND CHEMICAL PROPERTIES

Purity of polyurethane was used in our production is 98 %. Purity has decided based on our unit process and market value. Physical and chemical properties polyurethane is shown in Table 1.1.

Table 1.1 Physical and Chemical Properties of Polyurethane

Properties	**Polyurethane**
Physical state	Solid
Boiling point	137°C
Specific gravity	1.17
Density	1.17 g/cm^3
Odor, Colour, Grade	Mild xylene odor
Thermal Conductivity	0.14 – 0.5 W/m.K
Molecular formula	$C_{27}H_{36}N_2O_{10}$
Molecular weight	7.6 x 10^{12} g/mol

Source: Material Safety Data Sheet Polyurethane, 2013

1.3 USAGE OF POLYURETHANE

Polyurethanes (PU) is a class of polymers with organic molecules joined with urethanes linkage. Polyurethane's versatility allows them to be used to solve the problems. It molds into unexpected shapes and improve the industrial and consumer products. Most polyurethanes are in the foam form, which is the most material that has been used in furniture, cushioning, medical application, automotive, marine, packaging and hospital bedding (Das & Mahanwar, 2020).

In medical application, polyurethanes are commonly used in production of blood contacting device such as heart valves, artificial, and arteries. Polyurethanes have properties such as durability, flexibility, fatigue resistance and tolerance in body during healing make these material played a major role in medical development. Chemical group of polyurethanes structure allow for bulk and surface modification via hydrophilic or hydrophobic balancing or attachments of physiologically active species such as anticoagulants and bio recognizable group. These alterations are intended to help the devices to be accepted and heal more quickly (Zdrahala et al., 1999).

Polyurethane has been a great addition in marine technology along with epoxy. It's not only great building material but also great for marine coating. PU protects the product from corrosion and water erosion, as well as preventing aquatic life from settling and growing on the ship or boat hull. PU marine coating has anti-fouling and algae protection. It also uses in boats and ships because it provides excellent insulation as well as great noise reduction. Boat parts that manufactured from PU are lighter than metal counterparts and improve the efficiency of the engine (Muminovic, 2016).

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CHAPTER II

ECONOMIC ANALYSIS

2.1 THE SUPPLY AND DEMAND OF POLYURETHANE

The global polyurethane market demand at 16.00 million tonnes in 2016 and is expected to grow at a compound annual growth rate (CAGR) of 5.22% from 2017 to 2025. The expected value of polyurethane demand in 2025 is 25.29 million tonnes. The polyurethane chemistry allows it to be molded into unusual shapes and enhance industrial and consumer products by adding comfort and convenience.

Polyurethanes are formed by reacting polyols with a diisocyanate or a polymeric isocyanate in the presence of suitable catalysts and additives. A variety of products are manufactured based on wide range of polyols to meet the needs of specific applications. Polyurethane products are used in wide range of consumer goods used in day-to-day life (Polyurethane Market, 2017).

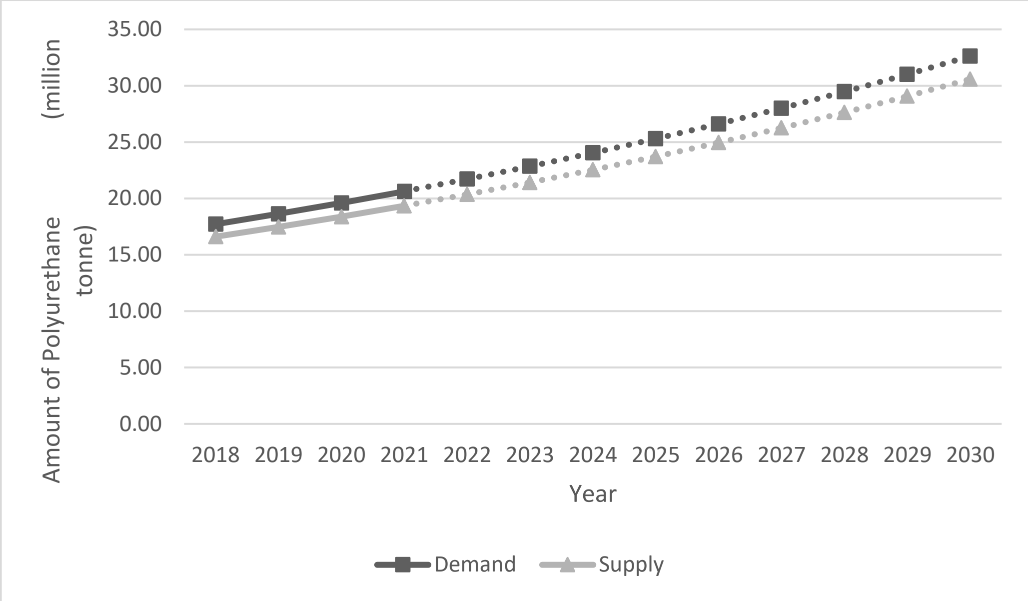

Figure 2.1 Graph of supply and demand of polyurethane from 2016 to 2025

Source: Polyurethane production, pricing, and market demand. Plastics Insight, 2021

2.2 LIST OF COMPANY PRODUCING POLYURETHANE

Many companies around the globe nowadays that produced the Polyurethane. Because of it promising market potential, the companies will keep produce it because it will be benefit for both sides, the companies and the consumer. These were the top five polyurethane market vendors, BASF SE, Covestro Ag, DowDuPont, Hunstman International LLC and Recticel NV (Technavio, 2019). Other than that, there are also many companies that produced the Polyurethane. The list of Polyurethane production companies is shown in the table below:

Table 2.1 List of Company Producing Polyurethane

Company	Location
Ultimate Panel (M) sdn. bhd.	Rawang, Malaysia
American Urethane	USA
Yayasan Al Huffaz	Alor Star, Malaysia
Falline Corporation	California, USA

Source: Bizdirect, 2018

The list of Polyurethane production by country is shown in the table 2.2. From the data, European Union is the largest producer of polyurethanes.

Table 2.2 List of Country Producing Polyurethane

Country	Production Capacity, kg
European Union	456, 840, 000
Germany	389, 431, 000
Italy	198, 150, 000
Malaysia	22, 688, 500

Source: WorldIntegratedTradeSolution, 2018

2.3 MARKET PRICE OF POLYURETHANE

Polyurethanes has been affected by recent logistical challenges, which have limited supply and as a result, driven up prices. Key factors that are driving the market and price growth include government restrictions, lockdowns and factories being shut-down because of Covid-19 (Mordor Intelligence, 2021). Then, the market price for 98% purity of polyurethane is \$12000 per metric ton and \$12 per kilogram (Polyurethane Pricing Dashboard, 2020). Assumption has been considered that the market price for polyurethane will be same all around the world which is match to the industrial standards. Figure 2.2 below shows the price of polyethylene in year 2017.

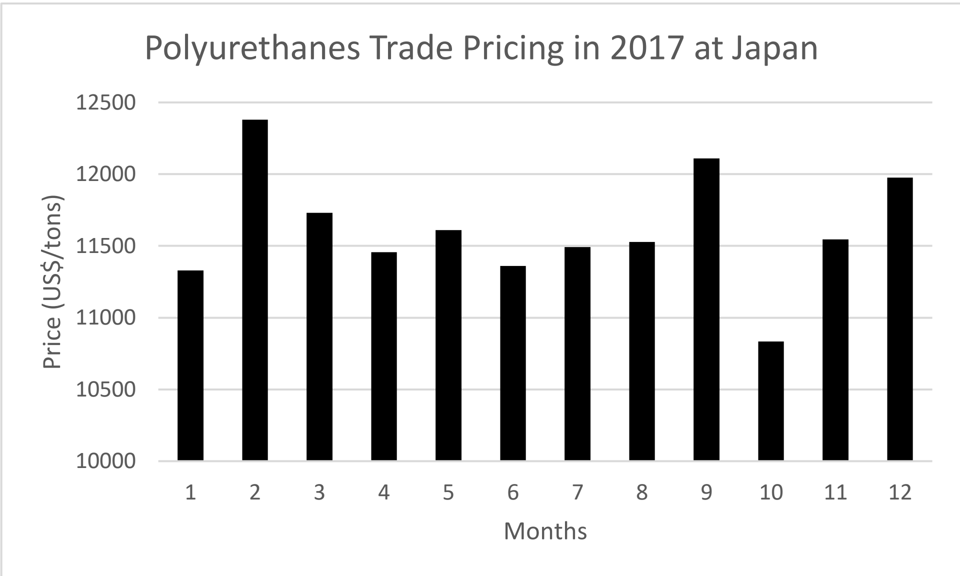

Figure 2.2 Price of Polyurethane in 2017 at Japan

Source: Plastic Insight, 2018

Currency rate: 1 US dollar = 4.15 Malaysian Ringgit (October 27, 2021)

2.4 PLANT CAPACITY

Based on the figure 2.1, the demand for Polyurethane in 2025 are expected to be at 25.29 million tonnes per year, while the supply for that year is expected at 23.71 million tonnes per year. For our Polyurethane production on the year 2025, we decided to fulfill for 2.5% of the deficiency (1.58 million tonnes), which means we produced about 39,500 tonnes per year and equals to 4,770.5 kg per hour. The chemical plant will operate for 345 days with 20 days left for maintenance purposes.

Plant Capacity for year 2025:

Demand	=	25 290 000 tonnes/ year
Supply	=	23 710 000 tonnes/ year
Deficient	=	Demand – Supply
	=	25 290 000 – 23 710 000
	=	1 580 000 tonnes/ year

Production time	=	(365 – 20 maintenance days) days × 24 hours
	=	8 280 hours

Our production fulfills 2.5% from the deficient.

Plant Capacity	=	0.025 × 1 580 000
	=	39 500 tonnes/year
	=	39 500 000 kg/year
	=	39 5000 000 ÷ 8 280
	=	4 770.5 kg/ hour

Hence, the production rate is estimated at 4,770.5 kg/ hour.

2.5 FUTURE MARKET ANALYSIS

The future market potential for Polyurethane showing a promising positive trend because as the CAGR grow at 5.22% from 2017 to 2025. As the year goes by, more and more production companies will compete to produce the Polyurethane and to fulfill the global demand.

The key factor that drives the increasing demand for Polyurethane is the increasing demand from the building and construction industry (Polyurethane Market - Growth, Trends, COVID-19 Impact, and Forecasts (2021 - 2026), 2021). This is because the Polyurethane has many advantages such as it insulation properties, durability, and versatility. One of the usages of Polyurethane in building and construction are rigid polyurethane foam (RPUF). It has been produced in large number because of its outstanding performance (Wang et al., 2019).

Other than that, a part of the world, the Asia-Pacific region will dominate the Polyurethane market. The increasing construction activities in the country such as China and India will increase the usage of Polyurethane in that region (Polyurethane Market - Growth, Trends, COVID-19 Impact, and Forecasts (2021 - 2026), 2021). Other than that, the electronics market has experienced the increasing demand with market size increase from USD 145 billion to USD 215 billion (Electronics System Design & Manufacturing (ESDM) Industry in India, 2020). In India also shows the increasing demand in electronics. It also the factor for the promising future market potential for Polyurethane as it also used in electronics sector.

CHAPTER III

PROCESS DESCRIPTION

3.1 INTRODUCTION

Polyurethanes can be Synthesis using Aminolysis of Poly (ethylene terephthalate) (PET) which one of the most used in study and industry. (PET) recycling has been carried out in many ways like Mechanical recycling, Chemical Recycling, and Energy recovery method. There are many stages in producing Polyurethanes. Chemical recycling use in this project include aminolysis using ethanolamine. (More et al. 2013). The synthesis of PET produce BHETA which is has potential to undergo further reaction to yield secondary value-added products.

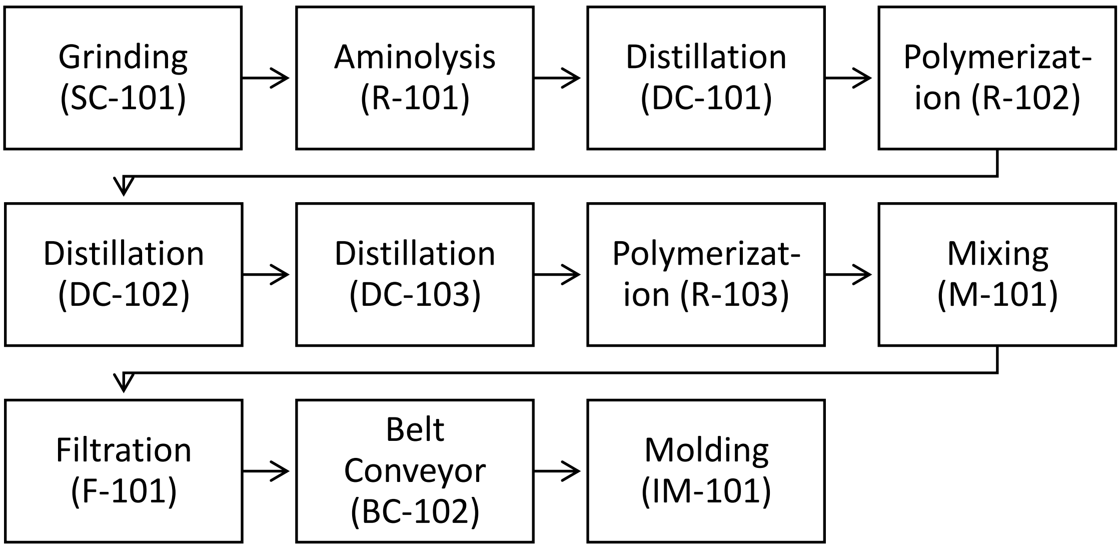

Figure 3.1 Simplified process diagram in block diagram

3.2 PROCESS DESCRIPTION

3.2.1 Grinding (SC-101)

The clean PET waste enters the screw conveyor to form the PET waste into small particles.

3.2.2 Aminolysis (R-101)

Aminolytic degradation of PET with ethanolamine produce bis(2-hydroxyethyl) terephthalamide (BHETA) and Ethylene Glycol (EG). The ratio between PET and ethanolamine is 1:4 (w/w) % with 3-hour reaction at 160°C and 1 atm under reflux in presence of zinc acetate as catalyst (Azman et al. 2018) in nitrogen atmosphere in the reactor 1. PET enter the reactor from screw conveyor with temperature 93°C. In this reaction, ethanolamine has two nucleophilic centres, while nitrogen is more electronegative than oxygen. The amine group from ethanolamine will attacks the ester linkage of PET and produce BHETA (85%) while EG as side product (Azman et al. 2019).

$$C_{10}H_8O_4 + 2C_2H_7NO \xrightarrow{\text{zinc acetate}} C_{12}H_{16}O_4N_2 + C_2H_6O_2$$

3.2.3 Distillation (DC-101)

The mixture of the product from first reaction which is BHETA and EG will be cooling down using heat exchanger and then separated in Distillation column at 197°C because both product which is BHETA and EG are liquid. Since the boiling point of BHETA is higher than EG which is 446.5 °C, the top product should be EG (boiling point 197°C) and unreacted reactant which PET and ethanolamine while BHETA is the bottom product.

3.2.4 Polymerization (R-102)

BHETA was further reacted with Caprolactone through ring opening polymerization at 130°C and 1 atm with Dibutyltin dilaurate (DBTDL) 1% wt as a catalyst in the second reactor (Packed bed reactor) with nitrogen gas inlet. The product obtained is Polyester polyol with 2 hydroxyl group (More et al.2013).

$$C_{12}H_{16}N_2 + 2C_6H_{10}O_2 \xrightarrow{DBTDL} C_{24}H_{34}O_6N_2(OH)_2$$

3.2.5 Distillation (DC-102)

The temperature mixture from the reactor 2 polyester polyol and unreacted reactant (BHETA and caprolactone) was reduced by to heat exchanger 70°C and the mixture were separated in distillation column (D-102) at 300°C and above. The top product is caprolactone since its boiling point is 241°C and polyol (boiling point 300°C) while bottom product is BHETA.

3.2.6 Distillation (DC-103)

To separate the Polyol and caprolactone, this mixture will enter the Distillation column (D-103) again at 241°C to separate the caprolactone and polyol and the top product is Caprolactone while polyol is Bottom product.

3.2.7 Polymerization (R-103)

Polyurethanes polymer formed through step-Growth polymerization by reacting the polyester polyol with two hydroxyl group Polyester Hexamethylene Diisocyanate (HDI) with two isocyanate group by forming urethanes linkage. (Mir et al. n.d.). There are 3 basic components in this reaction diisocyanate, short chain diol (Chain extender) and long chain diol (OH-OH). This reaction occurs at 110°C at 1 atm in CSTR which is the Polyol react with Hexamethylene Diisocyanate (HDI) to form liquid polyurethanes with DMF as a solvent.

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_8N_4$$

3.2.8 Mixing (M-101)

The polyurethanes from reactor 3 were cooling down to 70°C in heat exchanger. To obtain the polyurethanes in solid form, the liquid polyurethanes were mixed with water in mixer to separate the polyurethanes from DMF solvent. (Wiley 2008)

3.2.9 Filtration (F-101)

The mixture was undergoing filtration in the filter to separated wastewater and Polyurethanes. The wastewater will undergo pre-treatment in wastewater treatment plant.

3.2.10 Belt Conveyor (BC-101)

Move the solid polyurethanes after filtration to injection molding to make a desire shape.

3.2.11 Molding (IM-101)

The last process of this production is injection molding which is to give a shape desire of solid polyurethanes. There are 4 stages in injection molding which is clamping, injection, cooling, and ejection stages. The clamping unit is what piece together the mold and then follow up by injection. The two sides of the mold are placed into the unit and then pushes the two halves together. The mold is left alone so that the polyurethanes can cool and start form as solid inside the mold. The final step is ejection which reveals the final product from mold (Jason, 2016).

3.3 PROCESS FLOW DIAGRAM

Refer to the attachment

P-101 Pump 1
P-102 Pump 2
P-103 Pump 3
P-104 Pump 4
P-105 Pump 5
SC-101 Screw Conveyor
R-101 Reactor 1
C-101 Cooler 1
P-106 Pump 6
DC-101 Distillation Column 1
P-107 Pump 7
C-102 Cooler 2
FX-101 Reflux 1
RB-101 Reboiler 1
B-101 Blower 1
RB-102 Reboiler 2
CD-101 Condenser 1
R-102 Reactor 2
P-108 Pump 8
P-109 Pump 9
CD-102 Condenser 2
FX-102 Reflux 2
DC-102 Distillation Column 2
DC-103 Distillation Column 2
CD-103 Condenser 3
FX-103 Reflux 3
RB-103 Reboiler 3
R-103 Reactor 3
C-103 Cooler 3
P-110 Pump 10
F-101 Filter 1
BC-102 Belt Conveyer
IM-101 Injection Molding 1
C-104 Cooler 4
C-105 Cooler 5
C-106 Cooler 6

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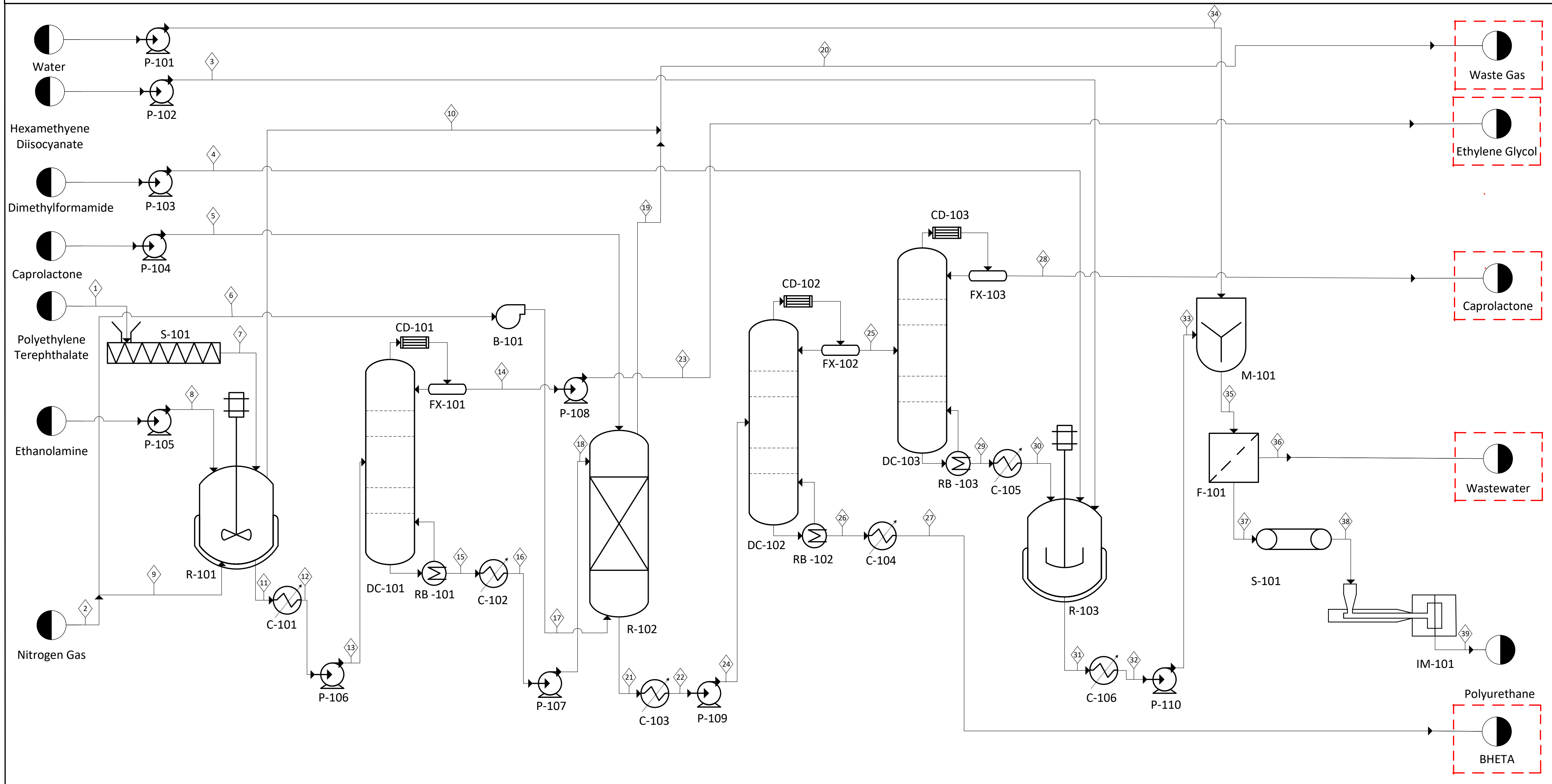
The National University of Malaysia

Title: Production of Polyurethane from Polyethylene Terephthalate



Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Temperature (℃)	25	25	25	25	25	25	93	25	25	160	160	70	70	50	197	70	25	70	130
Pressure (bar)	1.0	1.0	2.0	2.0	2.0	1.0	1.0	1.2	1.0	1.2	1.0	1.0	2.0	1.2	1.2	1.2	2.0	2.0	1.2
Phase	S	G	L	L	L	G	L	L	G	G	L	L	L	L	L	L	G	L	G
Water (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hexamethyene Diisocyanate (kg/h)	0.00	0.00	1352.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dimethylformamide (kg/h)	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Caprolactone (kg/h)	0.00	0.00	0.00	0.00	2040.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Polyethylene Terephthalate (kg/h)	2021.27	0.00	0.00	0.00	0.00	0.00	2021.27	0.00	0.00	0.00	303.19	303.19	303.19	300.03	3.16	3.16	0.00	3.16	0.00
Ethanolamine (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1284.35	0.00	0.00	192.65	192.65	192.65	190.55	2.11	2.11	0.00	2.11	0.00
Nitrogen Gas (kg/h)	0.00	200.00	0.00	0.00	0.00	100.00	0.00	0.00	100.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	0.00	100.00
Ethylene Glycol (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	554.80	554.80	554.80	552.69	2.11	2.11	0.00	2.11	0.00
Polyol (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Polyurethane (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BHETA (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2254.98	2254.98	2254.98	0.00	2254.98	2254.98	0.00	2254.98	0.00
Total flow rate (kg/h)	2021.27	200.00	1352.99	100.00	2040.22	100.00	2021.27	1284.35	100.00	100.00	3305.62	3305.62	3305.62	1043.27	2262.35	2262.35	100.00	2262.35	100.00

Stream	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
Temperature (℃)	145	130	70	50	70	50	300	30	50	241	70	110	70	70	25	48	48	48	60	60
Pressure (bar)	1.2	1.0	1.0	2.0	2.0	1.0	1.0	1.0	1.0	1.0	1.2	1.2	1.0	2.0	2.0	1.0	1.0	1.0	1.0	1.0
Phase	G	L	L	L	L	L	L	L	L	L	L	L	L	L	L	S/L	L	S	S	S
Water (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	300.00	300.00	300.00	0.00	0.00	0.00
Hexamethyene Diisocyanate (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	135.30	135.30	135.30	0.00	135.30	126.35	8.95	8.95	8.95
Dimethylformamide (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	100.00	100.00	0.00	100.00	100.00	0.00	0.00	0.00
Caprolactone (kg/h)	0.00	204.02	204.02	0.00	204.02	201.92	2.11	2.11	199.81	2.11	2.11	2.11	2.11	2.11	0.00	2.11	2.11	0.00	0.00	0.00
Polyethylene Terephthalate (kg/h)	0.00	3.16	3.16	300.03	3.16	1.58	1.58	1.58	0.00	1.58	1.58	1.58	1.58	1.58	0.00	1.58	0.00	1.58	1.58	1.58
Ethanolamine (kg/h)	0.00	2.11	2.11	190.55	2.11	2.11	0.00	0.00	2.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen Gas (kg/h)	200.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene Glycol (kg/h)	0.00	2.11	2.11	552.69	2.11	2.11	0.00	0.00	2.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Polyol (kg/h)	0.00	3865.69	3865.69	0.00	3865.69	3865.69	0.00	0.00	0.00	3865.69	3865.69	386.57	386.57	386.57	0.00	386.57	323.40	63.16	63.16	63.16
Polyurethane (kg/h)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4696.81	4696.81	4696.81	0.00	4696.81	0.00	4696.81	4696.81	4696.81
BHETA (kg/h)	0.00	225.50	225.50	0.00	225.50	0.00	225.50	225.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total flow rate (kg/h)	200.00	4302.57	4302.57	1043.27	4302.57	4073.39	229.18	229.18	204.02	3869.37	3869.37	5322.36	5322.36	5322.36	300.00	5622.36	851.86	4770.50	4770.50	4770.50

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Input
Output
Stream number

Date : 19th January 2022

CHAPTER IV

MASS AND ENERGY BALANCE

4.1 INTRODUCTION

A mass balance is used widely in production industry. It's used to compare the overall inputs and overall outputs of the process because mass that enter a system must equal to mass that flow out of the system. In our Polyurethane production from waste PET, reaction takes place at batch reactor (R-101), packed bed reactor (R-102) and continuous stirred tank reactor (CSTR).

4.2 MASS BALANCE

Plant capacity for our production as below:

Plant capacity = 4770.5 kg/hr

The reaction occurred in the production:

$$C_{10}H_8O_4 + 2C_2H_7NO \xrightarrow{\text{zinc acetate}} C_{12}H_{16}O_4N_2 + C_2H_6O_2 \quad \ldots (4.1)$$

$$C_{12}H_{16}N_2 + 2C_6H_{10}O_2 \xrightarrow{\text{DBTDL}} C_{24}H_{34}O_6N_2(OH)_2 \quad \ldots (4.2)$$

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_8N_4 \quad \ldots (4.3)$$

In our material balance calculation, we used forward calculation and get the ratio of the plant capacity with the obtained final flow rate hence all the flow rate has been multiplied by the scale factor 0.105274656. In the end of the calculations, the mass flow rate of Polyurethane is 4770.5 kg/hr, where we achieved our plant capacity.

4.2.1 Batch Reactor (R-101)

Aminolytic degradation of PET with ethanolamine produce bis(2-hydroxyethyl) terephthalamide (BHETA) and Ethylene Glycol (EG) as by-product happen in reactor (R-101). The chemical reaction equation is as below:

$$C_{10}H_8O_4 + 2C_2H_7NO \xrightarrow{\text{zinc acetate}} C_{12}H_{16}O_4N_2 + C_2H_6O_2$$

Assumption:

Conversion of PET = 85%

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

With N_{iP} equals to 100 kmole/hr.

So, rate of reaction for reactor (R-101), r_1 = 85 kmol/hr

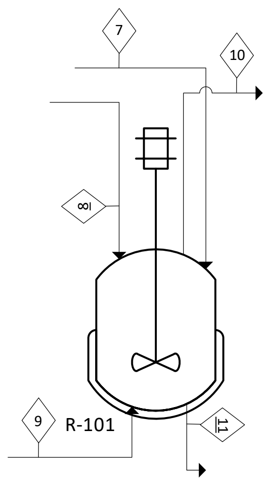


Figure 4.1 Batch Reactor (R-101)

Table 4.1 Summarized Inlet Flow Rate of Component in reactor (R-101)

Components	Inlet stream 7 Mass flow rate (kg/hr)	Inlet stream 8 Mass flow rate (kg/hr)	Inlet stream 9 Mass flow rate (kg/hr)
PET	2021.27	0	0
Ethanolamine	0	1284.35	0
Nitrogen Gas	0	0	100
BHETA	0	0	0
Ethylene Glycol	0	0	0
Total	2021.27	1284.35	100

Table 4.2 Summarized Outlet Flow Rate of Component in reactor (R-101)

Components	**Outlet stream 11 Mass flow rate (kg/hr)**	**Outlet stream 10 Mass flow rate (kg/hr)**
PET	303.19	0
Ethanolamine	192.65	0
Nitrogen Gas	0	100
BHETA	2254.98	0
Ethylene Glycol	554.80	0
Total	3305.62	100

Overall mass balance for R-101:

$$\sum F_{in} = \sum F_{out}$$

$$2021.27 + 1284.35 + 100 = 3305.62 + 100$$

$$3405.62 \text{kg/hr} = 3405.62 \text{ kg/hr (Balanced)}$$

4.2.2 Distillation Column (DC-101)

The mixture of the product from first reaction which is BHETA and EG with the excess of reactant will be separated in Distillation Column (D-101). BHETA with the highest boiling point will be the bottom product.

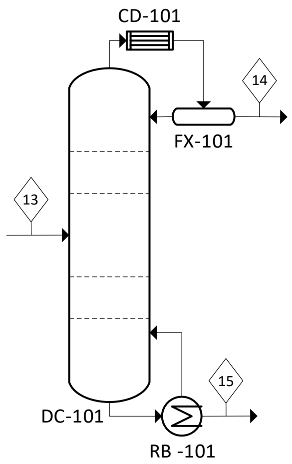


Figure 4.2 Distillation Column (DC-101)

Table 4.3 Summarized of stream table of components in Distillation Column (D-101)

Components	Inlet stream 13 Mass flow rate (kg/hr)	Outlet stream 14 Mass flow rate (kg/hr)	Outlet stream 15 Mass flow rate (kg/hr)
PET	303.19	300.03	3.16
Ethanolamine	192.65	190.55	2.11
BHETA	2254.98	0	2254.98
Ethylene Glycol	554.80	552.69	2.11
Total	3305.62	1043.27	2262.35

Overall mass balance for D-101:

$$\sum F_{in} = \sum F_{out}$$

$$3305.62 = 1043.267 + 2262.348$$

$$3305.62 \text{ kg/hr} = 3305.62 \text{ kg/hr (Balanced)}$$

4.2.3 Packed Bed Reactor (R-102)

BHETA was further reacted with Caprolactone through ring opening polymerization with Dibutyltin dilaurate (DBTDL) as a catalyst in the packed bed reactor (R-102) with nitrogen gas inlet. The product obtained is Polyester polyol with 2 hydroxyl group (More et al.2013). The chemical reaction equation is as below:

$$C_{12}H_{16}N_2 + 2C_6H_{10}O_2 \xrightarrow{DBTDL} C_{24}H_{34}O_6N_2(OH)_2$$

Assumption:

Conversion of BHETA = 90%

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

With N_{iB} equals to 85 kmole/hr.

So, rate of reaction for reactor (R-102), r_2 = 76.5 kmol/hr

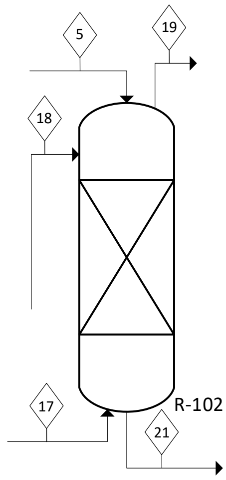


Figure 4.3 Packed Bed Reactor (R-102)

Table 4.4 Summarized Inlet Flow Rate of Component in reactor R-102

Components	Inlet stream 18 Mass flow rate (kg/hr)	Inlet stream 5 Mass flow rate (kg/hr)	Inlet stream 17 Mass flow rate (kg/hr)
BHETA	2254.98	0	0
PET	3.158	0	0
Ethanolamine	2.11	0	0
Ethylene Glycol	2.11	0	0
Caprolactone	0	2040.22	0
Nitrogen Gas	0	0	100
Total	2262.35	2040.22	100

Table 4.5 Summarized Outlet Flow Rate of Component in reactor R-102

Components	Outlet stream 21 Mass flow rate (kg/hr)	Outlet stream 20 Mass flow rate (kg/hr)
BHETA	225.50	0
PET	3.16	0
Ethanolamine	2.11	0
Ethylene Glycol	2.11	0
Caprolactone	204.02	0
Nitrogen Gas	0	100
Polyol	3865.69	0
Total	4302.57	100

Overall mass balance for R-102:

$$\sum F_{in} = \sum F_{out}$$

$$2262.348 + 2040.22 + 100 = 4302.57 + 100$$

$$4402.57 \text{ g/hr} = 4402.57 \text{ kg/hr (Balanced)}$$

4.2.4 Distillation Column (DC-102)

The product from the reaction which is Polyol with the excess of reactant will be separated in Distillation Column (D-102). Caprolactone with the lowest boiling point will be the top product. BHETA and Polyol will go to another Distillation Column for another separation process.

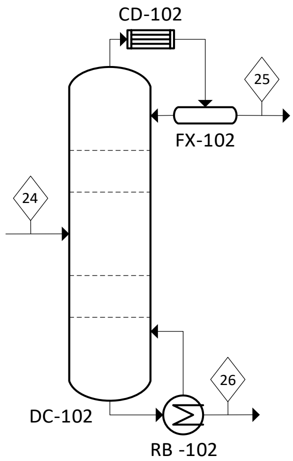


Figure 4.4 Distillation Column (D-102)

Table 4.6 Summarized of stream table of components in Distillation Column (D-102)

Components	**Inlet stream 24 Mass flow rate (kg/hr)**	**Outlet stream 25 Mass flow rate (kg/hr)**	**Outlet stream 26 Mass flow rate (kg/hr)**
BHETA	225.50	0	225.50
PET	3.16	1.58	1.58
Ethanolamine	2.11	2.11	0
Ethylene Glycol	2.11	2.11	0
Caprolactone	204.02	201.92	2.11
Polyol	3865.69	3865.69	0
Total	4302.57	4073.39	229.18

Overall mass balance for D-102:

$$\sum F_{in} = \sum F_{out}$$

$$4302.57 = 4073.39 + 229.182$$

$$4302.57 \text{ kg/hr} = 4302.57 \text{ kg/hr (Balanced)}$$

4.2.5 Distillation Column (DC-103)

The product from D-102 which is Polyol with the excess of BHETA will be separated in Distillation Column (D-103). BHETA with the highest boiling point will be the bottom product. The top product which is Polyol will be condensed to get the liquid form.

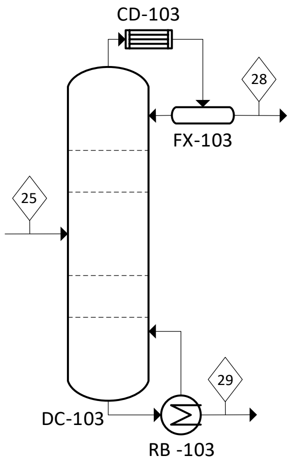


Figure 4.5 Distillation Column (DC-103)

Table 4.7 Summarized of stream table of components in Distillation Column (D-103)

Components	Inlet stream 25 Mass flow rate (kg/hr)	Outlet stream 28 Mass flow rate (kg/hr)	Outlet stream 29 Mass flow rate (kg/hr)
PET	1.58	0	1.58
Ethanolamine	2.11	2.11	0
Ethylene Glycol	2.11	2.11	0
Caprolactone	201.92	199.81	2.11
Polyol	3865.69	0	3865.69
Total	4073.39	204.02	3869.37

Overall mass balance for D-103:

$$\sum F_{in} = \sum F_{out}$$

$$4073.39 = 204.02 + 3869.369$$

$$4073.39 \text{ kg/hr} = 4073.39 \text{ kg/hr (Balanced)}$$

4.2.6 Continuous Stirred-Tank Reactor (R-103)

Polyurethanes polymer formed through step-Growth polymerization by reacting the polyester polyol with two hydroxyl group Polyester Hexamethylene Diisocyanate (HDI) with two isocyanate group by forming urethanes linkage. (Mir et al., n.d.). The Dimethylformamide (DMF) also will flow into the reactor (R-103) to act as solvent to obtain liquid Polyurethane. The chemical reaction equation is as below:

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_8N_4$$

Assumption:

Conversion of Polyol = 90%

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

With N_{iP} equals to 76.5 kmole/hr.

So, rate of reaction for reactor (R-103), r_3 = 68.85 kmol/hr

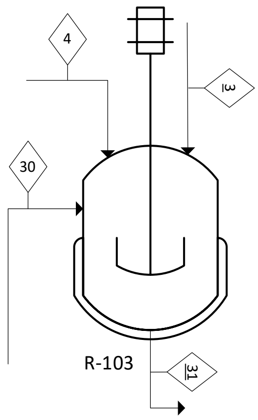


Figure 4.6 Continuous Stirred Tank (R-103)

Table 4.8 Summarized Inlet Flow Rate of Component in reactor R-103

Components	Inlet stream 30 Mass flow rate (kg/hr)	Inlet stream 3 Mass flow rate (kg/hr)	Inlet stream 4 Mass flow rate (kg/hr)
Polyol	3865.69	0	0
Caprolactone	2.11	0	0
PET	1.58	0	0
HDI	0	1352.99	0
DMF	0	0	100
Total	3869.37	1352.99	100

Table 4.9 Summarized Outlet Flow Rate of Component in reactor R-103

Components	Outlet stream 31 Mass flow rate (kg/hr)
Polyol	386.57
Caprolactone	2.11
PET	1.58
HDI	135.30
DMF	100
Polyurethane	4696.81
Total	5322.36

Overall mass balance for R-103:

$$\sum F_{in} = \sum F_{out}$$

$$3869.369 + 1352.99 + 100 = 5322.36$$

$$5322.36 \text{ kg/hr} = 5322.36 \text{ kg/hr (Balanced)}$$

4.2.7 Mixer (M-101)

To obtain the polyurethanes in solid form, the liquid polyurethanes were mixed with water in mixer to precipitate the Polyurethane.

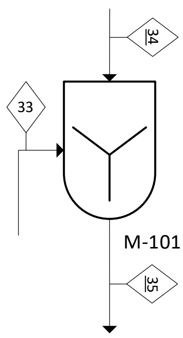


Figure 4.7 Mixer (M-101)

Table 4.10 Summarized of stream table of components in Mixer (M-101)

Components	Inlet stream 33 Mass flow rate (kg/hr)	Inlet Stream 34 Mass flow rate (kg/hr)	Outlet stream 35 Mass flow rate (kg/hr)
Polyol	386.57	0	386.57
Caprolactone	2.11	0	2.11
PET	1.58	0	1.58
HDI	135.30	0	135.30
DMF	100	0	100
Polyurethane	4696.81	0	4696.81
Water	0	300	300
Total	5322.36	300	5622.36

Overall mass balance for M-101:

$$\sum F_{in} = \sum F_{out}$$

$$5322.36 = 300 + 5622.36$$

$$5322.36 \text{ kg/hr} = 5322.36 \text{ kg/hr (Balanced)}$$

4.2.8 Filter (F-101)

The mixture was undergoing filtration in the filter to separated wastewater and Polyurethanes. The wastewater will undergo pre-treatment in wastewater treatment plant.

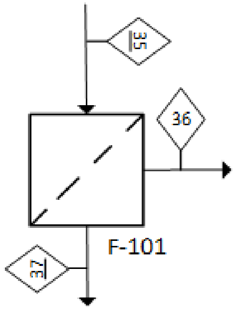


Figure 4.8 Filter (F-101)

Table 4.11 Summarized of stream table of components in Filter (F-101)

Components	Inlet stream 35 Mass flow rate (kg/hr)	Outlet stream 36 Mass flow rate (kg/hr)	Outlet stream 37 Mass flow rate (kg/hr)
Polyol	386.57	323.40	63.16
Caprolactone	2.11	2.11	0
PET	1.58	0	1.58
HDI	135.30	126.35	8.95
DMF	100	100	0
Polyurethane	4696.81	0	4696.81
Water	300	300	0
Total	5622.36	851.86	4770.50

Overall mass balance for F-101:

$$\sum F_{in} = \sum F_{out}$$

$$5622.36 = 851.855 + 4770.5$$

$$5622.36 \text{ kg/hr} = 5622.36 \text{ kg/hr (Balanced)}$$

4.2.9 Overall Mass Balance

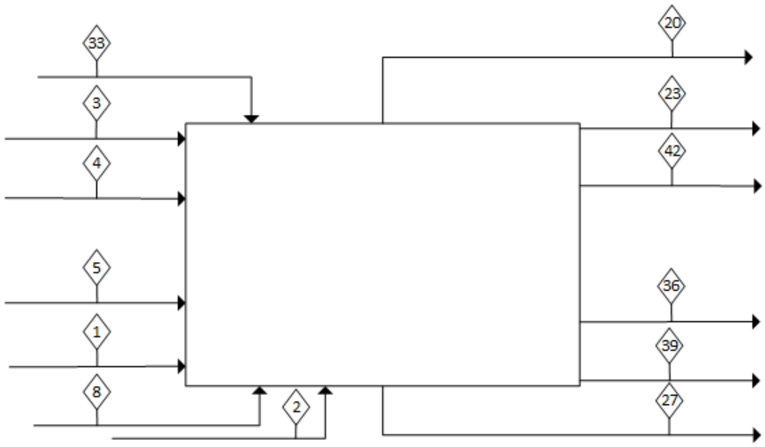


Figure 4.9 Overall Mass Balance

Overall mass balance:

$$\sum F_{in} = \sum F_{out}$$

$$2021.27 + 200 + 1284.35 + 1352.99 + 100 + 2040.22 + 300 = 200 + 1043.267 + 204.02 + 4770.5 + 851.855 + 229.182$$

$$7299 \text{ kg/hr} = 7299 \text{ kg/hr}$$

(Balanced)

All the calculation at **Appendix A**.

4.3 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°C 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 heat capacity of component.

Table 4.12 Heat capacity of each component

Component	Cp (J/mol.K)
PET	305.4
Ethanolamine	107.21
BHETA	303.26
Ethylene Glycol	167.88
Caprolactone	196.8
Polyol	907.2
Diisocyanate	299.2
Polyurethanes	637.0

Source: Busnel, 2006

Table 4.13 Heat of formation of each component

Component	Cp (J/mol.K)
PET	-270.518
Ethanolamine	-507.50
BHETA	-396.30
Ethylene Glycol	-455.20
Caprolactone	-458.00
Polyol	-210.52
Diisocyanate	-219.27
Polyurethanes	77.00

Source: Bross, 2016

Reference temperature=298.15K

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

ΔH_{rxn} can be calculated by using this formula,

$$\Delta H_{rxn} = \Delta H_{product} - \Delta H_{reactant}$$

4.3.1 Batch Reactor (R-101)

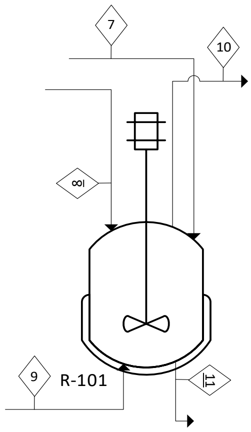


Figure 4.10 Batch Reactor (R-101)

The equations with each rate of reaction that occurs in the batch reactor are shown as below:

$$C_{10}H_8O_4 + 2C_2H_7NO \xrightarrow{\text{zinc acetate}} C_{12}H_{16}O_4N_2 + C_2H_6O_2$$

$$r_1 = 85 \text{ kmol/hr}$$

Temperature = 160˚C

Inlet Enthalpy

Stream 7
$\Delta H_{PET} = 20767.2$ J/mol

Stream 8
$\Delta H_{Ethanolamine} = 0$ J/mol

Outlet Enthalpy

Stream 11
$\Delta H_{BHETA} = 40940$ J/mol
$\Delta H_{Ethylene\ glycol} = 22663$ J/mol
$\Delta H_{unreacted\ PET} = 41229$ J/mol
$\Delta H_{unreacted\ Ethanolamine} = 14473$ J/mol

Total Enthalpy inlet and outlet

$\Delta H_{outlet} = 679947.94\ kJ$/h
$\Delta H_{inlet} = 21756.66\ kJ$/h

Heat of reaction,

$$\Delta Hrxn = \Sigma\Delta vp\Delta Hf\ Product{-}\Sigma\Delta vr\Delta Hf\ Reactant$$
$$\Delta Hrxn = 434.018\ kJ/mol$$

$$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r\Delta H_{rxn}$$
$$Q = (679947.94\ \text{-}21756.66) + 85(434.018)$$
$$Q = 21934.81\ kJ/h$$

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

4.3.2 Packed Bed Reactor (R-102)

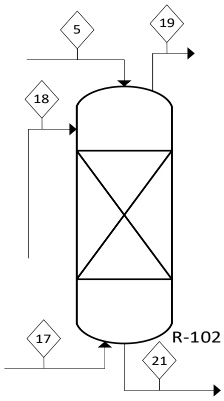


Figure 4.11 Packed Bed Reactor (R-102)

The equations with each rate of reaction that occurs in the batch reactor are shown as below:

$$C_{12}H_{16}N_2 + 2C_6H_{10}O_2 \xrightarrow{DBTDL} C_{24}H_{34}O_6N_2(OH)_2$$

r_2 = 76.5 kmol/hr

Temperature=160°C

Inlet Enthalpy

Stream 18
ΔH_{BHETA} = 13646.7J/mol

Stream 5
$\Delta H_{Caprolactone}$ = 0 J/mol

Outlet Enthalpy

Stream 21
ΔH_{polyol} = 95256 J/mol
ΔH_{BHETA} = 31842.3 J/mol
$\Delta H_{caprolactone}$ = 20644 J/mol

Total Enthalpy inlet and outlet

$\Delta H_{outlet} = \sum N\Delta H$
$\Delta H_{outlet} = 832618.78\ kJ/\text{h}$
$\Delta H_{inlet} = \sum N\Delta H$
$\Delta H_{inlet} = 122108.50\ kJ/\text{h}$

Heat of reaction,

$$\Delta Hrxn = \Sigma\Delta vp\Delta Hf\ Product - \Sigma\Delta vr\Delta Hf\ Reactant$$
$$\Delta Hrxn = 1101.78\ kJ/mol$$

$$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r\Delta H_{rxn}$$
$$Q = (832618.78 - 122108.50) + 76.5(1101.78)$$
$$Q = 794796.45\ kJ/h$$

Hence reaction in packed bed Reactor (R-102) is endothermic reaction because of positive value of Q. Thus, the heat is absorbed.

4.3.3 Continuous Stirred-Tank Reactor (R-103)

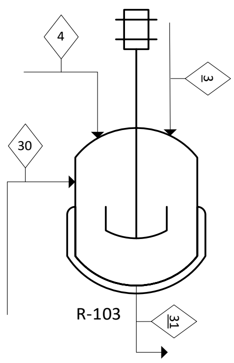


Figure 4.12 Continuous Stirred Tank (R-103)

The equations with each rate of reaction that occurs in the batch reactor are shown as below:

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_8N_4$$
$$r_2 = 68.855\ kmol/hr$$

Temperature = 110°C

Inlet Enthalpy

Stream 30
ΔH_{polyol} = 40824 J/mol

Stream 3
ΔH_{HDI} = 0 J/mol

Outlet Enthalpy

Stream 31
$\Delta H_{polyurethanes}$ = 2580 J/mol
ΔH_{polyol} = 77112 J/mol
ΔH_{HDI} = 25432 J/mol

Total Enthalpy inlet and outlet

$\Delta H_{outlet} = \sum N\Delta H$
ΔH_{outlet} = 783305.27 kJ/h
$\Delta H_{inlet} = \sum N\Delta H$
ΔH_{inlet} = 328776.084 kJ/h

Heat of reaction,

$$\Delta Hrxn = \Sigma\Delta vp\Delta Hf\ Product - \Sigma\Delta vr\Delta Hf\ Reactant$$

$$\Delta Hrxn = 506.69\ kJ/mol$$

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

$$Q = (783305.27 - 328776.084) + 68.855(506.79)$$

$$Q = 489424.2115\ kJ/h$$

Hence reaction in packed bed Reactor (R-103) is exothermic reaction because of negative value of Q. Thus, the heat is released

All the calculation at **Appendix A**.

CHAPTER V

SAFETY AND ENVIRONMENTAL ISSUES

5.1 SAFETY ISSUES OF RAW MATERIAL AND PRODUCT

Table 5.1 shows few of safety issues such as first aid measures and personal precautions on raw materials and product that we must considered. This is to ensure the risks in workplace can be minimized so that employers and workers can be safe at their workplace and activities at the workplace can be done at ease.

Table 5.1 First aid precautions and personal precautions

Component	First Aid Measures	Personal precautions	References
Polyethylene Terephthalate (PET)	▪ Skin contact: cool skin rapidly with cold water after contact with molten polymer. Do not try to peel molten polymer from the skin. ▪ Eye contact: Immediately flush eyes with plenty of clean water or eye wash solution.	▪ No action shall be taken involving any personal risk or without suitable training. ▪ Evacuate surrounding areas. ▪ Keep unprotected personnel from approaching or entering. ▪ Do not touch or walk-through spilled material. ▪ Wear suitable personal protective equipment.	Material safety data sheet
Ethanolamine	▪ Eye contact: Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. ▪ Ingestion: Do not induce vomiting. Never give anything by mouth to an unconscious person. Clean mouth with water.	▪ Use personal protective equipment as required. ▪ Evacuate personnel to safe areas. ▪ Keep people away from and upwind of spill/leak. ▪ Ensure adequate ventilation. ▪ Remove all sources of ignition. ▪ Take precautionary measures against static discharges.	Material safety data sheet
Caprolactone	▪ Skin contact: Take off immediately all contaminated clothing. Rinse skin with water.	▪ Do not breathe vapours, aerosols. ▪ Avoid substance contact. ▪ Ensure adequate ventilation.	Material safety data sheet

	▪ Eye contact: Rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.	▪ Evacuate the danger area, observe emergency procedures, consult an expert.	
Dimethylformamide	▪ Skin contact: Take off immediately all contaminated clothing. Rinse skin with water. Consult with physician. ▪ Inhalation: Inhale fresh air after inhalation occurred. Contact physician	▪ Do not breathe vapours, aerosols. Avoid substance contact. ▪ Ensure adequate ventilation. ▪ Keep away from heat and sources of ignition. ▪ Evacuate the danger area, observe emergency procedures, consult an expert.	Material safety data sheet
Polyester hexamethylene diisocyanate	▪ Eye contact: Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice ▪ Skin contact: Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.	▪ Evacuate non-essential personnel. ▪ Shut off sources of ignition. ▪ Put on personal protective equipment. ▪ Control source of leak ventilated. ▪ Contain the spill to prevent spread to drains, sewers, water supplies or soil. ▪ Pour decontamination solution over spill and allow to react for at least 15 minutes. ▪ Collect material in open containers with further amounts of decontamination solution. ▪ Wash down spill area of decontamination solution.	Material safety data sheet
Polyuretha ne	▪ Eye contact: In case of contact with the dust from this product, flush eyes with plenty of lukewarm water. Get medical attention if irritation develops. ▪ Inhalation: Inhale fresh air in case of accidental inhalation of dust or fumes from overheating or combustion. Get medical attention if irritation develops.	▪ No action shall be taken without appropriate training or involving any personal risk. ▪ Keep unnecessary and unprotected personnel away from the spillage. ▪ Wear protective clothing. ▪ Follow precautions for safe handling. ▪ Wash thoroughly after dealing with a spillage. ▪ Ensure procedures and training for emergency decontamination and disposal are in place	Material safety data sheet

5.2 METHODS TO HANDLE RAW MATERIAL AND PRODUCT

There are procedures in handling raw materials and product as shown in Table 5.2. The most important step when handling the materials in the production of polyurethane is to wear complete and proper personal protective equipment such as glove, safety glasses and protective clothing.

Table 5.2 Procedures in handling raw materials and product

Materials	Handling procedure	Storage requirement	References
PET	▪ Eating, drinking, and smoking should be prohibited in areas where the material is stored, handled, and processed. ▪ Removed any contaminated clothing and personal protective equipment before entering eating area. ▪ Provide exhaust ventilation at places where dust is formed.	▪ Store in original containers. Keep containers tightly closed in a dry, cool and well-ventilated area, away from incompatible materials. ▪ Protect from direct sunlight, UV light, high temperatures and rain. Containers that have been opened should be carefully resealed after use and kept upright to prevent leakage. ▪ Do not store in unlabelled containers.	Material safety data sheet
Ethanolamine	▪ Use only under a chemical fume hood. ▪ Do not get in eyes, on skin or on clothing. ▪ Keep away from open flames, hot surfaces and sources of ignition	▪ Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area. ▪ Keep away from heat and sources of ignition. Store under an inert atmosphere.	Material safety data sheet
Caprolactone	▪ Wash skin thoroughly after handling material. ▪ Wear proper personal protective equipment	▪ Keep containers tightly closed in a dry, cool and well-ventilated place. ▪ Store below the temperature of 30°C	Material safety data sheet
Dimethylformamide	▪ Work under chemical fume hood. Do not inhale substance/mixture ▪ Keep away from open flames hot surfaces and sources of ignition	▪ Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. ▪ Keep locked up or in an area accessible only to qualified or authorized persons. ▪ Recommended storage temperature see product label.	Material safety data sheet
Polyester hexamethylene diisocyanate	▪ Do not get in eyes, on skin or on clothing. ▪ Use only under a chemical fume hood ▪	▪ Store in cool, well-ventilated areas. Keep away from heat and open flames. ▪ Avoid prolonged inhalation of heated vapours or mists. Avoid prolonged skin contact. ▪ Use non-sparking tools and grounding cables when transferring. ▪ Containers maybe hazardous when empty	Material safety data sheet
Polyurethane	▪ Avoid creating dust ▪ Wash thoroughly after handling substance	▪ Store away from incompatible materials. Store in accordance with local regulations. ▪ Keep away from oxidising materials, heat, and flames. Keep only in the original container. ▪ Keep container tightly closed, in a cool, well-ventilated place.	Material safety data sheet

5.3 WASTE GENERATION

In the production of Polyurethane from waste PET, there will be a few by-products that known as waste will be generated. The waste product generated may be harmful to the environment, so the waste product needs to be treat first before it can be released to the surrounding. The waste product that will be generated in the production of Polyurethane are Ethylene Glycol, waste BHETA, waste Caprolactone and wastewater. Table below shows the waste generation in the production process.

Table 5.3 Waste Generation from Production of Polyurethane from Waste PET

Waste	Waste Generation
Ethylene Glycol	The Ethylene Glycol was extracted from the BHETA in a distillation column (DC-101). It's because we need BHETA for Polyol production, and Ethylene Glycol is a by-product of the reactor reaction (R-101).
Waste BHETA	In the reactor (R-101), BHETA is generated for use in the polyol synthesis. The unreacted BHETA, on the other hand, was expelled from the distillation column (DC-102).
Waste Caprolactone	Polyol was made using Caprolactone as a reactant material. In reactor (R-102), it will react with BHETA to synthesis Polyol. Two distillation columns will separate unreacted Caprolactone from Polyol and unreacted BHETA (DC-102 & DC-103).
Waste Gas	Nitrogen gas has been injected into the reactors (R-101 and R-102) to help with the polymerization process by changing the atmosphere into nitrogen atmosphere. Before being released into the atmosphere, the wasted waste gas will be treated first.
Wastewater	Water is used in the production process to precipitate solid Polyurethane. After the product has solidified, at the filter (F-101) at the end of production, the wastewater is discharged.

5.4 WASTE TREATMENT

The waste that produced during production of Polyurethanes need to be treated after the production took place. Table 5.4 below shows the waste that produce during the processes and the treatment for waste generated during the processes.

Table 5.4: Waste treatment from Production of Polyurethane from Waste PET

Waste	Description
Ethylene Glycol	Biological process usually used to manage EG waste and good performance were achieved with an influent chemical oxygen demand range between 1000 to 3000 mg/L. Anaerobic treatment is preferred cause of its simplicity, reduced sludge production and very low consumption. Formation of Microbial granules is a key factor for successful operation of Anaerobic reactor. The plant for EG treatment generally operates with a reduce loading rate (OLR). (Jin et al., 2016).
Caprolactone	Caprolactone also known as Biodegradable Polymer are mainly used in Biomedical engineering, tissues scaffolds and gene, drug, and protein-delivery vehicles. So that we can gain profit by selling its.

Wastewater	Treatment for wastewater is sewage treatment. Sewage treatment is one way to impurities the wastewater before reach the natural river, lakes, or daily use. Wastewater follow a determined treatment path to achieve water quality standards. Wastewater is normally called influent as it passes through the wastewater treatment facility. Wastewater treatment plants help nature to defend water from excessive pollution. The degree and type of wastewater decides the nature of treatment and the engineering scale of the plant (AZoCleantech, 2008). Most wastewater treatment plants consist of primary and secondary treatment.
BHETA	The unreacted BHETA will be disposed in disposal landfill. Criteria for land treatment or sanitary landfill disposal practices to significant revision. Prior implementing land disposal of waste residue, need to consult with environmental regulatory agencies for guidance on acceptable disposal practices.
Waste gases	Waste gases will be treating in Burn/Wet Technology. Waste gases will be fed into ring-shaped burner apparatus, depend on the chemical composition of the waste gases. Our waste gas contains mostly Nitrogen gas, various rection take place such as Oxidation, reduction. (DAS, 2017).

5.5 ENVIRONMENTAL ACT

To keep the ecosystem and environment in great shape, Malaysia has regulations in place to prevent pollution, preserve the environment, and ensure environmental quality. The Ministry of Energy, Science, Technology, and Climate Change oversees the Department of Environment that responsible for pollution prevention and control, as well as industrial waste management in Malaysia. Department of Environment has done so by establishing rules and regulations, as well as encouraging industry to invest more in greener technologies which can minimize hazardous waste. The following are some of the environmental laws in Malaysia that are mentioned in the Environmental Quality Act 1974:

1. Environmental Quality (Licensing) Regulations 1977
2. Environmental Quality (Sewage and Industrial Effluents) Regulations 1979
3. Environmental Quality (Schedule Wastes) Regulations 1989
4. Environmental Quality (Sewage and Industrial Effluents) (Amendment) Regulations 2000

All the acts mentioned can improve environmental quality, limit pollution from all sources, and prevent the establishment or operation of any industrial facility on environmental grounds.

CHAPTER VI

CHEMICAL ENGINEERING COMPUTATION II

6.1 INTRODUCTION

In this computational part, we are required to design a MATLAB or Octave coding to compute the steady state value of all parameters such as concentration and temperature in one major unit operation in both mass balance and energy balance of our project which is production of Polyurethane.

In our project, we have used MATLAB to calculate the mass balance and energy balance of the process.

6.2 DEVELOPING MATLAB PROGRAMMING

6.2.1 Mass Balance

Prompting the user

Figure 6.1 shows a graphic user interface (GUI) that user will see once they run the program. The program will ask for user to input the mass flowrate in of Polyol and HDI in kg/h as shown in Figure 6.2.

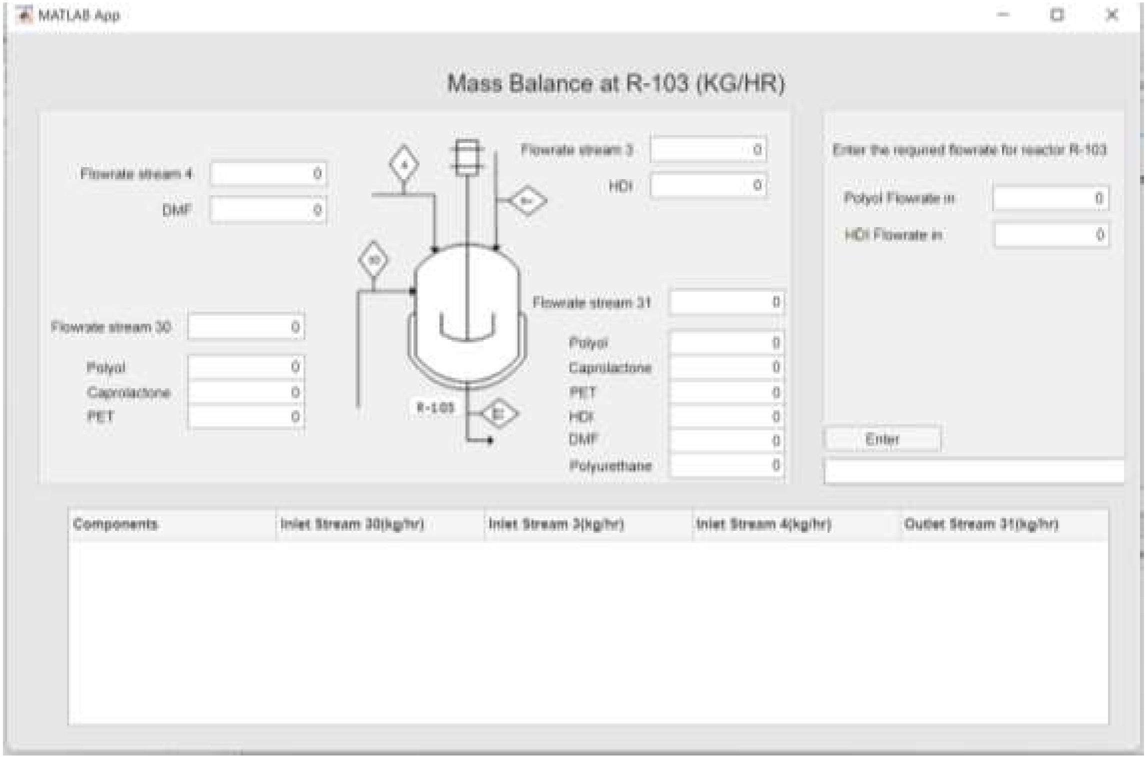


Figure 6.1 GUI from MATLAB Programming

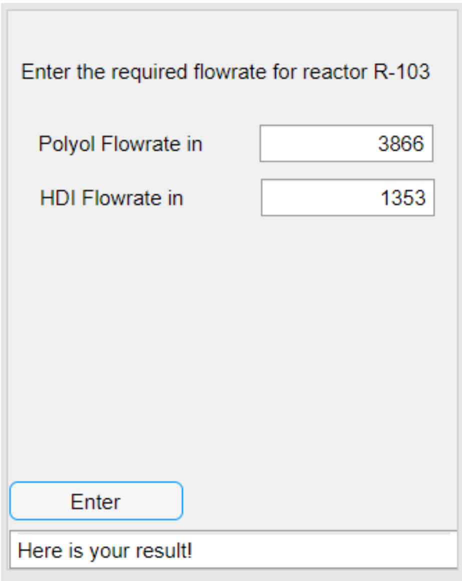


Figure 6.2 Prompting user to input value

6.2.2 The Result

After pressed the button 'Enter', the program will calculate the mass balance of components in CSTR R-103 and it will display 'Here is your result!'. In Figure 6.3 shown the result after the calculation that had been made. At the top of the GUI shows the flowrate in and flowrate out for each component. At the bottom shows the mass balance for each component in inlet streams 30, inlet stream 3, inlet stream 4 and outlet stream 31. As you can see, the result shows it is in a steady state. The variable, which is the flowrate does not change with time.

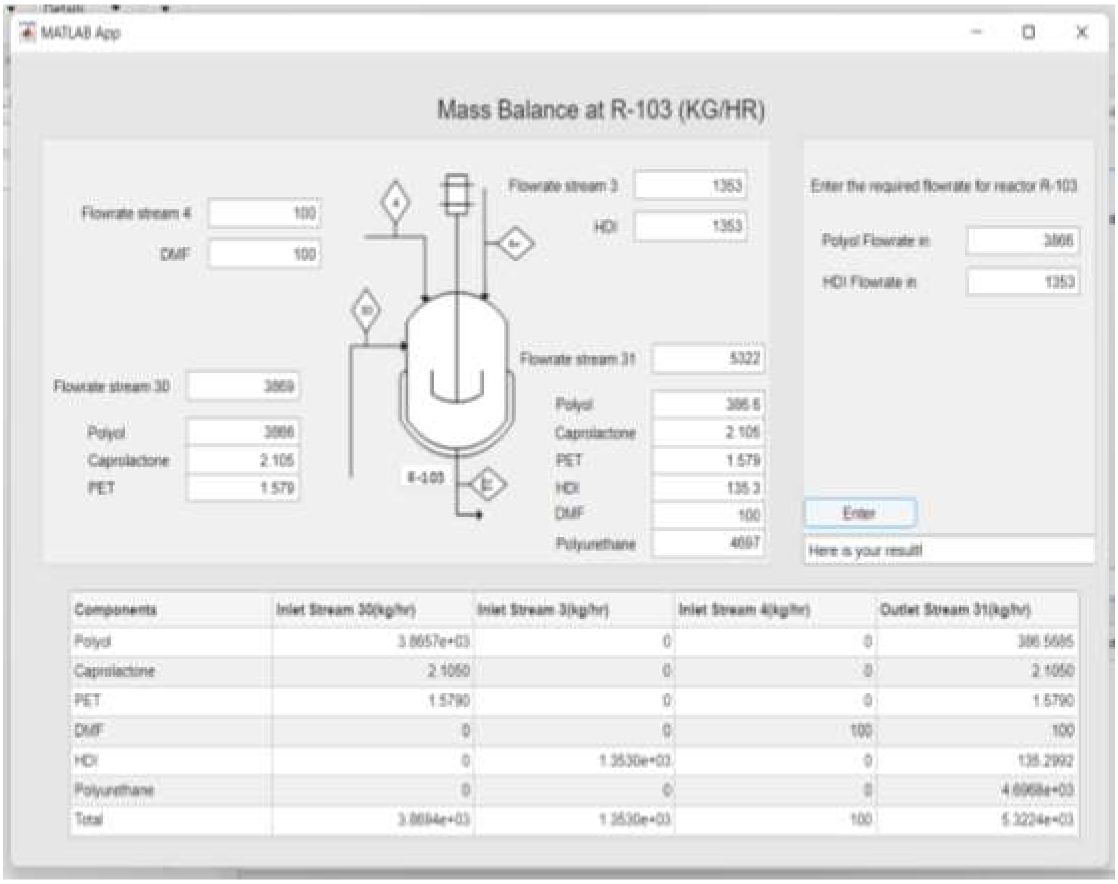


Figure 6.3 Result from MATLAB Programming

6.2.3 Energy Balance

Prompting the user

Figure 6.4 shows another GUI that user will see once they run the program. The program will ask for user to input the temperature in inlet stream 30 and 31 in °C as shown in Figure 6.5. The other stream which is stream 3 already stated the value in MATLAB.

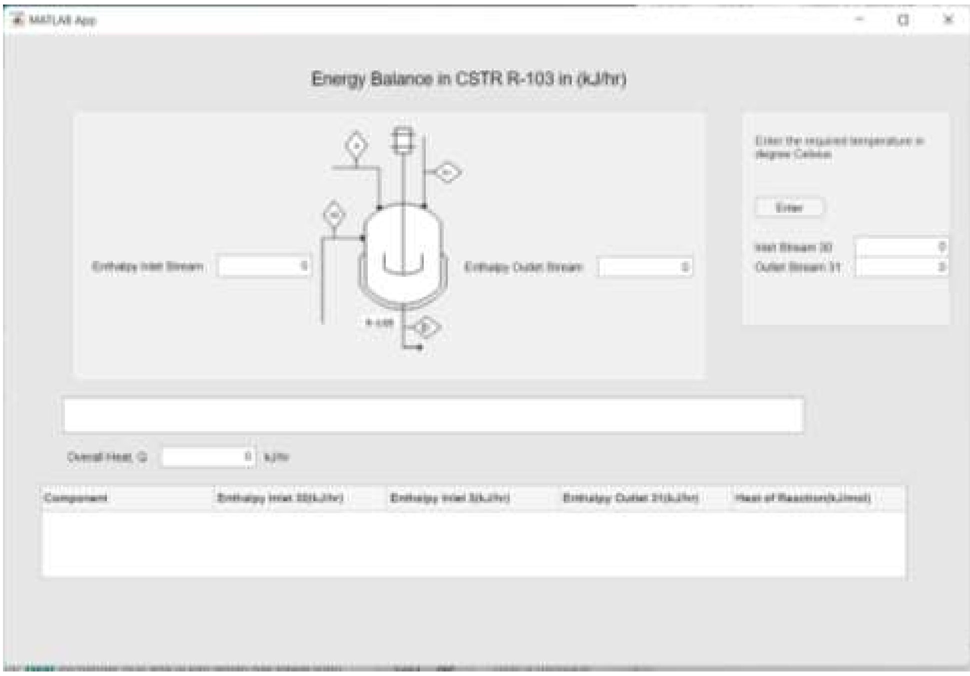


Figure 6.4 GUI from MATLAB Programming

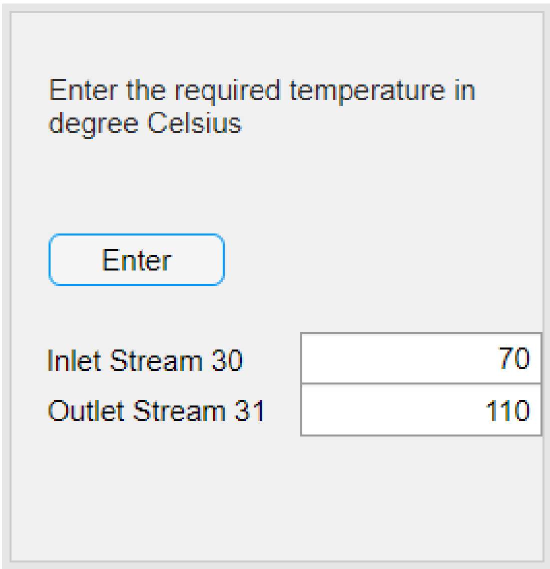


Figure 6.5 Prompting user to input value

6.2.4 The Result

After pressed the button ‘Enter’, the program will calculate the enthalpy change of components and heat energy, Q in CSTR R-103. In Figure 6.6 shown the result after the calculation that had been made. At the top of the GUI shows the enthalpy change inlet stream and outlet stream. At the bottom shows the table of enthalpy change and heat reaction for each component in inlet streams 30, inlet stream 3 and outlet stream 31. The program will also tell us if the reaction is endothermic or exothermic as shown in Figure 6.7

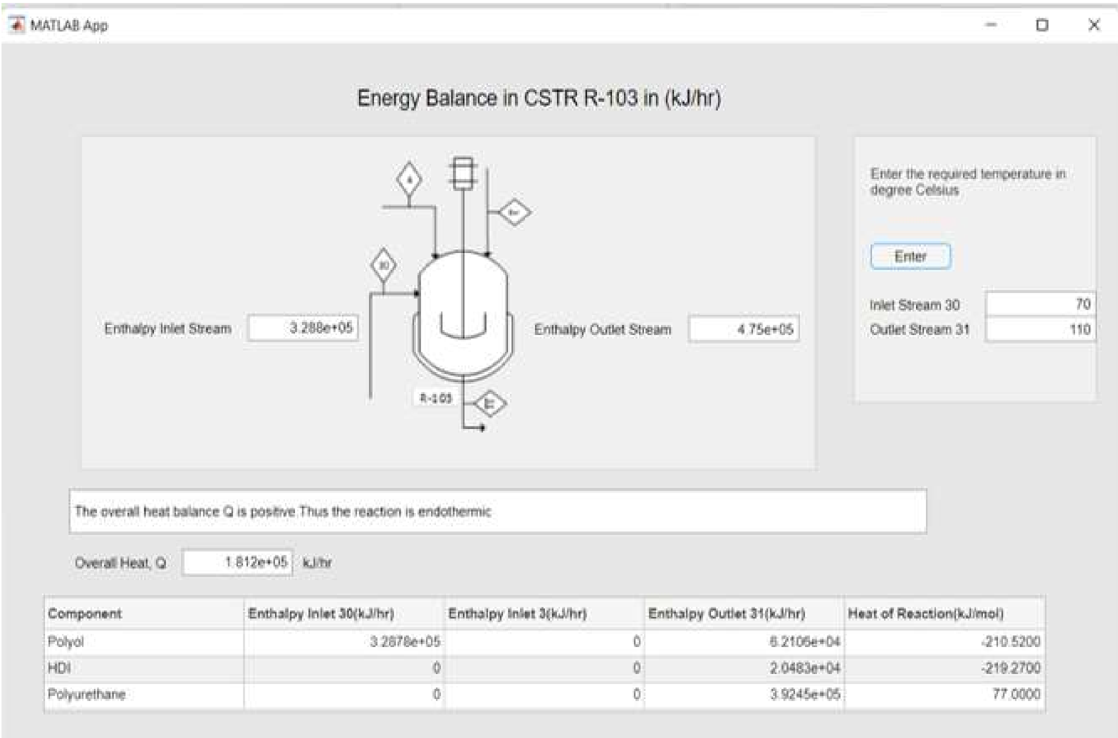


Figure 6.6 The result from MATLAB programming

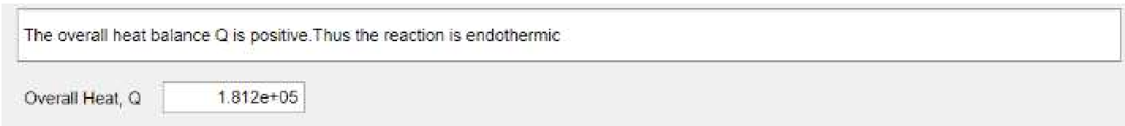


Figure 6.7 Display reaction is endothermic or exothermic reaction

6.2.5 Handling the Error

For the mass balance, the flowrate should not be in negative value in this program. So, the program will display ‘Error! Please Enter a Positive Value’ when the user inputs a negative value as shown in Figure 6.8. When user input the value 0, it will display ‘Error! Please Enter A Value Greater Than Zero’ as shown in Figure 6.9. This way user will not enter the invalid value to make sure there is no mistake in mass balance calculation.

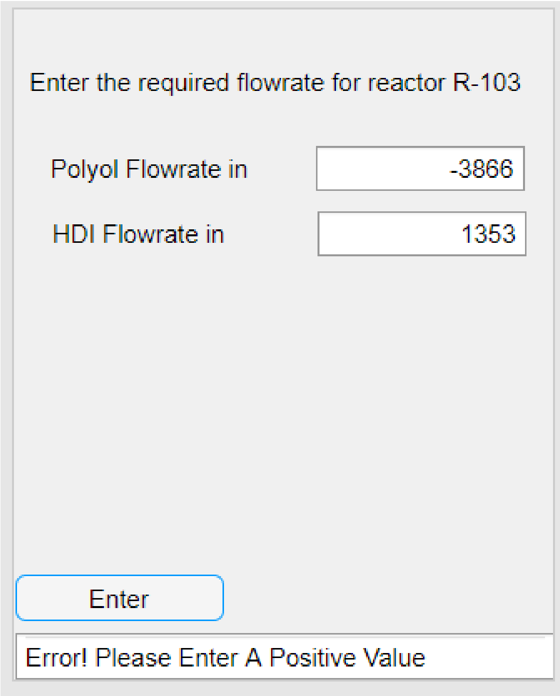


Figure 6.8 Error caused due to wrong input or invalid answer

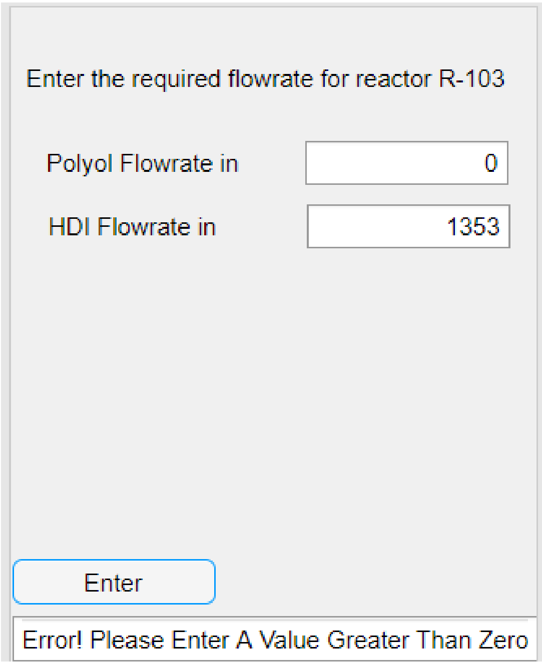


Figure 6.9 Error caused due to user input value

6.3 NUMERICAL METHOD

Numerical method used in finding the root based on the equation obtained from the reactor R-103 is Trapezoidal Rule. The equation is to find the enthalpy out for polyurethane, where the root I is representing the parameter. The result shows that the value obtained is the same as the value that we obtained from the energy balance in the previous chapter.

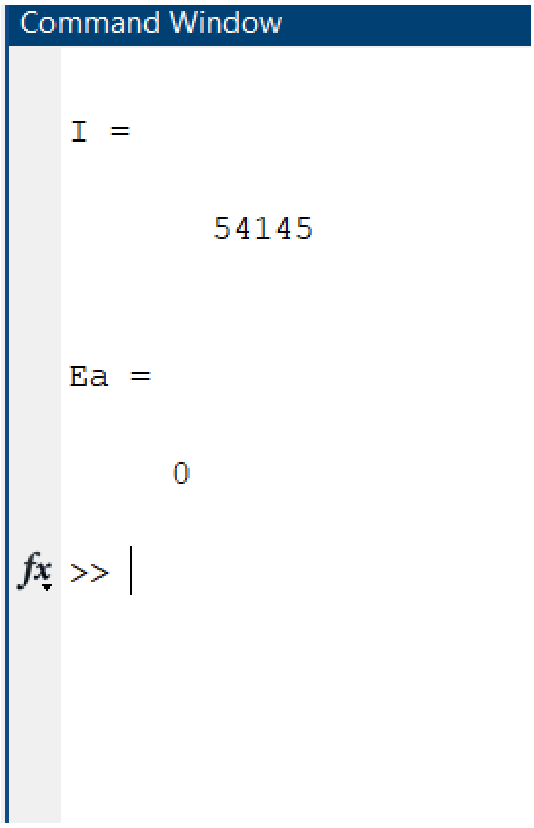


Figure 6.10 Result from calculation of enthalpy out for Polyurethane using Trapezoidal Rule Method

The value of I and error, Ea are then calculated and being displayed. The result shows that the value obtained is the same as the value that we obtained from the energy balance from the manual calculation which is 54145 kJ/kmol.

All the coding at **Appendix B**.

CHAPTER VII

CHEMICAL REACTION ENGINEERING II

7.1 INTORDUCTION

In this part, it will discuss the application of chemical reaction engineering in these processes. Chemical reaction engineering is the industrial chemical that dealing with chemical reactor, but in this part the Continuous-stirred tank reactor (CSTR) was chosen. The term specifically to catalytic reaction either homogenous or heterogenous is present in the reactor. Chemical reaction engineering also applied chemicals kinetics rate and to determine how far the certain reaction proceed at what rate, process condition and final product be approached.

7.2 SELECTION PROCESS

Polyurethanes are linear polymers with carbamate groups in their molecular backbone. A chemical reaction between a Diisocyanate and polyol produces theses group, which are known as urethane. There are many commercial methods for synthesis Polyurethanes from PET waste such as Glycolysis and Aminolysis. In this process, Aminolysis were used using ethanolamine, it consists of 3 main reactions. The first process involving raw material PET waste, Ethanolamine, nitrogen gas and zinc acetate as a catalyst at high temperature. The reaction produced bis(2-hydroxyethyl) terephthalamide (BHETA) and ethylene glycol (EG). The Caprolactone were used as a raw material for second reaction with BHETA produced Polyester polyol. The caprolactone were to get Biodegradable Polyurethanes. The polyester polyol with two hydroxyl group Polyester Hexamethylene Diisocyanate (HDI) with two isocyanate group by forming urethanes linkage. All the process of synthesis polyurethanes produced highest yield of production but the only different in this process is we used Caprolactone for second reaction. To make sure the reaction occurs perfectly, the nitrogen gas is feed into first reactor and second reactor to remove air (Al-Sabagh et al., 2016).

7.3 RAW MATERIAL SELECTION

There are seven raw materials in this process which is polyethylene terephthalate (PET), ethanolamine, caprolactone, hexamethylene diisocyanate, dimethylformamide (DMF), water and nitrogen gas. Polyethylene terephthalate (PET) was used using as a main material and our main source of polyethylene terephthalate (PET) is from plastic waste, PET is the common thermoplastic resin of the polymer. As the production of PET as synthetic fibres growth the waste of PET waste also increase. To reduce the waste for environmental sake, it will cycle for production of polyurethanes. Ethanolamine was used for the aminolysis of PET to produce Bis (2-hydroxy ethylene) terephthalamide (BHETA) and ethylene glycol (Mir Mohamad Sadeghi et al., 2011).

Then, caprolactone will react with BHETA to obtain polyol. It will undergo ring opening polymerization process. These reactions typically demand anhydrous reagent and inert atmosphere (Atta et al., 2021). Caprolactone were chosen to set the biodegradable component. While the hexamethylene diisocyanate were used to react with polyol to produce polyurethane. Diisocyanate is an organic compound 25 with two isocyanate groups. Different types of diisocyanate like toluene diisocyanate dan methylene phenyl diisocyanate will produce different types of polyurethane if reacted with polyol (Akindoyo et al., 2016). All the raw materials are supplied in liquid form except for nitrogen gas that used to remove the air in the reactor.

7.4 REACTOR SELECTION

To maximize the plant capacity, the selection of the reactor is very important. The main reactor in this process is Continuous Stirred-Tank Reactor (CSTR). CSTR is typically used for homogeneous liquid phase reactions, but it also accepted for a gas-liquid reaction (Show & Lee, 2013). CSTR have a large reactor volume because of slow reaction rates inside it and CSTR provide higher conversions (Show & Lee, 2013). CSTR is used in third chemical reaction because it conditions don't require time duration and catalyst. An ideal CSTR is assume with uniform composition and temperature everywhere in the reactor, the effluent composition is same as in the tank. This reactor operates at steady state.

7.5 SELECTION CATALYST

As we know, catalyst is a Chemical substance that can speed up the chemical reaction or increase the reaction rate by lowering the activation energy of reaction without being consumed by the reaction. In this process, there are two catalysts were used which is zinc acetate and dibutyltin dilaurate (DBTDL). Zinc acetate were used in the first reaction in batch reactor (R-101) because zinc acetate is very excellent catalyst in producing the best depolymerization rate of the first reaction between PET and ethanolamine under nitrogen atmosphere and 160 °C condition (Leonardo dos Santos et al., 2012).

Then, DBTDL were used as catalyst for second reaction between BHETA and caprolactone in PBR (R-102). DBTDL helps chemically curing systems dry faster by favoring the Isocyanate or polyol reaction over the side reaction like isocyanate or water. Scratch resistance, hardness and mechanical qualities are all improves. So, DBTDL can help polyurethanes cure faster. Other than that, DBTDL are very suitable to accelerate the cross-linking process of solvent-based two component in polyurethane's production. (*Dibutyltin Dilaurate*, 2020).

7.6 GENERAL MASS BALANCE FOR CSTR

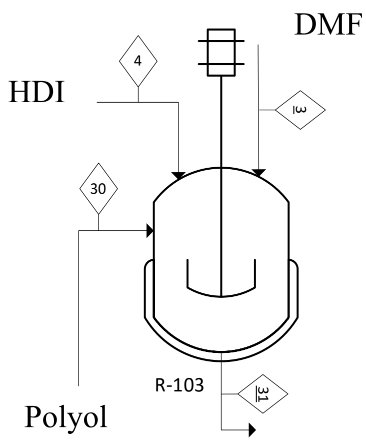


Figure 7.1 Mass Balance at CSTR

7.6.1 General Mole Balance for CSTR:

$$In - Out + Generation = Accumulation$$

$$F_{AO} - F_A + \int_0^V r_A \, dV = \frac{dN_A}{dt}$$

Assumption:

1. $Steady\ state, \frac{dN_A}{dt} = 0$
2. No time dependence or position dependence of temperature, concentration, and reaction rate.

Thus,

$$\int_0^V r_A \, dV = r_A \int_0^V dV = r_A . V$$

By substituting the equation,

$$F_{AO} - F_A + r_A.V = 0$$

$$V = \frac{F_{A0} - F_A}{-r_A}$$

$$F_{AO} = C_{AO} v_o \quad F_A = C_A v$$

$$V = \frac{C_{AO} v_o - C_A v}{-r_A}$$

In term of conversion,

$$X = \frac{moles\ of\ A\ reacted}{moles\ of\ A\ fed\ to\ reactor}$$

$$X = \frac{F_{A0} - F_A}{F_{A0}}$$
$$X = \frac{F_{A0}X}{-r_A}$$

7.6.2 Kinetic Rate Expression:

Main reaction:

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_8N_4$$

Let:

$$A \quad + \quad B \longrightarrow C$$

Reaction stoichiometry:

$$-r_A = -r_B = r_C$$

Based on the equation, rate law is

$$-r_A = KC_AC_B$$

Table 7.1 Stoichiometric table

Species	Symbol	Initial rate (kmol/h)	Change (kmol/h)	Effluent rate (kmol/h)	Concentration (kmol/L)
$C_{24}H_{34}O_6N_2(OH)_2$	A	F_{AO}	$-F_{AO}X$	$F_A = F_{AO}(1-X)$	$C_A = C_{AO}(1-X)$
$C_6H_{12}(NCO)_2$	B	$F_{BO} = \theta_B F_{AO}$	$-F_{BO}X$	$F_B = F_{AO}(\theta_B-X)$	$C_B = C_{AO}(\theta_B-X)$
$C_{32}H_{48}O_8N_4$	C	0	$F_{CO}X$	$F_C = F_{AO}(\theta_C+X)$	$C_C = C_{AO}(\theta_C+X)$

Volumetric flowrate,

$$v_o = 1.755\ m^3/h$$
$$v_o = 4.875 \times 10^{-4}\ m^3/s$$

Molar flowrate of A from mass balance, $N_A = 8.0535$ mol/h

Concentration of A,

$$C_A = \frac{molar\ flowrate}{volumetric\ flowrate}$$
$$C_A = 4588.9\ mol/m^3$$

Conversion of Polyol

$$X = \frac{F_{A0} - F_A}{F_{A0}}$$

$$X = \frac{3685.685 - 386.57}{3685.685}$$

$$= 0.9$$

Concentration of A,

$$C_A = C_{A0}(1 - X)$$

$$C_{A0} = 45888.9 \text{ mol/m}^3$$

Calculation of k constant value,

$$k = ln\frac{C_{AO}}{C_A}$$

$$k = 6.396 \times 10^{-4} \text{ s}^{-1}$$

The volume of the reactor,

$$V = \frac{v_o X}{k(1 - X)}$$

$$V = 6.86\, m^3$$

Figure show graph X against Volumes.

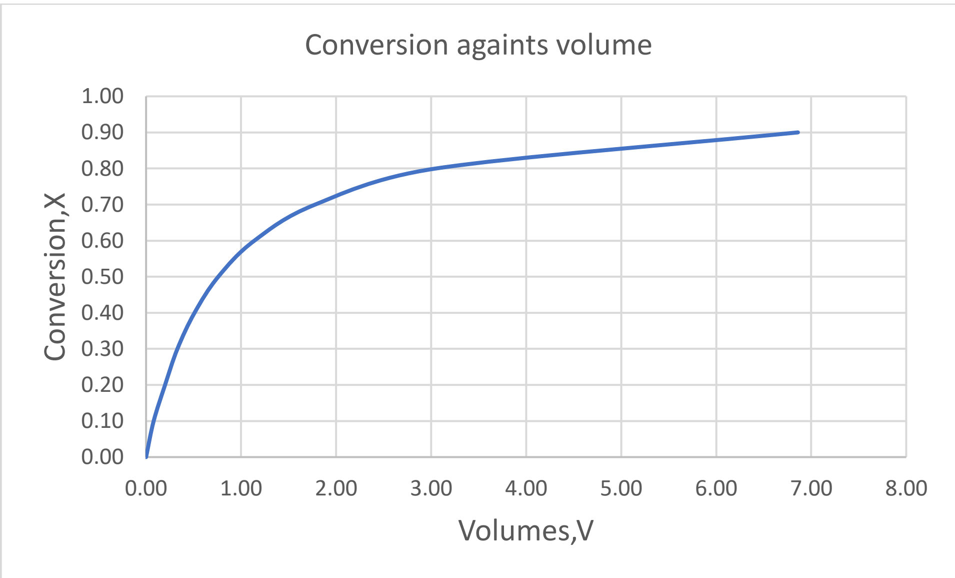


Figure 7.2 Graph conversion and Volume against t

Detailed calculation in **Appendix C**

CHAPTER VIII

SEPARATION PROCESS

8.1 INTRODUCTION

In Chemical Engineering, separation processes were used to separate a mixture of various components into a pure result. We have three separating processes for our Polyurethane manufacture. This is to ensure that our product is as pure as possible. In this production, the separation procedure is carried out in the distillation column (DC-101, DC-102 & DC-103).

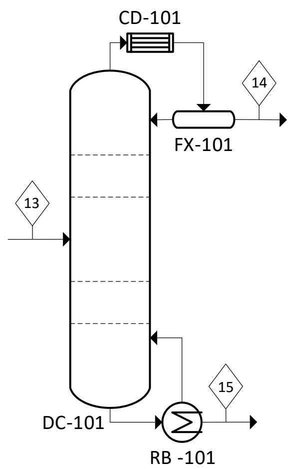


Figure 8.1 Distillation Column (DC-101)

The calculations for the separation process at DC-101 are shown and performed in this chapter. Four components were separated using DC-101: BHETA, PET, Ethylene Glycol, and Ethanolamine. PET, Ethylene Glycol, and Ethanolamine are the light keys, top product in the DC-101, while BHETA is the heavy key bottom product.

The separation process operates according to the volatility of the components. Volatility is defined as how easily a substance will vaporize (The MSDS HyperGlossary: Volatility, 2016). The high volatility, lower boiling point components will evaporate and out as top product and the low volatility, high boiling point component will out as bottom product.

8.2 SELECTION OF SEPARATION UNIT

The distillation operation that we choose is tray tower. Tray tower are designed to offer liquid hold up so that the distillation process can accomplish the correct vapor-liquid mass transfer required for separation (Costello, 2016). Holdup is a process that allow the liquid to run across a tray. It also allows the upward travelling vapours and downward moving liquid across the trays.

The type of trays that we used is sieve tray type. It is a plate with a hole that allows a vapor to go upward. The velocity of the vapour will keep the liquid from flowing down through the holes. The sieve tray also will ensure to lesser the pressure drop due to the number of hole and tray thickness. Other than that, the entrainment also higher than valve tray (Kolmetz, 2011).

Figure 8.2 Sieve Tray

8.3 PROCESS DESIGN

In our separation process at DC-101, we want to separate BHETA and other components. Mass flowrate for feed is 3305.62 kg/hr while the mass flowrate for steam is 1043.267 kg/hr. Distillation column is used to purify the mixture. The composition of BHETA, PET, Ethylene Glycol and Ethanolamine are shown below.

Table 8.1 Summarized of stream table of components in Distillation Column (D-101)

Components	Inlet stream 13 Mass flow rate (kg/hr)	Outlet stream 14 Mass flow rate (kg/hr)	Outlet stream 15 Mass flow rate (kg/hr)
PET	303.19	300.03	3.158
Ethanolamine	192.65	190.547	2.105
BHETA	2254.98	0	2254.98
Ethylene Glycol	554.80	552.69	2.105
Total	3305.62	1043.267	2262.348

8.4 COMPARISON WITH SUPERPRO CALCULATION

Stream Name	S-107	S-108	S-109
Source	INPUT	P-2	P-2
Destination	P-2	OUTPUT	OUTPUT
Stream Properties			
Activity (U/ml)	0.00	0.00	0.00
Temperature (°C)	160.00	170.00	241.00
Pressure (bar)	1.01	1.01	1.01
Density (g/L)	672.98	366.90	959.00
Total Enthalpy (kW-h)	134.82	82.91	92.20
Specific Enthalpy (kcal/kg)	35.09	68.32	35.07
Heat Capacity (kcal/kg-°C)	0.26	0.47	0.16
Component Flowrates (kg/h averaged)			
bis(2-hydroxyet	2,254.979	0.225	2,254.754
Ethanolamine	192.654	190.554	2.100
Ethylene Glycol	555.405	553.294	2.111
Polyethylene Te	303.191	300.037	3.153
TOTAL (kg/h)	3,306.228	1,044.111	2,262.117
TOTAL (L/h)	4,912.784	2,845.745	2,358.832

Figure 8.3 SuperPro Result for Mass Balance at DC-101

Table 8.2 Percentage Error between Manual and SuperPro calculation for Mass Balance

Component	Manual calculation (kg/h)		SuperPro calculation (kg/h)		Percentage Error (%)	
	Top product	Bottom product	Top product	Bottom product	Top product	Bottom product
BHETA	0	2254.98	0.23	2254.75	100	0.01
Ethanolamine	192.55	2.11	190.55	2.10	1.05	0.24
Ethylene Glycol	552.69	2.11	553.29	2.11	0.11	0.28
Polyethylene Terephthalate	300.03	3.16	300.04	3.15	0.01	0.16

8.5 SHORT-CUT METHOD

8.5.1 Number of Stages, N

The fenske equation is used to determine the minimum number of stages needed in the distillation column.

$$N_{min} = \frac{\ln\left(\frac{d_i}{d_j}\right)\left(\frac{b_j}{b_i}\right)}{\log\,(\alpha_m)}$$

d_i = Light key at distillate

d_j = Heavy key at distillate

b_i = Light key at bottom

b_j = Heavy key at bottom

α_m = Mean Relative Volatility

Mean Relative Volatility calculation:

$$\alpha_m = (\left(\alpha_{i,j}\right)_N \left(\alpha_{i,j}\right)_1)^{\frac{1}{2}}$$

$$\alpha_m = \left((1.2)(2.3)(2.25)\right)^{\frac{1}{2}}$$

$$\alpha_m = 2.49$$

Table 8.3 Vapor pressure for each component

Components	PET	BHETA	Ethylene Glycol	Ethanolamine
Vapor Pressure (mmHg)	0.9	0.4	0.92	0.48

Table 8.4 Relative Volatility for each component

Components	PET	BHETA	Ethylene Glycol	Ethanolamine
Relative votality	2.25	1	2.3	1.2

$$N_{min} = \frac{\ln\left(\frac{0.288}{0.001}\right)\left(\frac{0.99}{0.0014}\right)}{\ln\,(2.49)}$$

$$N_{min} = 13.4$$

$$N_{min} \approx 14$$

8.5.2 Minimum Reflux Ration Calculation

First Underwood Equation

$$\sum \frac{\left(\alpha_{i,r}\right) z_{i,f}}{(\alpha_{i,r}) - \varphi} = 1 - q$$

Feed is liquid, q = 1

$$\frac{(2.25)(0.092)}{2.25 - \varphi} + \frac{(1.2)(0.058)}{1.2 - \varphi} + \frac{(2.3)(0.168)}{2.3 - \varphi} + \frac{(1)(0.68)}{1 - \varphi} = 0$$

$$\varphi = 2.268$$

Second Underwood Equation

$$\sum \frac{\left(\alpha_{i,r}\right) x_{i/d}}{(\alpha_{i,r}) - \varphi} = 1 + R_{min}$$

$$R_{min} = 1.03$$

Assumption:

$$R = 2R_{min}$$

$$R = 2(1.03)$$

$$R = 2.06$$

8.5.3 Gilliland Correlation

By applying the correlation,

$$X = \frac{R - R_{min}}{R + 1}$$

$$X = 0.337$$

$$Y = 1 - e^{\left(\left(\frac{1 + 54.4X}{11 + 117.2X}\right)\left(\frac{X-1}{X^{0.5}}\right)\right)}$$

$$Y = 0.354$$

$$Y = \frac{N - N_{min}}{N + 1}$$

$$0.354 = \frac{N - 13.4}{N + 1}$$

$$N = 21.29$$

$$N \approx 22$$

The actual stages are 22

8.5.4 Efficiency

$$E = \frac{N_{min}}{N} \times 100\%$$
$$E = 63.63\%$$

8.6 DIAMETER AND HEIGHT OF DISTILLATION COLUMN

Diameter of distillation column formula:

$$D_T = \sqrt{\frac{4VM_v}{fU_f\pi(1 - \frac{A_d}{A})\rho_v}}$$

The parameters:

1. L = 2262.348 kg/hr = 9.033 kmol/hr
2. V = 1043.267 kg/hr = 13.6 kmol/hr
3. Tray spacing = 24 inch

   Because of the ease of maintenance, most trays have been spaced at 24 inch intervals (Seader, J.D et. al., 2011). So we decided to use 24 inch tray spacing.
4. Liquid surface tension, σ = 47.3
5. Density of Vapor:

$$\rho_v = \frac{PM_v}{RT}$$
$$M_v = (0.287)(192) + (0.53)(62) + (0.183)(61) + (0.001)(252)$$
$$M_v = 99.15\ kg/kmol$$
$$\rho_v = \frac{(200)(99.15)}{(8.314)(623)}$$
$$\rho_v = 3.828\ kg/m^3$$

Density of Liquid:

Table 8.5 Density for each component

Components	PET	BHETA	Ethylene Glycol	Ethanolamine
Density (kg/m^3)	1380	1300	1110	1010

$$M_L = (0.0014)(192) + (0.0009)(62) + (0.0009)(61) + (0.998)(252)$$
$$M_L = 251.88\ kg/kmol$$

$$\rho_L = (0.0014)(1380) + (0.0009)(1110) + (0.0009)(1010) + (0.998)(1300)$$
$$\rho_L = 1301.24\ kg/m^3$$

Flood factor: f = 0.8

Abscissa Ratio:

$$F_{LV} = (\frac{LM_L}{VM_V})(\frac{\rho_v}{\rho_L})^{0.5}$$
$$F_{LV} = 0.0915 \ \leq 1.0$$

Since $F_{LV} < 1.0$,

$$\frac{A_d}{A} = 0.1$$

Flooding Velocity, U_f:

$$U_f = C(\frac{\rho_L - \rho_v}{\rho_v})^{0.5}$$
$$C = F_{st}F_F F_{HA} C_F$$

F_{ST} = surface tension factor, $(\sigma/20)^{0.2}$ = 1.19

F_F = 1

F_{HA} = 1.0

C_F = 0.36 ft/s

The value of C_F is obtained from the graph of entrainment flooding capacity in a trayed tower from figure 6.23 at Separation Process Principle (Seader, J.D et. al., 2011).

$$C = (1.19)(1)(1)(0.36)$$
$$C = 0.4284\ ft/s$$

So,

$$U_f = 0.4284(\frac{\rho_L - \rho_v}{\rho_v})^{0.5}$$
$$U_f = 7.887\ ft/s$$

The diameter of distillation column:

$$D_T = \sqrt{\frac{4VM_v}{fU_f\pi(1-\frac{A_d}{A})\rho_v}}$$

$$D_T = \sqrt{\frac{4(13.6/3600)(99.15)}{(0.8)\left(\frac{7.887}{3.28}\right)\pi(1-0.1)(3.828)}}$$

$$D_T = 0.82\ m = 2.62\ ft$$

The height of distillation column:

$$H = Tray\ spacing\ \times N$$
$$H = 24\ \times 22$$
$$H = 528\ inches$$
$$H = 13.41\ m = 44\ ft$$

We must consider for the top and bottom tray spacing. The bottom side of the distillation column tower must be tall enough to function as a liquid reservoir. Around 15% of the height, 44 ft need to be added for the bottom and top spaces. So:

$$H_{new} = (15\%\ \times 44\ ft) + 44\ ft$$
$$H_{new} = 50.6\ ft$$

8.7 HEIGHT OF DIAMETER RATIO

$$\frac{H_{new}}{D_T} = \frac{50.6}{2.62}$$

$$\frac{H_{new}}{D_T} = 19.4$$

The suitable ration should be less than 20 to 30 (Linninger et al., n.d.).

8.8 HEAT DUTY

Total Heat Duty = $Q_{sensible} + Q_{latent}$

$T_1 = 298$ K

$T_2 = 443$ K

Table 8.6 Specific heat for each component

Components	PET	BHETA	Ethylene Glycol	Ethanolamine
Specific Heat (J/mol)	305.4	303.26	167.88	107.2

Table 8.7 Heat of vaporization for each component

Components	PET	BHETA	Ethylene Glycol	Ethanolamine
Heat of Vaporization (kJ/mol)	74.3	78.6	50.5	49.9

$$\sum Q_{sensible} = N_i \int_{T1}^{T2} Cp_i \, dT$$

$$\sum Q_{sensible} = 1.58 \int_{298}^{443} 305.4 \, dT$$

$$+ \; 3.19 \int_{298}^{443} 107.2 \, dT + \; 8.95 \int_{298}^{443} 167.88 \, dT + \; 8.95 \int_{298}^{443} 303.29 \, dT$$

$$\sum Q_{sensible} = 730.97 \; kJ/mol$$

$$\sum Q_{latent} = N_i . \Delta H^{vap,i}$$

$$\sum Q_{latent} = (1.58)(74.3) + (3.19)(49.9) + (8.95)(50.5) + (8.95)(78.6)$$

$$\sum Q_{latent} = 1432.02 \; kJ/mol$$

Total Heat Duty = 730.97 + 1432.02 = 2162.99 kL/mol

CHAPTER IX

COMPUTER AIDED PLANT DESIGN

9.1 INTRODUCTION

In this chapter, we will be discussing on then use of SuperPro Designer and Symmetry to test the mass balance for the production of polyurethane from PET. The mass balance and energy balance are tested for all unit operations used in the process with SuperPro. Designer. There are some unit operation is using Symmetry to calculate mass and energy balance which are batch reactor (R-101), and packed-bed reactor (PBR) (R-102) in this process. At R-101 and R-102, we will compared the error between SuperPro calculation and Symmtery calculation.

9.2 AMINOLYSIS, (R-101)

Aminolytic degradation of PET with ethanolamine produce bis(2-hydroxyethyl) terephthalamide (BHETA) and ethylene glycol (EG) as by-product happen in reactor (R-101). The conversion of PET is 85%. Symmetry simulation was used to calculate mass and enegry balance by using conversion reactor. Conversion reactor was used to provide shortcut material and energy balance models for actual reactors. Then, SuperPro simulation was used stoichiometry equation reactor.

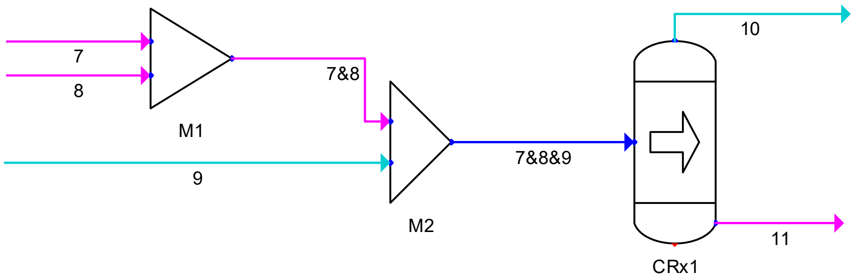


Figure 9.1 Conversion reactor at R-101 on Syymetry simulation

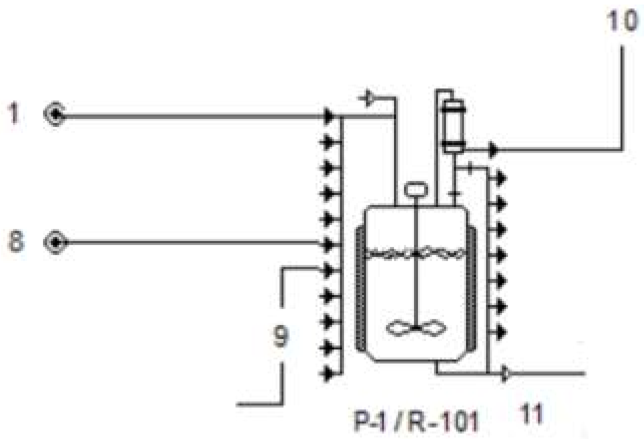


Figure 9.2 Stoichiometry reaction reactor at R-101 on SuperPro simulation

9.2.1 Mass Balance using Symmetry at R-101.

Table 9.1 shows percentage error at output stream 11 for mass balance. The percentage error was calculated between manual calculation and simulation calculation which are SuperPro and Symmetry

Table 9.1 Percentage error at output stream 11 for mass balance

Component	Manual calculation (kg/h)	Symmetry Simulation		SuperPro Simulation	
		Calculation (kg/h)	Percentage Error (%)	Calculation (kg/h)	Percentage Error (%)
BHETA	2254.98	2327.76	3.13	2254.98	0
Ethanolamine	192.65	158.67	21.42	192.65	0.04
Ethylene Glycol	554.80	505.23	9.81	555.41	0.11
Polyethylene Terephthalate	303.19	313.67	3.34	303.19	0

Table 9.2 shows the differences of percentage error between SuperPro and Symmetry simulation. There are some differences for both simulations, especially at mass balance of ethanolamine. This is due to the difference type reactor was used in the simulation.

Table 9.2 Percentage error difference between SuperPro and Symmetry simulation.

Component	**Symmetry Simulation Percentage Error (%)**	**SuperPro Simulation Percentage Error (%)**	**Difference**
BHETA	3.13	0	3.13
Ethanolamine	21.42	0.04	21.38
Ethylene Glycol	9.81	0.11	9.7
Polyethylene Terephthalate	3.34	0	3.34

9.2.2 Energy Balance using Symmetry at R-101

Table 9.3 shows the percentage error for energy balance at reactor 1. The percentage error was calculated between manual calculation and simulation calculation which are SuperPro and Symmetry The higher percentage error due to the assumption was made in manual calculation cannot be made in the simulation process.

Table 9.3 Percentage error at output reactor (R-101) for energy balance.

			Symmetry Simulation		**SuperPro Simulation**	
	Stream number	**Manual calculation (kJ/h)**	**Calculation (kJ/h)**	**Percentage Error (%)**	**Calculation (kJ/h)**	**Percentage Error (%)**
Inlet	9	21756.66	-706320.00	96.92	89483.31	75.69
Outlet	11	679947.94	-537120.00	26.59	485342.18	40.00

Table 9.4 shows the differences of percentage error between SuperPro and Symmetry simulation for energy balance. There are some differences for both simulations because both simulations used the difference type of reactor.

Table 9.4 Percentage error difference between SuperPro and Symmetry simulation.

Stream number	Symmetry Simulation Percentage Error (%)	SuperPro Simulation Percentage Error (%)	Difference
9	96.92	75.69	21.23
11	26.59	40.00	13.41

9.3 POLYMERIZATION, (R-102)

BHETA was further reacted with Caprolactone through ring opening polymerization with Dibutyltin dilaurate (DBTDL) as a catalyst in the packed bed reactor (R-102) with nitrogen gas inlet. The product obtained is Polyester polyol with 2 hydroxyl group (More et al.2013). The conversion of BHETA is 90%. Symmetry simulation was used to calculate mass and enegry balance by using conversion reactor. Conversion reactor was used to provide shortcut material and energy balance models for actual reactors. Then, SuperPro simulation was used stoichiometry equation reactor.

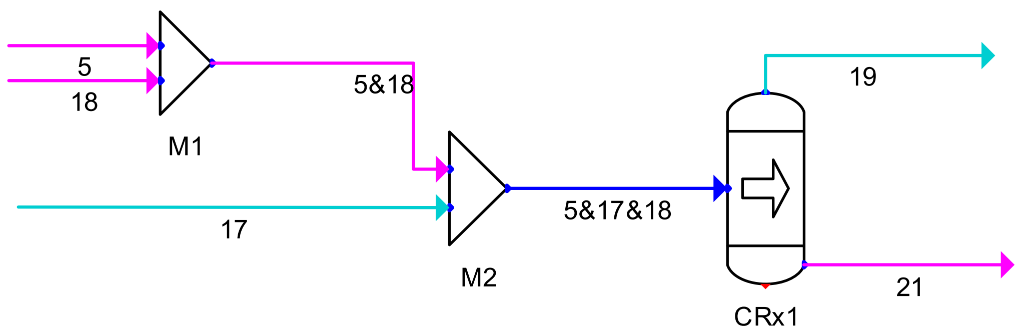


Figure 9.3 Conversion reactor at R-101 on Syymetry simulation

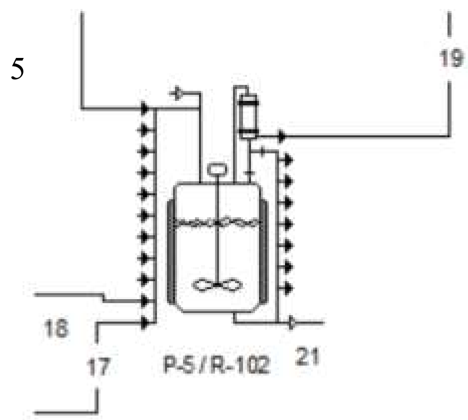


Figure 9.4 Stoichiometry reaction reactor at R-102 on SuperPro simulation

9.3.1 Mass Balance using Symmetry at R-102

Table 9.5 shows percentage error at output stream 21 for mass balance. The percentage error was calculated between manual calculation and simulation calculation which are SuperPro and Symmetry.

Table 9.5 Percentage error at output stream 21 for mass balance

		Symmetry Simulation		SuperPro Simulation	
Component	**Manual calculation (kg/h)**	**Calculation (kg/h)**	**Percentage Error (%)**	**Calculation (kg/h)**	**Percentage Error (%)**
BHETA	225.50	225.60	0.04	225.48	0.01
Caprolactone	204.02	199.89	2.07	204.21	0.09
Ethanolamine	2.11	1.64	28.66	2.10	0.24
Ethylene Glycol	2.11	1.44	46.53	2.11	0.28
Polyester Polyol	3865.69	3870.39	0.12	3865.29	0.01
Polyethylene Terephthalate	3.16	3.17	0.32	3.15	0.16

Table 9.6 shows the differences of percentage error between SuperPro and Symmetry simulation. There are some differences for both simulations, especially at mass balance of ethanolamine and ethylene glycol. This is due to the difference type reactor was used in the simulation.

Table 9.6 Percentage error difference between SuperPro and Symmetry simulation.

Component	**Symmetry Simulation Percentage Error (%)**	**SuperPro Simulation Percentage Error (%)**	**Difference**
BHETA	0.04	0.01	0.03
Caprolactone	2.07	0.09	1.98
Ethanolamine	28.66	0.24	28.42
Ethylene Glycol	46.53	0.28	46.25
Polyester Polyol	0.12	0.01	0.11
Polyethylene Terephthalate	0.32	0.16	0.16

9.3.2 Energy Balance using SuperPro at R-102

Table 9.7 shows the percentage error for energy balance at reactor 2. The percentage error was calculated between manual calculation and simulation calculation which are SuperPro and Symmetry The higher percentage error due to the assumption was made in manual calculation cannot be made in the simulation process.

Table 9.7 Percentage error at output reactor (R-102) for energy balance.

			Symmetry Simulation		SuperPro Simulation	
	Stream number	**Manual calculation (kJ/h)**	**Calculation (kJ/h)**	**Percentage Error (%)**	**Calculation (kJ/h)**	**Percentage Error (%)**
Inlet	18	122108.50	-1792440	93.19	335117	63.56
Outlet	21	832618.78	995760	16.38	117657	60.76

Table 9.8 shows the differences of percentage error between SuperPro and Symmetry simulation for energy balance. There are some differences for both simulations because both simulations used the difference type of reactor.

Table 9.8 Percentage error difference between SuperPro and Symmetry simulation.

Stream number	Symmetry Simulation Percentage Error (%)	SuperPro Simulation Percentage Error (%)	Difference
9	96.92	75.69	21.23
11	26.59	40.00	13.41

9.4 POLYMERIZATION, (R-103)

Polyurethanes polymer formed through step-Growth polymerization by reacting the polyester polyol with two hydroxyl group Polyester Hexamethylene Diisocyanate (HDI) with two isocyanate group by forming urethanes linkage. (Mir et al., n.d.). The Dimethylformamide (DMF) also will flow into the reactor (R-103) to act as solvent to obtain liquid Polyurethane.The conversion of Polyol is 90%. SuperPro simulation was used to calculate mass and energy balance of CSTR (R-103).

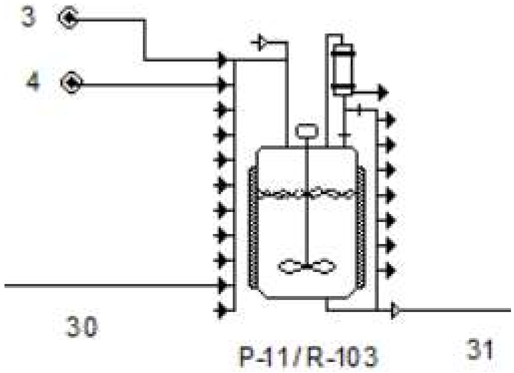
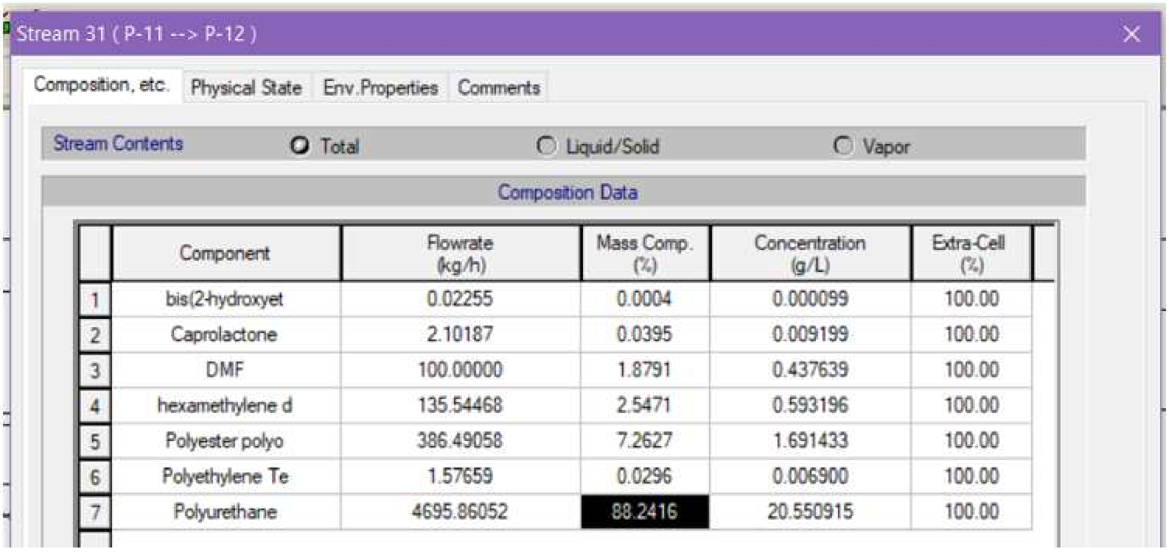


Figure 9.5 SuperPro simulation for third reaction at R-103

9.4.1 Mass Balance using SuperPro at R-103



	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	0.02255	0.0004	0.000099	100.00
2	Caprolactone	2.10187	0.0395	0.009199	100.00
3	DMF	100.00000	1.8791	0.437639	100.00
4	hexamethylene d	135.54468	2.5471	0.593196	100.00
5	Polyester polyo	386.49058	7.2627	1.691433	100.00
6	Polyethylene Te	1.57659	0.0296	0.006900	100.00
7	Polyurethane	4695.86052	88.2416	20.550915	100.00

Figure 9.6 Mass Balance for R-103 on SuperPro simulation

Table 9.9 Percentage Error between Manual and SuperPro calculation for Mass Balance

Component	Manual calculation (kg/h)	SuperPro calculation (kg/h)	Percentage Error (%)
BHETA	0	0.02	100
Caprolactone	2.11	2.10	0.48
DMF	100	100	0
HDI	135.30	135.54	0.18
Polyurethane	4696.81	4695.86	0.02
Polyester Polyol	386.57	386.49	0.02
Polyethylene Terephthalate	1.58	1.58	0

9.3.2 Energy Balance using SuperPro at R-103

Input stream 3

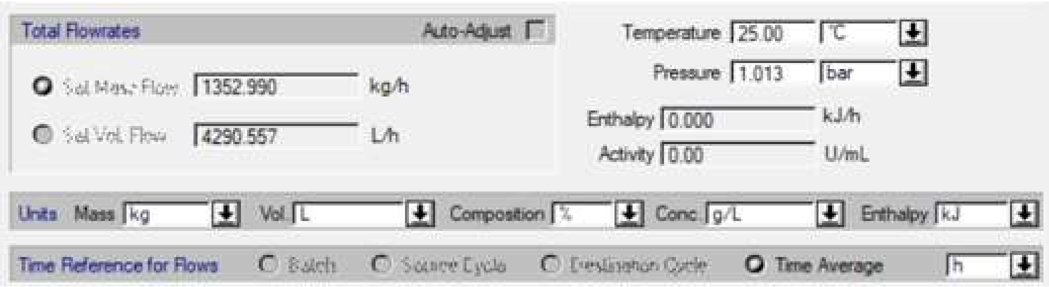


Figure 9.7 SuperPro result for energy balance input stream R-103

Input stream 4

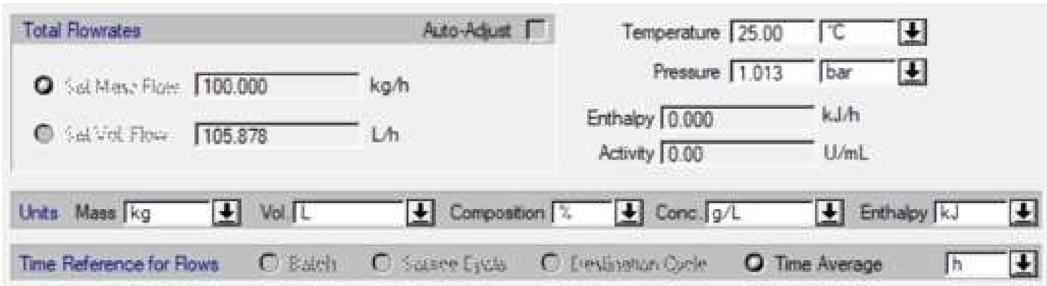


Figure 9.8 SuperPro result for energy balance input stream R-103

Input stream 30

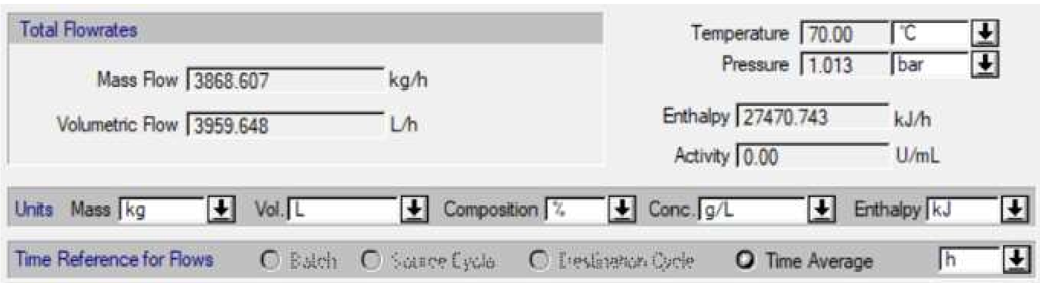


Figure 9.9 SuperPro result for energy balance input stream R-103

Oulet stream 31

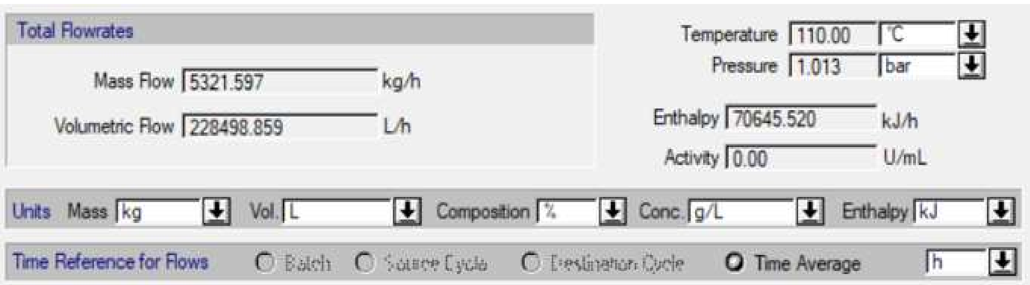


Figure 9.10 SuperPro result for energy balance output stream R-103

Table 9.10 Percentage error at conversion reactor (R-102) for energy balance

	Stream number	Manual calculation (kJ/h)	SuperPro calculation (kJ/h)	Percentage Error (%)
Inlet	3	0	0	0
	4	0	0	0
	30	328776.08	27470.74	91.64
Outlet	31	783305.27	70645.52	90.98

9.5 DISTILLATION, (DC-101)

The mixture of the product from first reaction which is BHETA and EG with the excess of reactant will be separated in Distillation Column (D-101). BHETA with the highest boiling point will be the bottom product. SuperPro simulation was used to calculate mass and energy balance of Distillation Column (DC-101).

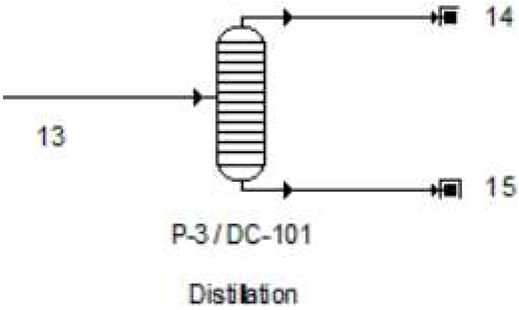
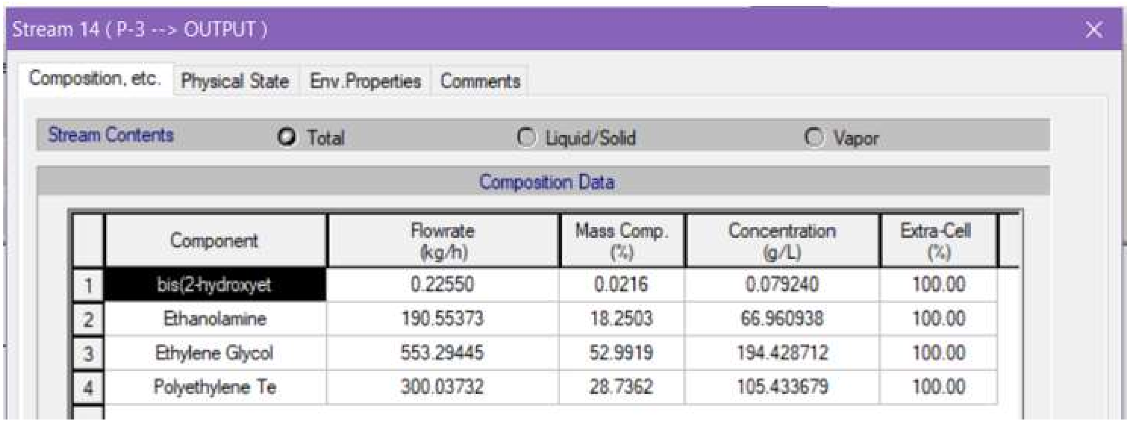


Figure 9.11 SuperPro simulation for DC-101

9.5.1 Mass Balance using SuperPro at DC-101

Oulet stream 14


Stream 14 (P-3 --> OUTPUT)

Composition, etc. | Physical State | Env.Properties | Comments

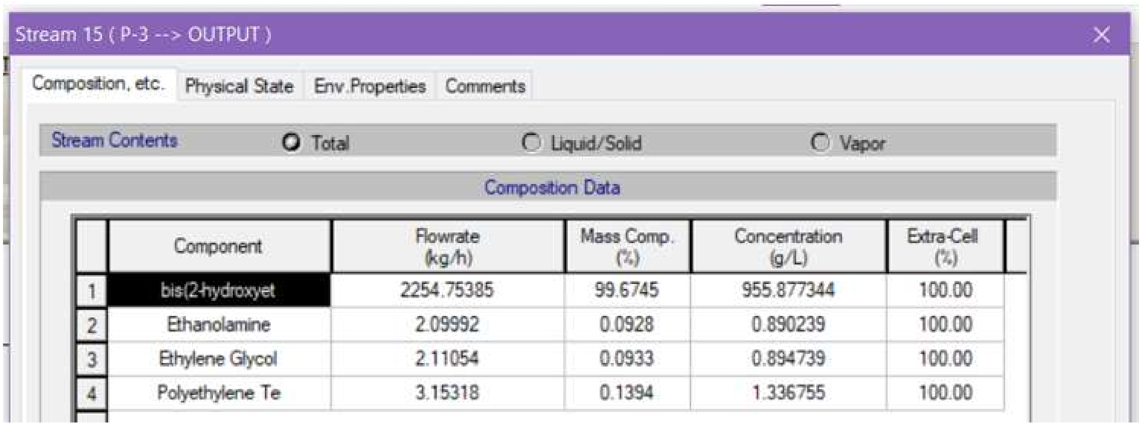
Stream Contents — Total — Liquid/Solid — Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	0.22550	0.0216	0.079240	100.00
2	Ethanolamine	190.55373	18.2503	66.960938	100.00
3	Ethylene Glycol	553.29445	52.9919	194.428712	100.00
4	Polyethylene Te	300.03732	28.7362	105.433679	100.00

Figure 9.12 Mass Balance for DC-101 on SuperPro simulation at top product

Oulet stream 15


Stream 15 (P-3 --> OUTPUT)

Composition, etc. | Physical State | Env.Properties | Comments

Stream Contents: Total / Liquid/Solid / Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	2254.75385	99.6745	955.877344	100.00
2	Ethanolamine	2.09992	0.0928	0.890239	100.00
3	Ethylene Glycol	2.11054	0.0933	0.894739	100.00
4	Polyethylene Te	3.15318	0.1394	1.336755	100.00

Figure 9.13 Mass Balance for DC-101 on SuperPro simulation at bottom product

Table 9.11 Percentage Error between Manual and SuperPro calculation for Mass Balance

Component	Manual calculation (kg/h)		SuperPro calculation (kg/h)		Percentage Error (%)	
	Top product	Bottom product	Top product	Bottom product	Top product	Bottom product
BHETA	0	2254.98	0.23	2254.75	100	0.01
Ethanolamine	192.55	2.11	190.55	2.10	1.05	0.24
Ethylene Glycol	552.69	2.11	553.29	2.11	0.11	0.28
Polyethylene Terephthalate	300.03	3.16	300.04	3.15	0.01	0.16

9.6 OVERALL MASS BALANCE

Overall mass balance was calculated using SuperPro simulation. Figure 9.14 shows overall process flow diagram of plant using SuperPro.

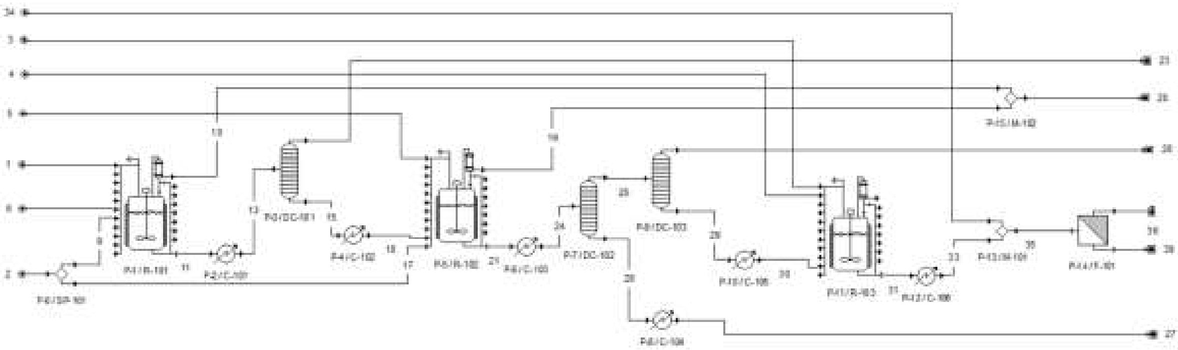


Figure 9.14 SuperPro simulation for overall process

4. OVERALL COMPONENT BALANCE (kg/h)

COMPONENT	IN	OUT	IN-OUT
bis(2-hydroxyet	0.000	225.701	- 225.701
Caprolactone	2,040.220	204.206	1,836.014
DMF	100.000	100.000	0.000
Ethanolamine	1,284.350	192.654	1,091.696
Ethylene Glycol	0.000	555.405	- 555.405
hexamethylene d	1,352.990	135.545	1,217.445
Nitrogen	200.000	200.000	0.000
Polyester polyo	0.000	386.877	- 386.877
Polyethylene Te	2,021.270	303.191	1,718.080
Polyurethane	0.000	4,695.861	- 4,695.861
Water	300.000	300.000	0.000
TOTAL	7,298.830	7,299.438	0.608

Figure 9.15 Mass Balance for overall process on SuperPro simulation

Table 9.12 shows our percentage error is 0.01% for overall mass balance between manual calculation and SuperPro simulation. So, we can said that our manual calculation is accurate because the percentage error very low for mass balance.

Table 9.12 Percentage Error between Manual and SuperPro calculation for Mass Balance

Component	Manual calculation (kg/h)	SuperPro calculation (kg/h)	Percentage Error (%)
BHETA	225.50	225.70	0.09
Caprolactone	204.03	204.21	0.09
DMF	100	100	0
Ethanolamine	192.66	192.65	0
Ethylene Glycol	554.8	555.41	0.11
HDI	135.30	135.55	0.18
Nitrogen	200	200	0
Polyurethane	4696.81	4695.86	0.02
Polyester Polyol	386.56	386.88	0.08
Polyethylene Terephthalate	303.19	303.19	0
Water	300	300	0
Overall	7298.850.	7299.44	0.01

In conclusion, energy balance for overall process cannot be compared because the manual calculation cannot be calculated. Then, the higher percentage error might happen due to several reasons. Such as the assumptions made in the manual calculations is not accurate and cannot be set in the both simulation. For example, enthalpy is automatically calculated in simulation while in manual calculation, it needed data like heat capacity and others to be calculate. So, the value might be inaccurate.

All the data for Symmetry dan SuperPro simulation is at **Appendix D**.

CONCLUSION

Polyurethane are plastic polymers made by combining diisocynates with polyols with chemical formula C3H8N2O it also known as polyform plastic sponge. It was produced by the exothermic reaction between those chemicals which are polyol and diisocyanates. It was used in many industries which is aviation, railway, architecture, and sports. It also used in manufacture of plastic products, synthesis rubber product, synthetic fiber, hard and soft foam plastics, adhesives, and coating. The usage of polyurethanes extensive during World War II, when it was utilized as a replacement for rubber because at that time rubber was expensive and hardly to obtain.

The global market indicated the demand of Polyurethane is steadily increased over the year from 2016 to 2025 with estimated CAGR of 5.22%. In order to fulfil the global demand market, we have come up with a production plant that produces about 1.58 million tonnes tonnes of Polyurethane per year (1.58×10^6 kg per year). With a 2.5% market deficiency and the plant operates for 345 days which 8280 hours per year gives us the plant capacity for production of Polyurethane is 4770.5 kg/hour.

The method for calculation of mass balance used is forward calculation where assuming the molar flowrate in for PET, N_{iP} as 100 kmol/hour. Then, scaling the molar and mass flowrate of each component including our product Propylene Glycol to 0.105274656 in order to achieve our required plant capacity of 4770.5 kg/hour. The energy balance at each reactor was calculated.

The raw material selection and reactor selection have been made. Continuous stirred tank reactor (CSTR) is chosen for general mole balance and calculation of volume for the tank. The volume for the CSTR is 6.86 m^3. For separation process I part, unit selection for the separator was made. We did the process design for the required separator and obtained various value such as minimum stages, N_{min}, minimum reflux ratio, R_{min} and the efficiency of the separator unit. For computational part, MATLAB program had been made to calculate the mass and energy balance for R-103 and numerical method was used to calculate the enthalpy out for Polyurethane is Trapezoidal Rule method. Furthermore, we had made calculation for mass balance in a simulation which is SuperPro and Symmetry The values obtained from the simulation are then compared with the manual calculation.

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APPENDIX A

MASS AND ENERGY BALANCE

PART I: MASS BALANCE

In the material balance calculation, we used forward calculation and get the ratio of the plant capacity with the obtained final flow rate hence all the flow rate has been multiplied by the scale factor 0.1069264.

Mass Balance on Reactor (R-101)

$$C_{10}H_8O_4 + 2C_2H_7NO \xrightarrow{\text{Zink acetate}} C_{12}H_{16}O_4N_2 + C_2H_6O_2$$

The PET conversion = 85%

$N_{i,PET}$ = 100 kmole/h

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

$$0.85 = \frac{-(-1)r}{100}$$

$$r = 85\ kmole/h$$

Calculation:

PET Balance

$F_{i,PET}$ = (100 kmole/h)(192 g/mole)

$F_{i,PET}$ = 19200 kg/h

$N_i = N_o - \alpha r$

100 k/mole/h = $N_{o,PET}$ – (-1)(85 kmole/h)

$N_{o,PET}$ = 15 kmole/h

$F_{o,PET}$ = (15 kmole/h)(192 g/mole)

$F_{o,PET}$ = 2880 kg/h

Ethanolamine Balance

$N_{i,ET} = 200$ kmole/h

$F_{i,\,ET} = (200\ \text{kmole/h})(61\ \text{g/mole})$

$F_{i,\,ET} = 12{,}200$ kg/h

$N_i = N_o - \alpha r$

$200\ \text{kmole/h} = N_{o,ET} - (-2)(85\ \text{kmole/h})$

$N_{o,ET} = 30$ kmole/h

$F_{o,ET} = (30\ \text{kmole/h})(61\ \text{g/mole})$

$F_{o,ET} = 1830$ kg/h

BHETA Balance

$N_i = N_o - \alpha r$

$0\ \text{kmole/h} = N_{o,B} - (-1)(85\ \text{kmole/h})$

$N_{o,B} = 85$ kmole/h

$F_{o,B} = (85\ \text{kmole/h})(252\ \text{g/mole})$

$F_{o,B} = 21420$ kg/h

Ethylene Glycol Balance

$N_i = N_o - \alpha r$

$0\ \text{kmole/h} = N_{o,EG} - (-1)(85\ \text{kmole/h})$

$N_{o,EG} = 85$ kmole/h

$F_{o,EG} = (85\ \text{kmole/h})(62\ \text{g/mole})$

$F_{o,EG} = 5270$ kg/h

Scale down the flow rate by multiply it with the scale factor 0.105274656.

$F_{i,PET} = (19200\ \text{kg/h})(0.105274656) = 2052.99$ kg/h

$F_{o,PET} = (2880\ \text{kg/h})(0.105274656) = 303.19$ kg/h

$F_{i,\,ET} = (12{,}200\ \text{kg/h})(0.105274656) = 1284.35$ kg/h

$F_{o,ET}$ = (1830 kg/h)(0.105274656) = 192.65 kg/h

$F_{o,B}$ = (21420 kg/h)(0.105274656) = 2254.98 kg/h

$F_{o,EG}$ = (5270 kg/h)(0.105274656) = 554.80 kg/h

Mass Balance on Distillation Column (DC-101)

Mass balance calculation at Distillation Column:

$$F_{zF} = x_D D + x_B B$$

Rearrange the equation:

$$D = F[\frac{z_F - x_B}{x_D - x_B}]$$

$$D = 3305.62 \left[\frac{0.0917 - 1.3959 \times 10^{-3}}{0.2876 - 1.3959 \times 10^{-3}}\right]$$

$$D = 1043.267$$

$$F = D + B$$

$$B = F - D$$

$$B = 3305.62 - 1043.267$$

$$B = 2262.348$$

Mass Balance at Distillate

Mass flow rate for light key, PET at distillate:

$F_{PET} = x_D D$

F_{PET} = (0.2876)(1043.267)

F_{PET} = 300.03

Mass flow rate for light non key, Ethylene Glycol at distillate:

F_{EG} = (0.53)(1043.267)

F_{EG} = 552.69

Mass flow rate for light non key, Ethanolamine at distillate:

$F_{ET} = (0.183)(1043.267)$

$F_{ET} = 190.547$

Mass Balance at Bottom

Mass flow rate for light key, PET at bottom:

$F_{PET} = x_B B$

$F_{PET} = (1.3959 \text{ x } 10^{-3})(2262.348)$

$F_{PET} = 3.158$

Mass flow rate for light non key, Ethylene Glycol at bottom:

$F_{EG} = (9.3044 \text{ x } 10^{-4})(2262.348)$

$F_{EG} = 2.105$

Mass flow rate for light non key, Ethanolamine at bottom:

$F_{ET} = (9.3044 \text{ x } 10^{-4})(2262.348)$

$F_{ET} = 2.105$

Mass flow rate for heavy key, BHETA at bottom:

$F_B = (0.9967)(2262.348)$

$F_B = 2254.98$

Mass Balance on Reactor (R-102)

$$C_{12}H_{16}O_4N_2 + 2C_6H_{10}O_2 \xrightarrow{\text{DBTDL}} C_{24}H_{34}O_6N_2(OH)_2$$

The BHETA conversion = 90%

$N_{i,B} = 85$ kmole/h

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

$$0.90 = \frac{-(-1)r}{85}$$

$$r = 76.5\ kmole/h$$

Calculation:

BHETA Balance

$F_{i,B}$ = (85 kmole/h)(252 g/mole)

$F_{i,B}$ = 21420 kg/h

$N_i = N_o - \alpha r$

85 k/mole/h = $N_{o,B}$ – (-1)(76.5 kmole/h)

$N_{o,B}$ = 8.5 kmole/h

$F_{o,B}$ = (8.5 kmole/h)(252 g/mole)

$F_{o,B}$ = 2142 kg/h

Caprolactam Balance

$N_{i,CP}$ = 170 kmole/h

$F_{i,\ CP}$ = (170 kmole/h)(114 g/mole)

$F_{i,\ CP}$ = 19380 kg/h

$N_i = N_o - \alpha r$

170 kmole/h = $N_{o,CP}$ – (-2)(76.5 kmole/h)

$N_{o,CP}$ = 17 kmole/h

$F_{o,CP}$ = (17 kmole/h)(114 g/mole)

$F_{o,CP}$ = 1938 kg/h

Polyol Balance

$N_i = N_o - \alpha r$

0 kmole/h = $N_{o,PO}$ – (-1)(76.5 kmole/h)

$N_{o,PO}$ = 76.5 kmole/h

$F_{o,PO}$ = (76.5 kmole/h)(480 g/mole)

$F_{o,PO}$ = 36720 kg/h

Scale down the flow rate by multiply it with the scale factor 0.105274656.

$F_{i,B}$ = (21420 kg/h)(0.105274656) = 2254.98 kg/h

$F_{o,B}$ = (2142 kg/h)(0.105274656) = 225.498 kg/h

$F_{i,\ CP}$ = (19380 kg/h)(0.105274656) = 2040.22 kg/h

$F_{o,CP}$ = (1938 kg/h)(0.105274656) = 204.02 kg/h

$F_{o,PO}$ = (36720 kg/h)(0.105274656) = 3865.685 kg/h

Mass Balance on Distillation Column (DC-102)

Mass balance calculation at Distillation Column:

$$F_{zF} = x_D D + x_B B$$

Rearrange the equation:

$$D = F[\frac{z_F - x_B}{x_D - x_B}]$$

$$D = 4302.57\left[\frac{0.0474 - 9.1848 \times 10^{-3}}{0.0496 - 9.1848 \times 10^{-3}}\right]$$

$$D = 4073.39$$

$$F = D + B$$

$$B = F - D$$

$$B = 4302.57 - 4073.39$$

$$B = 229.18$$

Mass Balance at Distillate

Mass flow rate for light key, Caprolactam at distillate:

$F_{CP} = x_D D$

F_{CP} = (0.0496)(4073.39)

F_{CP} = 201.916

Mass flow rate for light non key, Ethylene Glycol at distillate:

$F_{EG} = (5.1677 \times 10^{-4})(4073.39)$

$F_{EG} = 2.105$

Mass flow rate for light non key, Ethanolamine at distillate:

$F_{ET} = (5.1677 \times 10^{-4})(4073.39)$

$F_{ET} = 2.105$

Mass flow rate for light non key, PET at distillate:

$F_{PET} = (3.8764 \times 10^{-4})(4073.39)$

$F_{PET} = 1.579$

Mass flow rate for light non key, Polyol at distillate:

$F_{PO} = (0.949)(4073.39)$

$F_{PO} = 3865.685$

Mass Balance at Bottom

Mass flow rate for light key, Caprolactam at bottom:

$F_{CP} = x_B B$

$F_{CP} = (9.1848 \times 10^{-3})(229.182)$

$F_{CP} = 2.105$

Mass flow rate for light non key, PET at bottom:

$F_{PET} = (6.8897 \times 10^{-3})(229.182)$

$F_{PET} = 1.579$

Mass flow rate for heavy key, BHETA at bottom:

$F_B = (0.984)(229.182)$

$F_B = 225.498$

Mass Balance on Distillation Column (DC-103)

Mass balance calculation at Distillation Column:

$$F_{zF} = x_D D + x_B B$$

Rearrange the equation:

$$D = F[\frac{z_F - x_B}{x_D - x_B}]$$

$$D = 4073.39\left[\frac{0.0496 - 5.440 \times 10^{-4}}{0.9794 - 5.440 \times 10^{-4}}\right]$$

$$D = 204.02$$

$$F = D + B$$

$$B = F - D$$

$$B = 4073.39 - 204.02$$

$$B = 3869.369$$

<u>Mass Balance at Distillate</u>

Mass flow rate for light key, Caprolactam at distillate:

$F_{CP} = x_D D$

$F_{CP} = (0.9794)(204.02)$

$F_{CP} = 199.81$

Mass flow rate for light non key, Ethylene Glycol at distillate:

$F_{EG} = (0.0103)(204.02)$

$F_{EG} = 2.105$

Mass flow rate for light non key, Ethanolamine at distillate:

$F_{ET} = (0.0103)(204.02)$

$F_{ET} = 2.105$

<u>Mass Balance at Bottom</u>

Mass flow rate for light key, Caprolactam at bottom:

$F_{CP} = x_B B$

$F_{CP} = (5.440 \times 10^{-4})(3869.369)$

$F_{CP} = 2.105$

Mass flow rate for light non key, PET at bottom:

$F_{PET} = (4.0808 \times 10^{-4})(3869.369)$

$F_{PET} = 1.579$

Mass flow rate for heavy key, Polyol at bottom:

$F_{PO} = (0.9990)(3869.369)$

$F_{PO} = 3865.685$

Mass Balance on Reactor (R-103)

$$C_{24}H_{34}O_6N_2(OH)_2 + C_6H_{12}(NCO)_2 \longrightarrow C_{32}H_{48}O_{10}N_4$$

The Polyol conversion = 90%

$N_{i,PO} = 76.5$ kmole/h

The formula to obtain the rate of reaction, r is as below:

$$X = \frac{-\alpha r}{N}$$

$$0.90 = \frac{-(-1)r}{76.5}$$

$$r = 68.85\frac{kmole}{h}$$

Calculation:

Polyol Balance

$F_{i,PO} = (76.5 \text{ kmole/h})(480 \text{ g/mole})$

$F_{i,PO} = 36720$ kg/h

$N_i = N_o - \alpha r$

76.5 k/mole/h $= N_{o,PO} - (-1)(68.85 \text{ kmole/h})$

$N_{o,PO} = 7.65$ kmole/h

$F_{o,PO} = (7.65\ kmole/h)(480\ g/mole)$

$F_{o,PO} = 3672\ kg/h$

HDI Balance

$N_{i,H} = 76.5\ kmole/h$

$F_{i,\ H} = (76.5\ kmole/h)(168\ g/mole)$

$F_{i,\ H} = 12852\ kg/h$

$N_i = N_o - \alpha r$

$76.5\ kmole/h = N_{o,H} - (-1)(68.85\ kmole/h)$

$N_{o,H} = 7.65\ kmole/h$

$F_{o,H} = (7.65\ kmole/h)(168\ g/mole)$

$F_{o,H} = 1285.2\ kg/h$

Polyurethane Balance

$N_i = N_o - \alpha r$

$0\ kmole/h = N_{o,PU} - (-1)(68.85\ kmole/h)$

$N_{o,PU} = 68.85\ kmole/h$

$F_{o,PU} = (68.85\ kmole/h)(648\ g/mole)$

$F_{o,PU} = 44614.8\ kg/h$

Scale down the flow rate by multiply it with the scale factor 0.105274656.

$F_{i,PO} = (36720\ kg/h)(0.105274656) = 3865.685\ kg/h$

$F_{o,PO} = (3672kg/h)(0.105274656) = 386.57\ kg/h$

$F_{i,\ H} = (12852\ kg/h)(0.105274656) = 1352.99\ kg/h$

$F_{o,H} = (1285.2\ kg/h)(0.105274656) = 135.299\ kg/h$

$F_{o,PU} = (44614.8\ kg/h)(0.105274656) = 4696.81\ kg/h$

<u>Mass Balance on Mixer (M-101)</u>

Components Balance Inlet Stream 33

$F_{i,PO}$ = 386.57 kg/h

$F_{i,CP}$ = 2.105 kg/h

$F_{i,PET}$ = 1.579 kg/h

$F_{i,H}$ = 135.299 kg/h

$F_{i,DMF}$ = 100 kg/h

$F_{i,PU}$ = 4696.81 kg/h

Components Balance Inlet Stream 34

$F_{i,W}$ = 300 kg/h

Components Balance Outlet Stream 35

$F_{o,PO}$ = 386.57 kg/h

$F_{o,CP}$ = 2.105 kg/h

$F_{o,PET}$ = 1.579 kg/h

$F_{o,H}$ = 135.299 kg/h

$F_{o,DMF}$ = 100 kg/h

$F_{o,PU}$ = 4696.81 kg/h

$F_{o,W}$ = 300 kg/h

<u>Mass Balance on Mixer (M-101)</u>

Components Balance Inlet Stream 35

$F_{i,PO}$ = 386.57 kg/h

$F_{i,CP}$ = 2.105 kg/h

$F_{i,PET}$ = 1.579 kg/h

$F_{i,H}$ = 135.299 kg/h

$F_{i,DMF}$ = 100 kg/h

$F_{i,PU}$ = 4696.81 kg/h

$F_{i,W}$ = 300 kg/h

Components Balance Outlet Stream 36

$F_{o,PO} = 323.4$ kg/h

$F_{o,CP} = 2.105$ kg/h

$F_{o,H} = 126.35$ kg/h

$F_{o,DMF} = 100$ kg/h

$F_{o,W} = 300$ kg/h

Components Balance Outlet Stream 37

$F_{o,PO} = 63.16$ kg/h

$F_{o,PET} = 1.579$ kg/h

$F_{o,H} = 8.948$ kg/h

$F_{o,PU} = 4696.81$ kg/h

PART II: ENERGY BALANCE

Energy Balance on Batch Reactor (R-101)

$$\begin{aligned}\Delta Hrxn &= \Sigma\Delta vp\Delta Hf\ Product - \Sigma\Delta vr\Delta Hf\ Reactant \\ &= [1(-396.3) + (-455.20)] - [1(-270.518) + 2(-507.50) \\ &= 434.018\ kJ/mol\end{aligned}$$

Inlet Enthalpy:

Stream 7

$$\Delta H_{PET} = \int_{298.15}^{366.15} 305.4\ \mathrm{dT} = 20767.2\ \mathrm{J/mol}$$

Stream 8

$$\Delta H_{Ethanolamine} = \int_{298}^{298} 107.21\ \mathrm{dT} = 0\ \mathrm{J/mol}$$

Outlet Enthalpy:

Stream 11

$$\Delta H_{BHETA} = \int_{298.15}^{433.15} 303.26\ dT = 40940\ \mathrm{J/mol}$$

$$\Delta H_{EG} = \int_{298.15}^{433.15} 167.88 = 22663\ \mathrm{J/mol}$$

$$\Delta H_{unreacted\ PET} = \int_{298.15}^{433.15} 305.4\, dT = 41229\ \mathrm{J/mol}$$

$$\Delta H_{unreacted\ Ethanolamine} = \int_{298.15}^{433.15} 107.2\, dT = 14473\ \mathrm{J/mol}$$

Total Enthalpy outlet:

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

ΔH_{outlet} = 8.9483(40940) + 8.9483(22663) + 1.5791(41229) + 3.1582(14473)

ΔH_{outlet} = 679947.94 kJ/h

Total Enthalpy inlet:

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

ΔH_{inlet} = 10.5247(20767.2)

ΔH_{inlet} = 21756.66 kJ/h

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

Q = (679947.94 -21756.66) + 85(434.018)

Q = 21934.81 kJ/h

<u>Energy Balance on Packed Bed Reactor (R-102)</u>

$\Delta Hrxn = \Sigma\Delta vp\Delta Hf\ Product - \Sigma\Delta vr\Delta Hf\ Reactant$

$= [1(-210.52)] - [2(-458) + (-396.3)]$

$= 1101.78\ kJ/mol$

<u>Inlet Enthalpy:</u>

Stream 18

$\Delta H_{BHETA} = \int_{298.15}^{343.15} 303.26\ dT$ = 13646.7 J/mol

Stream 5

$\Delta H_{Caprolactone} = \int_{298.15}^{298.15} 196.8$ = 0 J/mol

<u>Outlet Enthalpy:</u>

Stream 21

$\Delta H_{polyol} = \int_{298.15}^{403.15} 907.2\ dT$ = 95256 J/mol

$\Delta H_{BHETA} = \int_{298.15}^{403.15} 303.26\ dT$ = 31842.3 J/mol

$\Delta H_{caprolactone} = \int_{298.15}^{403.15} 196.8\,dT$ = 20644 J/moL

Total Enthalpy outlet:

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

ΔH_{outlet} = 8.0535(95256) + 0.8948(31842) + 1.7897(20664)

ΔH_{outlet} = 832618.78 kJ/h

Total Enthalpy inlet:

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

ΔH_{inlet} = 8.9483(13646) +17.8967(0)

ΔH_{inlet} = 122108.50 kJ/h

$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r \Delta H_{rxn}$
Q = (832618.78 -122108.50) + 76.5(1101.78)
$Q = 794796.45\ kJ/h$

<u>Energy Balance on Continuous Stirred-Tank Reactor (R-103)</u>

$\Delta Hrxn = \Sigma \Delta vp \Delta Hf\ Product - \Sigma \Delta vr \Delta Hf\ Reactant$
$= [1(77)] - [(-210.52) + (-219.27)]$
$= 506.79\ kJ/mol$

<u>Inlet Enthalpy:</u>

Stream 30
$\Delta H_{polyol} = \int_{298.15}^{343.15} 907.2\ dT$ = 40824 J/mol

Stream 3
$\Delta H_{HDI} = \int_{298.15}^{298.15} 299.2\ dT$ = 0 J/mol

<u>Outlet Enthalpy:</u>

Stream 31

$\Delta H_{polyurethanes} = \int_{298.15}^{383.15} 637\ dT$ = 25480 J/mol
$\Delta H_{polyol} = \int_{298.15}^{383.15} 907.2\ dT$ = 77112 J/mol
$\Delta H_{HDI} = \int_{298.15}^{383.15} 299.2\, dT$ = 25432 J/mol

Total Enthalpy outlet:
$\Delta H_{outlet} = \sum N \Delta H$
ΔH_{outlet} = 7.2482(25480) + 0.8054(77112) + 0.8054(25432)
ΔH_{outlet} = 783305.27 kJ/h

Total Enthalpy inlet:
$\Delta H_{inlet} = \sum N \Delta H$
ΔH_{inlet} = 8.0535(40824) +(0)
ΔH_{inlet} = 328776.084 kJ/h

$Q = \Delta H_{out}(N_{out}) - \Delta H_{in}(N_{in}) + \sum r \Delta H_{rxn}$
Q = (783305.27 - 328776.084) + 68.855(506.79)
$Q = 489424.2115\ kJ/h$

APPENDIX B

CHEMICAL ENGINEERING COMPUTATION II

PART I: MASS BALANCE CODING

```
classdef IP3rdyear_massBalance < matlab.apps.AppBase

    % Properties that correspond to app components
    properties (Access = public)
        UIFigure                        matlab.ui.Figure
        UITable
matlab.ui.control.Table
        MassBalanceatR103KGHRLabel
matlab.ui.control.Label
        Panel
matlab.ui.container.Panel
        EditField
matlab.ui.control.EditField
        EnterButton
matlab.ui.control.Button
        EntertherequiredflowrateforreactorR103Label
matlab.ui.control.Label
        HDIFlowrateinLabel
matlab.ui.control.Label
        FlowrateInHDI
matlab.ui.control.NumericEditField
        PolyolFlowrateinLabel
matlab.ui.control.Label
        FlowrateInPolyol
matlab.ui.control.NumericEditField
        Panel_2
matlab.ui.container.Panel
        Image
matlab.ui.control.Image
        DMFEditField_2Label
matlab.ui.control.Label
        DMFOutEditField
matlab.ui.control.NumericEditField
        HDIEditField_2Label
matlab.ui.control.Label
        HDIOutEditField
matlab.ui.control.NumericEditField
        PETEditField_2Label
matlab.ui.control.Label
        PETOutEditField
matlab.ui.control.NumericEditField
        PolyolEditField_2Label
matlab.ui.control.Label
```

```
        PolyolOutEditField
matlab.ui.control.NumericEditField
        PolyurethaneEditFieldLabel
matlab.ui.control.Label
        PolyurethaneEditField
matlab.ui.control.NumericEditField
        CaprolactoneEditField_2Label
matlab.ui.control.Label
        CaprolactoneOutEditField
matlab.ui.control.NumericEditField
        Flowratestream31EditFieldLabel
matlab.ui.control.Label
        Flowratestream31EditField
matlab.ui.control.NumericEditField
        HDIEditFieldLabel
matlab.ui.control.Label
        HDIEditField
matlab.ui.control.NumericEditField
        Flowratestream3EditFieldLabel
matlab.ui.control.Label
        Flowratestream3EditField
matlab.ui.control.NumericEditField
        DMFEditFieldLabel
matlab.ui.control.Label
        DMFEditField
matlab.ui.control.NumericEditField
        PETEditFieldLabel
matlab.ui.control.Label
        PETEditField
matlab.ui.control.NumericEditField
        PolyolEditFieldLabel
matlab.ui.control.Label
        PolyolEditField
matlab.ui.control.NumericEditField
        CaprolactoneEditFieldLabel
matlab.ui.control.Label
        CaprolactoneEditField
matlab.ui.control.NumericEditField
        Flowratestream4EditFieldLabel
matlab.ui.control.Label
        Flowratestream4EditField
matlab.ui.control.NumericEditField
        Flowratestream30EditFieldLabel
matlab.ui.control.Label
        Flowratestream30EditField
matlab.ui.control.NumericEditField
    end

    % Callbacks that handle component events
    methods (Access = private)
```

```
        % Button pushed function: EnterButton
        function EnterButtonPushed(app, event)
            %Stoichiometric coefficient of components for the
reaction
            aPO =-1;
            aHDI=-1;
            aPU = 1;

            %Conversion of polyol
            X=0.9;



            Fi30PO=app.FlowrateInPolyol.Value;
            Fi3HDI=app.FlowrateInHDI.Value;
            app.EditField.Value= '';
            if (Fi3HDI<0 || Fi30PO<0)
                app.EditField.Value= 'Error! Please Enter A
Positive Value';
            elseif (Fi3HDI==0 || Fi30PO==0)
                    app.EditField.Value= 'Error! Please Enter
A Value Greater Than Zero';
            else
                app.EditField.Value= 'Here is your result!';


                %Molar Flowrate of each reacted Components
                %Inlet Stream 4
                NiHDI=Fi3HDI/168;

                %Inlet Stream 30
                NiPO=Fi30PO/480;

                %Outlet STream 31
                NiPU=0;


                %Using the conversion of polyol, X=0.90
                NoPO= NiPO - (X*NiPO);
                %Find the rate of reaction, r
                r=(X*NiPO)/-aPO;
                NoHDI= NiHDI + (aHDI*r);
                NoPU= NiPU + (aPU*r);



                %MW(PO)= 480, MW(HDI)= 168, MW(PU)= 648,
                %Fi30= input mass flowrate stream 30
                Fi30DMF=0;
                Fi30HDI=0;
                Fi30PU=0;
```

```
                Fi30CL = 2.105;
                Fi30PET = 1.579;

                %Fi3=Input mass flowrate stream 3
                Fi3PO= 0;
                Fi3DMF= 0;
                Fi3PU= 0;
                Fi3PET=0;
                Fi3CL=0;

                %Fi4=Input mass flowrate stream 4
                Fi4PO= 0;
                Fi4HDI= 0;
                Fi4PU= 0;
                Fi4PET=0;
                Fi4CL=0;
                Fi4DMF=100;

                %Fo31= Output mass flowrate
                Fo31PO= NoPO*480;
                Fo31HDI= NoHDI*168;
                Fo31PU= NoPU*648;
                Fo31DMF=Fi4DMF;
                Fo31PET=Fi30PET;
                Fo31CL=Fi30CL;


                %Display Mass Flowrate In and Out of Each
Components
                %Mass Flowrate in
                app.HDIEditField.Value=Fi3HDI;
                app.DMFEditField.Value=Fi4DMF;
                app.PolyolEditField.Value=Fi30PO;
                app.PETEditField.Value=Fi30PET;
                app.CaprolactoneEditField.Value=Fi30CL;

                %Mass Flowrate Out
                app.PolyolOutEditField.Value=Fo31PO;
                app.HDIOutEditField.Value=Fo31HDI;
                app.PETOutEditField.Value=Fo31PET;
                app.CaprolactoneOutEditField.Value=Fo31CL;
                app.DMFOutEditField.Value=Fo31DMF;
                app.PolyurethaneEditField.Value=Fo31PU;

                %Calculation of total mass flowrate

Fo31=Fo31PO+Fo31CL+Fo31PET+Fo31DMF+Fo31HDI+Fo31PU;
                Fi30=Fi30PO+Fi30CL+Fi30PET;
                Fi3=Fi3HDI;
                Fi4=Fi4DMF;
                app.Flowratestream31EditField.Value=Fo31;
```

```
                app.Flowratestream30EditField.Value=Fi30;
                app.Flowratestream3EditField.Value=Fi3HDI;
                app.Flowratestream4EditField.Value=Fi4DMF;

                %Tabulate the data
                flowrate_in_01 =
[Fi30PO;Fi30CL;Fi30PET;Fi30DMF;Fi30HDI;Fi30PU;Fi30;];
                flowrate_in_02 =
[Fi3PO;Fi3CL;Fi3PET;Fi3DMF;Fi3HDI;Fi3PU;Fi3;];
                flowrate_in_03 =
[Fi4PO;Fi4CL;Fi4PET;Fi4DMF;Fi4HDI;Fi4PU;Fi4;];
                flowrate_out =
[Fo31PO;Fo31CL;Fo31PET;Fo31DMF;Fo31HDI;Fo31PU;Fo31;];
                Component =
{'Polyol';'Caprolactone';'PET';'DMF';'HDI';'Polyurethane';'Tot
al'};
                table1 =
table(Component,flowrate_in_01,flowrate_in_02,flowrate_in_03,f
lowrate_out);
                app.UITable.Data= table1;

            end

        end
    end

    % Component initialization
    methods (Access = private)

        % Create UIFigure and components
        function createComponents(app)

            % Create UIFigure and hide until all components
are created
            app.UIFigure = uifigure('Visible', 'off');
            app.UIFigure.Color = [0.902 0.902 0.902];
            app.UIFigure.Position = [100 100 973 616];
            app.UIFigure.Name = 'MATLAB App';

            % Create UITable
            app.UITable = uitable(app.UIFigure);
            app.UITable.ColumnName = {'Components'; 'Inlet
Stream 30(kg/hr)'; 'Inlet Stream 3(kg/hr)'; 'Inlet Stream
4(kg/hr)'; 'Outlet Stream 31(kg/hr)'};
            app.UITable.RowName = {};
            app.UITable.ColumnSortable = true;
            app.UITable.Position = [54 23 893 187];

            % Create MassBalanceatR103KGHRLabel
            app.MassBalanceatR103KGHRLabel =
uilabel(app.UIFigure);
```

```
            app.MassBalanceatR103KGHRLabel.HorizontalAlignment
= 'center';
            app.MassBalanceatR103KGHRLabel.FontSize = 20;
            app.MassBalanceatR103KGHRLabel.FontColor = [0.149
0.149 0.149];
            app.MassBalanceatR103KGHRLabel.Position = [280 551
488 45];
            app.MassBalanceatR103KGHRLabel.Text = 'Mass
Balance at R-103 (KG/HR)';

            % Create Panel
            app.Panel = uipanel(app.UIFigure);
            app.Panel.BackgroundColor = [0.9412 0.9412
0.9412];
            app.Panel.Position = [702 229 260 323];

            % Create EditField
            app.EditField = uieditfield(app.Panel, 'text');
            app.EditField.Position = [1 1 259 22];

            % Create EnterButton
            app.EnterButton = uibutton(app.Panel, 'push');
            app.EnterButton.ButtonPushedFcn =
createCallbackFcn(app, @EnterButtonPushed, true);
            app.EnterButton.Position = [1 29 100 22];
            app.EnterButton.Text = 'Enter';

            % Create
EntertherequiredflowrateforreactorR103Label
            app.EntertherequiredflowrateforreactorR103Label =
uilabel(app.Panel);

app.EntertherequiredflowrateforreactorR103Label.Position = [8
277 243 22];

app.EntertherequiredflowrateforreactorR103Label.Text = 'Enter
the required flowrate for reactor R-103';

            % Create HDIFlowrateinLabel
            app.HDIFlowrateinLabel = uilabel(app.Panel);
            app.HDIFlowrateinLabel.Position = [19 204 88 22];
            app.HDIFlowrateinLabel.Text = 'HDI Flowrate in';

            % Create FlowrateInHDI
            app.FlowrateInHDI = uieditfield(app.Panel,
'numeric');
            app.FlowrateInHDI.Position = [146 204 100 22];

            % Create PolyolFlowrateinLabel
            app.PolyolFlowrateinLabel = uilabel(app.Panel);
```

```
            app.PolyolFlowrateinLabel.Position = [18 235 100
22];
            app.PolyolFlowrateinLabel.Text = 'Polyol Flowrate
in';

            % Create FlowrateInPolyol
            app.FlowrateInPolyol = uieditfield(app.Panel,
'numeric');
            app.FlowrateInPolyol.Position = [145 235 100 22];

            % Create Panel_2
            app.Panel_2 = uipanel(app.UIFigure);
            app.Panel_2.ForegroundColor = [1 1 1];
            app.Panel_2.BackgroundColor = [0.9412 0.9412
0.9412];
            app.Panel_2.Position = [28 229 647 323];

            % Create Image
            app.Image = uiimage(app.Panel_2);
            app.Image.Position = [265 27 224 290];
            app.Image.ImageSource = 'cstr.png';

            % Create DMFEditField_2Label
            app.DMFEditField_2Label = uilabel(app.Panel_2);
            app.DMFEditField_2Label.HorizontalAlignment =
'right';
            app.DMFEditField_2Label.Position = [451 29 31 22];
            app.DMFEditField_2Label.Text = 'DMF';

            % Create DMFOutEditField
            app.DMFOutEditField = uieditfield(app.Panel_2,
'numeric');
            app.DMFOutEditField.Position = [542 27 100 22];

            % Create HDIEditField_2Label
            app.HDIEditField_2Label = uilabel(app.Panel_2);
            app.HDIEditField_2Label.HorizontalAlignment =
'right';
            app.HDIEditField_2Label.Position = [451 48 26 22];
            app.HDIEditField_2Label.Text = 'HDI';

            % Create HDIOutEditField
            app.HDIOutEditField = uieditfield(app.Panel_2,
'numeric');
            app.HDIOutEditField.Position = [542 48 100 22];

            % Create PETEditField_2Label
            app.PETEditField_2Label = uilabel(app.Panel_2);
            app.PETEditField_2Label.HorizontalAlignment =
'right';
            app.PETEditField_2Label.Position = [451 69 29 22];
```

```
            app.PETEditField_2Label.Text = 'PET';

            % Create PETOutEditField
            app.PETOutEditField = uieditfield(app.Panel_2,
'numeric');
            app.PETOutEditField.Position = [542 69 100 22];

            % Create PolyolEditField_2Label
            app.PolyolEditField_2Label = uilabel(app.Panel_2);
            app.PolyolEditField_2Label.HorizontalAlignment =
'right';
            app.PolyolEditField_2Label.Position = [451 111 38
22];
            app.PolyolEditField_2Label.Text = 'Polyol';

            % Create PolyolOutEditField
            app.PolyolOutEditField = uieditfield(app.Panel_2,
'numeric');
            app.PolyolOutEditField.Position = [542 111 100
22];

            % Create PolyurethaneEditFieldLabel
            app.PolyurethaneEditFieldLabel =
uilabel(app.Panel_2);
            app.PolyurethaneEditFieldLabel.HorizontalAlignment
= 'right';
            app.PolyurethaneEditFieldLabel.Position = [451 6
76 22];
            app.PolyurethaneEditFieldLabel.Text =
'Polyurethane';

            % Create PolyurethaneEditField
            app.PolyurethaneEditField =
uieditfield(app.Panel_2, 'numeric');
            app.PolyurethaneEditField.Position = [542 6 100
22];

            % Create CaprolactoneEditField_2Label
            app.CaprolactoneEditField_2Label =
uilabel(app.Panel_2);

app.CaprolactoneEditField_2Label.HorizontalAlignment =
'right';
            app.CaprolactoneEditField_2Label.Position = [450
90 77 22];
            app.CaprolactoneEditField_2Label.Text =
'Caprolactone';

            % Create CaprolactoneOutEditField
            app.CaprolactoneOutEditField =
uieditfield(app.Panel_2, 'numeric');
```

```
            app.CaprolactoneOutEditField.Position = [542 90
100 22];

            % Create Flowratestream31EditFieldLabel
            app.Flowratestream31EditFieldLabel =
uilabel(app.Panel_2);

app.Flowratestream31EditFieldLabel.HorizontalAlignment =
'right';
            app.Flowratestream31EditFieldLabel.Position = [419
146 108 22];
            app.Flowratestream31EditFieldLabel.Text =
'Flowrate stream 31';

            % Create Flowratestream31EditField
            app.Flowratestream31EditField =
uieditfield(app.Panel_2, 'numeric');
            app.Flowratestream31EditField.Position = [542 146
100 22];

            % Create HDIEditFieldLabel
            app.HDIEditFieldLabel = uilabel(app.Panel_2);
            app.HDIEditFieldLabel.HorizontalAlignment =
'right';
            app.HDIEditFieldLabel.Position = [485 246 26 22];
            app.HDIEditFieldLabel.Text = 'HDI';

            % Create HDIEditField
            app.HDIEditField = uieditfield(app.Panel_2,
'numeric');
            app.HDIEditField.Position = [526 246 100 22];

            % Create Flowratestream3EditFieldLabel
            app.Flowratestream3EditFieldLabel =
uilabel(app.Panel_2);

app.Flowratestream3EditFieldLabel.HorizontalAlignment =
'right';
            app.Flowratestream3EditFieldLabel.Position = [409
277 102 22];
            app.Flowratestream3EditFieldLabel.Text = 'Flowrate
stream 3';

            % Create Flowratestream3EditField
            app.Flowratestream3EditField =
uieditfield(app.Panel_2, 'numeric');
            app.Flowratestream3EditField.Position = [526 277
100 22];

            % Create DMFEditFieldLabel
            app.DMFEditFieldLabel = uilabel(app.Panel_2);
```

```
            app.DMFEditFieldLabel.HorizontalAlignment =
'right';
            app.DMFEditFieldLabel.Position = [102 225 31 22];
            app.DMFEditFieldLabel.Text = 'DMF';

            % Create DMFEditField
            app.DMFEditField = uieditfield(app.Panel_2,
'numeric');
            app.DMFEditField.Position = [148 225 100 22];

            % Create PETEditFieldLabel
            app.PETEditFieldLabel = uilabel(app.Panel_2);
            app.PETEditFieldLabel.HorizontalAlignment =
'right';
            app.PETEditFieldLabel.Position = [37 48 29 22];
            app.PETEditFieldLabel.Text = 'PET';

            % Create PETEditField
            app.PETEditField = uieditfield(app.Panel_2,
'numeric');
            app.PETEditField.Position = [129 48 100 22];

            % Create PolyolEditFieldLabel
            app.PolyolEditFieldLabel = uilabel(app.Panel_2);
            app.PolyolEditFieldLabel.HorizontalAlignment =
'right';
            app.PolyolEditFieldLabel.Position = [37 90 38 22];
            app.PolyolEditFieldLabel.Text = 'Polyol';

            % Create PolyolEditField
            app.PolyolEditField = uieditfield(app.Panel_2,
'numeric');
            app.PolyolEditField.Position = [129 90 100 22];

            % Create CaprolactoneEditFieldLabel
            app.CaprolactoneEditFieldLabel =
uilabel(app.Panel_2);
            app.CaprolactoneEditFieldLabel.HorizontalAlignment
= 'right';
            app.CaprolactoneEditFieldLabel.Position = [37 69
77 22];
            app.CaprolactoneEditFieldLabel.Text =
'Caprolactone';

            % Create CaprolactoneEditField
            app.CaprolactoneEditField =
uieditfield(app.Panel_2, 'numeric');
            app.CaprolactoneEditField.Position = [129 69 100
22];

            % Create Flowratestream4EditFieldLabel
```

```
            app.Flowratestream4EditFieldLabel =
uilabel(app.Panel_2);

app.Flowratestream4EditFieldLabel.HorizontalAlignment =
'right';
            app.Flowratestream4EditFieldLabel.Position = [31
256 102 22];
            app.Flowratestream4EditFieldLabel.Text = 'Flowrate
stream 4';

            % Create Flowratestream4EditField
            app.Flowratestream4EditField =
uieditfield(app.Panel_2, 'numeric');
            app.Flowratestream4EditField.Position = [148 256
100 22];

            % Create Flowratestream30EditFieldLabel
            app.Flowratestream30EditFieldLabel =
uilabel(app.Panel_2);

app.Flowratestream30EditFieldLabel.HorizontalAlignment =
'right';
            app.Flowratestream30EditFieldLabel.Position = [6
125 108 22];
            app.Flowratestream30EditFieldLabel.Text =
'Flowrate stream 30';

            % Create Flowratestream30EditField
            app.Flowratestream30EditField =
uieditfield(app.Panel_2, 'numeric');
            app.Flowratestream30EditField.Position = [129 125
100 22];

            % Show the figure after all components are created
            app.UIFigure.Visible = 'on';
        end
    end

    % App creation and deletion
    methods (Access = public)

        % Construct app
        function app = IP3rdyear_massBalance

            % Create UIFigure and components
            createComponents(app)

            % Register the app with App Designer
            registerApp(app, app.UIFigure)

            if nargout == 0
```

```
                clear app
            end
        end

        % Code that executes before app deletion
        function delete(app)

            % Delete UIFigure when app is deleted
            delete(app.UIFigure)
        end
    end
end
```

PART II: MASS BALANCE CODING

```
classdef IP3rdyear_energyBalance_ < matlab.apps.AppBase

    % Properties that correspond to app components
    properties (Access = public)
        UIFigure                        matlab.ui.Figure
        UITable
matlab.ui.control.Table
        Panel
matlab.ui.container.Panel
        EnthalpyInletStreamEditFieldLabel
matlab.ui.control.Label
        EnthalpyInletStreamEditField
matlab.ui.control.NumericEditField
        Image
matlab.ui.control.Image
        EnthalpyOutletStreamEditFieldLabel
matlab.ui.control.Label
        EnthalpyOutletStreamEditField
matlab.ui.control.NumericEditField
        Panel_2
matlab.ui.container.Panel
        EnterButton
matlab.ui.control.Button
        InletStream30EditField_2Label
matlab.ui.control.Label
        TempInletStream30
matlab.ui.control.NumericEditField
        OutletStream31EditField_2Label
matlab.ui.control.Label
        TempOutletStream31
matlab.ui.control.NumericEditField
        EntertherequiredtemperatureindegreeCelsiusLabel
matlab.ui.control.Label
        EditField
matlab.ui.control.EditField
```

```
        OverallHeatQEditFieldLabel
matlab.ui.control.Label
        OverallHeatQEditField
matlab.ui.control.NumericEditField
        EnergyBalanceinCSTRR103inkJhrLabel
matlab.ui.control.Label
        kJhrLabel
matlab.ui.control.Label
    end



    % Callbacks that handle component events
    methods (Access = private)

        % Button pushed function: EnterButton
        function EnterButtonPushed(app, event)
            %Heat of Reaction for Each Components
            HRxnPO=-210.52;
            HRxnHDI=-219.27;
            HRxnPU=77;


            r=68.85;
            %Heat_of reaction = Hrxn_Product-Hrxn_Reactant
            HeatReaction=HRxnPU-(HRxnPO+HRxnHDI);

            %Heat Change Calculation,Temperature
Reference,T=298.15K
            T3=298.15;
            T30=app.TempInletStream30.Value +273.15;
            T31=app.TempOutletStream31.Value +273.15;
            %CpHDI=299.2, CpDMF=148.46, CpPolyol=907.2
            %CpPolyurethane=637


            %Heat Change inlet Stream
            HRInlet30PO=907.2*(T30-298.15)*8.0535;
            HRInlet30HDI=0;
            HRInlet30PU=0;
            HRInlet3PO=0;
            HRInlet3HDI=299.2*(T3-298.15)*8.0535;
            HRInlet3PU=0;

            %Heat Change Outlet Stream
            HROutlet31HDI=299.2*(T31-298.15)*0.8054;
            HROutlet31PO=907.2*(T31-298.15)*0.8054;
            HROutlet31PU=637*(T31-298.15)*7.2482;

            %Heat,Q of each components
```

```
            Qin=HRInlet3HDI+HRInlet30PO;
            Qout=HROutlet31PU+HROutlet31PO+HROutlet31HDI;
            Heat_Balance= Qout - Qin + r*HeatReaction;
            app.OverallHeatQEditField.Value=Heat_Balance;
            if (Heat_Balance<0)
                app.EditField.Value='The overall heat balance
Q is negative.Thus the reaction is exothermic';
            else
                app.EditField.Value='The overall heat balance
Q is positive.Thus the reaction is endothermic';
            end

            %Display Heat Change
            app.EnthalpyInletStreamEditField.Value=HRInlet30PO
+ HRInlet3HDI;


app.EnthalpyOutletStreamEditField.Value=HROutlet31PU+HROutlet3
1PO+HROutlet31HDI;

            %Tabulate the data
            flowrate_in_01 =
[HRInlet30PO;HRInlet30HDI;HRInlet30PU;];
            flowrate_in_02 =
[HRInlet3PO;HRInlet3HDI;HRInlet3PU;];
            flowrate_out =
[HROutlet31PO;HROutlet31HDI;HROutlet31PU;];
            Heat_Reaction =[HRxnPO;HRxnHDI;HRxnPU;];
            Component = {'Polyol';'HDI';'Polyurethane';};
            table1 =
table(Component,flowrate_in_01,flowrate_in_02,flowrate_out,Hea
t_Reaction);
                app.UITable.Data= table1;

        end
    end

    % Component initialization
    methods (Access = private)

        % Create UIFigure and components
        function createComponents(app)

            % Create UIFigure and hide until all components
are created
            app.UIFigure = uifigure('Visible', 'off');
            app.UIFigure.Color = [0.902 0.902 0.902];
            app.UIFigure.Position = [100 100 1014 663];
            app.UIFigure.Name = 'MATLAB App';
```

```
            % Create UITable
            app.UITable = uitable(app.UIFigure);
            app.UITable.ColumnName = {'Component'; 'Enthalpy
Inlet 30(kJ/hr)'; 'Enthalpy Inlet 3(kJ/hr)'; 'Enthalpy Outlet
31(kJ/hr)'; 'Heat of Reaction(kJ/mol)'};
            app.UITable.RowName = {};
            app.UITable.Position = [40 94 907 98];

            % Create Panel
            app.Panel = uipanel(app.UIFigure);
            app.Panel.BackgroundColor = [0.9412 0.9412
0.9412];
            app.Panel.Position = [73 300 666 286];

            % Create EnthalpyInletStreamEditFieldLabel
            app.EnthalpyInletStreamEditFieldLabel =
uilabel(app.Panel);

app.EnthalpyInletStreamEditFieldLabel.HorizontalAlignment =
'right';
            app.EnthalpyInletStreamEditFieldLabel.Position =
[17 111 120 22];
            app.EnthalpyInletStreamEditFieldLabel.Text =
'Enthalpy Inlet Stream';

            % Create EnthalpyInletStreamEditField
            app.EnthalpyInletStreamEditField =
uieditfield(app.Panel, 'numeric');
            app.EnthalpyInletStreamEditField.Position = [152
111 100.30572597137 22];

            % Create Image
            app.Image = uiimage(app.Panel);
            app.Image.Position = [251 27 207 259];
            app.Image.ImageSource = 'cstr.png';

            % Create EnthalpyOutletStreamEditFieldLabel
            app.EnthalpyOutletStreamEditFieldLabel =
uilabel(app.Panel);

app.EnthalpyOutletStreamEditFieldLabel.HorizontalAlignment =
'right';
            app.EnthalpyOutletStreamEditFieldLabel.Position =
[406 110 130 22];
            app.EnthalpyOutletStreamEditFieldLabel.Text =
'Enthalpy Outlet Stream';

            % Create EnthalpyOutletStreamEditField
            app.EnthalpyOutletStreamEditField =
uieditfield(app.Panel, 'numeric');
```

```
            app.EnthalpyOutletStreamEditField.Position = [551
110 100 22];

            % Create Panel_2
            app.Panel_2 = uipanel(app.UIFigure);
            app.Panel_2.BackgroundColor = [0.9412 0.9412
0.9412];
            app.Panel_2.Position = [773 358 221 228];

            % Create EnterButton
            app.EnterButton = uibutton(app.Panel_2, 'push');
            app.EnterButton.ButtonPushedFcn =
createCallbackFcn(app, @EnterButtonPushed, true);
            app.EnterButton.Position = [16 114 73 22];
            app.EnterButton.Text = 'Enter';

            % Create InletStream30EditField_2Label
            app.InletStream30EditField_2Label =
uilabel(app.Panel_2);

app.InletStream30EditField_2Label.HorizontalAlignment =
'right';
            app.InletStream30EditField_2Label.Position = [10
73 87 22];
            app.InletStream30EditField_2Label.Text = 'Inlet
Stream 30';

            % Create TempInletStream30
            app.TempInletStream30 = uieditfield(app.Panel_2,
'numeric');
            app.TempInletStream30.Position = [120 73 100 22];

            % Create OutletStream31EditField_2Label
            app.OutletStream31EditField_2Label =
uilabel(app.Panel_2);

app.OutletStream31EditField_2Label.HorizontalAlignment =
'right';
            app.OutletStream31EditField_2Label.Position = [10
52 96 22];
            app.OutletStream31EditField_2Label.Text = 'Outlet
Stream 31';

            % Create TempOutletStream31
            app.TempOutletStream31 = uieditfield(app.Panel_2,
'numeric');
            app.TempOutletStream31.Position = [120 52 100 22];

            % Create
EntertherequiredtemperatureindegreeCelsiusLabel
```

```
app.EntertherequiredtemperatureindegreeCelsiusLabel =
uilabel(app.Panel_2);

app.EntertherequiredtemperatureindegreeCelsiusLabel.FontColor
= [0.149 0.149 0.149];

app.EntertherequiredtemperatureindegreeCelsiusLabel.Position =
[16 170 190 36];

app.EntertherequiredtemperatureindegreeCelsiusLabel.Text =
{'Enter the required temperature in '; 'degree Celsius'};

            % Create EditField
            app.EditField = uieditfield(app.UIFigure, 'text');
            app.EditField.Position = [63 247 777 37];

            % Create OverallHeatQEditFieldLabel
            app.OverallHeatQEditFieldLabel =
uilabel(app.UIFigure);
            app.OverallHeatQEditFieldLabel.HorizontalAlignment
= 'right';
            app.OverallHeatQEditFieldLabel.Position = [63 211
88 22];
            app.OverallHeatQEditFieldLabel.Text = 'Overall
Heat, Q';

            % Create OverallHeatQEditField
            app.OverallHeatQEditField =
uieditfield(app.UIFigure, 'numeric');
            app.OverallHeatQEditField.Position = [166 211 100
22];

            % Create EnergyBalanceinCSTRR103inkJhrLabel
            app.EnergyBalanceinCSTRR103inkJhrLabel =
uilabel(app.UIFigure);
            app.EnergyBalanceinCSTRR103inkJhrLabel.FontSize =
18;
            app.EnergyBalanceinCSTRR103inkJhrLabel.Position =
[324 593 340 48];
            app.EnergyBalanceinCSTRR103inkJhrLabel.Text =
'Energy Balance in CSTR R-103 in (kJ/hr)';

            % Create kJhrLabel
            app.kJhrLabel = uilabel(app.UIFigure);
            app.kJhrLabel.Position = [275 211 31 22];
            app.kJhrLabel.Text = 'kJ/hr';

            % Show the figure after all components are created
            app.UIFigure.Visible = 'on';
        end
```

```
    end

    % App creation and deletion
    methods (Access = public)

        % Construct app
        function app = IP3rdyear_energyBalance_

            % Create UIFigure and components
            createComponents(app)

            % Register the app with App Designer
            registerApp(app, app.UIFigure)

            if nargout == 0
                clear app
            end
        end

        % Code that executes before app deletion
        function delete(app)

            % Delete UIFigure when app is deleted
            delete(app.UIFigure)
        end
    end
end
```

Numerical Method coding -Trapezoidal Rule

```
%% Newton cotes trapezoidal single
%This program is to determine the enthalpy out for
Polyurethane
close all
clear all
clc
f = @(x) 637;
a = 298.15;
b = 383.15;
I = (b-a)* ((f(a)+f(b))/2)
%Integrate using formula, I
syms x
f1= diff(f,x);
f2= diff(f1,x); %Find 2nd derivative
ff = int(f2,x,a,b);
%Integrate the 2nd derivative within limit a and b
favg = ff/(b-a);
m = double(favg);
```

```
assume(x,'clear')
Ea = (-1/12)*(m*(b-a).^3)
```

APPENDIX C

CHEMICAL REACTION ENGINEERING II

Volumetric flowrate, v_o

$v_o = \frac{mass\ flowrate\ A}{density\ of\ A} = \frac{3685.685\ kg/h}{2100\ \text{kg/m3}}$

$v_o = 1.755\ m^3/h$

$v_o = 4.875 \times 10^{-4}\ m^3/s$

Molar flowrate from mass balance, N_A

$N_A = \frac{Mass\ flowrate\ of\ A}{Molar\ mass\ of\ A}$

$= \frac{3865.685}{0.480}$

$N_A = 8053.51$ mol/h

Concentration Calculation,

$C_A = \frac{molar\ flowrate}{volumetric\ flowrate}$

$C_A = \frac{8053.51\ mol/h}{1.755\ \text{m3/h}}$

$C_A = 4588.9$ mol/m^3

Concentration of A, Conversion of polyol is 90%,

$C_A = C_{A0}(1 - X)$

$2.292 = C_{A0}(1\text{-}0.9)$

$C_{A0} = 45888.9$ mol/m^3

Calculation of k constant value,

$k = ln\frac{C_{AO}}{C_A}$

$k = \left(ln\frac{45888.9}{4588.9}\right) x \left(\frac{1}{3600}\right)$

$k = 6.396 \times 10^{-4}\ s^{-1}$

The volume of the reactor,

$V = \frac{v_o X}{k(1-X)}$

$V = \frac{4.875x10^{-4}(0.9)}{6.396x10^{-4}(1-0.9)}$

$V = 6.86\ m^3$

$V = 6860\ L$

Polymath:

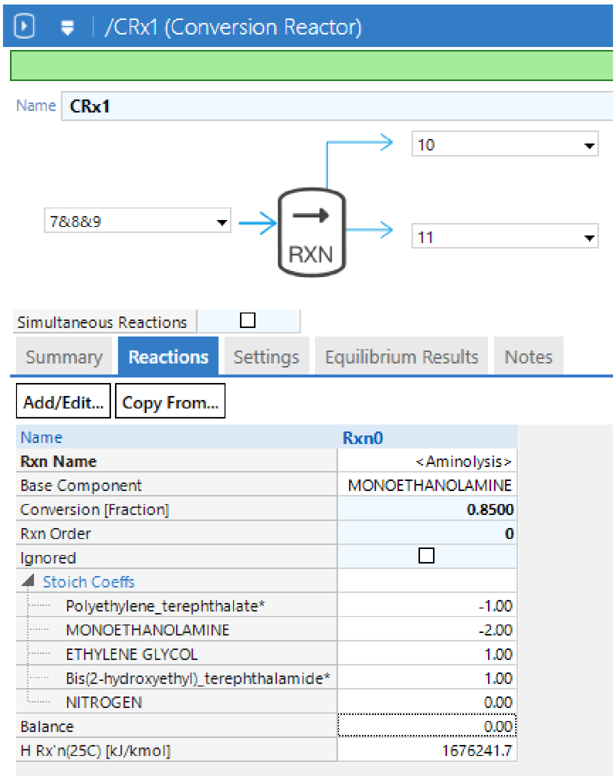
```
d(Na)/d(t)=Cao*vo-Ca*vo+rA*V
d(Nb)/d(t)=Cbo*vo-Cb*vo+rA*V
d(Nc)/d(t)=-Cc*vo+rA*V
Na(0)=805.4
Nb(0)=805.4
Nc(0)=7248.2
t(0)=0
t(f)=30

Ca=Cao*(1-X)
Cb=Cao*(1-X)
Cbo=Cb
Cc=Cao*(0.315+X)
vo=0.0004875
rA=k*Ca*Cb
Cao=45888.9
k=0.0006396
X=(Fao-Fa)/Fao
Fao=3685.685
Fa=386.57
V=(vo*X)/k*(1-X)
```

APPENDIX D

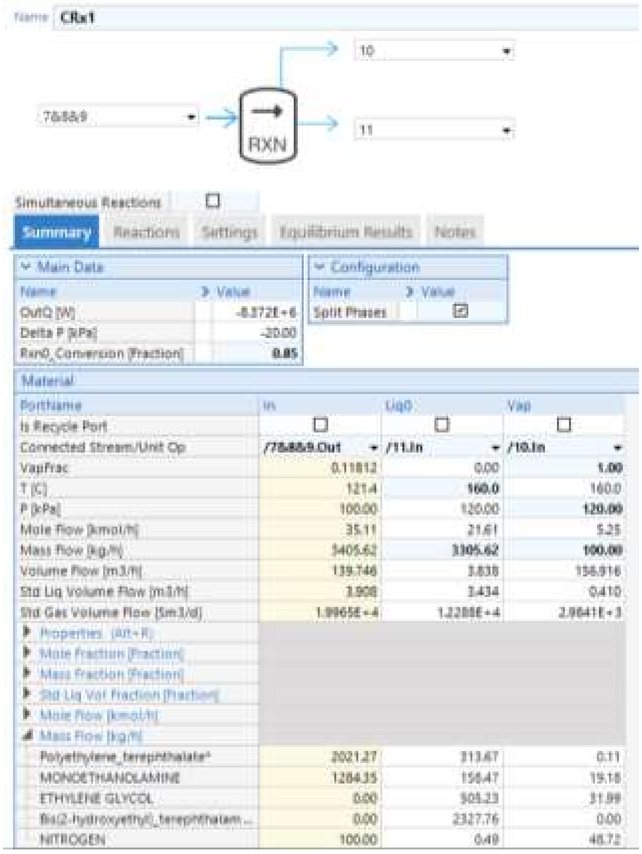
COMPUTER AIDED PLANT DESIGN

<u>AMINOLYSIS, (R-101) AT SYMMETRY SIMULATION</u>

Insert the all data inside the conversion reactor such ass stochiomtery coefficient, base component and make sure it is balance.



Mass balance for reactor (R-101) in the Symmetry simulation.



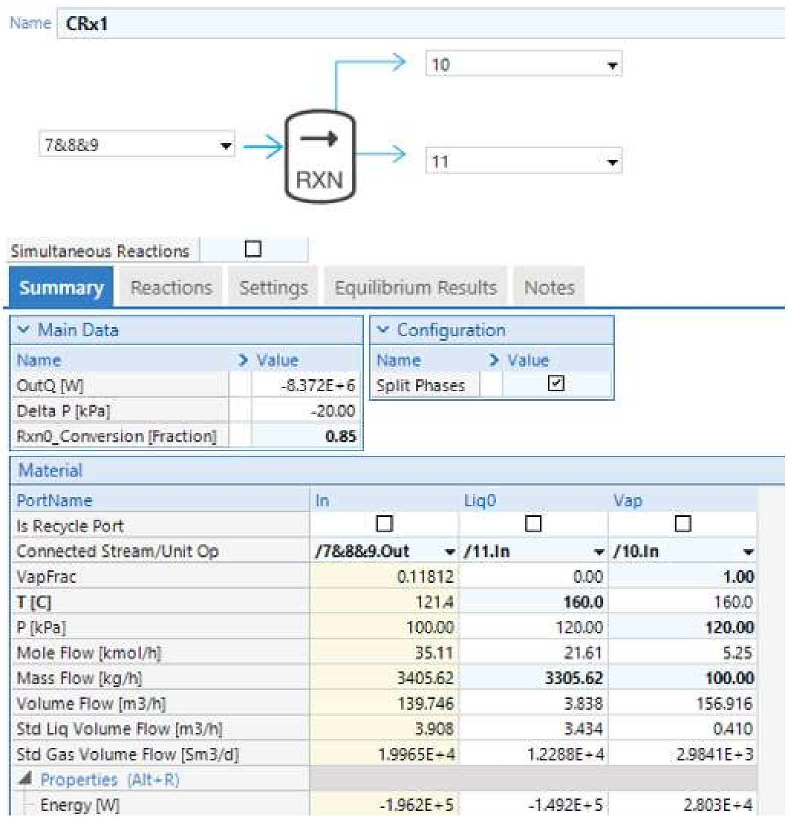
Name	Value
OutQ [W]	-8.372E+6
Delta P [kPa]	-20.00
Rxn0_Conversion [Fraction]	0.85

Name	Value
Split Phases	☑

Material

PortName	In	Liq0	Vap
Is Recycle Port	☐	☐	☐
Connected Stream/Unit Op	/7&8&9.Out	/11.In	/10.In
VapFrac	0.11812	0.00	1.00
T [C]	121.4	160.0	160.0
P [kPa]	100.00	120.00	120.00
Mole Flow [kmol/h]	35.11	21.61	5.25
Mass Flow [kg/h]	3405.62	3305.62	100.00
Volume Flow [m3/h]	139.746	3.838	156.916
Std Liq Volume Flow [m3/h]	3.908	3.434	0.410
Std Gas Volume Flow [Sm3/d]	1.9965E+4	1.2288E+4	2.9841E+3
Properties (Alt+R)			
Mole Fraction [Fraction]			
Mass Fraction [Fraction]			
Std Liq Vol Fraction [Fraction]			
Mole Flow [kmol/h]			
Mass Flow [kg/h]			
Polyethylene_terephthalate*	2021.27	313.67	0.11
MONOETHANOLAMINE	1284.35	158.47	19.18
ETHYLENE GLYCOL	0.00	505.23	31.99
Bis(2-hydroxyethyl)_terephthalam...	0.00	2327.76	0.00
NITROGEN	100.00	0.49	48.72

Mass balance for reactor (R-101) in the Symmetry simulation.



Name	Value
OutQ [W]	-8.372E+6
Delta P [kPa]	-20.00
Rxn0_Conversion [Fraction]	0.85

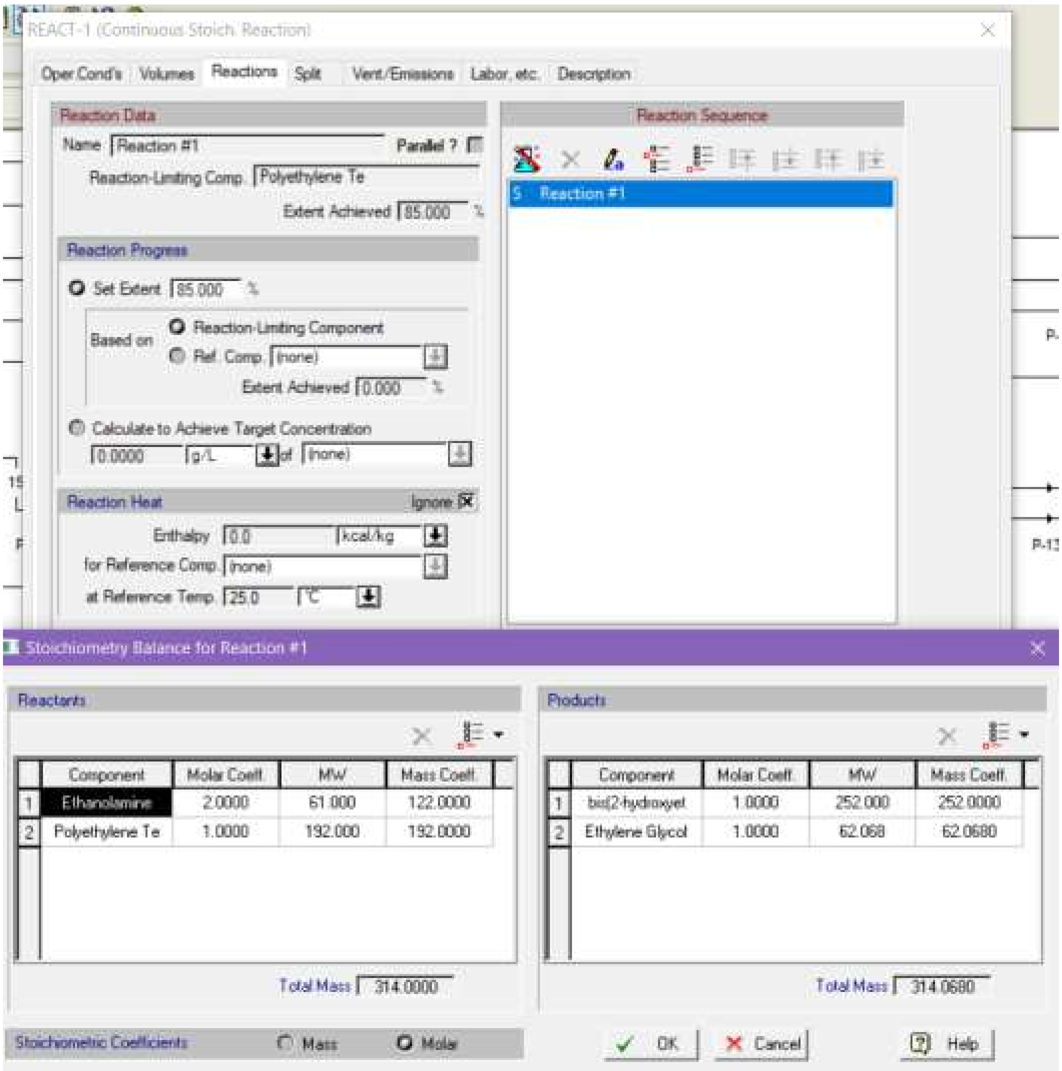
Name	Value
Split Phases	☑

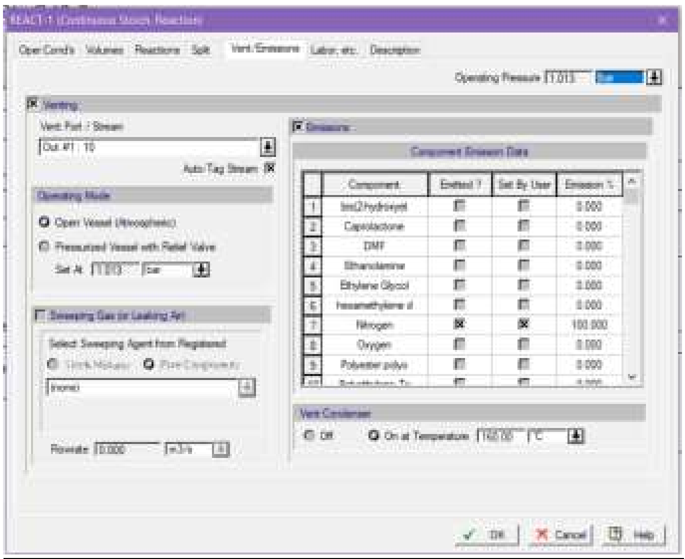
Material

PortName	In	Liq0	Vap
Is Recycle Port	☐	☐	☐
Connected Stream/Unit Op	/7&8&9.Out	/11.In	/10.In
VapFrac	0.11812	0.00	1.00
T [C]	121.4	160.0	160.0
P [kPa]	100.00	120.00	120.00
Mole Flow [kmol/h]	35.11	21.61	5.25
Mass Flow [kg/h]	3405.62	3305.62	100.00
Volume Flow [m3/h]	139.746	3.838	156.916
Std Liq Volume Flow [m3/h]	3.908	3.434	0.410
Std Gas Volume Flow [Sm3/d]	1.9965E+4	1.2288E+4	2.9841E+3
Properties (Alt+R)			
Energy [W]	-1.962E+5	-1.492E+5	2.803E+4

AMINOLYSIS, (R-101) AT SUPERPRO SIMULATION

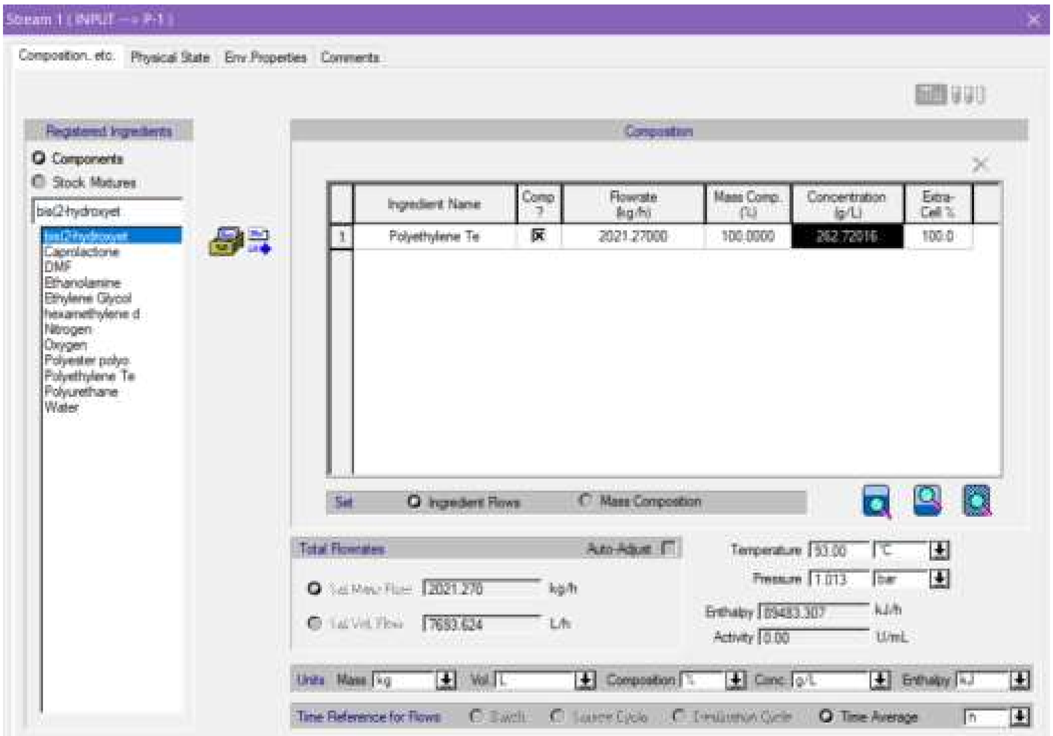
Insert the all data inside the conversion reactor such ass stochiomtery coefficient, base component and make sure it is balance.



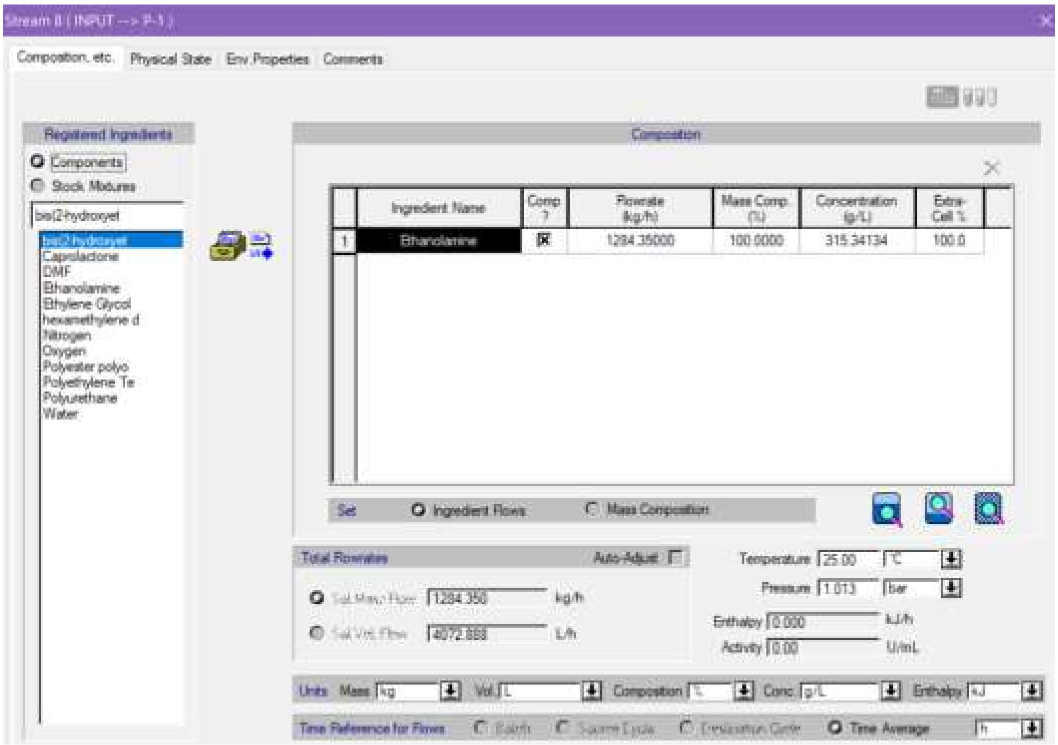


Input mass balance and energy balance on Reactor (R-101)

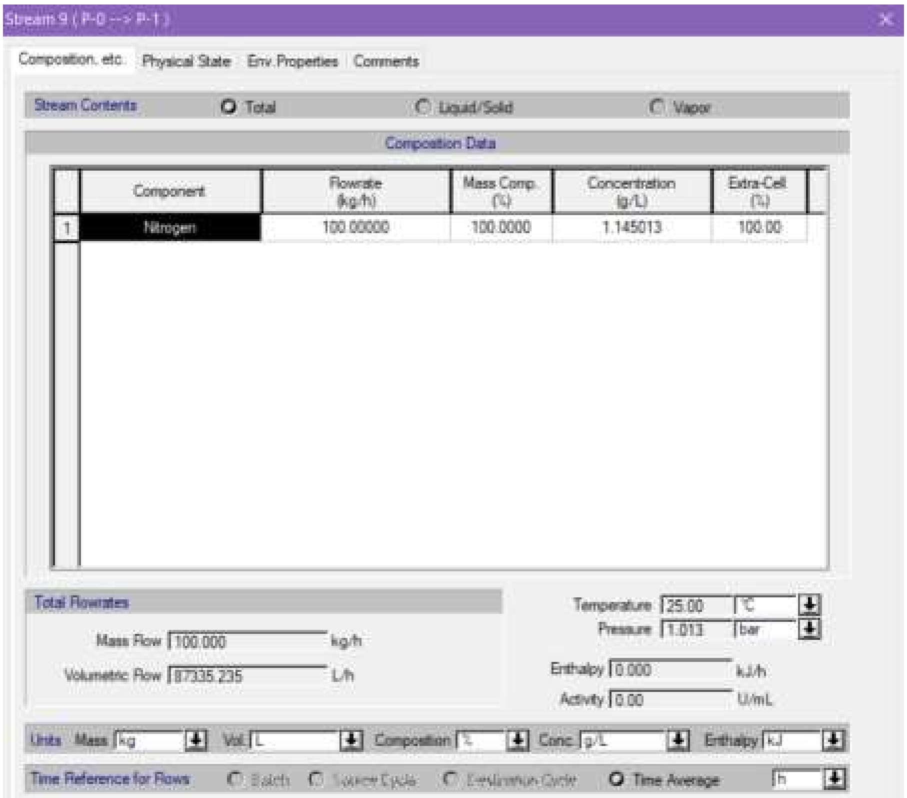
Stream 1



Stream 8

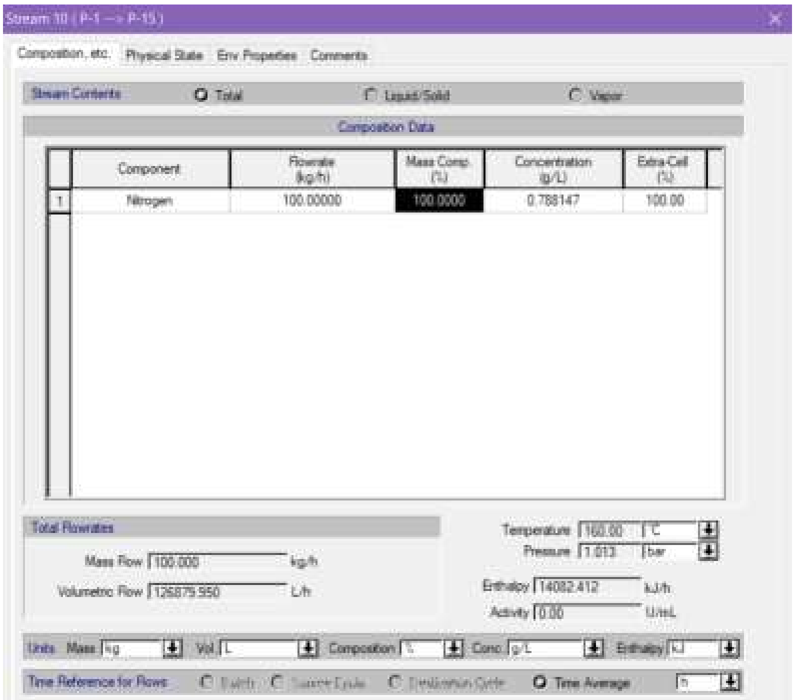


Stream 9

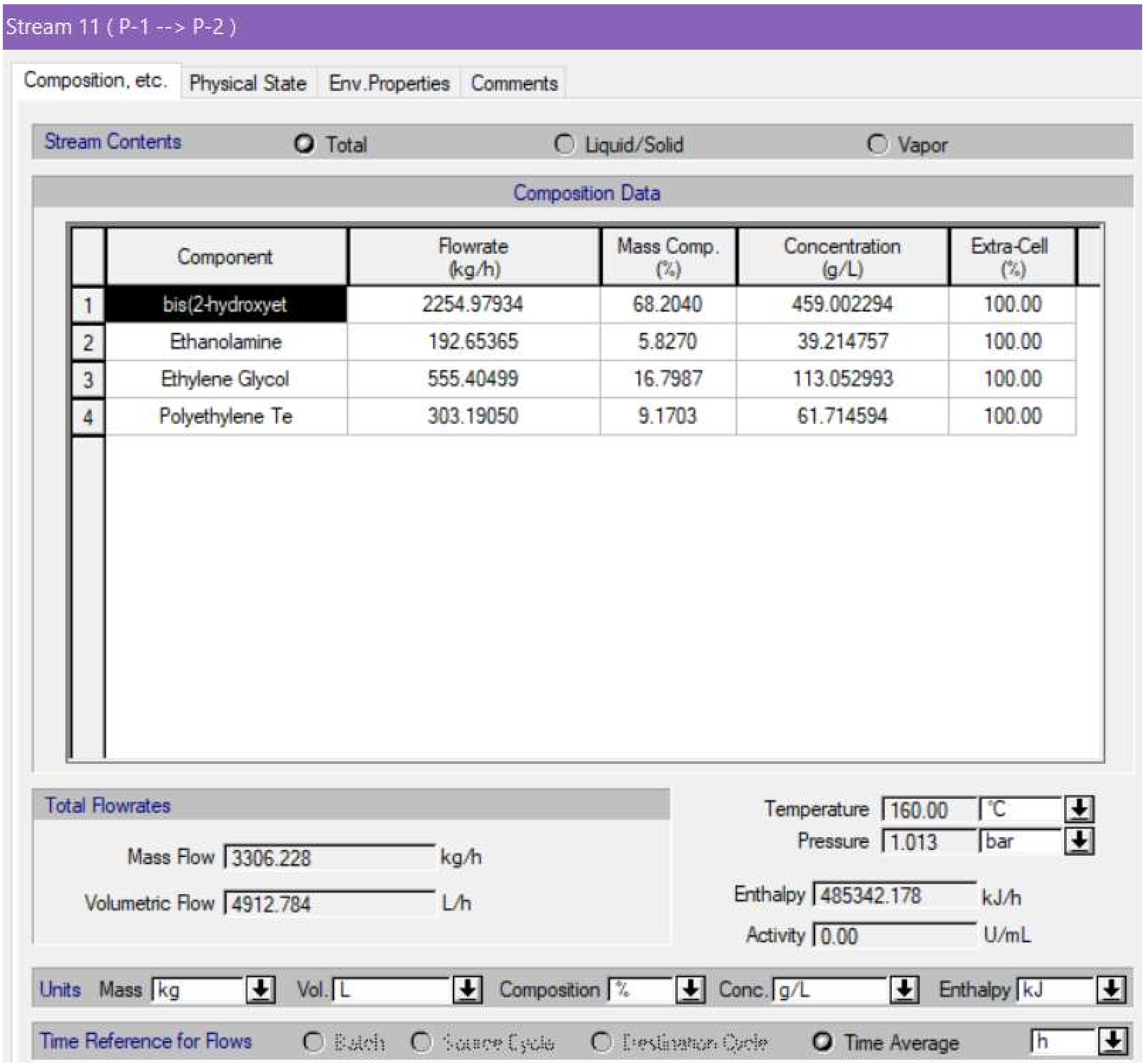


Output mass balance and energy balance on Reactor (R-101)

Stream 10



Stream 11



Stream 11 (P-1 --> P-2)

Composition, etc. | Physical State | Env.Properties | Comments

Stream Contents: Total / Liquid/Solid / Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	2254.97934	68.2040	459.002294	100.00
2	Ethanolamine	192.65365	5.8270	39.214757	100.00
3	Ethylene Glycol	555.40499	16.7987	113.052993	100.00
4	Polyethylene Te	303.19050	9.1703	61.714594	100.00

Total Flowrates

Mass Flow 3306.228 kg/h

Volumetric Flow 4912.784 L/h

Temperature 160.00 °C

Pressure 1.013 bar

Enthalpy 485342.178 kJ/h

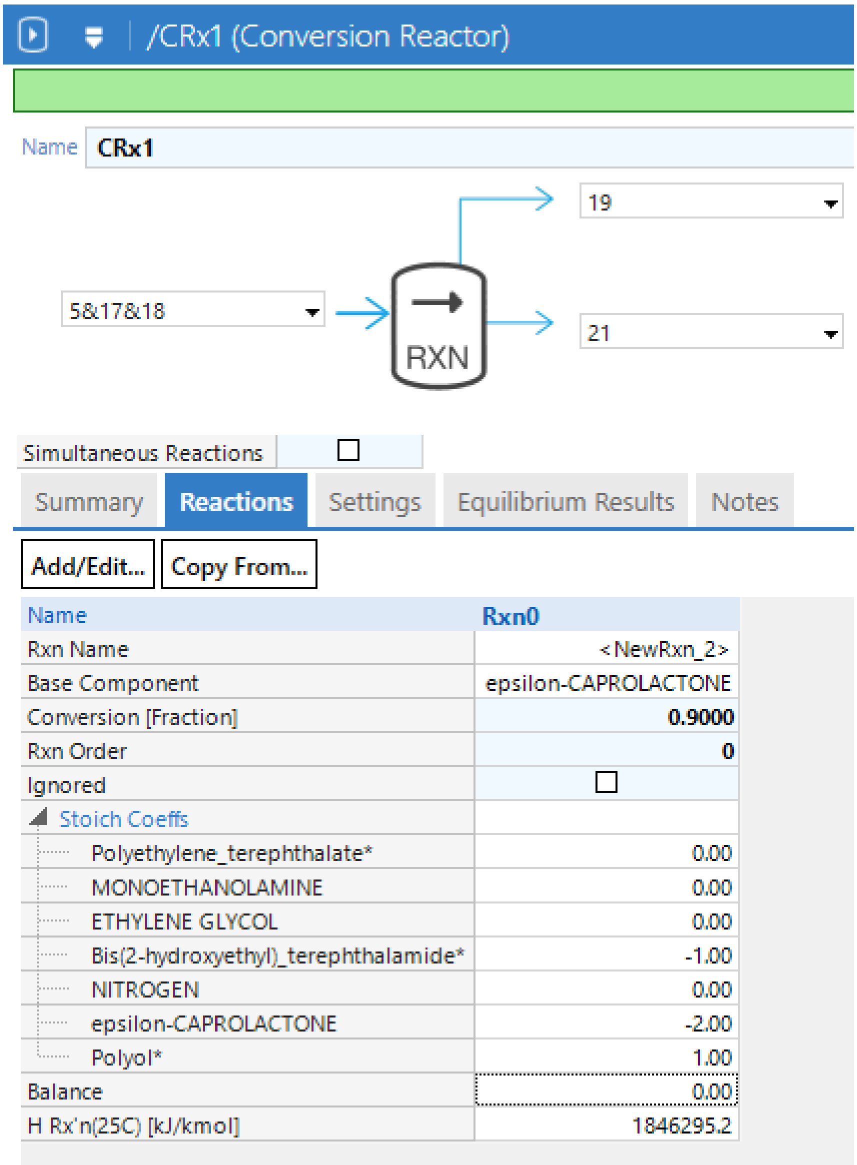
Activity 0.00 U/mL

Units Mass kg Vol. L Composition % Conc. g/L Enthalpy kJ

Time Reference for Flows: Batch / Source Cycle / Destination Cycle / Time Average h

POLYMERIZATION, (R-102) AT SYMMETRY SIMULATION

Insert the all data inside the conversion reactor such ass stochiomtery coefficient, base component and make sure it is balance.



Mass balance for reactor (R-102) in the Symmetry simulation.

Simultaneous Reactions ☐

Summary | Reactions | Settings | Equilibrium Results | Notes

Main Data	
Name	Value
OutQ [W]	-8.970E+6
Delta P [kPa]	80.00
Rxn0_Conversion [Fraction]	**0.90**

Configuration	
Name	Value
Split Phases	☑

Material			
PortName	In	Liq0	Vap
Is Recycle Port	☐	☐	☐
Connected Stream/Unit Op	**/5&17&18.Out**	**/21.In**	**/19.In**
VapFrac	0.11583	**0.00**	**1.00**
T [C]	51.7	**130.0**	130.0
P [kPa]	200.00	**120.00**	120.00
Mole Flow [kmol/h]	30.46	10.79	3.62
Mass Flow [kg/h]	4402.35	**4302.57**	**100.00**
Volume Flow [m3/h]	52.021	5.197	101.096
Std Liq Volume Flow [m3/h]	4.606	5.017	0.323
Std Gas Volume Flow [Sm3/d]	1.7321E+4	6.1356E+3	2.0577E+3
Properties (Alt+R)			
Mole Fraction [Fraction]			
Mass Fraction [Fraction]			
Std Liq Vol Fraction [Fracti...			
Mole Flow [kmol/h]			
Mass Flow [kg/h]			
Polyethylene_terephthalate*	3.17	3.17	0.00
MONOETHANOLAMINE	2.04	1.64	0.36
ETHYLENE GLYCOL	2.04	1.44	0.55
Bis(2-hydroxyethyl)_tereph...	2255.11	225.60	0.00
NITROGEN	100.00	0.45	90.97
epsilon-CAPROLACTONE	2040.00	199.89	4.17
Polyol*	0.00	3870.39	3.95

Mass balance for reactor (R-101) in the Symmetry simulation.

Name **CRx1**

Simultaneous Reactions ☐

Summary | Reactions | Settings | Equilibrium Results | Notes

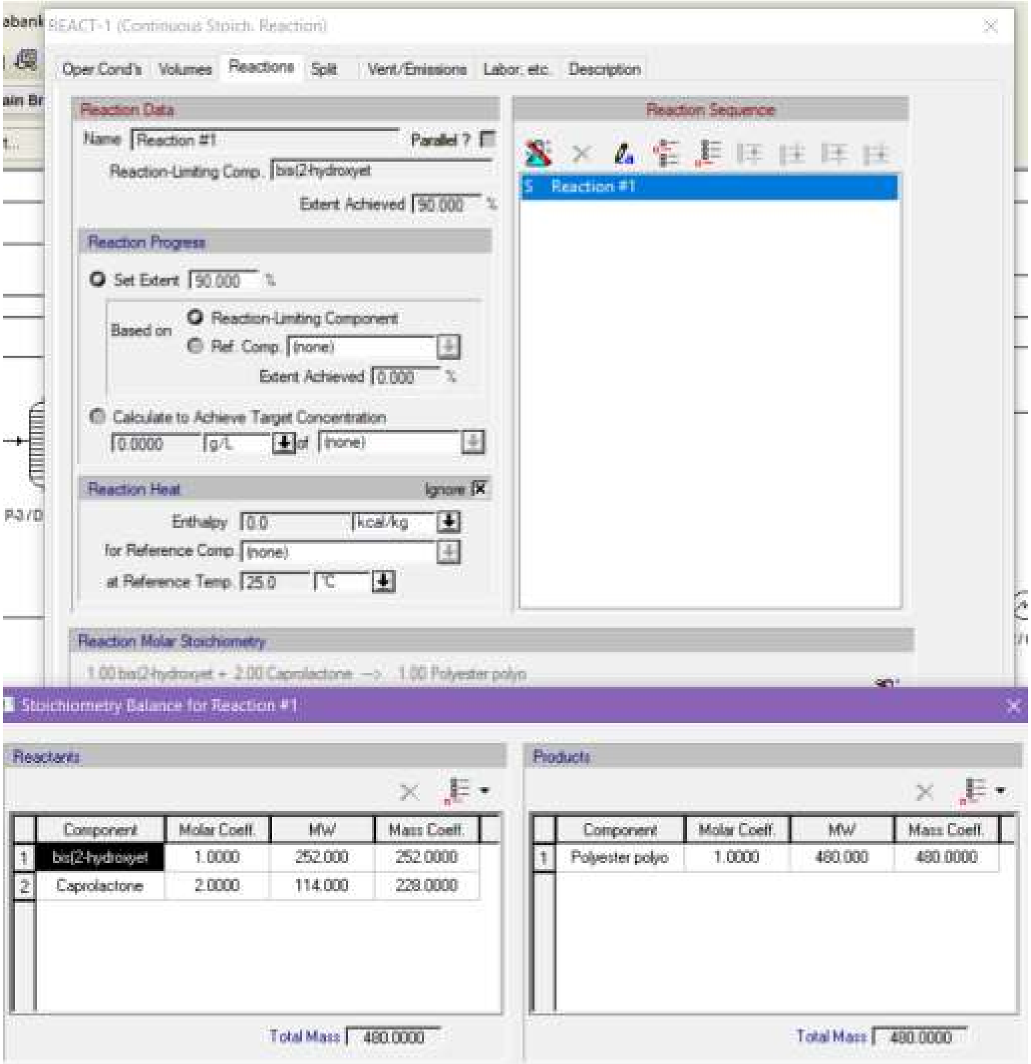
Main Data	
Name	Value
OutQ [W]	-8.970E+6
Delta P [kPa]	80.00
Rxn0_Conversion [Fraction]	**0.90**

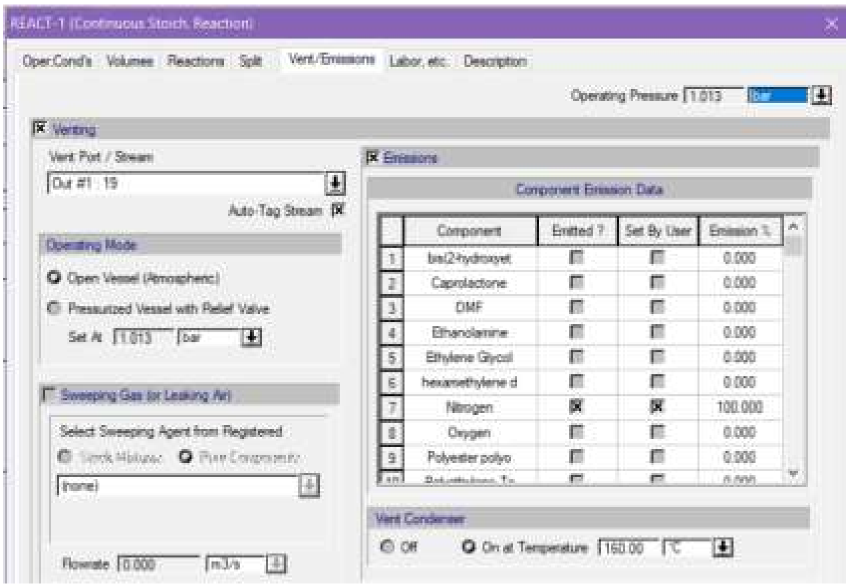
Configuration	
Name	Value
Split Phases	☑

Material			
PortName	**In**	Liq0	Vap
Is Recycle Port	☐	☐	☐
Connected Stream/Unit Op	**/5&17&18.Out**	**/21.In**	**/19.In**
VapFrac	0.11583	**0.00**	**1.00**
T [C]	51.7	**130.0**	130.0
P [kPa]	200.00	**120.00**	120.00
Mole Flow [kmol/h]	30.46	10.79	3.62
Mass Flow [kg/h]	4402.35	**4302.57**	**100.00**
Volume Flow [m3/h]	52.021	5.197	101.096
Std Liq Volume Flow [m3/h]	4.606	5.017	0.323
Std Gas Volume Flow [Sm3/d]	1.7321E+4	6.1356E+3	2.0577E+3
Properties (Alt+R)			
Energy [W]	-4.979E+5	2.766E+5	1.252E+4

POLYMERIZATION, (R-102) AT SUPERPRO SIMULATION

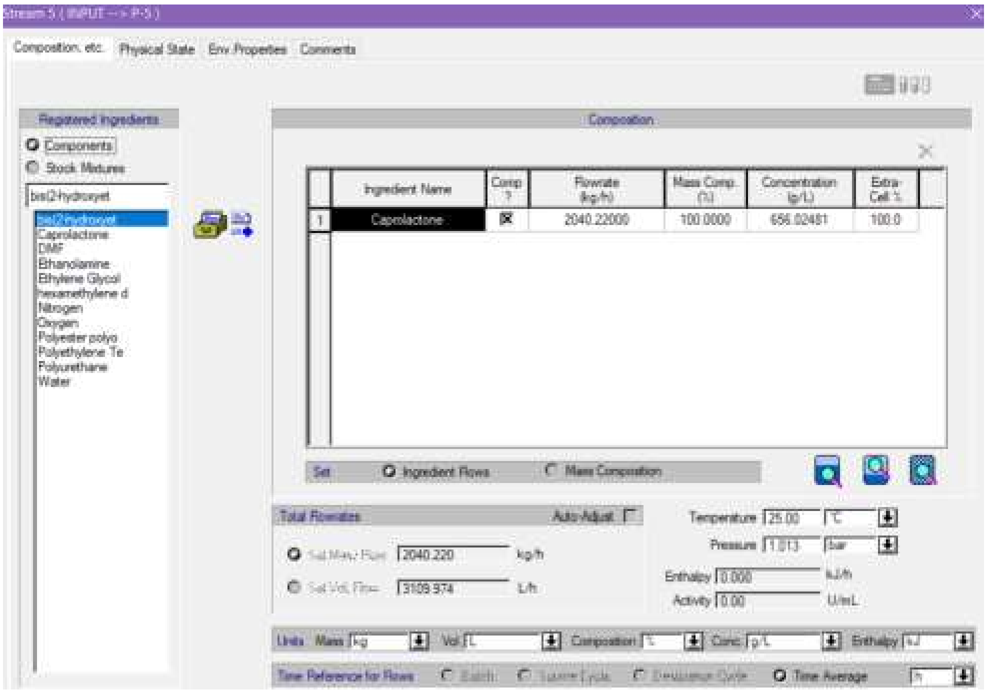
Insert the all data inside the conversion reactor such ass stochiomtery coefficient, base component and make sure it is balance.



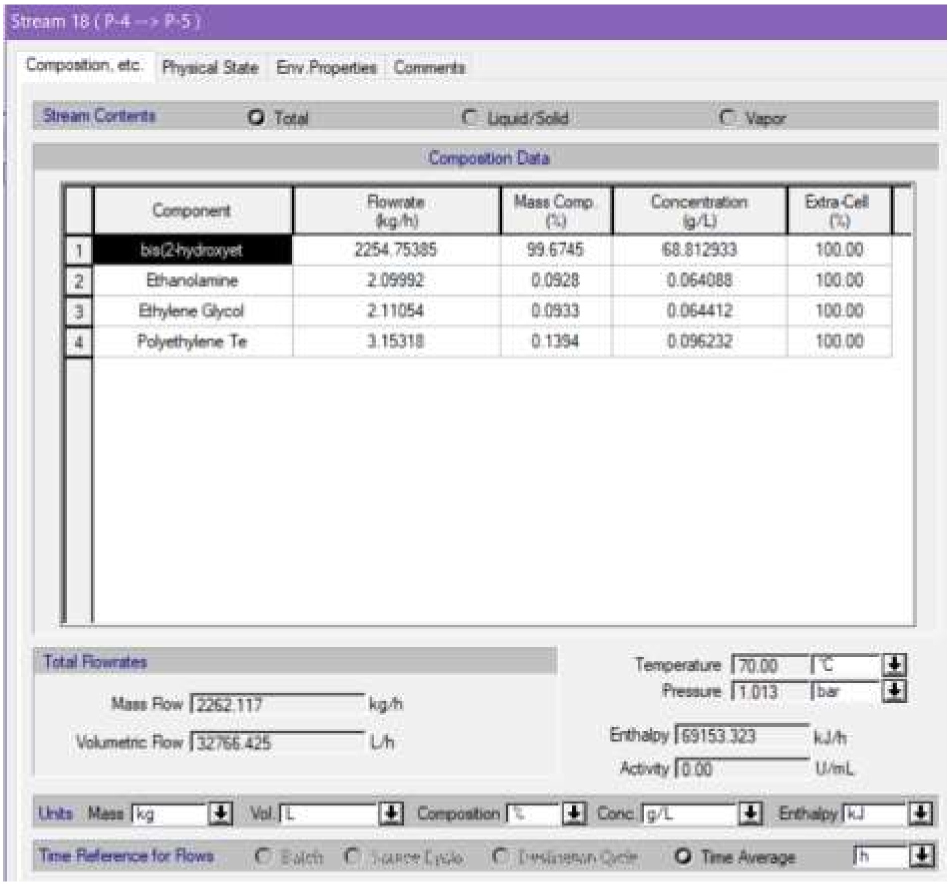


Input mass balance and energy balance on Reactor (R-102)

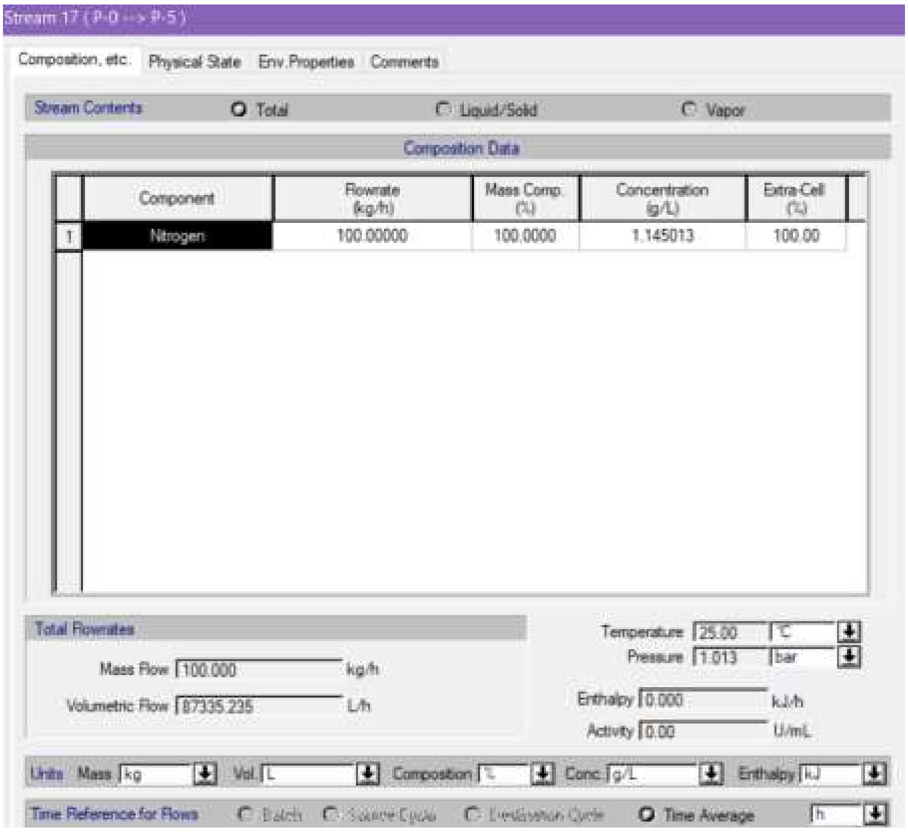
Stream 5



Stream 18

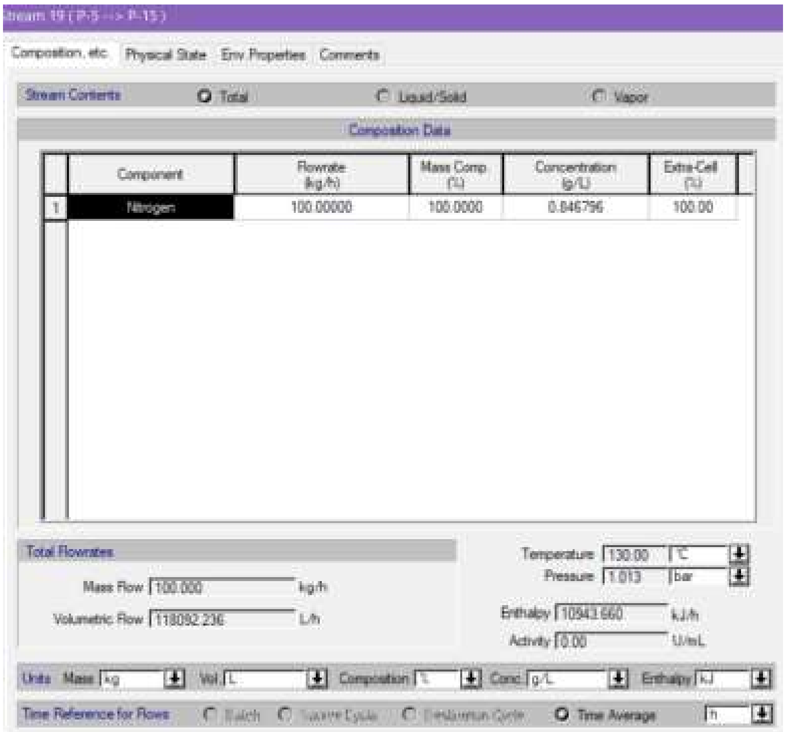


Stream 17



Output mass balance and energy balance on Reactor (R-102)

Stream 19



Stream 21

Stream 21 (P-5 --> P-6)

Composition, etc. | Physical State | Env.Properties | Comments

Stream Contents: Total (selected) / Liquid/Solid / Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	225.47538	5.2408	48.489094	100.00
2	Caprolactone	204.20615	4.7464	43.915089	100.00
3	Ethanolamine	2.09992	0.0488	0.451595	100.00
4	Ethylene Glycol	2.11054	0.0491	0.453877	100.00
5	Polyester polyo	3865.29231	89.8417	831.241619	100.00
6	Polyethylene Te	3.15318	0.0733	0.678100	100.00

Total Flowrates

Mass Flow 4302.337 kg/h

Volumetric Flow 4650.023 L/h

Temperature 130.00 °C

Pressure 1.013 bar

Enthalpy 117657.916 kJ/h

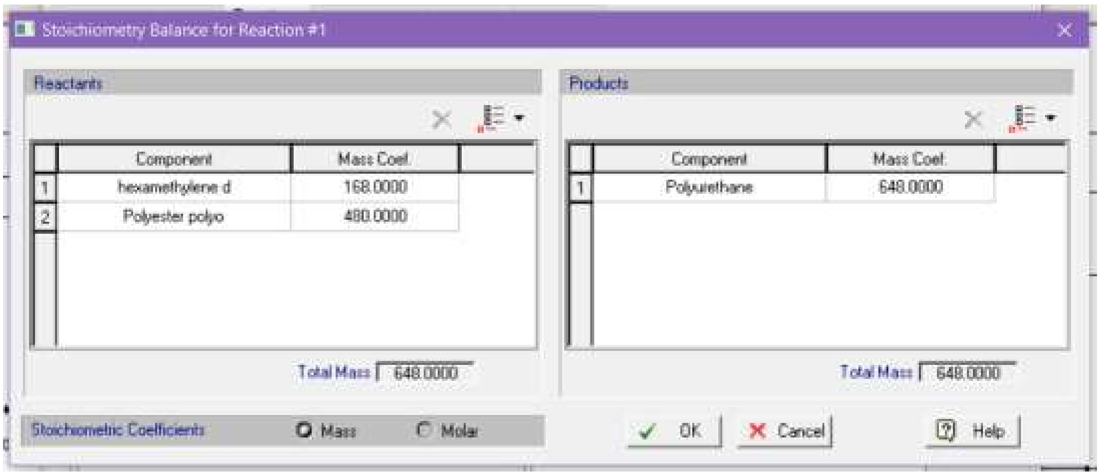
Activity 0.00 U/mL

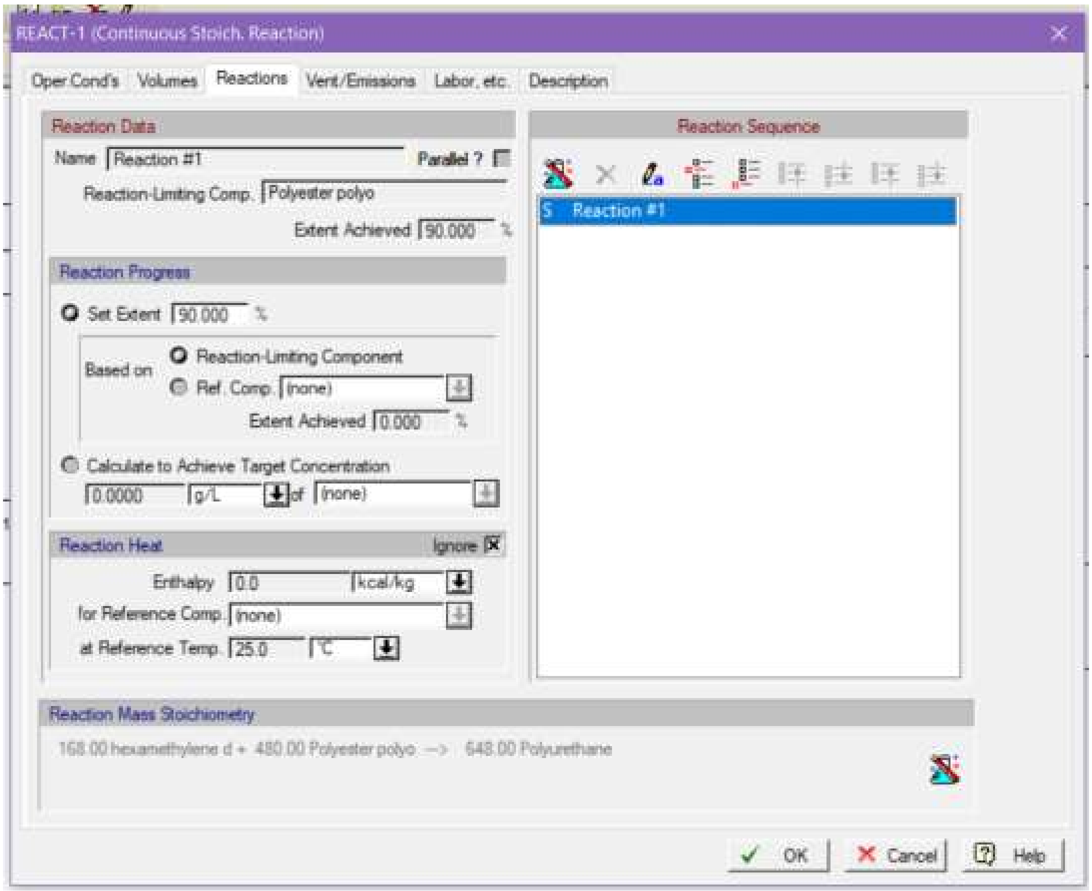
Units: Mass kg; Vol. L; Composition %; Conc. g/L; Enthalpy kJ

Time Reference for Flows: Batch / Source Cycle / Destination Cycle / Time Average (selected) h

POLYMERIZATION, (R-103) AT SUPERPRO SIMULATION

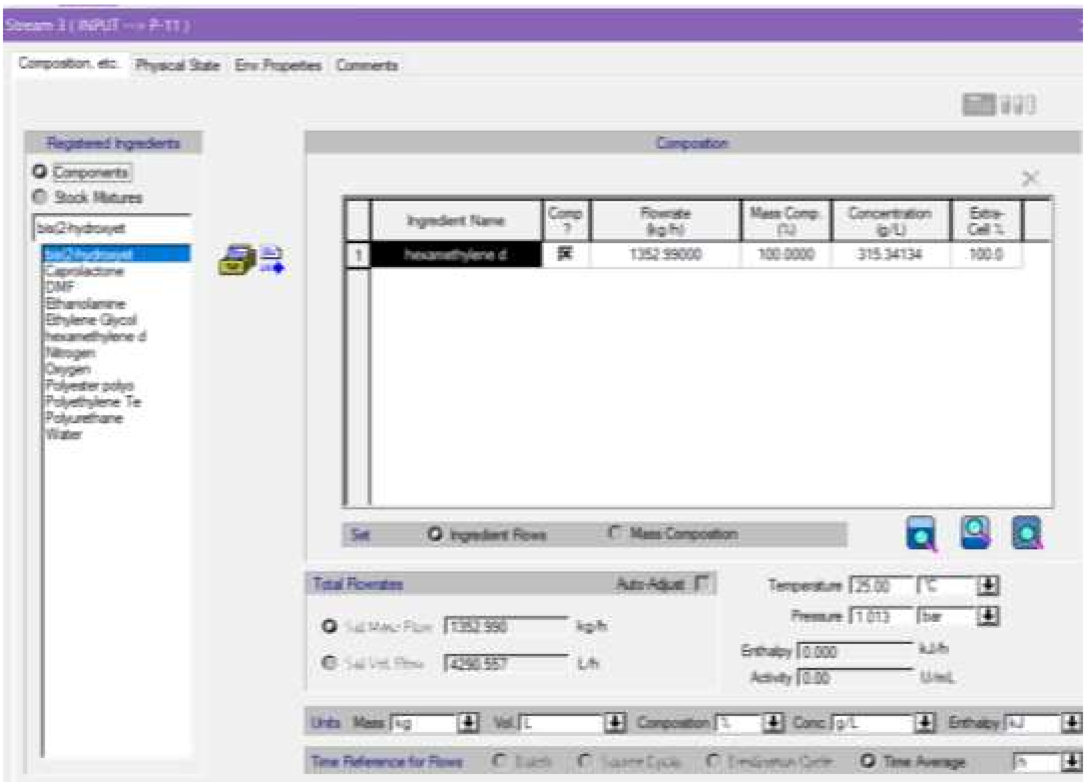
Insert the all data inside the conversion reactor such ass stochiomtery coefficient, base component and make sure it is balance.



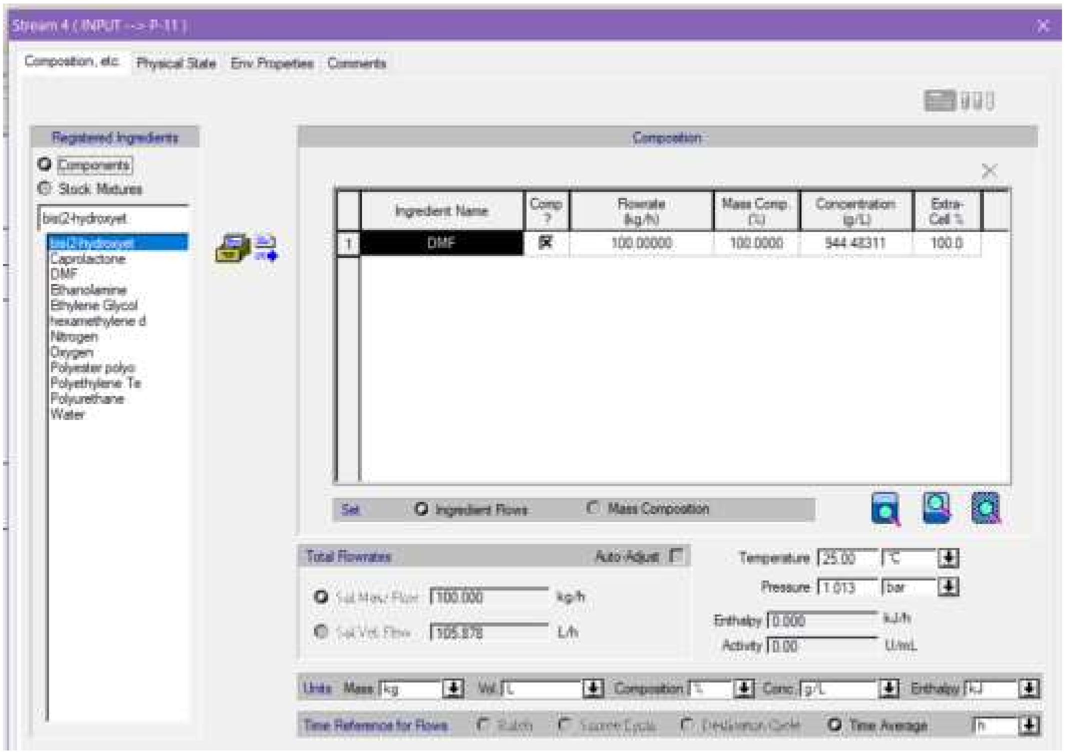


Input mass balance and energy balance on Reactor (R-103)

Stream 3



Stream 4



Stream 30

Stream 30 (P-10 --> P-11)

Composition, etc. | Physical State | Env Properties | Comments

Stream Contents: Total / Liquid/Solid / Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	0.02255	0.0006	0.005694	100.00
2	Caprolactone	2.10187	0.0543	0.530822	100.00
3	Polyester polyo	3864.90578	99.9043	976.072962	100.00
4	Polyethylene Te	1.57659	0.0408	0.398164	100.00

Total Flowrates

Mass Flow 3868.607 kg/h

Volumetric Flow 3959.648 L/h

Temperature 70.00 °C

Pressure 1.013 bar

Enthalpy 27470.743 kJ/h

Activity 0.00 U/mL

Units: Mass kg; Vol L; Composition %; Conc. g/L; Enthalpy kJ

Time Reference for Flows: Batch / Source Cycle / Destination Cycle / Time Average h

Output mass balance and energy balance on Reactor (R-103)

Stream 31

Stream 31 (P-11 --> P-12)

Composition, etc. | Physical State | Env Properties | Comments

Stream Contents: Total / Liquid/Solid / Vapor

Composition Data

	Component	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	0.02255	0.0004	0.000099	100.00
2	Caprolactone	2.10187	0.0395	0.009199	100.00
3	DMF	100.00000	1.8791	0.437639	100.00
4	hexamethylene d	135.54468	2.5471	0.593196	100.00
5	Polyester polyo	386.49058	7.2627	1.691433	100.00
6	Polyethylene Te	1.57659	0.0296	0.006900	100.00
7	Polyurethane	4695.86052	88.2416	20.550915	100.00

Total Flowrates

Mass Flow 5321.597 kg/h

Volumetric Flow 228498.859 L/h

Temperature 110.00 °C

Pressure 1.013 bar

Enthalpy 70645.520 kJ/h

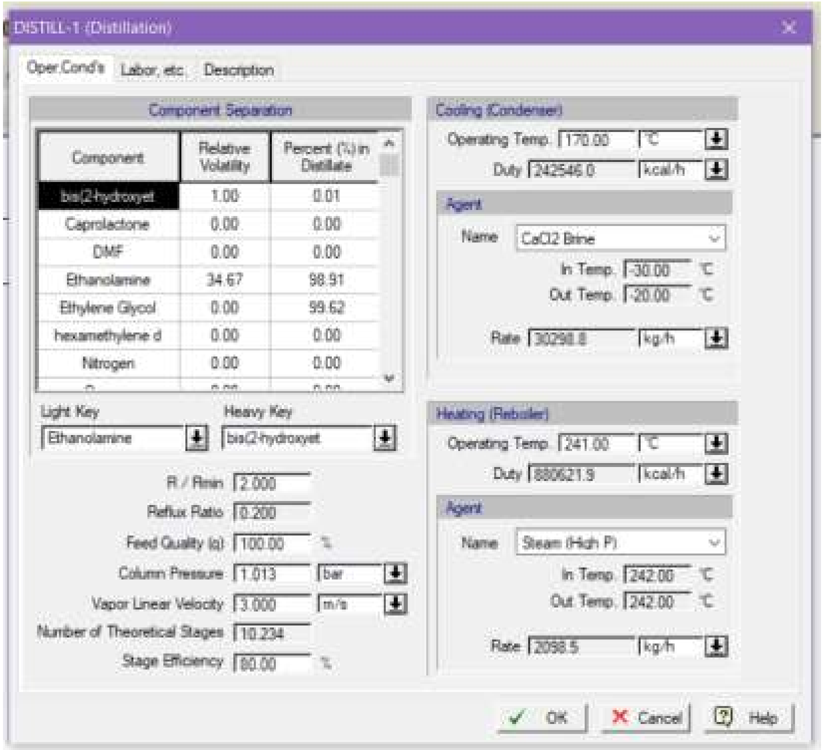
Activity 0.00 U/mL

Units: Mass kg; Vol L; Composition %; Conc. g/L; Enthalpy kJ

Time Reference for Flows: Batch / Source Cycle / Destination Cycle / Time Average h

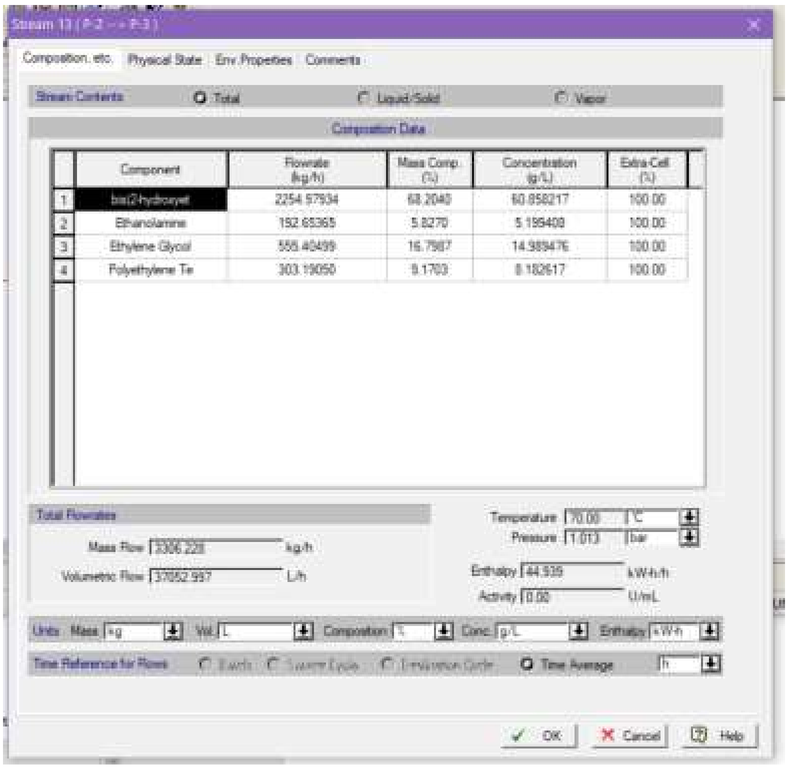
SEPARTION , (DC-101) AT SUPERPRO SIMULATION

Make sure heavy top and light key component is right



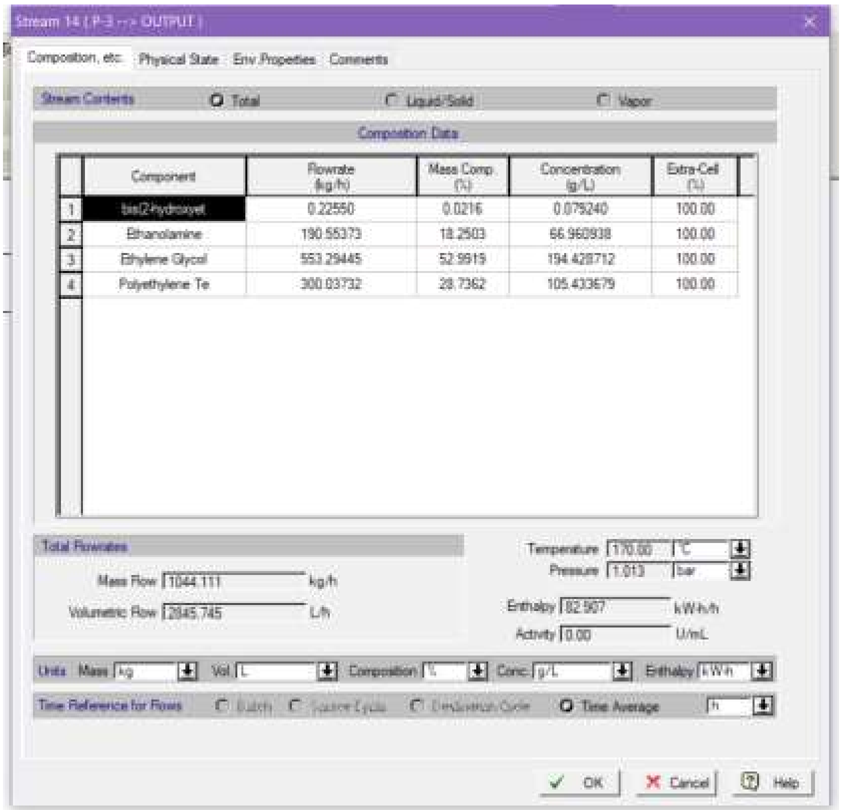
Input mass balance and energy balance on DC-101

Stream 13



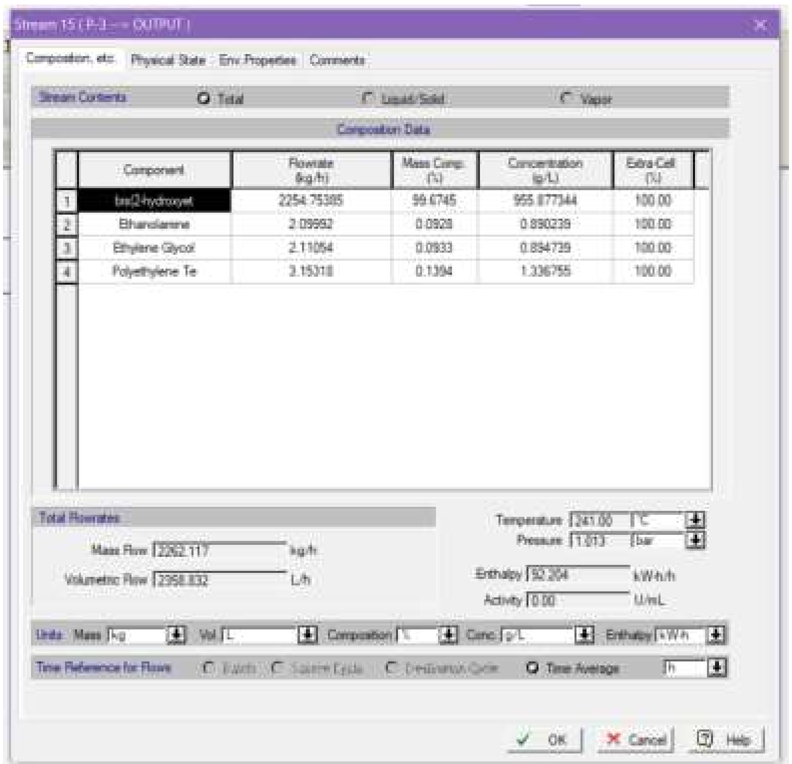
Output mass balance and energy balance on DC-101

Stream 14



	Component	Flowrate (kg/h)	Mass Comp (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	0.22550	0.0216	0.079240	100.00
2	Ethanolamine	190.55373	18.2503	66.960938	100.00
3	Ethylene Glycol	553.29445	52.9919	194.428712	100.00
4	Polyethylene Te	300.03732	28.7362	105.433679	100.00

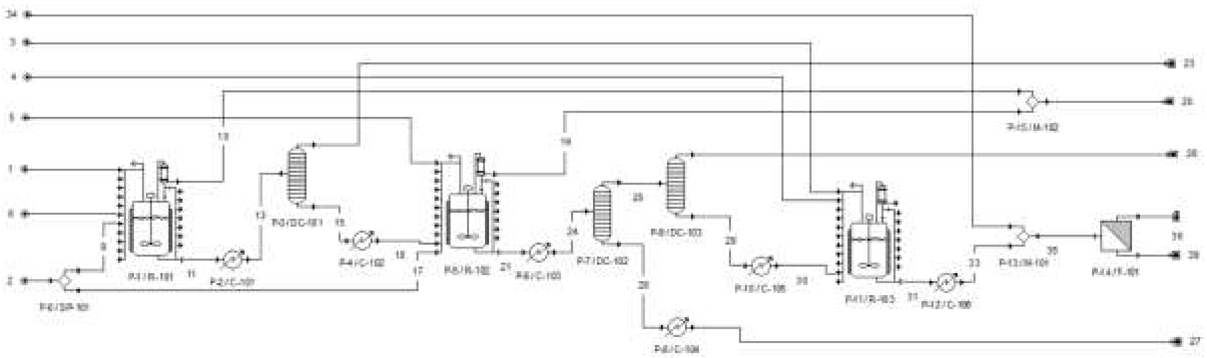
Stream 15



	Component	Flowrate (kg/h)	Mass Comp (%)	Concentration (g/L)	Extra-Cell (%)
1	bis(2-hydroxyet	2254.75385	99.6745	955.877344	100.00
2	Ethanolamine	2.09992	0.0928	0.890239	100.00
3	Ethylene Glycol	2.11054	0.0933	0.894739	100.00
4	Polyethylene Te	3.15318	0.1394	1.336755	100.00

Overall Process at SuperPro simulation

Process flow diagram in SuperPro simulation.



3. STREAM DETAILS

Stream Name	2	9	17	1
Source	INPUT	P-0	P-0	INPUT
Destination	P-0	P-1	P-5	P-1
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	25.00	25.00	93.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	1.15	1.15	1.15	262.72
Total Enthalpy (kW-h)	0.00	0.00	0.00	24.86
Specific Enthalpy (kcal/kg)	0.00	0.00	0.00	10.58
Heat Capacity (kcal/kg-°C)	0.25	0.25	0.25	0.16
Component Flowrates (kg/h averaged)				
Nitrogen	200.000	100.000	100.000	0.000
Polyethylene Te	0.000	0.000	0.000	2,021.270
TOTAL (kg/h)	200.000	100.000	100.000	2,021.270
TOTAL (L/h)	174,670.470	87,335.235	87,335.235	7,693.624

Stream Name	8	10	11	13
Source	INPUT	P-1	P-1	P-2
Destination	P-1	P-15	P-2	P-3
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	25.00	160.00	160.00	70.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	315.34	0.79	672.98	89.23
Total Enthalpy (kW-h)	0.00	3.91	134.82	44.94
Specific Enthalpy (kcal/kg)	0.00	33.66	35.09	11.70
Heat Capacity (kcal/kg-°C)	0.67	0.25	0.26	0.26
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.000	0.000	2,254.979	2,254.979
Ethanolamine	1,284.350	0.000	192.654	192.654
Ethylene Glycol	0.000	0.000	555.405	555.405
Nitrogen	0.000	100.000	0.000	0.000
Polyethylene Te	0.000	0.000	303.191	303.191
TOTAL (kg/h)	1,284.350	100.000	3,306.228	3,306.228
TOTAL (L/h)	4,072.888	126,879.950	4,912.784	37,052.997

Stream Name	23	15	18	5
Source	P-3	P-3	P-4	INPUT
Destination	OUTPUT	P-4	P-5	P-5
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	170.00	241.00	70.00	25.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	366.90	959.00	69.04	656.02
Total Enthalpy (kW-h)	82.91	92.20	19.21	0.00
Specific Enthalpy (kcal/kg)	68.32	35.07	7.31	0.00
Heat Capacity (kcal/kg-°C)	0.47	0.16	0.16	0.41
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.225	2,254.754	2,254.754	0.000
Caprolactone	0.000	0.000	0.000	2,040.220
Ethanolamine	190.554	2.100	2.100	0.000
Ethylene Glycol	553.294	2.111	2.111	0.000
Polyethylene Te	300.037	3.153	3.153	0.000
TOTAL (kg/h)	1,044.111	2,262.117	2,262.117	2,040.220
TOTAL (L/h)	2,845.745	2,358.832	32,766.425	3,109.974

Stream Name	19	21	20	24
Source	P-5	P-5	P-15	P-6
Destination	P-15	P-6	OUTPUT	P-7
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	130.00	130.00	145.01	70.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	0.85	925.23	0.82	566.24
Total Enthalpy (kW-h)	3.04	32.68	6.95	14.01
Specific Enthalpy (kcal/kg)	26.16	6.54	29.91	2.80
Heat Capacity (kcal/kg-°C)	0.25	0.06	0.25	0.06
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.000	225.475	0.000	225.475
Caprolactone	0.000	204.206	0.000	204.206
Ethanolamine	0.000	2.100	0.000	2.100
Ethylene Glycol	0.000	2.111	0.000	2.111
Nitrogen	100.000	0.000	200.000	0.000
Polyester polyo	0.000	3,865.292	0.000	3,865.292
Polyethylene Te	0.000	3.153	0.000	3.153
TOTAL (kg/h)	100.000	4,302.337	200.000	4,302.337
TOTAL (L/h)	118,092.236	4,650.023	244,978.291	7,598.115

Stream Name	25	26	27	28
Source	P-7	P-7	P-8	P-9
Destination	P-9	P-8	OUTPUT	OUTPUT
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	170.00	241.00	30.00	170.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	904.40	818.64	289.85	531.19
Total Enthalpy (kW-h)	38.81	9.42	0.22	14.22
Specific Enthalpy (kcal/kg)	8.20	35.37	0.82	59.81
Heat Capacity (kcal/kg-°C)	0.06	0.16	0.16	0.41
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.023	225.453	225.453	0.000
Caprolactone	202.103	2.103	2.103	200.001
Ethanolamine	2.100	0.000	0.000	2.100
Ethylene Glycol	2.111	0.000	0.000	2.111
Polyester polyo	3,865.292	0.000	0.000	0.387
Polyethylene Te	1.577	1.577	1.577	0.000
TOTAL (kg/h)	4,073.205	229.133	229.133	204.598
TOTAL (L/h)	4,503.774	279.896	790.527	385.168

Stream Name	29	30	3	4
Source	P-9	P-10	INPUT	INPUT
Destination	P-10	P-11	P-11	P-11
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	241.00	70.00	25.00	25.00
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	905.17	977.01	315.34	944.48
Total Enthalpy (kW-h)	36.63	7.63	0.00	0.00
Specific Enthalpy (kcal/kg)	8.15	1.70	0.00	0.00
Heat Capacity (kcal/kg-°C)	0.04	0.04	0.24	0.49
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.023	0.023	0.000	0.000
Caprolactone	2.102	2.102	0.000	0.000
DMF	0.000	0.000	0.000	100.000
hexamethylene d	0.000	0.000	1,352.990	0.000
Polyester polyo	3,864.906	3,864.906	0.000	0.000
Polyethylene Te	1.577	1.577	0.000	0.000
TOTAL (kg/h)	3,868.607	3,868.607	1,352.990	100.000
TOTAL (L/h)	4,273.919	3,959.648	4,290.557	105.878

Stream Name	31	33	34	35
Source	P-11	P-12	INPUT	P-13
Destination	P-12	P-13	P-13	P-14
Stream Properties				
Activity (U/ml)	0.00	0.00	0.00	0.00
Temperature (°C)	110.00	70.00	25.00	50.53
Pressure (bar)	1.01	1.01	1.01	1.01
Density (g/L)	23.29	75.34	994.70	198.39
Total Enthalpy (kW-h)	19.62	20.53	0.00	20.53
Specific Enthalpy (kcal/kg)	3.17	3.32	0.00	3.14
Heat Capacity (kcal/kg-°C)	0.04	0.07	1.00	0.12
Component Flowrates (kg/h averaged)				
bis(2-hydroxyet	0.023	0.023	0.000	0.023
Caprolactone	2.102	2.102	0.000	2.102
DMF	100.000	100.000	0.000	100.000
hexamethylene d	135.545	135.545	0.000	135.545
Polyester polyo	386.491	386.491	0.000	386.491
Polyethylene Te	1.577	1.577	0.000	1.577
Polyurethane	4,695.861	4,695.861	0.000	4,695.861
Water	0.000	0.000	300.000	300.000
TOTAL (kg/h)	5,321.597	5,321.597	300.000	5,621.597
TOTAL (L/h)	228,498.859	70,633.411	301.597	28,335.785

Stream Name	36	39
Source	P-14	P-14
Destination	OUTPUT	OUTPUT
Stream Properties		
Activity (U/ml)	0.00	0.00
Temperature (°C)	52.50	52.50
Pressure (bar)	1.01	1.01
Density (g/L)	565.51	164.75
Total Enthalpy (kW-h)	12.69	9.43
Specific Enthalpy (kcal/kg)	11.79	1.73
Heat Capacity (kcal/kg-°C)	0.43	0.06
Component Flowrates (kg/h averaged)		
bis(2-hydroxyet	0.023	0.000
Caprolactone	2.102	0.000
DMF	100.000	0.000
hexamethylene d	135.545	0.000
Polyester polyo	386.491	0.000
Polyethylene Te	1.577	0.000
Polyurethane	0.000	4,695.861
Water	300.000	0.000
TOTAL (kg/h)	925.736	4,695.861
TOTAL (L/h)	1,637.004	28,503.178

4. OVERALL COMPONENT BALANCE (kg/h)

COMPONENT	IN	OUT	IN-OUT
bis(2-hydroxyet	0.000	225.701	- 225.701
Caprolactone	2,040.220	204.206	1,836.014
DMF	100.000	100.000	0.000
Ethanolamine	1,284.350	192.654	1,091.696
Ethylene Glycol	0.000	555.405	- 555.405
hexamethylene d	1,352.990	135.545	1,217.445
Nitrogen	200.000	200.000	0.000
Polyester polyo	0.000	386.877	- 386.877
Polyethylene Te	2,021.270	303.191	1,718.080
Polyurethane	0.000	4,695.861	- 4,695.861
Water	300.000	300.000	0.000
TOTAL	7,298.830	7,299.438	0.608

SAFETY DATA SHEET

Version 8.0
Revision Date 28.12.2020
Print Date 29.12.2020

SECTION 1: Identification of the hazardous chemical and of the supplier

1.1 Product identifiers

Product name	:	ε-Caprolactone for synthesis
Product Number	:	8.02801
Catalogue No.	:	802801
Brand	:	Millipore
CAS-No.	:	502-44-3

1.2 Other means of identification

No data available

1.3 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Chemical for synthesis

1.4 Details of the supplier of the safety data sheet

Company	:	Merck Sdn. Bhd. Co. No: 178145 No. 4, Jalan U1/26, Section U1, 40150 HICOM GLENMARIE INDUSTRIAL PARK,SHAH ALA MALAYSIA
Telephone	:	+60 (0)3-74943688
Fax	:	+60 (0)3-74910850

1.5 Emergency telephone

Emergency Phone # : 1-800-815-308 (CHEMTREC) * + 62 0800 140 1253 (Customer Call Centre)

Section 2: Hazard identification

2.1 GHS Classification

Classification according to CLASS regulations 2013
Serious eye damage/eye irritation (Category 2), H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Labelling according to CLASS regulations 2013
Pictogram

Signal word Warning

Hazard statement(s)
H319 Causes serious eye irritation.

Precautionary statement(s)

Prevention

P264	Wash skin thoroughly after handling.
P280	Wear eye protection/ face protection.

Response

P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.

Reduced Labeling (<= 125 ml)

Pictogram 

Signal word: Warning

Hazard statement(s): none

Precautionary statement(s): none

Refer to the Safety Data Sheet before use.

2.3 Other hazards - none

SECTION 3: Composition and information of the ingredients of the hazardous chemical

Substance / Mixture : Substance

3.1 Substances

Formula : C6H10O2
Molecular weight : 114.14 g/mol
CAS-No. : 502-44-3
EC-No. : 207-938-1

Hazardous ingredients

Component	Classification	Concentration
hexan-6-olide		
	2; H319	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO_2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
In the event of fire, wear self-contained breathing apparatus.

5.4 Further information
Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed.

Store below +30°C.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls and personal protection

8.1 Control parameters

Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Change contaminated clothing. Wash hands after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Full contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested:Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 30 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection
protective clothing

Respiratory protection
required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Color: colorless
b)	Odor	bitter almond
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -2.15 °C at 1,013 hPa Freezing point/ range: -25.15 °C at 1,013 hPa
f)	Initial boiling point and boiling range	98 - 99 °C at 3 hPa
g)	Flash point	109 °C - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	0.01 hPa at 20 °C
l)	Vapor density	3.94 - (Air = 1.0)
m)	Relative density	1.076 g/cm³
n)	Water solubility	1 g/l at 20 °C - OECD Test Guideline 105- completely soluble
o)	Partition coefficient: n-octanol/water	log Pow: 0.32 at 20 °C
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapor density	3.94 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity
Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents
alkalines
acids

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
Polyvinyl chloride

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 4,290 mg/kg
LD50 Dermal - Rabbit - male - 6,400 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Irritating to eyes.
(OECD Test Guideline 405)

Respiratory or skin sensitization
in vivo assay - Mouse
Result: negative
(OECD Test Guideline 429)
Remarks:
No data available

Germ cell mutagenicity
Chromosome aberration test in vitro
Chinese hamster fibroblasts
Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Poecilia reticulata (guppy) - 280 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 204 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	ErC50 - Desmodesmus subspicatus (green algae) - 2,616 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

SECTION 13: Disposal information

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and loc No mixing with other waste. Handle uncleaned containers like the product See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions. According to Quality Environment Regulation (Scheduled Waste) 2005, waste need to be sent to designated premise for

recycle, treatment or disposal. Please contact Kualiti Alam for waste classification and correct disposal method.

SECTION 14: Transportation information

14.1 UN number

ADR/RID: - IMDG: - IATA-DGR: -

14.2 UN proper shipping name

ADR/RID:	Not dangerous goods
IMDG:	Not dangerous goods
IATA-DGR:	Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: - IMDG: - IATA-DGR: -

14.4 Packaging group

ADR/RID: - IMDG: - IATA-DGR: -

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA-DGR: no

14.6 Special precautions for user

14.7 Incompatible materials

Polyvinyl chloride

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

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

Notification status

AICS:	On the inventory, or in compliance with the inventory
DSL:	All components of this product are on the Canadian DSL
ENCS:	On the inventory, or in compliance with the inventory
ISHL:	On the inventory, or in compliance with the inventory
KECI:	On the inventory, or in compliance with the inventory
NZIoC:	On the inventory, or in compliance with the inventory
PICCS:	On the inventory, or in compliance with the inventory

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H319 Causes serious eye irritation.

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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SAFETY DATA SHEET

Version 8.4
Revision Date 31.08.2021
Print Date 20.09.2021

SECTION 1: Identification of the hazardous chemical and of the supplier

1.1 Product identifiers

Product name	:	N,N-Dimethylformamide EMPARTA®
Product Number	:	1.03034
Catalogue No.	:	103034
Brand	:	Millipore
CAS-No.	:	68-12-2

1.2 Other means of identification

No data available

1.3 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Reagent for analysis, Chemical production

1.4 Details of the supplier of the safety data sheet

Company : Merck Sdn. Bhd.
Co. No: 178145
No. 4, Jalan U1/26, Section U1,
40150 HICOM GLENMARIE INDUSTRIAL PARK,SHAH ALA
MALAYSIA

Telephone : +60 (0)3-74943688
Fax : +60 (0)3-74910850

1.5 Emergency telephone

Emergency Phone # : 1-800-815-308 (CHEMTREC) * + 62 0800 140 1253 (Customer Call Centre)

Section 2: Hazard identification

2.1 GHS Classification

Classification according to CLASS regulations 2013
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Serious eye damage/eye irritation (Category 2), H319
Reproductive toxicity (Category 1B), H360D

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Labelling according to CLASS regulations 2013

Pictogram

Signal word Danger

Hazard statement(s)

H312 + H332 Harmful in contact with skin or if inhaled.

H319	Causes serious eye irritation.
H360D	May damage the unborn child.

Precautionary statement(s)

Prevention	
P201	Obtain special instructions before use.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P281	Use personal protective equipment as required.
Response	
P302 + P352 + P312	IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.

Reduced Labeling (<= 125 ml)

Pictogram

Signal word	Danger
Hazard statement(s)	none
Precautionary statement(s)	none

Refer to the Safety Data Sheet before use.

2.3 Other hazards - none

SECTION 3: Composition and information of the ingredients of the hazardous chemical

Substance / Mixture : Substance

3.1 Substances

Formula	:	C3H7NO
Molecular weight	:	73.09 g/mol
CAS-No.	:	68-12-2
EC-No.	:	200-679-5
Index-No.	:	616-001-00-X

Hazardous ingredients

Component	Classification	Concentration
N,N-dimethylformamide		
	Flam. Liq. 3; Acute Tox. 4; 2; Repr. 1B; H226, H332, H312, H319, H360D	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO_2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Combustible.
Fire may cause evolution of:
nitrogen oxides
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.
Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition.Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls and personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
N,N-dimethylformamide	68-12-2	TWA	10 ppm 30 mg/m3	Malaysia. Occupational Safety and Health (Use and Standards of Exposure of Chemicals Hazardous to Health) Regulations 2000.
	Remarks	Skin		

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Full contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested:Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Splash contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 240 min
Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Color: colorless
b)	Odor	amine-like
c)	Odor Threshold	0.329 ppm
d)	pH	7 at 200 g/l at 20 °C
e)	Melting point/freezing point	Melting point: -61 °C
f)	Initial boiling point and boiling range	153 °C at 1,013 hPa - DIN 53171

g)	Flash point	57.5 °C - closed cup - DIN 51755 Part 2
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 16 %(V) Lower explosion limit: 2.2 %(V)
k)	Vapor pressure	3.77 hPa at 20 °C
l)	Vapor density	2.52 - (Air = 1.0)
m)	Density	0.944 g/cm3 at 25 °C
	Relative density	No data available
n)	Water solubility	1,000 g/l at 20 °C completely miscible
o)	Partition coefficient: n-octanol/water	log Pow: -0.85 at 25 °C - Bioaccumulation is not expected.
p)	Autoignition temperature	435 °C at 1,013 hPa - DIN 51794
q)	Decomposition temperature	> 350 °C -
r)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 0.86 mPa.s at 20 °C
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

Relative vapor density	2.52 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 3,010 mg/kg
(OECD Test Guideline 401)
Symptoms: Gastrointestinal disturbance
Acute toxicity estimate Inhalation - 4 h - 11.1 mg/l
(Expert judgment)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)
LD50 Dermal - Rabbit - 1,500 mg/kg
Remarks: (Regulation (EC) No 1272/2008, Annex VI)
(IUCLID)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 20 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation
Remarks: (ECHA)
(Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: sister chromatid exchange assay
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)
Test Type: unscheduled DNA synthesis assay
Test system: human diploid fibroblasts
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal injection

Result: negative
Remarks: (ECHA)

Test Type: dominant lethal test
Species: Rat

Application Route: Inhalation

Result: negative
Remarks: (ECHA)

Test Type: dominant lethal test
Species: Mouse

Application Route: Intraperitoneal

Result: negative
Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse

Application Route: Intraperitoneal

Result: negative
Remarks: (ECHA)

Carcinogenicity
No data available

Reproductive toxicity
May damage the unborn child.

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 238 mg/kg - LOAEL (Lowest observed adverse effect level) - 475 mg/kg
Remarks: Subacute toxicity

Vomiting
Diarrhea
Abdominal pain
Warning: intolerance for alcohol can occur up to 4 days after dimethylformamide exposure.
N,N-dimethylformamide is considered to be a potent liver toxin.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Headache
Dizziness
Drowsiness

Damage to:

Kidney
Liver

This substance should be handled with particular care.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Lepomis macrochirus (Bluegill sunfish) - 7,100 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 13,100 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 1,000 mg/l - 72 h (DIN 38412)
Toxicity to bacteria	static test EC50 - Vibrio fischeri - 12,300 - 17,500 mg/l - 5 min Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 21 d Result: 100 % - Readily biodegradable. (OECD Test Guideline 301E)
Biochemical Oxygen Demand (BOD)	900 mg/g Remarks: (Lit.)
Theoretical oxygen demand	1,863 mg/g Remarks: (Lit.)

12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 56 d at 25 °C - 0.002 mg/l(N,N-dimethylformamide) Bioconcentration factor (BCF): 0.3 - 1.2 (OECD Test Guideline 305C) Remarks: Does not significantly accumulate in organisms.

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

Stability in water	- ca.50 d Remarks: reaction with hydroxyl radicals(calculated)(Lit.)

SECTION 13: Disposal information

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions. According to Quality Environment Regulation (Scheduled Waste) 2005, waste need to be sent to designated premise for recycle, treatment or disposal. Please contact Kualiti Alam for waste classification and correct disposal method.

SECTION 14: Transportation information

14.1 UN number

ADR/RID: 2265	IMDG: 2265	IATA-DGR: 2265

14.2 UN proper shipping name

ADR/RID:	N,N-DIMETHYLFORMAMIDE
IMDG:	N,N-DIMETHYLFORMAMIDE
IATA-DGR:	N,N-Dimethylformamide

14.3 Transport hazard class(es)

ADR/RID: 3	IMDG: 3	IATA-DGR: 3

14.4 Packaging group

ADR/RID: III	IMDG: III	IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no	IMDG Marine pollutant: no	IATA-DGR: no

14.6 Special precautions for user

None

14.7 Incompatible materials

Strong oxidizing agents

Other regulations

Hazchem Code : •2Y

SECTION 15: Regulatory information

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

Notification status

AICS:	On the inventory, or in compliance with the inventory
DSL:	All components of this product are on the Canadian DSL
ENCS:	On the inventory, or in compliance with the inventory
ISHL:	On the inventory, or in compliance with the inventory
KECI:	On the inventory, or in compliance with the inventory
NZIoC:	On the inventory, or in compliance with the inventory
PICCS:	On the inventory, or in compliance with the inventory

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H226	Flammable liquid and vapor.
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H360D	May damage the unborn child.

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Material Safety Data Sheet

According to EU Reg. 1907/2006 & 830/2015

Last review: JULY 2017

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY

1.1 Product identifier

Product Name	PoliPET
Product Identification Name	PoliPET 76W, PoliPET 80GP, PoliPET 84SD, PoliPET 84F PoliPET ECO 84SD, PoliPET ECO 84F
Name REACH	Polyethylene Terephthalate (copolymer)
CAS number	25038-59-9
EC number	N/A
REACH number	N/A
Molecular Formula	$(C_{10}H_8O_4)_n$
Synonyms	Poly(oxy-1,2-ethanedioloxycarbonyl-1,4phenylenecarbonyl)

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

Polyethylene terephthalate (PET) is an intermediate plastic used for food and non-food contact packaging, bottles and other relevant applications, by (not exhaustive methods): molding and extrusion processes. Do not use in medical applications involving permanent implantation in the human body.

1.3 Details of the supplier of the safety data sheet

Manufacturer/Supplier Polisan Hellas S.A
Industrial & Commercial Company of Pet Resin Production & Preforms
Head Office: B' Industrial Area of Volos, 37 500 Volos, Greece
Tel. HO: +30 24250 22250

1.4 Emergency telephone number

For emergency health, safety and environmental information, telephone:
+30 24250 22250

SECTION 2: HAZARDS IDENTIFICATION

2.1 Classification of substance and mixture

Polyethylene terephthalate (PET) is a polymer not classified as a hazardous substance according to Regulation (EC) No 1272/2008 (CLP). PET is not categorized as persistent, bio-accumulative or toxic (PBT). PET is not very persistent or very bio-accumulative (vPvB), as defined in REACH (Annex XIII) and is not included in the candidate list of substances of very high concern (SVHC).

In accordance with Regulation (EC) No 1907/2006 (REACH), there is no obligation to provide a material safety data sheet (MSDS) for PET products.

This Safety Data Sheet is provided only to ensure that, as a supplier (manufacturer of PET), we communicate safety information to the supply chain to facilitate safe use, handling, storage and transportation of PET products. Possible hazards of this product are associated mainly with its processing.

Resin particles, like other inert materials, are mechanically irritating to eyes. Molten polymer will adhere to the skin and can cause severe burn.

2.2 Label elements

Labeling not required according to Regulation (EC) 1272/2008 (CLP).

2.3 Other hazards

Polyethylene terephthalate (PET) is not categorized as persistent, bio-accumulative or toxic (PBT) according to Regulation (EC) 1907/2006, Annex XIII.
Hazards of this product may be associated with its processing: spilled pellets create a slipping hazard. Molten plastic can cause severe thermal burns. Fumes produced during the thermal processing of polymer melt may cause eye, skin and respiratory tract irritation. Treat in the same way as other thermal burns and wood smoke inhalation.

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

Substance: Mono-constituent substance **Mixtures:** Not applicable

Product name	CAS No	Content	REACH No	Classification according to Reg. (EC) 1272/2008 (CLP)
Polyethylene terephthalate (PET)	25038-59-9	100%	N/A	Not classified as hazardous

SECTION 4: FIRST AID MEASURES

4.1 Description of first aid measures

Inhalation: remove to fresh air and keep at rest in a position comfortable for breathing, in case of accidental inhalation of dust or fumes from overheating of combustion or melted substance. Drink water to clean the mouth and blow the nose to remove dust. Get medical attention if evidence of breathing problems or symptoms occur.
Skin contact: Cool skin rapidly with cold water after contact with molten polymer. Do not try to peel molten polymer from the skin. Put a sterile bandage on the wound and get medical advice.
Eye contact: Immediately flush eyes with plenty of clean water or eye wash solution, removing any contact lenses. Hold eyes open while flushing. If irritation occurs, get medical attention.
Ingestion: No toxicity hazard. This substance is biologically inactive. Wash out mouth with water. If material has been swallowed and the exposed person is conscious, provide small quantities of potable water to drink. If symptoms occur, get medical attention.
Protection of first-aiders: No action shall be taken involving any personal risk or without suitable training.

4.2 Most important symptoms and effects, both acute and delayed

Not known significant effects or critical hazards. Particles / dust are mechanically irritating to eyes. Molten polymer will adhere to the skin and can cause severe burn. If necessary treat symptomatically.

4.3 Indication of any immediate medical attention and special treatment method

Treat Symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable: In case of fire use water spray/aerosol, dry chemical, powder extinguishers, water/foam, CO2, A or B class fire extinguishers.
Not Suitable: Do not use water jet.

5.2 Special hazards arising from the substance or mixture

Hazards from the substance or mixture: No specific fire or explosion hazard. Low fire hazard. Only powdered material may form flammable / explosive dust-air-clouds mixture. High voltage static electricity build-up and discharge must be avoided when significant quantities of powdered material are present. During a fire, smoke may contain the original material in addition to combustion products of varying composition, which may be toxic and/or irritating.

Hazardous thermal decomposition products: Decomposition /combustion products may include and are not limited to carbon monoxide and carbon dioxide. In case of fire use breathing apparatus.

5.3 Advice for fire-fighters

Special protective actions for fire-fighters: Promptly isolate the scene by removing all persons from the vicinity of the incident, if there is a fire (solid polymer burns only with difficulty). No action shall be taken involving any personal risk or without suitable training.

Special protective equipment for fire-fighters: Fire-fighters must wear suitable personal protective equipment (clothing, helmet, protective boots, gloves conforming to EU standard EN 469), and self-contained breathing apparatus (SCBA).

Fire-fighting measures: Use self-contained apparatus if respirable dust and/or fumes/vapors occur. Use water spray to cool and disperse vapors and protect personnel.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unprotected personnel from approaching or entering. Do not touch or walk through spilled material. Wear suitable personal protective equipment.

For emergency responders: If specialized clothing is required to deal with spillage, consider information in Section 8 and information "For non-emergency personnel".

6.2 Environmental precautions

No special environmental precautions required. Avoid dispersion of spilled material. Clean up spills immediately.

6.3 Methods and materials for containment and cleaning up

Small spill: Vacuum or sweep spilled material and place in a designated, labeled waste container. Disposal handling must comply with the relevant environmental protection and waste disposal legislation and local authority requirements.

Large spill: Prevent entry into sewers, watercourses and confined areas. Vacuum or sweep spilled material and place in a designated, labeled waste container. Disposal handling must comply with the relevant environmental protection and waste disposal legislation and local authority requirements.

6.4 Reference to other

See Section 1 for emergency contact information.

See Section 8 for information on suitable personal protective equipment.

See Section 13 for additional waste treatment information.

SECTION 7: HANDLING AND STORAGE

7.1 Precautions for safe handling

Wear suitable personal protective equipment (see Section 8). Eating, drinking and smoking should be prohibited in areas where this material is stored, handled and processed. Wash hands and face before eating, drinking and smoking. Remove any contaminated clothing and personal protective equipment before entering eating area. Provide exhaust ventilation at places where dust is formed. Take precautionary measures against static discharges, where dust is formed.

7.2 Conditions for safe storage, including any incompatibilities

Store in accordance with local regulations.
Store in original containers. Keep containers tightly closed in a dry, cool and well ventilated area, away from incompatible materials (see Section 10). Protect from direct sunlight, UV light, high temperatures and rain. Containers that have been opened should be carefully resealed after use and kept upright to prevent leakage. Do not store in unlabeled containers.

7.3 Specific end use(s)

Recommendations: Do not use in medical applications involving permanent implantation in the human body.

SECTION 8: EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters

Occupational exposure limits: No exposure limit value established (in case of dust, <10mg/m3 TLV-TWA 8h - 5mg/m3 respirable dust).
During processing of PET small amount of acetaldehyde, AA (CAS 75-07-0) is generated. Customers are advised to check exposure to workers and apply current workplace exposure limits. There are workplace exposure limits for aldehydes and the customer should ensure they use the measures appropriate to their workplace.
Derived effect levels: Not applicable
Predicted effect concentrations: Not applicable

8.2 Exposure controls

Individual protection measures
Hygiene measures: Wash hands and face before eating, drinking and smoking and at the end of workday. Remove any contaminated clothing and personal protective equipment before entering eating area.
Eye/face protection: Safety approved eyewear should be used as a good industrial practice and when a risk assessment indicates this as mandatory to avoid any possible exposure to material particles or dust. Full-face protection should be used when material is handled hot mass.
Hand protection: Approved protective gloves/clothing should be used as a good industrial practice. Thermal isolating gloves should be used when material is handled hot mass.
Body protection: Wear work clothing. Protective/thermal insulating gloves as above.
Other skin protection: Suitable approved protective footwear.
Respiratory protection: Respiratory protection should be worn when there is a potential to exceed the exposure limit requirements or guidelines. Dust protection mask or self-contained breathing apparatus. Do not breathe fumes evolved. Use an approved air-purifying respirator when vapors are generated at increased temperatures or when dust or mist is present. If there are no applicable exposure limit requirements or guidelines, wear respiratory protection when adverse effects, such as respiratory irritation or discomfort have been experienced, or where indicated by your risk assessment process.
Appropriate engineering controls: Use of local exhaust ventilation system (or other engineering controls), efficient to maintain airborne contaminants levels below exposure limit requirements or guidelines. If there are no applicable exposure limit requirements or guidelines, general ventilation should be sufficient for most operations.
Environmental exposure controls: Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels. Loose PET pellets produce a slipping hazard.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

Appearance (physical state)	Solid, cylindrical granules (pellets)
Color	White (in solid state)
Odor	Odorless
pH	Does not apply
Melting point	240 – 265°C
Initial boiling point and boiling range	Destruction at >380°C
Flash point	440°C
Flammability (solid, gas)	Slightly flammable in the presence of: open flames, static discharge and heat. Non-flammable under conditions: mechanical impacts, Oxidizing and reducing materials
Burning time	Not available
Vapor pressure	Does not apply
Vapor density	Does not apply
Solubility	Insoluble in water. Soluble in chlorinated hydrocarbons
Self-ignition point	500°C approx.
Viscosity (intrinsic)	0.74-0.86 dl/g
Explosive properties	Non-explosive
Dust explosiveness class	1
Limiting Oxygen Index	12%

SECTION 10: STABILITY AND REACTIVITY

Reactivity: None known. Stable/inert under normal use condition.
Chemical stability: Stable in normal ambient conditions.
Possibility of hazardous reactions: None, under normal conditions of storage and use.
Conditions to avoid: Avoid dust concentration with static discharges and high temperatures, flame or other sources of ignition. Temperatures above 150°C and/or long retention time must be avoided as product degradation and thermal decomposition can start.
Incompatible materials: strong oxidizing agents, mineral acids, organic solvents (acetic anhydride, acetone, aniline, benzene, chloroform, chromic acid, cyclohexanone, dimethylformamide, dioxin, ethyl acetate, methyl ethyl ketone, methylene chloride, phenol, tetrahydrofuran, trichloroethylene, triethanolamine, caustic soda).
Decomposition products: Above the decomposition temperature, the major volatiles will be carbon dioxide, carbon monoxide, acetaldehyde, terephthalic acid, oligomers of PET.

SECTION 11: TOXICOLOGICAL INFORMATION

Acute toxicity: Material is not hazardous or toxic at ambient conditions.
Skin corrosion/irritation: May cause physical abrasion in contact with skin. Molten polymer will adhere to the skin causing deep thermal burns.
Serious eye damage/irritation: May cause physical abrasion in contact with eyes.
Respiratory or skin sensitization: Not known
Mutagenicity: Not applicable
Carcinogenicity: Not applicable
Reproductive toxicity: Not applicable
STOT-repeated exposure: Not applicable
Aspiration hazard: Not applicable

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SECTION 12: ECOLOGICAL INFORMATION

12.1 Toxicity

Adverse effects would not be expected. Insoluble in water, nontoxic solid substance (no hazardous effect in water).

12.2 Persistence and degradability

Very minor degradability under impact of UV light. Material is solid with low volatility.

12.3 Bio accumulative potential

No evidence of hazardous effect on the environment.

12.4 Mobility in soil

Not applicable

12.5 Results of PBT and vPvB assessment

Not applicable (not PBT or vPvB)

12.5 Other adverse effects

Not applicable

SECTION 13: DISPOSAL CONSIDERATIONS

This is general advice information. Disposal handling must comply with the relevant environmental protection and waste disposal legislation and local authority requirements.

13.1 Waste treatment methods

Product: This product is not considered as hazardous waste, based on EU Directive 91/689. Like most thermoplastics, this product can be recycled. Recycling when possible is preferred to disposal or incineration. Disposal handling must comply with the relevant environmental protection and waste disposal legislation and local authority requirements.

Waste codes/waste designations according to LoW: proposed waste codes 12 01 05

12 - Wastes from shaping and surface treatment of metals and plastics

01 - Wastes from shaping (including forgoing, welding, pressing, drawing, turning, cutting and filing

05 - Plastics particles

Packaging: Waste packaging should be taken for recycling or waste disposal. Disposal handling must comply with the relevant environmental protection and waste disposal legislation and local authority requirements.

SECTION 14: TRANSPORT INFORMATION

Transport regulations do not apply. The product is not covered by international regulations on the transport of dangerous goods.

14.1 UN Number

Not classified as hazard for transport.

14.2 Proper shipping name

Not classified as hazard for transport.

14.3 Transport hazard class (es)

Not classified as hazard for transport, according the transport rules IMO, ADR/RID, ICAO.

14.4 Packaging group

Not classified as hazard for transport, according the transport rules IMO, ADR/RID, ICAO.

14.5 Packing group Environmental hazards

Not classified as hazard for transport, according the transport rules IMO, ADR/RID, ICAO.

14.6 Specials precautions for users

Always transport in closed containers that are upright and secure. Persons involved should know what to do if an accident or spillage occur.

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

Non-hazardous product, according to EU Regulations 1907/2006, 1272/2008 (REACH, CLP).

SVHC (substances of very high concern): none of the components are listed.

15.2 Chemical safety assessment

Not applicable

Safety, health and environmental regulations/legislation specific for the substance or mixture EU regulations for all EU Member states:

•Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006. Concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency with following amendments.

•Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008. On classification, labelling and packaging of substances and mixtures (CLP), amending and repealing Directives 67/548/EEC and 1999/45/EC and amending Regulation (EC) No 1907/2006.

•Regulation (EU) No 453/2010 of the Commission of 20 May 2010 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).

•Regulation (EC) No 2015/830 of 28 May 2015 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

•Regulation (EC) 649/2012 of the European Parliament and of the Council of 4 July 2012. Concerning the export and import of hazardous chemicals.

•European Agreement Concerning the International Carriage of Dangerous Goods by Road (ADR)

Authorisation and/or restrictions on use:

•Substances of very high concern (SVHC) according to Article 59(10) of the REACH Regulation

SECTION 16: OTHER INFORMATION

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 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.

For further information please contact Polisan Hellas:

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SAFETY DATA SHEET

Creation Date 11-Jun-2009 **Revision Date** 24-Dec-2021 **Revision Number** 5

1. Identification

Product Name	**Ethanolamine**
Cat No. :	**M251-1; M251-4**
CAS No	141-43-5
Synonyms	2-Aminoethanol, monoethanolamine
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 Company
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)

Flammable liquids	Category 4
Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word
Danger

Hazard Statements
Combustible liquid

Causes severe skin burns and eye damage
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Use only outdoors or in a well-ventilated area
Do not breathe dust/fume/gas/mist/vapors/spray
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep cool
Response
Immediately call a POISON CENTER or doctor/physician
Inhalation
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Skin
Wash contaminated clothing before reuse
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
Ingestion
Rinse mouth
Do NOT induce vomiting
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Storage
Store locked up
Store in a well-ventilated place. Keep container tightly closed
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
Harmful to aquatic life with long lasting effects

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Ethanolamine	141-43-5	>95

4. First-aid measures

General Advice Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required. Keep eye wide open while rinsing.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Remove and wash

	contaminated clothing and gloves, including the inside, before re-use. Call a physician immediately.
Inhalation	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. Remove from exposure, lie down. Call a physician immediately. If not breathing, give artificial respiration.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Clean mouth with water. Call a physician immediately.
Most important symptoms and effects	Difficulty in breathing. Causes burns by all exposure routes. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	CO_2, dry chemical, dry sand, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	92 °C / 197.6 °F
Method -	No information available
Autoignition Temperature	450 °C / 842 °F
Explosion Limits	
Upper	23.5% @ 140°C
Lower	3.0% @140°C
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. The product causes burns of eyes, skin and mucous membranes. Combustible material. Containers may explode when heated.

Hazardous Combustion Products
Carbon monoxide (CO). Carbon dioxide (CO_2). Nitrogen oxides (NOx). Thermal decomposition can lead to release of irritating gases and vapors.

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. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health	Flammability	Instability	Physical hazards
3	2	1	N/A

6. Accidental release measures

Personal Precautions	Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment. Do not flush into surface water or sanitary sewer system. See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage.

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

7. Handling and storage

Handling Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Do not breathe mist/vapors/spray. Keep away from open flames, hot surfaces and sources of ignition.

Storage. Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area. Keep away from heat, sparks and flame. Store under an inert atmosphere. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Ethanolamine	TWA: 3 ppm STEL: 6 ppm	(Vacated) TWA: 3 ppm (Vacated) TWA: 8 mg/m³ (Vacated) STEL: 6 ppm (Vacated) STEL: 15 mg/m³ TWA: 3 ppm TWA: 6 mg/m³	IDLH: 30 ppm TWA: 3 ppm TWA: 8 mg/m³ STEL: 6 ppm STEL: 15 mg/m³	TWA: 3 ppm TWA: 8 mg/m³ STEL: 6 ppm STEL: 15 mg/m³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists
OSHA - Occupational Safety and Health Administration
NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas.

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. Tight sealing safety goggles. Face protection shield.

Skin and body protection Wear impervious gloves and/or clothing if needed to prevent contact with the material.

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	Liquid
Appearance	Colorless
Odor	Fishy
Odor Threshold	No information available
pH	12 @ 20°C 20 g/l aq. sol
Melting Point/Range	10 °C / 50 °F
Boiling Point/Range	170 °C / 338 °F @ 760 mmHg
Flash Point	92 °C / 197.6 °F

Evaporation Rate	> 1 (Butyl Acetate = 1.0)
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	23.5% @ 140°C
Lower	3.0% @140°C
Vapor Pressure	0.48 mmHg @ 20°C
Vapor Density	2.1 (Air = 1.0)
Specific Gravity	1.012
Solubility	miscible
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	450 °C / 842 °F
Decomposition Temperature	No information available
Viscosity	24 cP at 20 °C
Molecular Formula	C2 H7 N O
Molecular Weight	61.08

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Hygroscopic. Air sensitive.

Conditions to Avoid Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Exposure to moist air or water.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2), Nitrogen oxides (NOx), Thermal decomposition can lead to release of irritating gases and vapors

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
Ethanolamine	1720 mg/kg (Rat)	1000 mg/kg (Rabbit) 1 mL/kg (Rabbit)	LC50 > 1.3 mg/L (Rat) 6 h

Toxicologically Synergistic Products No information available

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

Irritation Causes burns by all exposure routes

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
Ethanolamine	141-43-5	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 Respiratory system
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

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. Contains a substance which is:. Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Ethanolamine	EC50: 15 mg/L/72h	Leusiscus idus: LC50: >200 mg/L/48h Salmo gairdneri: LC50: 150 mg/L/96h	Pseudomonas putida: EC50: 110 mg/L/17 h Nitrosomonas: EC50: 12200 mg/L/2 h Photobacterium phosphoreum: EC50: 13.7 mg/L/30 min	EC50: 65 mg/L/48h

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

Bioaccumulation/ Accumulation No information available.

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

Component	log Pow
Ethanolamine	-1.91

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
UN-No UN2491
Proper Shipping Name ETHANOLAMINE
Hazard Class 8
Packing Group III

TDG
UN-No UN2491
Proper Shipping Name ETHANOLAMINE
Hazard Class 8
Packing Group III

IATA
UN-No UN2491
Proper Shipping Name ETHANOLAMINE
Hazard Class 8

Packing Group	III

IMDG/IMO

UN-No	UN2491
Proper Shipping Name	ETHANOLAMINE
Hazard Class	8
Packing Group	III

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Ethanolamine	141-43-5	X	ACTIVE	-

Legend:
TSCA US EPA (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), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Ethanolamine	141-43-5	X	-	205-483-3	X	X	X	X	X	X

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

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
Ethanolamine	X	X	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 This product does not contain any DHS chemicals.

Security

Other International Regulations

Mexico - Grade Slight risk, Grade 1

Authorisation/Restrictions according to EU REACH

Component	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Ethanolamine	-	Use restricted. See item 75. (see link for restriction details)	-

https://echa.europa.eu/substances-restricted-under-reach

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Ethanolamine	141-43-5	Listed	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Ethanolamine	141-43-5	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

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

Creation Date 11-Jun-2009
Revision Date 24-Dec-2021
Print Date 24-Dec-2021
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

SAFETY DATA SHEET

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY

MANUFACTURER'S NAME / ADDRESS

ARIZONA POLYMER FLOORING
4565 W WATKINS ST.
PHOENIX, AZ 85043 .

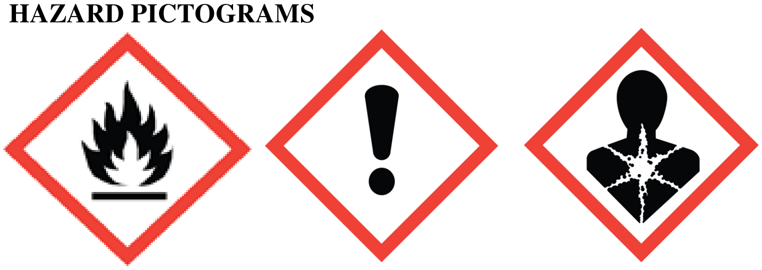
TRADE NAME: POLYURETHANE 250 PART B
COLOR: CLEAR
MAIN USE: SPECIALTY FLOORING CURATIVE

EMERGENCY TELEPHONE NUMBER: (800) 424-9300 (CHEMTREC)

SECTION 2: HAZARDS IDENTIFICATION

GLOBALLY HARMONIZED SYSTEM (GHS) CLASSIFICATION:
FLAMMABLE LIQUIDS: CATEGORY 3
ACUTE TOXICITY: CATEGORY 4 (INHALATION-MIST)
RESPIRATORY SENSITIZATION: CATEGORY 1
SKIN SENSITIZATION: CATEGORY 1
ACUTE AQUATIC TOXICITY: CATEGORY 2
CHRONIC AQUATIC TOXICITY: CATERGORY 3

GHS LABEL ELEMENTS
HAZARD PICTOGRAMS



SIGNAL WORD: DANGER!

HAZARD STATEMENTS:
H226: FLAMMABLE LIQUID AND VAPOR
H332: HARMFUL IF INHALED
H334: MAY CAUSE ALLERGY OR ASTHMA SYMPTOMS OR BREATHING DIFFICULTIES IF INHALED
H317: MAY CAUSE AN ALLERGIC SKIN REACTION
H304: MAY BE FATAL IF SWALLOWED AND ENTERS AIRWAY
H335: MAY CAUSE RESPIRATORY IRRITATION
H402: HARMFUL TO AQUATIC LIFE

PRECAUTIONARY STATEMENTS:

PREVENTION
P280: WEAR PROTECTIVE GLOVES/ PROTECTIVE CLOTHING/ EYE PROTECTION/ FACE PROTECTION
P271: USE ONLY OUTDOORS OR IN WELL VENTILATED AREA
P261: AVOID BREATHING MIST/VAPORS
P210: KEEP AWAY FROM HEAT, SPARKS, OPEN FLAMES, AND HOT SURFACES. NO SMOKING
P273: AVOID RELEASE TO THE ENVIRONMENT
P284: (IN CASE OF INADEQUATE VENTILATION) WEAR RESPIRATORY PROTECTION.
P240: GROUND/BOND CONTAINER AND RECEIVING EQUIPMENT
P241: USE EXPLOSION-PROOF ELECTRICAL, VENTILATING AND LIGHTING EQUIPMENT
P242: USE ONLY NON-SPARKING TOOLS
P243: TAKE PRECAUTIONARY MEASURES AGAINST STATIC DISCHARGE

SECTION 2: HAZARDS IDENTIFICATION CON'T.

P272: CONTAMINATED WORK CLOTHING SHOULD NOT BE ALLOWED OUT OF THE WORKPLACE

RESPONSE
P303+P361+353: **IF ON SKIN (OR HAIR):** REMOVE/TAKE OFF IMMEDIATELY ALL CONTAMINATED CLOTHING. RINSE SKIN WITH WATER/SHOWER
P333+P311: IF SKIN IRRITATION OR RASH OCCURS: CALL A POISON CENTER OR DOCTOR/PHYSICIAN
P304+P340: **IF INHALED:** REMOVE PERSON TO FRESH AIR AND KEEP COMFORTABLE FOR BREATHING
P362+P364: TAKE OFF CONTAMINATED CLOTHING AND WASH BEFORE REUSE.
P370+P378: IN CASE OF FIRE: USE DRY CHEMICAL, CARBON DIOXIDE (CO_2), FOAM, OR WATER SPRAY (FOR LARGE FIRES) TO EXTINGUISH

STORAGE
P403+P235: STORE IN A WELL-VENTILATED PLACE. KEEP COOL
P233: KEEP CONTAINER TIGHTLY CLOSED

DISPOSAL
P501: DISPOSE OF CONTENTS/CONTAINER TO AN APPROVED WASTE DISPOSAL PLANT

OTHER HAZARDS
NO DATA AVAILABLE

EMERGENCY OVERVIEW: DANGER!
HARMFUL IF INHALED
RESPIRATORY SENSITIZER
MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION
CONTAINS MATERIAL WHICH CAUSES DAMAGE TO THE FOLLOWING ORGANS: BLOOD, KIDNEYS, LIVER, GASTROINTESTINAL TRACT, RESPIRATORY TRACT, SKIN, NERVOUS SYSTEM, EYE, LENS OR CORNEA
FLAMMABLE LIQUID AND VAPOR
VAPOR MAY CAUSE FLASH FIRE
SKIN SENSITIZER

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

HAZARDOUS INGREDIENTS	Wt. %	CAS Number
HOMOPOLYMER OF HEXAMETHYLENE DIISOCYANATE	30-60	028182-81-2
ETHYL-3-ETHOXYPROPIONATE	30-60	000763-69-9
AROMATIC PETROLEUM DISTILLATES	30-60	064742-95-6
HEXAMETHYLENE-1,6- DIISOCYANATE	0.1-1.0	000822-06-0

SECTION 4: FIRST AID MEASURES

GENERAL: REMOVE PERSON FROM AFFECTED AREA AND MAKE COMFORTABLE. TREAT SYMPTOMATICALLY.

EYES: FLUSH WITH WATER FOR 15 MINUTES. GET MEDICAL ATTENTION.

SKIN: REMOVE PRODUCT AND FLUSH AFFECTED AREA WITH WATER FOR 15 MINUTES. IF IRRITATION PERSISTS GET MEDICAL ATTENTION.

INHALATION: MOVE TO FRESH AIR. GIVE ASSISTED RESPIRATION IF BREATHING HAS STOPPED OR IS LABORED (CALL A PHYSICIAN).

SECTION 4: FIRST AID MEASURES CON'T.

INGESTION: GIVE 3 – 4 GLASSES OF WATER OR MILK IF PERSON CONSCIOUS. **DO NOT INDUCE VOMITING!** OBTAIN MEDICAL CARE AND TREATMENT.

NOTES TO PHYSICIAN:
EYES: STAIN FOR EVIDENCE OF CORNEAL INJURY. IF CORNEA IS BURNED, INSTILL ANTIBIOTIC/STEROID PREPARATION AS NEEDED. WORKPLACE VAPORS COULD PRODUCE REVERSIBLE CORNEAL EPITHELIAL EDEMA IMPAIRING VISION.
SKIN: THIS COMPOUND IS A SKIN SENSITIZER. TREAT SYMPTOMATICALLY AS FOR CONTACT DERMATITIS OR THERMAL BURN.
INGESTION: TREAT SYMPTOMATICALLY. THERE IS NO SPECIFIC ANTIDOTE. INDUCING VOMITING IS CONTRAINDICATED BECAUSE OF THE IRRITATING NATURE OF THE COMPOUND.
INHALATION: TREATMENT IS ESSENTIALLY SYMPTOMATIC. AN INDIVIDUAL HAVING A DERMAL OR PULMONARY SENSITIZATION REACTION TO THIS MATERIAL SHOULD BE REMOVED FROM FURTHER EXPOSURE TO ANY ISOCYANATE.

SECTION 5: FIRE FIGHTING MEASURES

FLASH POINT: 43.3°C (110°F) TCC (SC #100)

CONDITIONS OF FLAMMABILITY: NA

FLAMMABLE LIMITS: **LEL**: 1.0% **UEL**: 7.0%

AUTO IGNITION TEMP.: 487.7°C (910°F)

OSHA CLASS: FLAMMABLE LIQUID, PACKING GROUP III

HAZARDOUS COMBUSTION PRODUCTS: CO, CO_2, ALDEHYDES, ACIDS

SENSITIVITY TO IMPACT: ND

SENSITIVITY TO STATIC DISCHARGE: ND

EXTINGUISHING MEDIA: IGNITION MAY GIVE RISE TO A CLASS B FIRE. IN CASE OF FIRE USE: WATER FOG, CARBON DIOXIDE, DRY CHEMICAL, ALCOHOL FOAM.

SPECIAL FIRE FIGHTING PROCEDURES: WEAR SELF-CONTAINED BREATHING APPARATUS AND PROTECTIVE CLOTHING. WATER SPRAY IS USEFUL IN COOLING FIRE-EXPOSED VESSELS AND IN DISPERSING VAPORS.

UNUSUAL FIRE AND EXPLOSIVE HAZARDS: MAY GENERATE TOXIC OR IRRITATING COMBUSTION PRODUCTS. SUDDEN REACTION AND FIRE MAY RESULT IF PRODUCT IS MIXED WITH AN OXIDIZING AGENT. SOLVENT VAPORS MAY BE HEAVIER THAN AIR. UNDER CONDITIONS OF STAGNANT AIR, VAPORS MAY BUILD UP AND TRAVEL ALONG THE GROUND TO AN IGNITION SOURCE.

SECTION 6: ACCIDENTAL RELEASE MEASURES

STEPS TO BE TAKEN IN CASE MATERIAL IS RELEASED OR SPILLED: EVACUATE NON-ESSENTIAL PERSONNEL. SHUT OFF SOURCES OF IGNITION. PUT ON PERSONAL PROTECTIVE EQUIPMENT. CONTROL SOURCE OF LEAK. VENTILATE. CONTAIN THE SPILL TO PREVENT SPREAD TO DRAINS, SEWERS, WATER SUPPLIES, OR SOIL. POUR DECONTAMINATION SOLUTION OVER SPILL AND ALLOW TO REACT FOR AT LEAST 15 MINUTES. COLLECT MATERIAL IN OPEN CONTAINERS WITH FURTHER AMOUNTS OF DECONTAMINATION SOLUTION. WASH DOWN SPILL AREA WITH DECONTAMINATION SOLUTION.

DECONTAMINATION SOLUTIONS: COLORIMETRIC LABORATORIES INC. (CLI) DECONTAMINATION SOLUTION OR 20% NON-IONIC SURFACTANT (TERGITOL TMN-10) WITH 80% WATER.

SECTION 7: HANDLING AND STORAGE

GENERAL: STORE IN COOL, WELL VENTILATED AREAS. KEEP AWAY FROM HEAT AND OPEN FLAMES. AVOID PROLONGED INHALATION OF HEATED VAPORS OR MISTS. AVOID PROLONGED SKIN CONTACT. USE NON-SPARKING TOOLS AND GROUNDING CABLES WHEN TRANSFERRING. CONTAINERS MAY BE HAZARDOUS WHEN EMPTY.

SECTION 7: HANDLING AND STORAGE CON'T.

STORAGE: AVOID TEMPERATURE EXTREMES. STORE AWAY FROM EXCESSIVE HEAT, FROM SOURCES OF IGNITION AND FROM REACTIVE MATERIALS. MATERIAL CAN BURN; LIMIT INDOOR STORAGE TO AREAS EQUIPPED WITH AUTOMATIC SPRINKLERS. STORE OUT OF DIRECT SUNLIGHT IN A COOL PLACE. KEEP CONTAINERS TIGHTLY CLOSED. GROUND ALL METAL CONTAINERS DURING STORAGE AND HANDLING.

SECTION 8: EXPOSURE CONTROL/PERSONAL PROTECTION

EXPOSURE LIMITS (ppm)

INGREDIENTS (CAS)	OSHA TWA	OSHA STEL	ACGIH TWA	ACGIH STEL	OTHER
028182-81-2	NE	NE	NE	NE	
000763-69-9	50	100	50	100	
064742-95-6	NE	NE	NE	NE	
000822-06-0	NE	NE	0.005	NE	

LEGEND: (M) MAX. EXPOSURE LIMIT; (S) OCCUPATIONAL EXP. LIMIT; (R) SUPPLIERS REC. LIMIT, (+) PERCUTANEOUS RISK
NOTE 1: VALUES MEANINGFUL ONLY WHEN HARDENED PRODUCT IS ABRADED, GROUND, ETC.

ENGINEERING CONTROLS: EXHAUST VENTILATION SUFFICIENT TO KEEP AIRBORNE CONCENTRATION OF THE SOLVENTS BELOW THEIR RESPECTIVE TLV'S. EXHAUST AIR MAY NEED TO BE CLEANED BY SCRUBBERS OR FILTERS TO REDUCE ENVIRONMENTAL CONTAMINATION.

PROTECTIVE GLOVES: NITRILE RUBBER

EYE PROTECTION: SPLASH-PROOF GOGGLES OR CHEMICAL SAFETY GLASSES

RESPIRATORY PROTECTION: A RESPIRATOR THAT IS RECOMMENDED FOR USE IN ISOCYANATE CONTAINING ENVIRONMENTS (AIR PURIFYING OR FRESH AIR SUPPLIED) MAY BE NECESSARY FOR SPRAY APPLICATIONS OR OTHER SITUATIONS SUCH AS HIGH TEMPERATURE USE WHICH MAY PRODUCE INHALATION EXPOSURES. A SUPPLIED AIR RESPIRATOR (EITHER POSITIVE PRESSURE TYPE OR CONTINUOUS FLOW TYPE) IS RECOMMENDED. BEFORE AN AIR PURIFYING RESPIRATOR CAN BE USED, AIR MONITORING MUST BE PERFORMED TO DETERMINE THE AIRBORNE CONCENTRATIONS OF HDI MONOMER, HDI POLYISOCYANATE AND ORGANIC SOLVENTS.

OTHER PROTECTIVE EQUIPMENT: LONG SLEEVED SHIRTS AND TROUSERS. EMERGENCY SHOWERS AND EYE WASH STATIONS SHOULD BE READILY ACCESSIBLE.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

BOILING POINT: >168°C (335°F)

SPECIFIC GRAVITY: 1.10-1.20

VAPOR PRESSURE: 2.1mmHg @ 20°C (68°F)

MELTING POINT: ND

VAPOR DENSITY: 4.50
(AIR = 1)

EVAPORATION RATE: 0.19 (SC #100)
(BUTYL ACETATE = 1)

SOLUBILITY IN WATER: INSOLUBLE, REACTS SLOWLY WITH WATER TO LIBERATE CO2 GAS

COEFFICIENT of WATER/OIL DISTRIBUTION: ND

ODOR THRESHOLD: ND

APPEARANCE AND ODOR: CLEAR LIQUID, AROMATIC SOLVENT ODOR

% VOLATILES BY VOLUME: 68.1%

%SOLIDS BY WEIGHT: 37.8%

SECTION 10: STABILITY AND REACTIVITY

STABILITY: STABLE; HOWEVER MAY FORM PEROXIDES OF UNKNOWN STABILITY

CONDITIONS TO AVOID: NOT APPLICABLE (MATERIAL IS STABLE).

INCOMPATIBILITY (MATERIALS TO AVOID)- WATER, AMINES, STRONG BASES, ALCOHOLS, METAL COMPOUNDS AND SURFACE ACTIVE MATERIALS.

HAZARDOUS DECOMPOSITION PRODUCTS: BY HIGH HEAT AND FIRE; CO, CO2, OXIDES OF NITROGEN, HCN, HDI.

HAZARDOUS POLYMERIZATION (REACTIVITY): MAY OCCUR. CONTACT WITH MOISTURE OR OTHER MATERIALS THAT REACT WITH ISOCYANATES OR TEMPERATURES OVER 400F (204C) MAY CAUSE POLYMERIZATION.

SECTION 11: TOXICOLOGICAL INFORMATION

PRIMARY ROUTES OF ENTRY: EYE CONTACT, SKIN CONTACT, INHALATION, INGESTION.

HEALTH HAZARDS (ACUTE AND CHRONIC EXPOSURES)

EYES:
ACUTE –VAPORS ARE IRRITATING AND CAN CAUSE PAIN, TEARING, REDDENING AND SWELLING. IF LEFT UNTREATED, CORNEAL DAMAGE CAN OCCUR AND INJURY IS SLOW TO HEAL. HOWEVER DAMAGE IS USUALLY REVERSIBLE
CHRONIC – MAY RESULT IN CORNEAL OPACITY. PROLONGED VAPOR CONTACT MAY CAUSE CONJUNCTIVITIS.

SKIN CONTACT:
ACUTE – ISOCYANATES REACT WITH SKIN PROTEIN AND MOISTURE AND CAN CAUSE IRRITATION. SYMPTOMS OF SKIN IRRITATION MAY BE REDDENING, SWELLING, RASH, SCALING OR BLISTERING. SOME PERSONS MAY DEVELOP SKIN SENSITIZATION FROM SKIN CONTACT. CURED MATERIAL IS DIFFICULT TO REMOVE. REPEATED OR PROLONGED SKIN CONTACT WITH SOLVENTS CAN RESULT IN DRY, DEFATTED AND CRACKED SKIN CAUSING INCREASED SUSCEPTIBILITY TO INFECTION. IN ADDITION IRRITATION MAY DEVELOP INTO DERMATITIS. SOLVENTS CAN PENETRATE THE SKIN AND MAY CAUSE EFFECTS SIMILAR TO THOSE IDENTIFIED UNDER ACUTE INHALATION SYMPTOMS.
CHRONIC – PROLONGED CONTACT WITH ISOCYANATES CAN CAUSE REDDENING, SWELLING, RASH, SCALING OR BLISTERING. IN THOSE WHO HAVE DEVELOPED A SKIN SENSITIZATION, THESE SYMPTOMS CAN DEVELOP AS A RESULT OF CONTACT WITH VERY SMALL AMOUNTS OF LIQUID OR EVEN AS A RESULT OF VAPOR-ONLY EXPOSURE. SOLVENTS CAN PENETRATE THE SKIN AND MAY CAUSE SYSTEMIC EFFECTS SIMILAR TO THOSE IDENTIFIED UNDER CHRONIC INHALATION EFFECTS.

SKIN ABSORPTION:
ACUTE—ND
CHRONIC-- ND

INHALATION:
ACUTE –HDI AEROSOLS OR VAPORS AT CONCENTRATIONS ABOVE THE APPLICABLE EXPOSURE LIMITS CAN IRRITATE THE MUCOUS MEMBRANES IN THE RESPIRATORY TRACT CAUSING RUNNY NOSE, SORE THROAT, COUGHING, CHEST DISCOMFORT, SHORTNESS OF BREATH AND REDUCED LUNG FUNCTION. PERSONS WITH PRE-EXISTING NONSPECIFIC BRONCHIAL HYPER REACTIVITY CAN RESPOND TO CONCENTRATIONS BELOW THE EXPOSURE LIMITS WITH SIMILAR SYMPTOMS AS WELL AS AN ASTHMA ATTACK. EXPOSURE WELL ABOVE THE EXPOSURE LIMITS MAY LEAD TO BRONCHITIS, BRONCHIAL SPASM AND PULMONARY EDEMA. CHEMICAL OR HYPERSENSITIVE PNEUMONITIS HAS ALSO BEEN REPORTED. SOLVENT VAPORS ARE IRRITATING TO THE EYES NOSE AND THROAT. SYMPTOMS OF IRRITATION MAY INCLUDE RED, ITCHY EYES, DRYNESS OF THE THROAT AND A FEELING OF TIGHTNESS IN THE CHEST.

SECTION 11: TOXICOLOGICAL INFORMATION CON'T.

OTHER POSSIBLE SYMPTOMS OF OVEREXPOSURE INCLUDE: HEADACHE, DIZZINESS, NAUSEA, NARCOSIS, FATIGUE AND LOSS OF APPETITE.
CHRONIC – AS A RESULT OF PREVIOUS REPEATED OVEREXPOSURES OR A SINGLE LARGE DOSE, CERTAIN INDIVIDUALS WILL DEVELOP ISOCYANTE SENSITIZATION (CHEMICAL ASTHMA) WHICH WILL CAUSE THEM TO REACT TO A LATER EXPOSURE TO ISOCYANATES AT LEVELS WELL BELOW APPLICABLE EXPOSURE LIMITS. THESE SYMPTOMS, WHICH INCLUDE CHEST TIGHTNESS, WHEEZING, COUGH, SHORTNESS OF BREATH OR ASTHMATIC ATTACK, COULD BE IMMEDIATE OR DELAYED UP TO SEVERAL HOURS AFTER EXPOSURE. SIMILAR TO MANY NON-SPECIFIC ASTHMATIC RESPONSES, THERE ARE REPORTS THAT ONCE SENSITIZED AN INDIVIDUAL CAN EXPERIENCE THESE SYMPTOMS UPON EXPOSURE TO DUST, COLD AIR OR OTHER IRRITANTS. THIS INCREASED LUNG SENSITIVITY CAN PERSIST FOR WEEKS AND IN SEVERE CASES FOR SEVERAL YEARS.

CHRONIC OVEREXPOSURE TO ISOCYANTES HAS ALSO BEEN REPORTED TO CAUSE LUNG DAMAGE, INCLUDING DECREASE IN LUNG FUNCTION, WHICH MAY BE PERMANENT. SENSITIZATION MAY BE EITHER TEMPORARY OR PERMANENT. CHRONIC EXPOSURE TO ORGANIC SOLVENTS HAS BEEN ASSOCIATED WITH VARIOUS NEUROTOXIC EFFECTS INCLUDING PERMANENT BRAIN AND NERVOUS SYSTEM DAMAGE. SYMPTOMS INCLUDE LOSS OF MEMORY, LOSS OF INTELLECTUAL ABILITY AND LOSS OF COORDINATION.

INGESTION:
ACUTE – CAN RESULT IN IRRITATION AND POSSIBLE CORROSIVE ACTION IN THE MOUTH, STOMACH TISSUE AND DIGESTIVE TRACT. SYMPTOMS CAN INCLUDE SORE THROAT, ABDOMINAL PAIN, NAUSEA, VOMITING AND DIARRHEA. VOMITING MAY CAUSE ASPIRATION OF SOLVENT RESULTING IN CHEMICAL PNEUMONITIS
CHRONIC -- ND

CONDITIONS AGGRAVATED BY EXPOSURE: ASTHMA AND OTHER RESPIRATORY DISORDERS, SKIN ALLERGIES, ECZEMA

ACUTE TOXICITY: NO DATA ON THE PRODUCT ITSELF

ACUTE ORAL TOXICITY- COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	LD50: >2500mg/kg	SPECIES: RAT
AROMATIC PETROLEUM DISTILLATES	LD50: 8400 mg/kg	SPECIES: RAT
ETHYL-3-ETHOXYPROPIONATE	LD50: >5000 mg/kg	SPECIES: RAT

ACUTE DERMAL TOXICITY- COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	LD50: >2000 mg/kg	SPECIES: RAT
AROMATIC PETROLEUM DISTILLATES	LD50: >2000 mg/kg	SPECIES: RABBIT
ETHYL-3-ETHOXYPROPIONATE	LD50: 4080 mg/kg	SPECIES: RAT

ACUTE INHALATION TOXICITY- COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	LC50: 0.467 mg/l
AROMATIC PETROLEUM DISTILLATES	LC50: 3400 ppm
ETHYL-3-ETHOXYPROPIONATE	LC50: >998 ppm OECD TEST GUIDLINE 403

SKIN CORROSION/IRRITATION
SLIGHTLY TO MODERATELY IRRITATING

SERIOUS EYE DAMAGE/EYE IRRITATION
SLIGHTLY TO MODERATELY IRRITATING

SECTION 11: TOXICOLOGICAL INFORMATION CON'T.

SENSITIZATION
PULMONARY AND DERMAL SENSITIZER IN ANIMALS AND HUMANS. EVIDENCE EXISTS THAT CROSS SENSITIZATION BETWEEN HDI AND OTHER ISOCYANATES, PARTICULARLY HYDROGENATED MDI AND TDI, CAN OCCUR.

SPECIFIC TARGET ORGAN SYSTEMIC TOXICITY (SINGLE EXPOSURE)
CATEGORY 3 (IRRITATING TO RESPIRATORY SYSTEM)

CARCINOGENIC DATA: **NTP**: NONE **OSHA**: NONE **IARC**: NONE

TERATOGENICITY: NO MUTAGENICITY: NO

EMBRYOTOXICITY: NO SYNERGISTIC MATERIAL: NO

SECTION 12: ECOLOGICAL INFORMATION

TOXICITY

AQUATIC TOXICITY: NO DATA ON THE PRODUCT ITSELF. BASED ON THE COMPONENTS THE PRODUCT IS ACUTELY HARMFUL FOR AQUATIC ORGANISMS.

ACUTE TOXICITY TO FISH- COMPONENTS

HEXAMETHYLENE-1,6-DIISOCYANATE	LC50 (96 HRS): 100 mg/l	SPECIES: FATHEAD MINNOW
AROMATIC PETROLEUM DISTILLATES	LC50 (96 HRS): 9.22 mg/l	SPECIES: FATHEAD MINNOW
ETHYL-3-ETHOXYPROPIONATE	LC50 (96 HRS): 55.3 mg/l	SPECIES: FATHEAD MINNOW

ACUTE TOXICITY TO AQUATIC INVERTEBRATES: COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	EC50 (48 HRS): 127 mg/l	SPECIES: DAPHNIA MAGNA
AROMATIC PETROLEUM DISTILLATES	EC50 (48 HRS): 6.14 mg/l	SPECIES: DAPHNIA MAGNA
ETHYL-3-ETHOXYPROPIONATE	EC50 (48 HRS): 479.7 mg/l	SPECIES: DAPHNIA MAGNA

ACUTE TOXICITY TO ALGAE/AQUATIC PLANTS: COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	EC50 (72 HRS): >1000 mg/l	SPECIES: GREEN ALGAE
AROMATIC PETROLEUM DISTILLATES	ND	
ETHYL-3-ETHOXYPROPIONATE	EC50 (72 HRS): 114.9 mg/l	SPECIES: GREEN ALGAE

TOXICITY TO BACTERIA: COMPONENTS

HEXAMETHYLENE-1,6- DIISOCYANATE	EC50: > 880mg/l	ACTIVATED SLUDGE
AROMATIC PETROLEUM DISTILLATES	ND	
ETHYL-3-ETHOXYPROPIONATE	EC50: > 5000mg/l	ACTIVATED SLUDGE

CHRONIC AQUATIC TOXICITY
CHRONIC TOXICITY TO AQUATIC INVERTEBRATES
LONG LASTING ADVERSE EFFECTS TO AQUATIC ORGANISMS

PERSISTANCE AND DEGRADABILITY
BIODEGRADABILITY: NOT READILY BIODEGRADABLE (BY OECD CRITERIA)

BIOACCUMULATIVE POTENTIAL
BIOACCUMULATION: ND
PARTITION COEFFECIENT: N-OCTANOL/WATER(LOG P_{OW}): ND

MOBILITY IN SOIL
ND

SECTION 13: DISPOSAL CONSIDERATIONS

WASTE DISPOSAL METHODS: INCINERATION IS PREFERED. THIS PRODUCT SHOULD NOT BE ALLOWED TO ENTER DRAINS, WATER COURSES OR THE SOIL. PLACE IN AN APPROPRIATE DISPOSAL FACILITY IN COMPLIANCE WITH ALL FEDERAL, STATE AND LOCAL REGULATIONS.

SECTION 14: TRANSPORT INFORMATION

DOT PROPER SHIPPING NAME: UN1866, RESIN SOLUTION, FLAMMABLE, (CONTAINS SC #100), 3, PG III

PACKAGING GROUP: III **DOT PRODUCT RQ LBS (KGS):** NA

HAZARD LABEL: FLAMMABLE LIQUID **HAZARD PLACARD:** FLAMMABLE LIQUID

IMO SHIPPING DATA: UN1866, RESIN SOLUTION, FLAMMABLE, (CONTAINS SC #100), 3, PG III

ICAO/IATA SHIPPING DATA: UN1866, RESIN SOLUTION, FLAMMABLE, (CONTAINS SC #100), 3, PG III

PASSENGER AIR MAX QUANTITY: 60L **PASSENGER PACKING INSTRUCTION:** 309

CARGO AIR- MAX QUANTITY: 220L **CARGO AIR INSTRUCTION NUMBER:** 310

SECTION 15: REGULATORY INFORMATION

VOC: COMPONENT = 115 gms/Liter **AS APPLIED** (Part of a multi-component system) = 350 gms/Liter

TSCA (TOXIC SUBSTANCE CONTROL ACT): ALL COMPONENTS ARE LISTED IN THE TSCA CHEMICAL SUBSTANCE INVENTORY.

CERCLA (COMPREHENSIVE RESPONSE COMPENSATION and LIABILITY ACT): REPORTABLE QUANTITY, MEK 5000 LBS.

SARA TITLE III

SECTION 312 HAZARD CLASS: IMMEDIATE (ACUTE) HEALTH HAZARD, DELAYED HEALTH HAZARD; FIRE HAZARD.

SECTION 313 LISTED INGREDIENTS: CAS# 822-06-0 HEXAMETHYLENE DIISOCYANATE

CALIFORNIA PROPOSITION 65: The below list of compounds is known to the State of California to cause cancer, birth defects or other reproductive harm: NONE.

SECTION 16: OTHER INFORMATION

INITIAL ISSUE DATE: MAY 27, 2015 **REVISION DATE:** **PREPARED BY:** J.W. ESSIG

HAZARD RATING

HMIS: **HEALTH 2** **FLAMMABILITY 1** **REACTIVITY 1**

LEGEND

ACGIH:	AMERICAN CONFERENCE OF GOVERNMENTAL INDUSTRIAL HYGIENISTS
OSHA:	OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION
STEL:	SHORT TERM EXPOSURE LIMIT
TWA:	TIME WEIGHTED AVERAGE
PEL:	PERMISSIBLE EXPOSURE LIMIT
TLV:	THRESHOLD LIMIT VALUE
NA:	NOT APPLICABLE
NE:	NOT ESTABLISHED
ND:	NO DATA

SAFETY DATA SHEET
Polyurethane Coating

According to Regulation (EC) No 1907/2006, Annex II, as amended. Commission Regulation (EU) No 2015/830 of 28 May 2015.

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

1.1. Product identifier

Product name Polyurethane Coating

Product number PUC-a, EPUC400, ZE

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

Identified uses Appliance protection.

Uses advised against No specific uses advised against are identified.

1.3. Details of the supplier of the safety data sheet

Supplier

ELECTROLUBE. A division of HK WENTWORTH LTD
ASHBY PARK, COALFIELD WAY,
ASHBY DE LA ZOUCH, LEICESTERSHIRE LE65 1JR
UNITED KINGDOM
+44 (0)1530 419600
+44 (0)1530 416640
info@hkw.co.uk

1.4. Emergency telephone number

Emergency telephone

IN CASE OF EMERGENCY CALL:
+44 1865 407333 (24hr, Provided by Carechem 24)
+353 (0)1 809 2166 (Beaumont Hospital, Republic of Ireland only, 8am-10pm, 7 days a week)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (EC 1272/2008)

Physical hazards Aerosol 1 - H222, H229

Health hazards STOT SE 3 - H336 STOT RE 1 - H372

Environmental hazards Aquatic Chronic 2 - H411

2.2. Label elements

Hazard pictograms

Signal word Danger

Polyurethane Coating

Hazard statements	EUH208 Contains 2-butanone oxime, 4,5-Dichloro-2-octyl-2H-isothiazol-3-one. May produce an allergic reaction. H222 Extremely flammable aerosol. H229 Pressurised container: may burst if heated. H336 May cause drowsiness or dizziness. H372 Causes damage to organs through prolonged or repeated exposure. H411 Toxic to aquatic life with long lasting effects.
Precautionary statements	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P211 Do not spray on an open flame or other ignition source. P251 Do not pierce or burn, even after use. P260 Do not breathe spray. P410+P412 Protect from sunlight. Do not expose to temperatures exceeding 50°C/122°F. P501 Dispose of contents/ container in accordance with national regulations.
Contains	Naphtha (petroleum), hydrodesulfurized heavy, Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Supplementary precautionary statements	P264 Wash contaminated skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P273 Avoid release to the environment. P314 Get medical advice/ attention if you feel unwell. P391 Collect spillage.

2.3. Other hazards

This product does not contain any substances classified as PBT or vPvB.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Petroleum gases, liquefied			**30-60%**
CAS number: 68476-85-7	EC number: 270-704-2		

Classification
Flam. Gas 1 - H220

Naphtha (petroleum), hydrodesulfurized heavy			**10-30%**
CAS number: 64742-82-1	EC number: 265-185-4	REACH registration number: 01-2119458049-33-XXXX	

Classification
Flam. Liq. 3 - H226
STOT SE 3 - H336
STOT RE 1 - H372
Asp. Tox. 1 - H304
Aquatic Chronic 2 - H411

Polyurethane Coating

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)		**10-30%**
CAS number: 64742-82-1	EC number: 919-446-0	REACH registration number: 01-2119458049-33-XXXX

Classification
Flam. Liq. 3 - H226
STOT SE 3 - H336
STOT RE 1 - H372
Asp. Tox. 1 - H304
Aquatic Chronic 2 - H411

2-butanone oxime		**0.1-1%**
CAS number: 96-29-7	EC number: 202-496-6	REACH registration number: 01-2119539477-28-XXXX

Classification
Acute Tox. 4 - H312
Eye Dam. 1 - H318
Skin Sens. 1 - H317
Carc. 2 - H351

Cobalt bis(2-ethylhexanoate)		**<0.1%**
CAS number: 136-52-7	EC number: 205-250-6	REACH registration number: 01-2119524678-29-XXXX
M factor (Acute) = 1		

Classification
Eye Irrit. 2 - H319
Skin Sens. 1 - H317
Repr. 2 - H361f
Aquatic Acute 1 - H400
Aquatic Chronic 3 - H412

4,5-Dichloro-2-octyl-2H-isothiazol-3-one		**<0.1%**
CAS number: 64359-81-5	EC number: 264-843-8	
M factor (Acute) = 100	M factor (Chronic) = 100	

Classification
Acute Tox. 4 - H302
Acute Tox. 4 - H312
Acute Tox. 2 - H330
Skin Corr. 1C - H314
Eye Dam. 1 - H318
Skin Sens. 1A - H317
STOT SE 3 - H335
Aquatic Acute 1 - H400
Aquatic Chronic 1 - H410

Polyurethane Coating

The full text for all hazard statements is displayed in Section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention immediately. Show this Safety Data Sheet to the medical personnel.
Inhalation	Remove affected person from source of contamination. Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Place unconscious person on their side in the recovery position and ensure breathing can take place.
Ingestion	Rinse mouth thoroughly with water. Remove any dentures. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Do not induce vomiting unless under the direction of medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Never give anything by mouth to an unconscious person. Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Place unconscious person on their side in the recovery position and ensure breathing can take place. Maintain an open airway. Loosen tight clothing such as collar, tie or belt.
Skin contact	Rinse with water.
Eye contact	Rinse immediately with plenty of water. Remove any contact lenses and open eyelids wide apart. Continue to rinse for at least 10 minutes.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue. Wash contaminated clothing thoroughly with water before removing it from the affected person, or wear gloves. It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.

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

General information	See Section 11 for additional information on health hazards. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Headache. Nausea, vomiting. Central nervous system depression. Drowsiness, dizziness, disorientation, vertigo. Narcotic effect.
Ingestion	Due to the physical nature of this product, it is unlikely that ingestion will occur.
Skin contact	Repeated exposure may cause skin dryness or cracking.
Eye contact	May be slightly irritating to eyes. May cause discomfort.

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

Notes for the doctor	Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	The product is flammable. Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Polyurethane Coating

Specific hazards Containers can burst violently or explode when heated, due to excessive pressure build-up. Bursting aerosol containers may be propelled from a fire at high speed. If aerosol cans are ruptured, care should be taken due to the rapid escape of the pressurised contents and propellant. Vapours may form explosive mixtures with air.

Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours.

5.3. Advice for firefighters

Protective actions during firefighting Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. If a leak or spill has not ignited, use water spray to disperse vapours and protect men stopping the leak. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions No action shall be taken without appropriate training or involving any personal risk. Keep unnecessary and unprotected personnel away from the spillage. Wear protective clothing as described in Section 8 of this safety data sheet. Follow precautions for safe handling described in this safety data sheet. Wash thoroughly after dealing with a spillage. Ensure procedures and training for emergency decontamination and disposal are in place. Do not touch or walk into spilled material. Evacuate area. Risk of explosion. Provide adequate ventilation. No smoking, sparks, flames or other sources of ignition near spillage. Promptly remove any clothing that becomes contaminated.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment. Large Spillages: Inform the relevant authorities if environmental pollution occurs (sewers, waterways, soil or air).

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Eliminate all ignition sources if safe to do so. No smoking, sparks, flames or other sources of ignition near spillage. Approach the spillage from upwind. Under normal conditions of handling and storage, spillages from aerosol containers are unlikely. If aerosol cans are ruptured, care should be taken due to the rapid escape of the pressurised contents and propellant. Small Spillages: Wipe up with an absorbent cloth and dispose of waste safely. Large Spillages: If the product is soluble in water, dilute the spillage with water and mop it up. Alternatively, or if it is not water-soluble, absorb the spillage with an inert, dry material and place it in a suitable waste disposal container. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority.

6.4. Reference to other sections

Polyurethane Coating

Reference to other sections	For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions	Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Avoid exposing aerosol containers to high temperatures or direct sunlight. The product is flammable. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not spray on an open flame or other ignition source. Do not pierce or burn, even after use. Spray will evaporate and cool rapidly and may cause frostbite or cold burns if in contact with skin. Avoid contact with eyes. Avoid inhalation of vapours and spray/mists.
Advice on general occupational hygiene	Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Wash at the end of each work shift and before eating, smoking and using the toilet. Change work clothing daily before leaving workplace.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions	Store away from incompatible materials (see Section 10). Store in accordance with local regulations. Keep away from oxidising materials, heat and flames. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage. Protect from sunlight. Do not store near heat sources or expose to high temperatures. Do not expose to temperatures exceeding 50°C/122°F. Bund storage facilities to prevent soil and water pollution in the event of spillage. The storage area floor should be leak-tight, jointless and not absorbent.
Storage class	Miscellaneous hazardous material storage.

7.3. Specific end use(s)

Specific end use(s)	The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

Occupational exposure limits

Petroleum gases, liquefied

Long-term exposure limit (8-hour TWA): WEL 1000 ppm 1750 mg/m³
Short-term exposure limit (15-minute): WEL 1250 ppm 2180 mg/m³

Cobalt bis(2-ethylhexanoate)

Long-term exposure limit (8-hour TWA): 0.1 mg/m³
WEL = Workplace Exposure Limit.

Cobalt bis(2-ethylhexanoate) (CAS: 136-52-7)

DNEL	Professional - Inhalation; Long term local effects: 0.24 mg/m³ Consumer - Oral; Long term systemic effects: 0.06 mg/kg/day Consumer - Inhalation; Long term local effects: 0.04 mg/m³

Polyurethane Coating

PNEC	Fresh water; 0 mg/l marine water; 0 mg/l Sediment (Freshwater); 9.5 mg/kg Sediment (Marinewater), Sediment (Marinewater); 9.5 mg/kg STP; 0.37 mg/l Soil; 7.9 mg/kg

8.2. Exposure controls

Protective equipment

Appropriate engineering controls
Provide adequate ventilation. Personal, workplace environment or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment. Use process enclosures, local exhaust ventilation or other engineering controls as the primary means to minimise worker exposure. Personal protective equipment should only be used if worker exposure cannot be controlled adequately by the engineering control measures. Ensure control measures are regularly inspected and maintained. Ensure operatives are trained to minimise exposure.

Eye/face protection
Eyewear complying with an approved standard should be worn if a risk assessment indicates eye contact is possible. Personal protective equipment for eye and face protection should comply with European Standard EN166. Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.

Hand protection
Chemical-resistant, impervious gloves complying with an approved standard should be worn if a risk assessment indicates skin contact is possible. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, gloves should comply with European Standard EN374. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.

Other skin and body protection
Appropriate footwear and additional protective clothing complying with an approved standard should be worn if a risk assessment indicates skin contamination is possible.

Hygiene measures
Provide eyewash station and safety shower. Contaminated work clothing should not be allowed out of the workplace. Wash contaminated clothing before reuse. Clean equipment and the work area every day. Good personal hygiene procedures should be implemented. Wash at the end of each work shift and before eating, smoking and using the toilet. When using do not eat, drink or smoke. Preventive industrial medical examinations should be carried out. Warn cleaning personnel of any hazardous properties of the product.

Respiratory protection
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

Environmental exposure controls
Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Polyurethane Coating

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Aerosol.
Colour	Clear. Amber.
Odour	Solvent.
pH	Not available.
Melting point	Not available.
Initial boiling point and range	Not available.
Flash point	-4°C/24.8°F
Evaporation rate	Not available.
Flammability (solid, gas)	Not available.
Upper/lower flammability or explosive limits	Not available.
Vapour pressure	Not available.
Vapour density	Not available.
Relative density	0.870 @ 20°C/68°F
Solubility(ies)	Not available.
Partition coefficient	Not available.
Auto-ignition temperature	Not available.
Decomposition Temperature	Not available.
Viscosity	Not available.
Explosive properties	Not considered to be explosive.
Oxidising properties	Does not meet the criteria for classification as oxidising.

9.2. Other information

SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	See the other subsections of this section for further details.

10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	The following materials may react strongly with the product: Oxidising agents.

10.4. Conditions to avoid

Conditions to avoid	Avoid exposing aerosol containers to high temperatures or direct sunlight. Pressurised container: may burst if heated

10.5. Incompatible materials

Polyurethane Coating

Materials to avoid No specific material or group of materials is likely to react with the product to produce a hazardous situation.

10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Notes (oral LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50}) Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity Based on available data the classification criteria are not met.

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Reproductive toxicity - development Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure STOT SE 3 - H336 May cause drowsiness or dizziness.

Target organs Central nervous system

Specific target organ toxicity - repeated exposure

STOT - repeated exposure STOT RE 1 - H372

Aspiration hazard

Aspiration hazard Based on available data the classification criteria are not met.

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation A single exposure may cause the following adverse effects: Headache. Nausea, vomiting. Central nervous system depression. Drowsiness, dizziness, disorientation, vertigo. Narcotic effect.

Ingestion Due to the physical nature of this product, it is unlikely that ingestion will occur.

Skin contact Repeated exposure may cause skin dryness or cracking.

Eye contact May be slightly irritating to eyes. May cause discomfort.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs Central nervous system

Toxicological information on ingredients.

Petroleum gases, liquefied

Toxicological effects Not regarded as a health hazard under current legislation.

Acute toxicity - oral

Notes (oral LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50}) Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro Based on available data the classification criteria are not met.

Genotoxicity - in vivo Chromosome aberration: Negative. REACH dossier information. Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity Based on available data the classification criteria are not met.

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Reproductive toxicity - development Based on available data the classification criteria are not met.

Polyurethane Coating

Specific target organ toxicity - single exposure

STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard Not relevant. Gas.

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation No specific symptoms known.

Ingestion Due to the physical nature of this product, it is unlikely that ingestion will occur.

Skin contact No specific symptoms known.

Eye contact No specific symptoms known.

Route of exposure Inhalation Skin and/or eye contact

Target organs No specific target organs known.

Naphtha (petroleum), hydrodesulfurized heavy

Acute toxicity - oral

Notes (oral LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50}) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50}) Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro May cause genetic defects.

Carcinogenicity

Carcinogenicity May cause cancer.

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

Polyurethane Coating

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure	Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure	STOT RE 1 - H372

Aspiration hazard

Aspiration hazard	Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways. Pneumonia may be the result if vomited material containing solvents reaches the lungs.

General information	May cause cancer after repeated exposure. Risk of cancer depends on duration and level of exposure. May cause genetic defects. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	No specific symptoms known.
Ingestion	Aspiration hazard if swallowed. Entry into the lungs following ingestion or vomiting may cause chemical pneumonitis.
Skin contact	No specific symptoms known.
Eye contact	No specific symptoms known.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Acute toxicity - oral

Notes (oral LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50})	Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data	Repeated exposure may cause skin dryness or cracking.

Serious eye damage/irritation

Serious eye damage/irritation	Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation	Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation	Based on available data the classification criteria are not met.

Polyurethane Coating

Germ cell mutagenicity

Genotoxicity - in vitro	Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure	STOT SE 3 - H336 May cause drowsiness or dizziness.
Target organs	Central nervous system

Specific target organ toxicity - repeated exposure

STOT - repeated exposure	STOT RE 1 - H372

Aspiration hazard

Aspiration hazard	Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways. Pneumonia may be the result if vomited material containing solvents reaches the lungs.

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Headache. Nausea, vomiting. Central nervous system depression. Drowsiness, dizziness, disorientation, vertigo. Narcotic effect.
Ingestion	Aspiration hazard if swallowed. Entry into the lungs following ingestion or vomiting may cause chemical pneumonitis.
Skin contact	Repeated exposure may cause skin dryness or cracking.
Eye contact	No specific symptoms known.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	Central nervous system

2-butanone oxime

Acute toxicity - oral

Notes (oral LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50})	Acute Tox. 4 - H312 Harmful in contact with skin.
ATE dermal (mg/kg)	1,100.0

Acute toxicity - inhalation

Notes (inhalation LC_{50})	Based on available data the classification criteria are not met.

Polyurethane Coating

Skin corrosion/irritation

Animal data	Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation	Eye Dam. 1 - H318 Causes serious eye damage.

Respiratory sensitisation

Respiratory sensitisation	Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation	May cause skin sensitisation or allergic reactions in sensitive individuals.

Germ cell mutagenicity

Genotoxicity - in vitro	Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity	Suspected of causing cancer.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure	Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure	Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard	Based on available data the classification criteria are not met.

General information	May cause cancer after repeated exposure. Risk of cancer depends on duration and level of exposure. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	No specific symptoms known.
Ingestion	May cause sensitisation or allergic reactions in sensitive individuals.
Skin contact	May cause skin sensitisation or allergic reactions in sensitive individuals. May cause discomfort.
Eye contact	Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.
Medical considerations	Skin disorders and allergies.

Polyurethane Coating

Benzene, C10-13-alkyl derivatives

Acute toxicity - oral

Notes (oral LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50})	Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data	Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation	Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation	Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation	Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro	Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure	Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure	Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard	Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways. Pneumonia may be the result if vomited material containing solvents reaches the lungs.

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	No specific symptoms known.
Ingestion	Aspiration hazard if swallowed. Entry into the lungs following ingestion or vomiting may cause chemical pneumonitis.

Polyurethane Coating

Skin contact	No specific symptoms known.
Eye contact	No specific symptoms known.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

2-Ethylhexanoic acid, zirconium salt

Acute toxicity - oral

Notes (oral LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - dermal

Notes (dermal LD_{50})	Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC_{50})	Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data	Irritating.

Serious eye damage/irritation

Serious eye damage/irritation	Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation	Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation	Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro	Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure	Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure	Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard	Based on available data the classification criteria are not met.

Polyurethane Coating

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	No specific symptoms known.
Ingestion	May cause irritation.
Skin contact	Redness. Irritating to skin.
Eye contact	No specific symptoms known.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Acute toxicity - oral

Notes (oral LD_{50})	Acute Tox. 4 - H302 Harmful if swallowed.
ATE oral (mg/kg)	500.0

Acute toxicity - dermal

Notes (dermal LD_{50})	Acute Tox. 4 - H312 Harmful in contact with skin.
ATE dermal (mg/kg)	1,100.0

Acute toxicity - inhalation

Acute toxicity inhalation (LC_{50} dust/mist mg/l)	0.26
Species	Rat
Notes (inhalation LC_{50})	Acute Tox. 2 - H330 Fatal if inhaled.
ATE inhalation (dusts/mists mg/l)	0.26

Skin corrosion/irritation

Animal data	Skin Corr. 1C - H314 Causes severe burns.

Serious eye damage/irritation

Serious eye damage/irritation	Eye Dam. 1 - H318 Corrosive to skin. Corrosivity to eyes is assumed.

Respiratory sensitisation

Respiratory sensitisation	Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation	May cause skin sensitisation or allergic reactions in sensitive individuals.

Germ cell mutagenicity

Genotoxicity - in vitro	Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

Polyurethane Coating

Reproductive toxicity - fertility	Based on available data the classification criteria are not met.
Reproductive toxicity - development	Based on available data the classification criteria are not met.

<u>Specific target organ toxicity - single exposure</u>

STOT - single exposure	STOT SE 3 - H335 May cause respiratory irritation.
Target organs	Respiratory system, lungs

<u>Specific target organ toxicity - repeated exposure</u>

STOT - repeated exposure	Not classified as a specific target organ toxicant after repeated exposure.

<u>Aspiration hazard</u>

Aspiration hazard	Not relevant. Solid.

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.
Ingestion	May cause sensitisation or allergic reactions in sensitive individuals. May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.
Skin contact	May cause skin sensitisation or allergic reactions in sensitive individuals. Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.
Eye contact	Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	Respiratory system, lungs
Medical considerations	Skin disorders and allergies.

SECTION 12: Ecological information

<u>Ecological information on ingredients.</u>

<u>Petroleum gases, liquefied</u>

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

<u>2-butanone oxime</u>

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

<u>Benzene, C10-13-alkyl derivatives</u>

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

Polyurethane Coating

2-Ethylhexanoic acid, zirconium salt

Ecotoxicity Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

Toxicity Aquatic Chronic 2 - H411 Toxic to aquatic life with long lasting effects.

Ecological information on ingredients.

Petroleum gases, liquefied

Toxicity Based on available data the classification criteria are not met.

Acute aquatic toxicity

Acute toxicity - fish LC_{50}, 96 hours: 147.54 mg/l, Freshwater fish
Estimated value.

Acute toxicity - aquatic invertebrates EC_{50}, 48 hours: 16.33 mg/l, Daphnia magna
Estimated value.

Acute toxicity - aquatic plants EC_{50}, 96 hours: 11.89 mg/l, Freshwater algae
Estimated value.

Naphtha (petroleum), hydrodesulfurized heavy

Toxicity Aquatic Chronic 2 - H411 Toxic to aquatic life with long lasting effects.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Toxicity Aquatic Chronic 2 - H411 Toxic to aquatic life with long lasting effects.

2-butanone oxime

Toxicity Based on available data the classification criteria are not met.

Benzene, C10-13-alkyl derivatives

Toxicity Based on available data the classification criteria are not met.

2-Ethylhexanoic acid, zirconium salt

Toxicity Based on available data the classification criteria are not met.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Toxicity Aquatic Acute 1 - H400 Very toxic to aquatic life. Aquatic Chronic 1 - H410 Very toxic to aquatic life with long lasting effects.

Acute aquatic toxicity

$LE(C)_{50}$ $0.001 < L(E)C50 \leq 0.01$

M factor (Acute) 100

Chronic aquatic toxicity

M factor (Chronic) 100

12.2. Persistence and degradability

Polyurethane Coating

Persistence and degradability The degradability of the product is not known.

Ecological information on ingredients.

Petroleum gases, liquefied

Persistence and degradability The degradability of the product is not known.

Biodegradation Water - Degradation 100%: 385.5 hours

Naphtha (petroleum), hydrodesulfurized heavy

Persistence and degradability The degradability of the product is not known.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Persistence and degradability The degradability of the product is not known.

2-butanone oxime

Persistence and degradability The degradability of the product is not known.

Benzene, C10-13-alkyl derivatives

Persistence and degradability The degradability of the product is not known.

2-Ethylhexanoic acid, zirconium salt

Persistence and degradability The degradability of the product is not known.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient Not available.

Ecological information on ingredients.

Petroleum gases, liquefied

Bioaccumulative potential No data available on bioaccumulation.

Naphtha (petroleum), hydrodesulfurized heavy

Bioaccumulative potential No data available on bioaccumulation.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Polyurethane Coating

Bioaccumulative potential No data available on bioaccumulation.

2-butanone oxime

Bioaccumulative potential No data available on bioaccumulation.

Benzene, C10-13-alkyl derivatives

Bioaccumulative potential No data available on bioaccumulation.

2-Ethylhexanoic acid, zirconium salt

Bioaccumulative potential No data available on bioaccumulation.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Bioaccumulative potential No data available on bioaccumulation.

12.4. Mobility in soil

Mobility The product contains volatile organic compounds (VOCs) which will evaporate easily from all surfaces.

Ecological information on ingredients.

Petroleum gases, liquefied

Mobility Not relevant.

Naphtha (petroleum), hydrodesulfurized heavy

Mobility No data available.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Mobility No data available.

2-butanone oxime

Mobility No data available.

Benzene, C10-13-alkyl derivatives

Mobility No data available.

2-Ethylhexanoic acid, zirconium salt

Mobility No data available.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Mobility No data available.

12.5. Results of PBT and vPvB assessment

Ecological information on ingredients.

Petroleum gases, liquefied

Polyurethane Coating

Results of PBT and vPvB assessment This substance is not classified as PBT or vPvB according to current EU criteria.

12.6. Other adverse effects

Other adverse effects None known.

Ecological information on ingredients.

Petroleum gases, liquefied

Other adverse effects None known.

Naphtha (petroleum), hydrodesulfurized heavy

Other adverse effects None known.

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Other adverse effects None known.

2-butanone oxime

Other adverse effects None known.

Benzene, C10-13-alkyl derivatives

Other adverse effects None known.

2-Ethylhexanoic acid, zirconium salt

Other adverse effects None known.

4,5-Dichloro-2-octyl-2H-isothiazol-3-one

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. Disposal of this product, process solutions, residues and by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any local authority requirements. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

Disposal methods Do not empty into drains. Empty containers must not be punctured or incinerated because of the risk of an explosion. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents.

SECTION 14: Transport information

General	For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID)	1950
UN No. (IMDG)	1950
UN No. (ICAO)	1950
UN No. (ADN)	1950

14.2. UN proper shipping name

Proper shipping name (ADR/RID)	AEROSOLS
Proper shipping name (IMDG)	AEROSOLS (CONTAINS Naphtha (petroleum), hydrodesulfurized heavy, Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%))
Proper shipping name (ICAO)	AEROSOLS
Proper shipping name (ADN)	AEROSOLS

14.3. Transport hazard class(es)

ADR/RID class	2.1
ADR/RID classification code	5F
ADR/RID label	2.1
IMDG class	2.1
ICAO class/division	2.1
ADN class	2.1

Transport labels

14.4. Packing group

ADR/RID packing group	None
IMDG packing group	None
ICAO packing group	None
ADN packing group	None

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS	F-D, S-U

Polyurethane Coating

ADR transport category	2
Tunnel restriction code	(D)

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

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not applicable.

SECTION 15: Regulatory information

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

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits. The Aerosol Dispensers Regulations 2009 (SI 2009 No. 2824).
EU legislation	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended). Commission Regulation (EU) No 2015/830 of 28 May 2015. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended). Council Directive of 20 May 1975 on the approximation of the laws of the Member States relating to aerosol dispensers (75/324/EEC) (as amended).

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC_{50}: Lethal Concentration to 50 % of a test population. LD_{50}: Lethal Dose to 50% of a test population (Median Lethal Dose). EC_{50}: 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.

Polyurethane Coating

Classification abbreviations and acronyms	Aerosol = Aerosol STOT RE = Specific target organ toxicity-repeated exposure STOT SE = Specific target organ toxicity-single exposure Aquatic Chronic = Hazardous to the aquatic environment (chronic)
Classification procedures according to Regulation (EC) 1272/2008	STOT RE 1 - H372: STOT SE 3 - H336: : Calculation method. Aquatic Chronic 2 - H411: : Calculation method. Aerosol 1 - H222, H229: : Expert judgement.
Training advice	Read and follow manufacturer's recommendations. Only trained personnel should use this material.
Issued by	Emily Kirk
Revision date	12/03/2020
Revision	1.3
SDS number	1155
Hazard statements in full	H220 Extremely flammable gas. H222 Extremely flammable aerosol. H226 Flammable liquid and vapour. H229 Pressurised container: may burst if heated. H302 Harmful if swallowed. H304 May be fatal if swallowed and enters airways. H312 Harmful in contact with skin. H314 Causes severe skin burns and eye damage. H317 May cause an allergic skin reaction. H318 Causes serious eye damage. H330 Fatal if inhaled. H335 May cause respiratory irritation. H336 May cause drowsiness or dizziness. H351 Suspected of causing cancer. H372 Causes damage to organs through prolonged or repeated exposure. H372 Causes damage to organs (Central nervous system) through prolonged or repeated exposure. H400 Very toxic to aquatic life. H410 Very toxic to aquatic life with long lasting effects. H411 Toxic to aquatic life with long lasting effects. EUH208 Contains 2-butanone oxime, 4,5-Dichloro-2-octyl-2H-isothiazol-3-one. May produce an allergic reaction.