



EKC 451 PROCESS DESIGN AND ANALYSIS
UNIVERSITI SAINS MALAYSIA
SCHOOL OF CHEMICAL ENGINEERING

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GROUP 3

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PLANT DESIGN FOR PRODUCTION OF ETHYLBENZENE

FINAL REPORT

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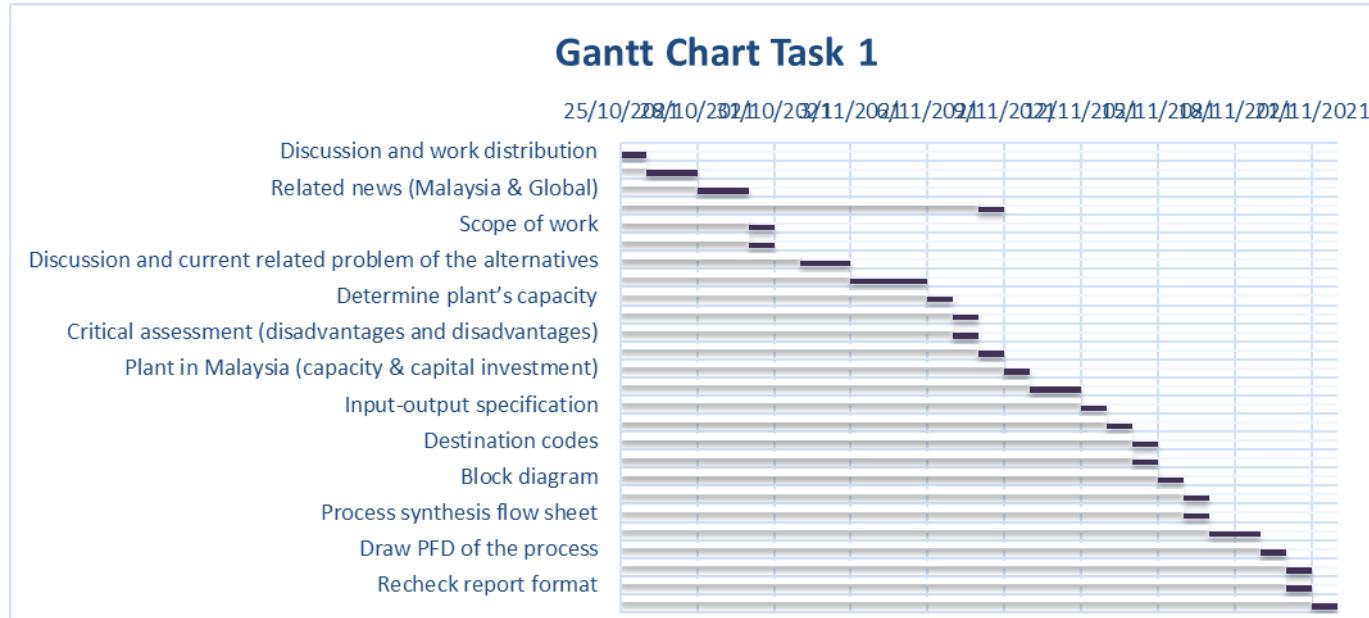
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CHAPTER 1

PROBLEM STATEMENT

1.1 Introduction to Ethylbenzene

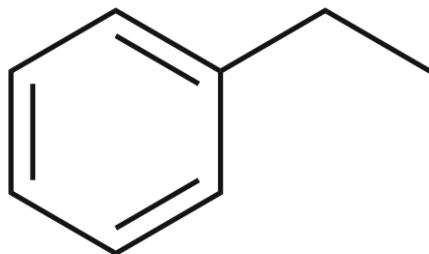


Figure 1.1 Chemical structure of ethylbenzene.

Ethylbenzene is an organic compound consisting of a benzene ring with an ethyl group attached to it. It is classified as an aromatic hydrocarbon with molecular formula of C_8H_{10} or $C_6H_5C_2H_5$. Ethylbenzene is a highly flammable and colourless liquid with a smell that resembles gasoline.

Mainly, ethylbenzene is used as an intermediate chemical to produce styrene monomer. Styrene monomer is important as it is a precursor to polystyrene, the common material for plastic manufacturing [1]. It is also used in fuels as a solvent and is an ingredient of commercial mixed xylenes. Examples of chemicals that used ethylbenzene as one of the ingredients are inks, pesticides, paint solvent, and tobacco products [2][3]. Ethylbenzene is also one of the chemicals in petroleum products and coal tar [4].

These are several processes to produce ethylbenzene [5]:

1. Catalytic alkylation of benzene with ethylene using zeolite catalyst
2. Isomer separation and catalytic isomerisation of mixed xylenes
3. Conversion of 1,3-butadiene to vinyl cyclohexane as intermediate and dehydrogenation of vinyl cyclohexane.

However, industrial ethylbenzene is produced mainly by alkylation of benzene with ethylene using zeolite catalyst. Addition to that, liquid alkylation of benzene with β -zeolite catalyst is better and more profitable compared to vapor alkylation with ZSM-5 catalyst [6].

1.2 Malaysia Chemical Industry Point of View

In 2017, ICIS reported that Malaysia's Idemitsu Styrene Monomer has been running its ethylbenzene unit with a capacity of 270,000 tonne/year. Meanwhile, the styrene monomer plant running rates also slightly increased, comparing 240,000 tonne/year in 2007 and 241,000 tonne/year in 2020 [7].

Besides, Malaysia was also spotted at 24th place of the largest crude oil reserves in the world. This will affect the supply of ethylbenzene as it is one of the petrochemicals produced in Malaysia. Malaysia also has a petrochemical zone in Pasir Gudang – Tanjung Langsat, Johor that produces ethylbenzene. Not only that, the capacity of raw material to produce ethylbenzene such as ethylene and benzene are among the largest compared to other chemicals. This shows the potential business market to industrially produce ethylbenzene in Malaysia [8].

1.3 Ethylbenzene Supply and Demand

According to Mordor Intelligence, during the forecast period from 2021 to 2026, the ethylbenzene market is expected to register a CAGR of over 4%. The demand for ethylbenzene market is negatively impacted by COVID-19 in 2020, which is mainly due to the temporarily stopped construction and automotive manufacturing activities during the government-imposed lockdown, leading to decrease in the demand for the ethylbenzene-based polymer and other products such as automotive dashboard, styrene-acrylic emulsions, exterior panels, solvent and reagent for paints and coatings, etc. Nevertheless, based on the ethylbenzene's derivative polystyrene from the food and e-commerce packaging segment, there is an increase in demand for packaging.

The aforementioned styrene-based polymers, elastomers, and resins are widely applied in various end-user industries, including electronics, packaging, petrochemicals, agriculture, and construction. Over the short term, the growth of ethylbenzene market is expected to be driven mainly by the increasing demand for styrene from various end-user industries as shown in Figure 1.2. The global electronics and IT industries production is estimated to have a growth rate of 7% year on year, hence the demand for ethylbenzene-

based polymer from electronics segment is expected to increase, which will lead to increase in the demand for the ethylbenzene market in the coming years.

Besides, due to the growth of the global construction industry, with a growth rate of approximately 4% compared to the previous year, there will be an increase of demand for various construction materials including styrene acrylic emulsions, acrylonitrile-butadiene-styrene, styrene-acrylonitrile resins, and others, thereby is expected to enhance the demand for ethylbenzene market. During 2021-2026, the construction industry dominated the market and is expected to grow due to the application of ethylbenzene as solvent and reagents in the production of various products, such as adhesives, and cleaning materials. On the other hand, the market's growth is expected to be hindered by strict regulations pertaining to the usage of ethylbenzene.

Based on Figure 1.3, the market across the world is dominated by Asia-Pacific region. The demand of ethylbenzene increased mainly in countries such as China, India, and Japan due to growing construction and packaging industries, and increasing application as solvent and reagents in paints and coatings, perfumes, inks, dyes, and synthetic rubber. During 2021-2026, the construction sector is expected to grow at a moderate pace over the next few years with increasing investments in public infrastructure, renewable energy, infrastructure, and commercial project. This will improve both consumer and investor confidence, which in turn enhancing the demand for ethylbenzene. Moreover, the growing demand for ethylbenzene is also due to the increased demand for lightweight automotive materials during this period, on account of the increased demand from the electric vehicles segment, as ethylbenzene-based polymers such as acrylonitrile-butadiene-styrene and others have functions in manufacturing of various automotive exterior and interior parts [9].



Figure 1.2 Ethylbenzene market, volume share (%), by application, global, 2020 [9].



Figure 1.3 Ethylbenzene market – growth rate by region, 2021-2026 [9].

1.4 Letter of Transmittal

Tetra Tech Sdn. Bhd,
Process Design and Analysis Department,
Bandar Cassia,
14110, Simpang Ampat,
Pulau Pinang

Profesor Dr. Mohd Azmier bin Ahmad
Plant Manager,
Chemical Malaysia Sdn. Bhd,
Jalan Transkrian.
14300, Nibong Tebal,
Pulau Pinang.

22 Nov 2021

Dear Sir,

Plant Design for the Production of Ethylbenzene through Alkylation Process

Referring to the above matter, the report is to present our proposed plant design for the production of ethylbenzene with a capacity of 100,000 tons per year. Ethylbenzene has high market demand around the world as it is an intermediate for the production of styrene. It is observed that Malaysia has a high potential business market of ethylbenzene as this country has one of the largest crude oil reserves in the world and has a high capacity of raw material to produce ethylbenzene.

2. Over the short term, the demand of ethylbenzene increased mainly in countries such as China, India, and Japan due to growing construction and packaging industries, and increasing application as solvent and reagents in paints and coatings, perfumes, inks, dyes, and synthetic rubber. The global electronics and IT industries production is estimated to have a growth rate of 7% year on year. Besides, there will be an increase of demand for various construction materials due to the growth of the global construction industry, with a growth rate of approximately 4% compared to the previous year.

3. We are comparing the production of ethylbenzene from liquid phase zeolite-based alkylation of benzene with ethylene, vapor phase alkylation of benzene with ethylene with ZSM-5 and kaolinite mixed catalyst and also isomer separation and catalytic isomerization of mixed xylenes. Alternative 1 has been chosen due to its positive green chemistry and sustainability, environmental impact, energy consumption, flexibility of operation, safety factor and waste management.

4. Kemasik, Terengganu is chosen as the most suitable place to locate the new ethylbenzene plant due to few criteria that help on the profitability of the project. The raw materials for the ethylbenzene production can be accessed easily as the ethylene and benzene is manufactured at Kertih, Terengganu, around 10 to 15km from Kemasik. In fact, it has efficient access to transportation and far from residential, school or recreation facilities. The plant is expected to produce 200,000 tons per year.

5. We have provided all information needed for the production of ethylbenzene, including its impact to the environment, process description, innovative approach and also process flow diagram. Hopefully our design plant meets all of the expectations needed with clear information. Regarding our plan, the plant is expected to be built by 2023 and it can be operated at the end of the year.

6. If there are comments regarding the proposed plant design, do not hesitate to contact us through email. Thank you in advance for your support and cooperation.

Sincerely,

KahHoe

(NG KAH HOE)

Plant Design Leader

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CHAPTER 2

PROCESS ALTERNATIVES

2.1 Three Process Alternatives for The Production Of Ethylbenzene

2.1.1 Alternative 1: Liquid Phase Alkylation of Benzene with Ethylene with EBZ-500 Zeolite Catalyst

Process Description

Ethylbenzene is produced by the catalytic alkylation of benzene with ethylene. In the early 1980s, Mobil/Badger developed a vapor phase alkylation using zeolite catalyst and this process offers higher yields and purity. More recently, liquid phase alkylation processes using zeolite catalysts have been established. These latest technologies offer low benzene-to-ethylene ratios, which reduces the size of equipment, and lowers the production of byproducts [10]. The alkylation process is maintained in liquid phase and uses multiple bed catalyst bed ethylene injection. Besides, the reactor almost operates isothermally [11].

Alkylation is an exothermic reaction which releases heat to the surrounding [11]. Since the reactor is nearly isothermal, the heat will not be lost to the surrounding. However, the heat released will be recovered and used to produce steam in distillation columns. Then the products formed will be sent to the distillation columns for separation to get the desirable product, ethylbenzene. The unreacted reactants (benzene and ethylene) will be recycled to the reactor for another time of reaction whereas the undesirable product will be removed as effluent.

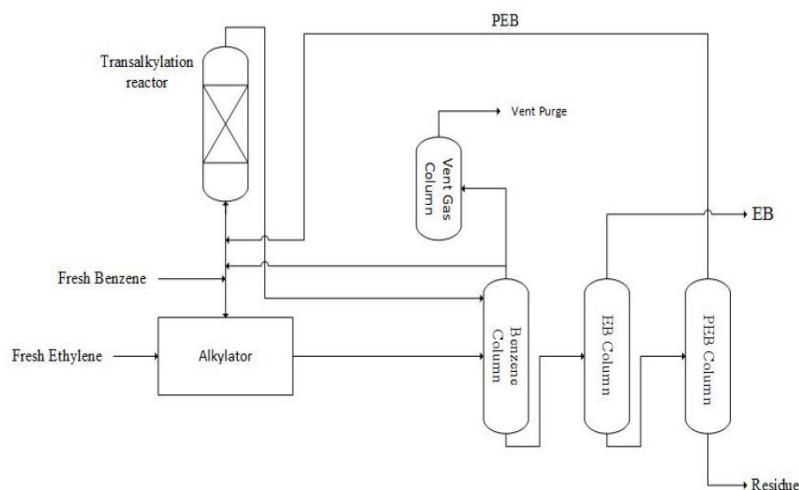


Figure 2.1 Simplified process flow diagram for liquid phase zeolite-based alkylation of benzene [3].

2.1.2 Alternative 2: Mixed Xylenes Isomerization and Ethylbenzene Produced by Xylenes Separation

Process Description

Xylene isomerization is one of the processes that focus on the process to turn ethylbenzene into additional xylenes which the standard unit operation, called as Universal Oil Product (UOP) process as shown in Figure 2.2. This process is important to achieve the target demand of xylene as the consumption rates around the world increases over the last few years. It involves the use of metal-acid catalysts where acid functions for the isomerization process and metal helps to improve the stability of the catalyst. Basically, the feed is added with hydrogen rich recycled gas, preheated with reactor effluent and then vaporized in the fired heater. It continued with the cooling process before undergoing a separation process in the product separator. The by-product of hydrogen gas is recycled back while the liquid is transferred to the deheptanizer column, to undergo the separation process. The concentration of naphthalene at the deheptanizer column should be constant but the loss of it at the top area must lead to the loss of aromatics, and it is assumed to synthesize more naphthalene. In terms of mathematical modelling, the hydrogen gas is ignored because the consumption is less than 2%.

For the xylene separation process, it has few methods but currently the best option is by using extractive distillation with p-dinitrobenzene as the ethylbenzene and p-xylene have a close boiling point [12]. The number of trays used for this process is inversely proportional to the reflux flow rate and the solvent is supplied at a rate of 5 times the feed rate. For solvent, p-nitrobenzene is being used as it has a similar structure of p-xylene but with higher boiling point so that it enhances the thermodynamic principle for the ternary system.

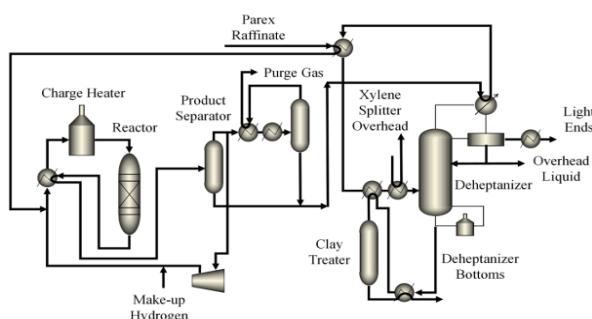


Figure 2.2 UOP's isomer process diagram [12].

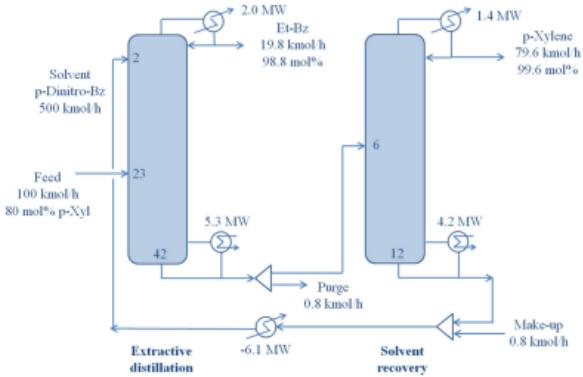


Figure 2.3 Schematic diagram of extractive distillation [12].

2.1.3 Alternative 3: Vapor Phase Alkylation of Benzene with Ethylene with ZSM-5 and Kaolinite Mixed Catalyst

Process Description

The Mobil-Badger developed, gas-phase alkylation of benzene with ethylene is the process used in the pilot plant as shown below. The plant consists of:

1. Two-way valve
2. Flow meter
3. Check valve
4. Pump
5. Three-way valve
6. Fixed bed reactor
7. Gas chromatography
8. Recorder

Each equipment has been labelled respectively in the figure below. This process is quite similar to liquid phase alkylation of benzene with ethylene. However, in this process, ethylene is supplied in the gas phase. The catalyst used in this ZSM-5 mixed with kaolinite with a 30:60 ratio to reduce the deactivation rate and formation of byproducts if using ZSM-5 alone. High content of kaolinite enables 1:1 benzene to ethylene ratio compared to conventional 5:1 or 6:1 and gives better stability. Addition kaolinite also reduce the usage of raw material and increase the conversion of benzene [13].

2-22 ml/min of mixture of benzene and ethylene is supplied for every 1.0 g catalyst loaded into the reactor. Meanwhile, the electrical furnace increases the temperature of the reactor while operating at atmospheric pressure. Temperature of the reactor ranging 300 – 450

°C and molar ratio of benzene to ethylene where the manipulated variables are used in this pilot plant. At the end of this project, maximum yield, conversion, and selectivity were observed at 1:1 benzene to ethylene ratio and 450 °C [13].

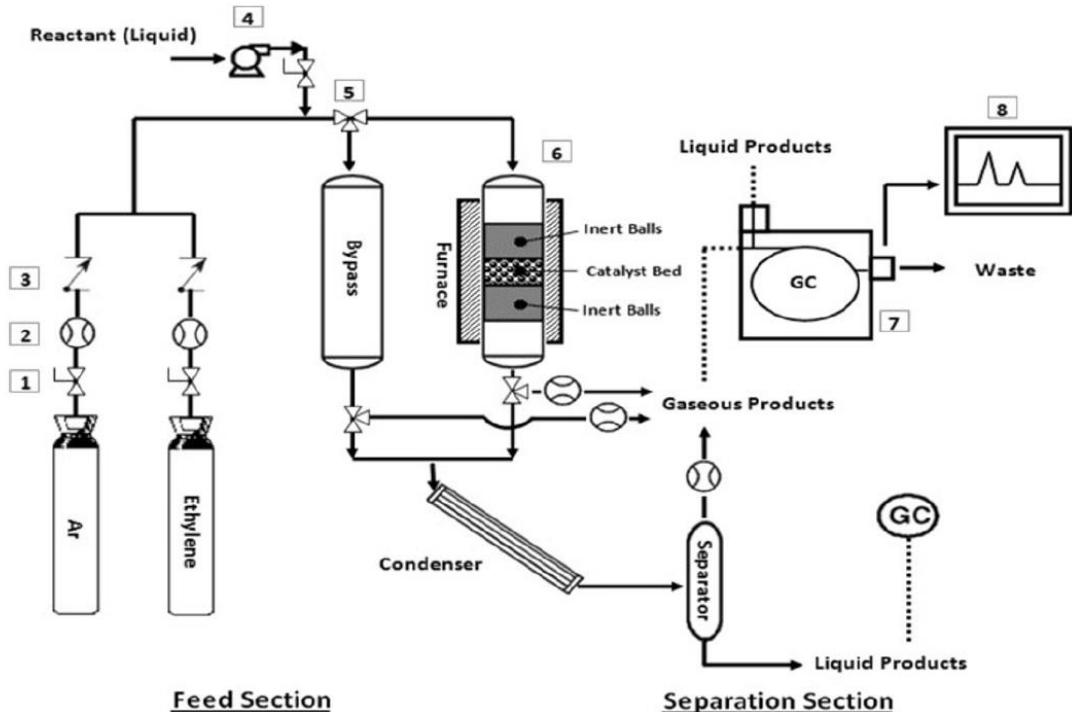
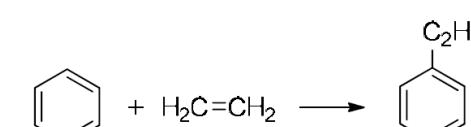


Figure 2.4 Bench-top pilot plant of ethylbenzene production [13].

2.2 Comparison of Three Process Alternatives for Production of Ethylbenzene

Table 2.1 Comparison of three process alternatives for the production of ethylbenzene.

Alternatives	Liquid Phase Alkylation of Benzene with Ethylene with EBZ-500 Zeolite Catalyst	Mixed Xylenes Isomerization and Ethylbenzene Produced by Xylenes Separation	Vapor Phase Alkylation of Benzene with Ethylene with ZSM-5 and Kaolinite Mixed Catalyst
Green Chemistry and Sustainability			
Raw materials	Benzene, ethylene [10]	Xylene (aromatics complex from Naphthalene), hydrogen [15]	Benzene, ethylene
Availability of raw materials	All are non-renewable. Benzene can be obtained through natural or industrial process. Whereas ethylene can be obtained through the extraction of natural gas and petroleum.	The raw material to produce xylenes are the non-renewable resources and it is assumed to be run out one day.	Benzene is one of the chemicals in crude oil and also a constituent of gasoline [21]. Besides, ethylene is found in a mix of natural gas and petroleum [22]. Both raw materials are not sustainable.
Chemical reaction	<p>Alkylation of benzene</p> <p>Main reaction: Benzene (l) + Ethylene (l) → Ethylbenzene (l)</p> <p>Side reaction: Ethylbenzene (l) + Ethylene (l) → Diethylbenzene (l)</p> <p>Transalkylation of benzene</p> <p>Diethylbenzene (l) + Benzene (l) → 2 Ethylbenzene (l)</p>	<p>Xylene isomerization with the used of acid catalyst: o-xylene + m-xylene → mixed p-xylene</p> <p>purification process: mixed p-xylene → ethylbenzene + p-xylene</p>	<u>Alkylation of benzene</u> <p><i>Benzene ethylation:</i></p> <p>Benzene (g) + Ethylene (g) → Ethylbenzene (g)</p>  <p><i>Side reaction:</i></p> <p>Ethylbenzene (g) + Ethylene (g) → Polyalkylbenzenes (g)</p>

			<p><i>Transalkylation of benzene:</i> Polyalkylbenzenes (g) + Benzene (g) → Ethylbenzene (g)</p>
Reactor	Multiple packed bed reactor [10], alkylation & transalkylation reactor [11]	N/A	Fixed-bed down-pass flow reactor
Operating condition	Temperature: 210 - 250 °C; Pressure: 32 - 40 bar	For isomerization [18]: Temperature: 655-755K Pressure: 1.68MPa Extractive distillation [12]: Temperature: 143-188K Pressure: 0.12MPa	Temperature: 350 – 450 °C Pressure: 1 atm
Catalyst used	EBZ-500 zeolite catalyst [10]	acid catalyst	ZSM-5 mixed with kaolinite
Catalyst life	2 – 5 years [11]	N/A	3 months – 1 year [23]
Conversion	99 – 100 % (*Ethylene as limiting reactant) [11]	99.9% ethylbenzene recovery [12]	63
Selectivity (%)	92	90% of production p-xylene by using ExxonMobil [18]	84.98
Yield (% wt.)	99.6	N/A	50
By-product	Diethylbenzene	p-xylene	Diethylbenzene isomers
Benzene/ethylene ratio	1.5 – 2.0 (on a molar basis) [11]	N/A	1:1, 3:1, & 6:1
Are the raw materials (benzene & ethylene) hazardous?	Long term exposure to benzene causes harmful effects on the bone	Yes. It is a carcinogen which needs to be handled with extreme caution	- Liquid ethylene can cause frostbite when contact with skin [25]

	marrow and can cause a decrease in red blood cells, leading to anemia [14] whereas exposure to ethylene will cause headache, dizziness, fatigue, lightheadedness, confusion, and unconsciousness [15].	because it can affect the inhalation when inhaled or passes through the skin. It is also flammable and a dangerous fire hazard [15].	- Benzene is carcinogenic [27]
Is the product (ethylbenzene) hazardous?	Yes. Short term exposure to ethylbenzene will result in respiratory effects, such as throat irritation and chest constriction, irritation of the eyes, and neurological effects such as dizziness. Long term exposure to ethylbenzene by inhalation in humans has shown conflicting results regarding its effects on the blood [16].	Yes. Short term exposure to ethylbenzene will result in respiratory effects while long term exposure to ethylbenzene by inhalation in humans has shown conflicting results regarding its effects on the blood. Exposure to xylene can lead to headache, dizziness or death but depends upon the dose, duration and work being done.	Short term exposure to ethylbenzene can cause respiratory reffect and neurological effects [3].
Environmental Impact			
Effect of the process (alkylation of benzene) to environment	<ul style="list-style-type: none"> - Runoff of ethylbenzene from spills, fire control and others should be diked to prevent it from entering streams or water supplies as it is toxic to aquatic life at relatively low concentration which is 10-100mg/kg [17] - Usage a lot of water during zeolite washing - Long catalyst life reduces disposal of spent catalyst annually 	<ul style="list-style-type: none"> - Isomerization process has a high potential to evaporate to the environment. It is a less constrained environment as it is rationalized by the weaker contribution of Van der Waals forces [20] 	<ul style="list-style-type: none"> - Usage a lot of water during zeolite washing [23] - Zeolite catalysts are abundant and considerably cheap to produce [26]
Energy Consumption			

Energy consumption	<ul style="list-style-type: none"> - Low operating temperature - Low benzene to ethylene ratio (large distillation capacity is not required) - Small reactor volume - Heat recovery for using in distillation column (no heat waste) 	<ul style="list-style-type: none"> - High operating temperature - Involve complex unit operation which increases the energy consumption 	<ul style="list-style-type: none"> - High reaction temperature - Usage of condenser and separator to purify the product
Flexibility of Operation			
Reaction	<ul style="list-style-type: none"> - Exothermic reaction - Reaction undergoes under high pressure (20 – 40 bar) in liquid phase at high temperature for a reasonable reaction rate. - Flexible temperature (420 – 470 K) and pressure (20 – 40 bar) range 	<ul style="list-style-type: none"> - Isomerization is chosen compared to dealkylation as it expenses higher conversion of p-xylene yields - Extractive distillation is chosen compared to crystallization due to its close boiling point 	<ul style="list-style-type: none"> - Highly exothermic reaction - Reactor using atmospheric pressure - Low conversion of benzene - Low yield of ethylbenzene - Higher rate of coke formation when temperature exceeds 400 °C
Raw material flexibility	Flexible. Raw material could be ethanol, propylene, olefin, etc	Raw material is flexible (any xylene)	Can be pure or diluted ethylene or ethanol [23]
Catalyst flexibility	Flexible.	Flexible of acidic catalyst but zeolite-type is the best catalyst for xylene isomerization (reduced reaction temperature, increased the activity and improved selectivity).	<ul style="list-style-type: none"> - Thermally and hydrothermally stable - Strength of acidity is flexible [23] - ZSM-5 based catalyst recorded to have high byproduct and rapid deactivation [13]
Safety Factors			
Safety concern	<ul style="list-style-type: none"> - Low operating temperature to minimize the risk of explosion - Since it is an exothermic reaction, heat transfer is required to prevent overheat - Benzene and ethylene are highly flammable so there is a risk of explosion 	<ul style="list-style-type: none"> - High operating temperature, risk of explosion - Naphthalene required extreme caution as it is highly flammable - Before entering a confined space with the presence of naphthalene, it is important to ensure explosive concentration does not exist [15] 	<ul style="list-style-type: none"> - Highly flammable reactant - Adequate atmospheric pressure during the process prevents over pressurization of the reactor - Reactors operating in high temperatures could lead to catastrophic failure
Healthy concern	<ul style="list-style-type: none"> - Zeolite catalyst will be harmful in contact with skin or inhaled 	<ul style="list-style-type: none"> - Zeolite catalyst is harmful which can cause respiratory irritation 	<ul style="list-style-type: none"> - Kaolin is considerably safe [24]

	<ul style="list-style-type: none"> - Zeolite may cause respiratory irritation - Benzene causes harmful effects on the bone marrow and can cause a decrease in red blood cells, leading to anemia - Ethylene will cause headache, dizziness, fatigue, lightheadedness, confusion, and unconsciousness 	<ul style="list-style-type: none"> - Exposure to Naphthalene can cause a skin allergy and may damage liver and kidneys 	<ul style="list-style-type: none"> - Meanwhile, zeolite can cause skin irritation and serious eye damage [24]
Waste Management			
Waste management	<ul style="list-style-type: none"> - Heat from exothermic reaction is recovered for use in distillation column - Residue stream is used to be fuel - Aqueous waste streams from aluminum chloride plants are avoided [8] 	<ul style="list-style-type: none"> - Waste of heat at the cooling process [18] - Used zeolite catalyst (higher catalyst life) to reduce waste - Treating clay isomerization: prolonging the life of catalyst [19] - Molecular sieve vessel: remove sulfur compound and water from hydrogen or hydrocarbons feed [19] 	<ul style="list-style-type: none"> - Templates of producing zeolite usually consist of nitrogen and only a part of the template can be recycled. [23] - After a maximum of one year of service as a catalyst, it becomes industrial waste. [23]

2.2.1 Green Chemistry and Sustainability

Alternative 1 and 3 require the same raw materials which are benzene and ethylene whereas the raw materials of Alternative 2 are xylene and hydrogen. Benzene can be obtained through natural or industrial processes while ethylene can be extracted from natural gas and petroleum. Both raw materials of Alternative 1 and 3 are non-renewable and non-sustainable. Xylene can be produced by catalytic reforming or by coal carbonisation in the manufacture of coke fuel while hydrogen can be produced from diverse, domestic resources including both non-renewable and renewable resources. Xylene is non-renewable while hydrogen is renewable and more sustainable. All these raw materials are hazardous at some point.

The chemical reactions involved in both Alternative 1 and 3 are alkylation and transalkylation of benzene whereas xylene isomerization with the use of acid catalyst and purification process are the chemical reactions in Alternative 2. All the three alternatives involve 2 chemical reactions. The operating condition for Alternative 1 is 420 – 470 K at 20 – 40 bar; for Alternative 2 is 655 - 755K at 16.8 bar while for Alternative 3 is 628 – 728 K at atmospheric pressure.

The enzymatic reaction of the three alternatives is compared mainly based on the yield, selectivity and conversion. The yield for Alternative 1 is higher than Alternative 3 which are 99.6 % wt. and 50 % wt. respectively while the yield for Alternative 2 is not known. Alternative 1 also has the highest selectivity among the three alternatives where selectivity for Alternative 1 is 92 %; for Alternative 2 is 90 % of production p-xylene by using ExxonMobil while for Alternative 3 is only 84.98 %. Besides, the conversion for each Alternative 1, 2 and 3 is 99 – 100 %, 99.9% ethylbenzene recovery and 63 % respectively.

The catalyst used in each Alternative 1, 2 and 3 is EBZ-500 zeolite catalyst, acid catalyst, and ZSM-5 mixed with kaolinite respectively. The catalyst life of Alternative 2 is unknown, thus by comparing between Alternative 1 and 3, the catalyst of Alternative 1 has a longer service life than Alternative 3 which is 2 - 5 years while the catalyst life of Alternative 3 is only 3 months – 1 year.

The reaction phase involved in Alternative 1 is only liquid phase whereas Alternative 2 and 3 involve both vapor and liquid phase. Thus, processes of Alternative 1 are simpler compared to the other two alternatives. Moreover, chemical reactions for each of the

alternatives result in by-products where the by-products of Alternative 1, 2 and 3 are diethylbenzene, p-xylene, and diethylbenzene isomers respectively. All these by-products can be used as feedstock to produce other products. Hence, there will be no wastage produced from all these processes.

2.2.2 Environmental Impact

It is observed that alternative 2 is the most dangerous method in producing ethylbenzene as it involves the isomerization process at high temperature. This matter could lead to the evaporation of chemicals to the environment, whereas danger to humans and the environment. Even this process is rationalized by the weaker contribution of Van der Waals forces, but high concentration of naphthalene or ethylbenzene to the environment could kill insects or repel animals, as well as formation of ozone depletion.

By comparing alternatives 1 and 3, it can be said that both alternatives give the most same impact to the environment as they are the same processes with different catalysts used. Both alternatives seem to use a lot of water for the washing of zeolite-based catalyst, which increases the amount of liquid disposal to any river. However, it is obtained that the catalyst life of EBZ-500 zeolite catalyst is longer than ZSM-5 mixed with kaolinite, which means that alternatives 1 is more preferable due to lesser waste that could contaminate the environment. It is because disposal of spent catalyst could be toxic to nature and affect the ecosystem.

2.2.3 Energy Consumption

In chemical reactions, Alternative 1 requires only a low benzene to ethylene ratio while Alternative 3 requires a high benzene to ethylene ratio which is up to 6:1. Low benzene to ethylene ratio indicates large distillation capacity is not needed which can save energy usage. Besides, Alternative 1 has the simplest unit operation as only a single liquid phase is involved in the reactions and small reactor volume is required; Alternative 2 has more complicated operation than that of Alternative 1 as two phases of substances are involved in the reactions whereas Alternative 3 involves complex unit operation which leads to increase in energy consumption.

Besides, Alternative 1 requires low operating temperature whereas Alternative 2 and 3 require high operating temperature where higher energy would be consumed. Furthermore,

for Alternative 1 and 3, exothermic heat from the chemical reactions is recovered to be used in the distillation column, hence, no heat energy is wasted.

2.2.4 Flexibility of Operation

The reactions in Alternative 1 need operating temperature within the range of 420 – 470 K and operating pressure within the range of 20 – 40 bar. The range of operating temperature in Alternative 2 is 655 - 755K at fixed pressure of 16.8 bar while the reactions in Alternative 3 operate at temperature within the range of 628 – 728 K at atmospheric pressure.

Besides, all the raw materials of the three alternatives are flexible. For Alternative 1, the raw material could be ethanol, propylene, olefin, etc. instead of ethylene; for Alternative 2, any xylene can be used as raw material while for Alternative 3, the raw material could be pure or diluted ethylene or ethanol. The catalyst for all the three alternatives is also flexible as long as an acidic catalyst is used.

In addition, all the three alternatives have a complex purification process where Alternative 1 and 3 more than 1 distillation column is needed while Alternative 2 involves extractive distillation.

2.2.5 Safety Factors

Safety and health are the two main concerns for safety factors. Regarding safety concern, Alternative 1 has low operating temperature, thus can minimize the risk of explosion, however, there is still a risk of explosion as benzene and ethylene are highly flammable. Moreover, overheating in the reactors can be prevented through heat transfer since the reactions are exothermic.

In Alternative 2, there is a higher risk of explosion than Alternative 1 due to high operating temperature. The usage of naphthalene in Alternative 2 requires extreme caution as the substance is highly flammable. Furthermore, it is crucial to ensure that explosive concentration does not exist before entering a confined space of the present of naphthalene.

Alternative 3 also operates in high temperatures which could lead to catastrophic failure. To prevent overpressure of the reactor, adequate atmospheric pressure must occur

during the process. Besides, the reactions also involve highly flammable reactants which are benzene and ethylene which needs extra caution when handling these substances.

Regarding health concerns, there are some substances which need to be taken into consideration for each alternative. For Alternative 1 and 3, zeolite catalyst is harmful in contact with skin or inhaled which may cause respiratory irritation and also serious eye damage. Benzene can bring harmful effects on the bone marrow and can cause a decrease in red blood cells, leading to anemia. Besides, exposure to ethylene can cause headache, dizziness, fatigue, lightheadedness, confusion, and unconsciousness. For Alternative 2, exposure to naphthalene can cause skin allergy and may damage liver and kidneys. Besides, respiratory irritation can be caused by acid catalysts.

2.2.6 Waste Management

The similarities that we can observe based on all three-process alternatives is that all processes used zeolite as the type of catalyst. The main concern related to the catalyst is the manufacturing of the catalyst and useful lifetime of it. Zeolite will consume plenty of water during its manufacturing and also the template to produce it will be disposed of as it cannot be reused after one time use. However, the useful lifetime of zeolite varies based on its properties and other combinations. For the vapor phase alkylation of benzene, the lifetime of the catalyst, ZSM-5 is quite short with up to 1 year. This will result in higher waste from this plant. In Contrast, zeolite catalysts in liquid phase alkylation of benzene last from 2 years to 5 years. This will greatly reduce the formation of waste.

Moving on, all the processes produce heat energy as waste due to its highly exothermic processes. The heat can be integrated to other streams to reduce its amount of wastage and supply it to the distillation column or heat exchanger. All processes also have isomer of xylene as a byproduct. Xylene is considered as hazardous waste; therefore, the chemical requires a proper downstream to be disposed of. One of the proper ways to dispose xylene is to burn it in an incinerator with afterburner and scrubber [28].

2.3 Current Related Problem to Environment and Society

Currently, there is a rapidly emerging crisis involving the access of clean drinking water due to the increasing release of various pollutants by industries to the environment. One of the main industries producing pollutants is ethylbenzene plants. Problems that might

be encountered in this plant are mostly related to the raw materials and main product. This is because some of these chemicals being used and produced are hazardous chemicals which may cause an impact to the environment and society.

First, let us discuss the problem of raw materials (benzene and ethylene) for the environment and society. In terms of environment, benzene can react with other chemicals to create smog when it is released into the atmosphere [29]. It might also attach to rain and snow and be carried to the ground to contaminate water and soil [29]. When benzene is being released to water, the aquatic ecosystem will be affected. Benzene will prevent aquatic animals from having babies whereas plants which are exposed to benzene in the soil their growth can be slowed, and they may even die [29]. On the other hand, the release of ethylene is not classified as hazardous to the environment [30]. Then, in term of *social*, long-term exposure to benzene causes harmful effects on the bone marrow and can cause a decrease in red blood cells, leading to anemia [14] whereas exposure to ethylene will cause headache, dizziness, fatigue, lightheadedness, confusion, and unconsciousness [15].

Then, we are going to discuss the impact of ethylbenzene on the environment and society. In terms of environment, if ethylbenzene drains off to the environment, it will contaminate the soil if it moves into the soil. However, ethylbenzene is rapidly broken down in air which is less than three days with the aid of sunlight. In terms of society, exposure to high levels of ethylbenzene in the air can cause eye and throat irritation whereas exposure to higher levels can result in vertigo and dizziness. It will also increase the risk of getting cancer if long-term exposure to high levels of ethylbenzene.

2.4 Choice of Process and its Justification

2.4.1 Safety Issues

Alternative 2 seems to be risky in the production of ethylbenzene compared to alternative 1 and 3 since it operates at high temperature which has the high tendency of explosion and also causes stress to the body. To ensure the process safety, it is important to have good ventilation and prepare a good emergency plan for the workers. The raw material of aromatic complex, Naphthalene also required extreme caution as it is highly flammable. Meanwhile, alternative 1 and 3 use the same raw materials, benzene and ethylene which

could affect the health when contact with skin. Therefore, the workers should wear complete personal protective equipment to minimize exposure to hazardous chemicals. The recorded data by National Occupational Exposure Safety (NOES, 1999) showed that around 200K workers in the United States were exposed to ethylbenzene [31].

2.4.2 Environmental Issues

The alkylation process of the chosen method, alternative 1 has the least issue on the environment compared to the other two alternatives. However, it is obtained that the emission of ethylbenzene gas to the surroundings could lead atmospheric transformation with photolytically generated hydroxyl radicals, dangerous to human and animal tissue. The release of ethylbenzene to water due to inappropriate disposal of waste could also contaminate the aquatic ecosystem. For the last few years, it is detected that ethylbenzene as one of the 58 most frequently detected chemical associated with groundwater contamination in United States after the analysis over 4% of surface water samples and 11% of the groundwater samples [31].

2.4.3 Public Issues

It is estimated about 970,000 kg of ethylbenzene emission from the xylene production plant in 1978 in the USA. However, there is not so much occupational exposure to the worker inside the styrene production plant [32]. The risk of exposure for the chosen process alternatives is quite high as all the processes contain benzene, a carcinogenic agent chemical. The production plants require careful measurement to control the discharge of each chemical involved. Not only that, discharge of the byproduct xylene also requires a systematic downstream process to handle the disposal of the chemical. Xylene will stay in the groundwater for months once it is discharged to the soil and eventually may be absorbed into the human food chain. High concentration of xylene consumed can hurt a human's liver [33]. Process alternative 1 produced the lowest byproduct % because of its high yield. Also, liquid phase alkylation of benzene may have the smallest effect to increment of surrounding temperature increase due to the plant running a highly exothermic process at a quite high temperature.

2.4.4 Market Analysis and Economic indicators

Overall cost of operating a plant must be taken into account when talking about the economy. The cost includes the total capital cost, operating cost, and maintenance. Price and availability for raw material as well as catalyst cost can also be an indicator of how economical the plant is.

Looking from the perspective of the catalyst used, all three process alternatives used zeolite-based catalysts. As process alternative 2 catalyst service life is unavailable, process alternative 1 has great advantage compared to process alternative 3. Process alternative 1 used EBZ-500 zeolite with a minimum of 2 years of service. Meanwhile process alternative 2 used ZSM-5 with only a maximum of 1 year of catalyst service life. By this comparison, we can say that process alternative 1 is more economical compared to process alternative 3 by using a lesser amount of catalyst and indirectly reducing the cost of maintenance for the plant.

Besides, availability of raw material used in plants is one of the important factors in choosing the most economical process alternative. Not only the amount, location of the supplier is also crucial in determining the overall price of obtaining the raw materials. Luckily, there are several companies in Malaysia that are supplying the desired raw material in all three process alternatives. Some of them are Titan Petchem (M) Sdn Bhd and Aromatics Malaysia Sdn Bhd that supply benzene and xylene. There are also petrochemical zones in Kertih, Terengganu that are able to supply raw materials for process alternatives 1 and 3 which are benzene and ethylene. On the other hand, ethylene has the most supply in Malaysia which makes its availability an advantage compared to other raw materials with 1.63 million metric ton annually. To add, PETRONAS Chemicals Ethylene Sdn. Bhd. Alone produced 400,000 metric tonnes of ethylene per year. [34] However, benzene and xylene also among the most supplied petrochemical product in Malaysia with 775 thousand metric tonnes per year for mixture of benzene, toluene, and xylene. [35] With that, the desired raw materials for all three process alternatives are available in Malaysia. To better distinguish the economy of the process, the price of raw materials has to be compared with one another and economical potential has to be calculated.

Prices of benzene, ethylene, and xylene are around RM4211/mt, RM3667/mt, and RM3746/mt respectively [36][37][38]. Based on the given price, it can be said that process

alternative 2 which used only xylene has slightly lower cost in term of raw material. On the other hand, process alternatives 1 and 3 which used similar types of chemical use more cost to buy the raw material. However, process alternative 2 is operating at such high operating temperature and has high potential to evaporate and lose its efficiency. However, process alternative 1 is able to utilize almost all of its material with a yield of 99.6%. Therefore, process alternative 1 produces better investment return compared to process alternative 2.

All in all, we have chosen process alternative 1 due to its availability of raw material in Malaysia which will reduce the cost of obtaining the raw material. Besides, process alternative 1 has the highest investment return considering the price of raw material and yield of the process.

2.3.5 Flexibility

The operating condition of reactions in Alternative 1 is temperature within the range of 420 – 470 K with pressure within the range of 20 – 40 bar. For Alternative 2, the reactions operating temperature is in the range of 655 - 755K with fixed pressure of 16.8 bar whereas for Alternative 3, the reactions operating condition is temperature within the range of 628 – 728 K at atmospheric pressure. All the three alternatives have flexible operating temperature. In terms of operating pressure, Alternative 1 has more flexibility compared to the other two alternatives with fixed operating pressure. Besides that, the usage of raw materials for the three alternatives are flexible. Instead of using ethylene, other raw materials such as ethanol, propylene, olefin, etc could also be used for Alternative 1; for Alternative 2, any xylene can be used while for Alternative 3, pure or diluted ethylene or ethanol could be the raw material.

Moreover, catalyst flexibility also exists in all the three alternatives. In Alternative 2, any acidic catalyst can be used, however, zeolite-type catalyst is the best catalyst for xylene isomerization as it can reduce the reaction temperature, increase the activity and selectivity. In Alternative 1 and 3, ethylbenzene can be synthesized over a wide range of zeolitic catalysts such as medium pore zeolites (ZSM-5, ZSM-11, ZSM-35) in vapor phase operation and large pore zeolites (β , Y, MCM-22, EBZ-500) in liquid phase operation [39]. In addition, zeolite has high thermal stability, thus, it can be applied to a wide range of operating temperature conditions [40]. Based on all these aspects, Alternative 1 is the most preferable alternative as it has the most flexible operation.

2.3.6 Controllability

In Alternative 3, higher temperature employed in vapor phase conditions yields considerable amount of xylene impurities which is ranging from 1200-1600 ppm [39] whereas in Alternative 1, lower operating temperature employed for liquid phase process typically yields less than 100 wppm xylene byproducts [39]. Since the boiling point of xylenes is very near to that of ethylbenzene, xylene impurities may co-boil with ethylbenzene which might affect the ethylbenzene quality and contaminate downstream products derived from ethylbenzene, such as styrene and polystyrene [39]. Hence, it is more difficult to control the quality of ethylbenzene in Alternative 3 than Alternative 1. For Alternative 2, since the raw material is xylene, it is much harder to control the quality of ethylbenzene. Moreover, in Alternative 1, operation in liquid phase can provide better thermal control [41]. Therefore, the operation of Alternative 1 is easiest to be controlled among the three alternatives

2.3.7 Conclusion

To choose the best alternative in the production of ethylbenzene, first and foremost, we must compare the terms of green chemistry and sustainability, source of raw materials, catalyst involved, operating conditions and produced waste. In term of green chemistry and sustainability, the existing environmental concerns associated with the disposal of AlCl₃ which gives significant waste production in Alternative 2 are eliminated by utilizing zeolite catalysts which are more environmental friendly as the zeolite catalyst can be easily regenerated in Alternative 1 and 3 whereas in term of safety issue, Alternative 2 seems to be risky in the production of ethylbenzene compared to Alternative 1 and 3. This is because it operates at high temperature which has the high tendency of explosion and also causes stress to the body. Besides, the operation of Alternative 2 exhibits higher risk as the piping and handling system is prone to corrosion due to the highly corrosive reaction mixture. However, zeolite catalyst is non-corrosive and non-hazardous in nature, thus, Alternative 1 and 3 are preferable in these aspects compared to Alternative 2.

Meanwhile in terms of energy consumption or in terms of economic factors, alternative 1 will be the best among these three alternatives. This is because Alternative 3 is carried out in liquid phase in the presence of a zeolite catalyst, thus, alternative 1 has the low operating temperature. Therefore, this will reduce energy costs and allow the use of carbon

steel as the material of construction. However, in Alternative 2 and 3, they need higher energy consumption due to numerous cooling systems required for the process of high operating temperature. Besides, Alternative 1 and 2 eliminate a large distillation capacity for benzene recovery since less excess benzene is recycled and circulated with the low benzene/ethylene (B/E) molar feed ratio to have a lower operating cost compared to Alternative 3 which requires high B/E molar ratio to increase ethylbenzene selectivity.

On the other hand, Alternative 1 has a longer catalyst lifetime than Alternative 3 which requires periodic regeneration. On the other hand, in terms of raw materials flexibility, although the usage of low-cost feedstock such as dilute ethylene from fluid catalytic cracking (FCC) off-gas or of lower-quality benzene is possible in Alternative 3 whereas it is strongly limited in alternativ Alternative 1 due to the lower catalyst tolerance to poisons under the low temperature operating conditions of liquid phase. However, Alternative 3 gives lower ethylbenzene yield probably due to the dilution of ethylene by benzene which leads to the lower probability of ethylene interaction with benzene.

In conclusion, Alternative 3 is chosen as the choice of the process as it does not impose harsh impact on the environment, provides a safer process system, lower operating cost, reduces energy consumption and operates at substantially lower temperature. All these process features result in lowered side reactions to produce high purified ethylbenzene of 99.9% with undetectable xylenes (by-products) production.

CHAPTER 3

CRITICAL ASSESSMENT OF THE PROCESS CHOSEN

3.1 Plant Capacity

Currently, the market demand for ethylbenzene chemical increased dramatically due to the high development of the plastic industry. This chemical is an intermediate for the production of styrene, which is the main ingredient for polystyrene products. Based on the engineering study of styrene, it can be produced through catalytic dehydrogenation ethylbenzene, oxidation of ethylbenzene to ethyl hyperoxide, side-chain of chlorination followed by dechlorination, side-chain chlorination of ethylbenzene hydrolysis to the corresponding alcohols followed by dehydration and pyrolysis of petroleum recovery from various petroleum processes followed by dechlorination [42]. Various methods of styrene production from ethylbenzene leads to the increasing world capacity of ethylbenzene around 20×10^6 t per year. After growing at a CAGR of 4.3% during 2020-2025, the market size of ethyl benzene could reach \$28.2 billion by 2023 [43].

From table 1, it is observed that the import amount of styrene monomer increased up to 160 thousand metric tons (KMts) in 2013 while the export amount is only 45 KMts. It means that Malaysia still could not afford to produce sufficient amounts of styrene due to the high amount of import styrene rather than the export value. Therefore, our designed plant for ethylbenzene production in Malaysia is expected to produce 100,000 tons per year, while targeting to reduce 2/3 of styrene imported to Malaysia as it can reduce risk while supplying locally. As reported by Independent Commodity Intelligent Services (I.C.I.S), Idemitsu's factory produced ethylbenzene at 220 tons per year and styrene at 200,000 tons per year [73]. We cannot go beyond 200,000 tons per year due high production and installation costs which perhaps risk the company.

Table 3.1 Malaysia Styrene Monomer Analysis [44].

Malaysia SM Capacity & Demand (Unit:KMts)

YEAR	2007	2008	2009	2010	2011	2012	2013
Demand	322	300	264	308	335	358	355
Capacity	240	240	240	240	240	240	240
Balance	-82	-60	-24	-68	-95	-118	-115
Import	146	135	102	162	160	160	160
Export	34	32	37	49	45	42	45

3.1.1 Site Selection

The most suitable location to build the ethylbenzene plant is at Kemasik, Terengganu due to few criteria that help on the profitability of the project. The raw materials for the ethylbenzene production can be accessed easily as the ethylene and benzene is manufactured at Kertih, Terengganu, around 10 to 15 km from Kemasik. It helps to minimize the transportation cost and any possible problem during delivery, which could affect the output production. In terms of raw material's price, the factory in Pasir Gudang offered pricey compared to the factory in Kertih. This location is also suitable for the transport of material and product to and from the plant, as well as the efficient access of air transport for any possibility of emergency or expansion of the plant.

In terms of effluent disposal, it is decided to be treated and re-used for the next cycle of manufacturing. By following the regulation by Occupational Safety and Health Administration (OSHA) regulation, the disposal of any toxic and harmful effluents will be recovered and enforcing the standards requirement. Next, this site is suitable for the proposed plant and quite far from any residential, schools or recreational facilities. It is an important consideration as the plant might lead to noise pollution. For the utilities, it is confirmed that there is no issue with the water and electricity. Water can be supplied by the Jabatan Air Terengganu or drawn from the Sungai Kertih. If the plant uses the water from the river, the production cost will be lower than expected and more profit for the company. The local authorities could also supply the electrical power even if it is required in large quantities.

3.2 Complete Description of Chosen Process

The production of ethylbenzene in the presence of liquid phase zeolite catalyst consists of reaction section and distillation section. There are two main reactions involved in the reaction section which are alkylation followed by transalkylation. The effluent stream from alkylation and transalkylation reactors are sent to the distillation section which consists of primarily three distillation columns. The first distillation column is a benzene column; the second column is an ethylbenzene column, and the third column is methane and ethane column.

The raw materials, fresh benzene and ethylene are fed from storage and are needed to be mixed before transported into the alkylator. Before mixing the two types of feeds, fresh benzene is firstly compressed to a pressure of approximately 35 bar, mixed with the recycled benzene from the first distillation column, and preheated to a temperature of 210 °C via heat exchanger. On the other hand, fresh ethylene is mixed with the recycled ethylene and transported in pipelines at 25°C and 40 bar. Prior to entering the alkylator, the benzene and ethylene are mixed together.

The alkylator is a fixed bed reactor contented with zeolite catalyst, which operates isothermally at pressure of 35 - 40 bar and temperature of 210 - 250 °C. The benzene/ethylene ratio for the alkylation reaction is 1.5 – 2.0 on molar basis [11]. Ethylene feed is essentially being converted completely in the fixed bed reactor with ethylene conversion of about 100 % and selectivity of 92.0 mol% towards ethylbenzene [45]. Since the alkylation reaction is exothermic, the exothermic heat of reaction is recovered and used to produce steams or as heat serves to the distillation columns. In addition, the bed outlet temperature of the alkylator should not exceed 270 °C in order to minimize radial temperature gradients [46]. The main product of the alkylation reaction is ethylbenzene and the side-product is diethylbenzene. The unreacted benzene is later being recovered in the distillation section and recycled back to the reaction section.

Another reaction, transalkylation is performed in a separate reactor, a single plug flow transalkylation reactor with zeolite catalyst [46]. In this transalkylator, the by-product, diethylbenzene recycled from the ethylbenzene column is transalkylated with fresh benzene and recycled benzene to produce more product, ethylbenzene. The benzene/diethylbenzene (B/DEB) ratio for this reaction is recommended at between 2 – 4 [45]. For optimizing the reaction rate, the operating condition of the transalkylator is the same as the alkylator, which operates isothermally at pressure of 32 – 35 bar and temperature of 210 – 250 °C. The unreacted benzene is also later being recovered in the distillation section and recycled back to the reaction section.

The effluent streams from alkylation and transalkylation reactors which consist of ethylbenzene, diethylbenzene, and unreacted benzene are being sent to the distillation section in order to recover the main product, ethylbenzene. The outlet streams from the reactors pass through liquid expander and heat exchanger for adjusting temperature and pressure to the respective inlet feed conditions in the downstream separation. The usage of

liquid expanders instead of valves is for the purpose of energy recovery. The combined stream enters the first distillation column which is the benzene column operating at temperature of between 85 °C and 120 °C with pressure of 1 bar. In benzene column, unconverted benzene is separated into the overhead stream which is being recycled to the reactors while the bottom stream which consists of liquid ethylbenzene and diethylbenzene is sent to the second column, which is the ethylbenzene column.

The bottom stream from the benzene column enters the ethylbenzene column which operates at temperature of between 145 °C and 170 °C and pressure of 1 bar. The overhead stream of ethylbenzene column is the desired product, ethylbenzene in vapor form while the bottom stream of the column, diethylbenzene is recycled back to the transalkylator to yield more ethylbenzene product. Furthermore, the methane and ethane distillation column which operates under temperature of 55 - 75 °C and pressure of 1 bar separates out the inerts which are methane and ethane from benzene. The sellable methane and ethane are then discharged as a purge stream.

3.3 Process Chemistry, Reactions and Kinetics

Process Chemistry

The process of alkylation is used to produce ethylbenzene as the main product. In this process, ethylbenzene is being produced through the reaction between benzene and ethylene by liquid phase alkylation. This reaction will be carried out in a packed bed reactor, fitted with a fixed bed of zeolite used as catalyst. Gaseous ethylene is sparged into the liquid phase of benzene mixture in the first reactor which is called alkylator. In this process, both reactors will operate under high pressure (32 – 40 bar) to maintain the liquid phase in the reactor at high temperature for a desirable reaction rate. To obtain maximum conversion of ethylene which is 100%, alkylator will operate at 210 to 250 °C. The operating temperature is relatively low compared to other processes as mentioned above (refer to Table 2.1). Therefore, lower operating temperature of liquid-phase operation generally results in decreased formation of by-products.

The reaction is exothermic under isothermal conditions. To prevent wasting unreacted reactant, benzene, the effluent from alkylator and transalkylator are fed to the benzene distillation column. Whereas, to separate the bottom product from the benzene

distillation column which is the mixture of ethylbenzene (main product) and di-ethylbenzene (side product), they will be fed to the second distillation column. Finally, ethylbenzene with high purity of about 99.88% will be produced as a distillate. Last but not least, in this process there is a flash drum for separating benzene from ethane and methane to prevent from wasting the benzene through the purge stream.

Reactions

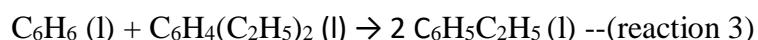
Alkylation (Main reaction):



Alkylation (Side reaction):



Transalkylation:



Rate Law

For (reaction 1),

$$r_1 = k_1 [\text{C}_6\text{H}_6] [\text{C}_2\text{H}_4]$$

For (reaction 2),

$$r_2 = k_2 [\text{C}_6\text{H}_5\text{C}_2\text{H}_5] [\text{C}_2\text{H}_4]$$

For (reaction 3),

$$r_3 = k_3 [\text{C}_6\text{H}_6] [\text{C}_6\text{H}_4(\text{C}_2\text{H}_5)_2]$$

Kinetic Model

- Assume reaction 1, 2, & 3 above is elementary reaction
- Assume the reaction is at steady state, $d[C_n]/dt = 0$ [37].
- Let benzene, ethylene, ethylbenzene and diethylbenzene be a, b, c, and d respectively
- $F(i)$ represent flow rate for i^{th} component
- Therefore, for alkylation:

$$\frac{dF(a)}{dw} = -r'_1 \quad * \text{For benzene}$$

$$\frac{dF(b)}{dw} = -r'_1 + (-r'_2) \quad * \text{For ethylene}$$

$$\frac{dF(c)}{dw} = r'_1 + (-r'_2) \quad * \text{For ethylbenzene}$$

$$\frac{dF(d)}{dw} = r'_2 \quad * \text{For diethylbenzene}$$

- Whereas, for transalkylation:

$$\frac{dF(a)}{dw} = -r'_3 \quad * \text{For benzene}$$

$$\frac{dF(d)}{dw} = -r'_3 \quad * \text{For diethylbenzene}$$

$$\frac{dF(c)}{dw} = r'_3 \quad * \text{For ethylbenzene}$$

Table 3.2 Kinetic parameters of alkylation and transalkylation reaction [46].

Rate Equation	Rate Constant, k
$r_1 = 1.528E + 06 \exp \frac{-7.113E + 04}{RT} [a][b]$	$k_1 = 1.528E + 06 \exp \frac{-7.113E + 04}{RT}$
$r_2 = 2.778E + 07 \exp \frac{-8.368E + 04}{RT} [c][b]$	$k_2 = 2.778E + 07 \exp \frac{-8.368E + 04}{RT}$
$r_3 = 1000 \exp \frac{-6.276E + 04}{RT} [d][a]$	$k_3 = 1000 \exp \frac{-6.276E + 04}{RT}$

3.4 Thermodynamic Data

Table 3.3 Heat capacity at constant pressure, C_p of organic liquid and ideal gas fit to hyperbolic function [J/(kmol.K)] [49].

Components	State	C1	C2	C3	C4	C5
Benzene	Gas, g	44767	230850	1479.20	168360	677.66
	Liquid, l	129440	-169.5	0.64781	N/A	N/A
Ethylene	Gas, g	33380	94790	1596	55100	740.8
	Liquid, l	247390	-4428	40.936	-0.1697	0.0002681 6
Ethylbenzene	Gas, g	78440	339900	1559	242600	702
	Liquid, l	154040	-142.29	0.80539	N/A	N/A
Methane	Gas, g	333300	79930	2086.9	41600	991.96
	Liquid, l	65.708	38883	-257.95	614.07	0
Ethane	Gas, g	40330	134220	1655.5	73220	752.87
	Liquid, l	44.009	89718	918.77	-1886	0

Table 3.4 Physical properties of benzene, ethylene, ethylbenzene, ethane, and methane [49][50].

Components	State	Formula weight	Specific gravity	Normal boiling point (°C)	Critical temperature, T _c (°C)	Critical pressure, P _c (atm)
Benzene	Liquid, l	78.11	0.879	80.1	289.45	48.6
Ethylene	Gas, g	28.05	0.57	-103.9	9.95	50.5
Ethylbenzene	Liquid, l	106.17	0.867	136.2	346.55	37
Ethane	Gas, g	30.07	0.546 ⁻⁸⁸	-88.8	32.25	48.2
Methane	Gas, g	16.04	0415 ⁻¹⁶⁴	-161.4	-82.45	45.8

Table 3.5 Heat capacities and physical properties of Diethylbenzene [49]/[51].

Components	State	Heat capacity, Cp [J/(kg.K)]	Formul a weight	Specific gravity	Normal boiling point (°C)	Critical temperature, Tc (°C)	Critical pressur e, Pc (atm)
Diethylbenzene	Liquid, l	1920.456	134.22	0.87	180	384.74	27.663

Table 3.6 Antoine constants of benzene and ethylbenzene; temperature in °C; vapor pressure in mmHg [50].

Components	Range (°C)	A	B	C
Benzene	14.5 – 80.9	6.89272	1203.531	219.888
Ethylbenzene	56.5-137.1	6.95650	1423.543	213.091

Table 3.7 Antoine constants of ethylene; temperature in kelvin; vapor pressure in bar [53].

Components	Range (K)	A	B	C
Ethylene	149.37 - 188.57	3.87261	584.146	-18.307
Ethane	91.33 -144.13	4.50706	791.3	6.422
Methane	90.99 - 189.99	3.9895	443.028	-0.49

Table 3.8 Vapor pressure of benzene, ethylene, & ethylbenzene in liquid form [49].

Components	Temperature range, (K)	C1	C2	C3	C4	C5
Benzene	278.68 – 562.05	83.107	-6486.2	-9.2194	6.9844E-06	2
Ethylene	104 – 282.34	53.963	-2443	-5.5643	1.9079E-05	2
Ethylbenzene	178.2 – 617.15	89.063	-7733.7	-9.917	5.9860E-06	2
Ethane	90.35 - 305.32	51.857	-2598.7	-5.1283	1.4913E-05	2
Methane	90.69 - 190.56	39.205	-1324.4	-3.4366	3.1019E-05	2

Table 3.9 Specific heat of vaporization at normal boiling point & specific heat of formation at 25 °C & specific heat of combustion at 25 °C & specific gibbs energy of formation at 25 °C for benzene, ethylene, ethylbenzene, ethane, and methane [49, 50].

Components	State	(ΔH _v /mole) at normal boiling temperature [kJ/mol]	(ΔG _f (25°C)/mole) [kJ/mol]	(ΔH _f (25°C)/mole) [kJ/mol]	(ΔH _c (25°C)/mole) [kJ/mol]
Benzene	Liquid, l	30.765	/	48.66 (l)	-3267.7 (l)
	Gas, g	/	129.6	82.93 (g)	3301.5 (g)
Ethylene	Liquid, l	13.54	/	/	/
	Gas, g	/	68.440	52.28 (g)	-1410.99 (g)
Ethylbenzene	Liquid, l	35.98	/	12.46 (l)	4564.9 (l)
	Gas, g	/	130.730	29.79 (g)	-4607.1 (g)
Ethane	Liquid, l	2.859	/	/	/
	Gas, g	/	-31.920	-84.67 (g)	-1559.9 (g)
Methane	Liquid, l	0.94	/	/	/
	Gas, g	/	-50.490	-74.85 (g)	-890.36 (g)

Table 3.10 Specific heat of vaporization at normal boiling point & specific heat of formation at 25 °C & specific heat of combustion at 25 °C & specific gibbs energy of formation at 25 °C for diethylbenzene [49, 52].

Components	State	(ΔH _v /mole) at 416.5 K [kJ/mol]	(ΔG _f (25°C)/mole) [kJ/mol]	(ΔH _f (25°C)/mole) [kJ/mol]	(ΔH _c (25°C)/mole) [kJ/mol]
Diethylbenzene	Liquid, l	45.80	/	-72.84 (l)	-5863.08 (l)
	Gas, g	/	136.10	-24.67 (g)	/

Table 3.11 Constants of heat of vaporization for benzene, ethylene, ethylbenzene, ethane , and methane [49].

Components	C1x10 ⁻⁷	C2	C3	C4	T _{min} , K	ΔH _v at T _{min} x 10 ⁻⁷	T _{max} , K	ΔH _v at T _{max}
Benzene	4.7500	0.45238	0.0534	-0.1181	278.68	3.4909	562.16	0
Ethylene	/	0.3746	0	0	104	1.6025	282.34	0

Ethylbenzene	5.4640	0.392	0	0	178.15	4.7811	617.2	0
Ethane	2.1091	0.60646	-0.55492	0.32799	90.35	1.7879	305.32	0
Methane	1.0194	0.26087	-0.14694	0.22154	90.69	0.8724	190.56	0

Calculation by Using Thermodynamics Data in Section 3.5

***Before using the calculation formula shown below, please check the unit and the range for the formulae to be applied. Otherwise, significant error will occur.

1) To calculate heat capacity of liquid raw materials and products at constant pressure for (a) liquid and (b) vapor/gas (use data in Table 3.1)

a) For liquid, C_{pl} (benzene, ethylene, & ethylbenzene, ethane, & methane),

$$C_{pl} = C1 + C2 \cdot T + C3 \cdot T^2 + C4 \cdot T^3 + C5 \cdot T^4 \quad \text{---Equation (1)}$$

b) For gas, C_{pv} (Assume ideal gas state fit to hyperbolic function)

$$C_{pv} = C1 + C2 \left[\frac{\frac{C3}{T}}{\sinh\left(\frac{C3}{T}\right)} \right]^2 + C4 \left[\frac{\frac{C5}{T}}{\cosh\left(\frac{C5}{T}\right)} \right]^2 \quad \text{---Equation (2)}$$

2) To calculate vapor pressure using Antoine constants (use data in Table 3.4 & 3.5)

a) For benzene & ethylbenzene,

$$\log_{10} p^* = A - \frac{B}{T+C} \quad \text{---Equation (3)}$$

Partial pressure, p^* in mmHg; Temperature, T in $^{\circ}\text{C}$

b) For ethylene, ethane, & methane

$$\log_{10} p^* = A - \frac{B}{T+C} \quad \text{---Equation (4)}$$

Partial pressure, p^* in bar; Temperature, T in Kelvin (K)

3) To calculate vapor pressure (use data in Table 3.6)

For benzene, ethylene, ethylbenzene, ethane & methane,

$$\ln P = C_1 + C_2/T + C_3 \ln T + C_4 T^{C_5} \text{ ---Equation (5)}$$

Pressure in Pascal (Pa), Temperature, T in Kelvin (K)

4) To calculate latent heat of vaporization at specific temperature, T

a) For benzene, ethylene, ethylbenzene, ethane & methane (use data in Table 3.9),

$$\Delta Hv(T) = C_1 \times (1-Tr)^{C_2 + C_3 \times Tr + C_4 \times Tr \times Tr + C_5 \times Tr \times Tr \times Tr} \text{ --- Equation (6)}$$

Heat of vaporization at specific temperature, $\Delta Hv(T)$ in J/kmol; Temperature in Kelvin (K);

reduced temperature, $Tr = T/T_c$

b) For diethylbenzene,

$$\ln \left(\frac{P_1}{P_2} \right) = \frac{\Delta Hv}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \text{ ---Equation (7)}$$

3.5 Physical and Chemical Properties Data

Table 3.12 Physical and chemical properties data of raw material and products.

PROPERTIES	BENZENE	1,4-DIETHYLBENZENE	ETHYLBENZENE	ETHANE	ETHYLENE	METHANE
	[54][55]	[56][57][58]	[4][59]	[54][60]	[54][61]	[54][62]
Molecular formula	C ₆ H ₆	CH ₃ CH ₂ (C ₆ H ₄)CH ₂ CH ₃	C ₆ H ₅ C ₂ H ₅	CH ₃ CH ₃	CH ₂ =CH ₃	CH ₄
Physical state at STP	Liquid	Liquid	Liquid	Gas	Gas	Gas
Molecular weight (g/mol)	78.11	134.22	106.16	30.07	29.05	16.04
Colour appearance	Clear & colourless	Colourless	Colourless	Colourless	Colourless	Colourless
Odour	Resembles gasoline	Resembles gasoline	Aromatic	Odourless	Sweet	Odourless
Vapor pressure, 25°C (mmHg)	94.8	1.06	9.6	1.06E+05	5.21E+04	4.66E+05
Specific gravity	0.879	0.86	0.867	0.546	1.047	0.554

Boiling point at 1 atm (°C)	80.1	183.7	136.1	-88.6	-103.9	-161.4
Melting point at 1 atm (°C)	5.5	-42.83	-94.9	-172	-169	-182.6
Solubility in water at 25°C (mg/l)	0.07	24.8	170	60.2	131	22
Flash point (°F)	12	132	59	-306	-213	-306
Viscosity (mPa.s)	0.604	3.6 X 10-3 Pa.s at 230.32 K	0.64 at 25 °C	9.4	0.01 at 20 °C	0.01107
Vapor density (air = 1)	2.7	4.64	3.7	1.05	1.98	0.6

3.6 Advantages and Disadvantages of the Process Chosen

3.6.1 Advantages of Alkylation of Benzene in Liquid-Phase Zeolite Catalyst

The advantages of the chosen process are listed as below:

- The operation of liquid phase zeolite catalyst process at substantially lower temperature largely decreases side reactions which results in high purity ethylbenzene product [11].
- Highly purified product makes the separation process simpler and saving operational cost.
- Excellent ethylbenzene yield of 99.6 wt% and high product purity of 99.9% with undetectable xylenes (by-products) are achieved with low production cost [69].
- The use of zeolite catalyst which is environment-friendly, has high activity and selectivity towards the production of ethylbenzene reduces side reactions which minimize the formation of undesired by-products.
- Mild carbon burn procedure for catalyst regeneration is relatively low-cost [11].
- Low benzene/ethylene ratio in the reactions minimizes recycling and energy consumption.
- Low turnaround and maintenance cost as the plant achieves high stream efficiency which is often higher than 99 % [11].
- The high temperature outlet effluents of the reactors due to exothermic heat of reaction serves as hot stream to heat up benzene fed to the alkylation reactor which can reduce the requirement of external heat and at the same time achieves cooling of the outlet stream.

3.6.2 Disadvantages of Alkylation of Benzene in Liquid-Phase Zeolite Catalyst

The disadvantages of the chosen process are listed as below:

- High operating pressure in the reactors is needed to maintain liquid phase operation.
- The feedstocks (benzene, ethylene) used for the ethylene production are non-renewable, where the price of the feedstock might be increased due to possibility of feedstock shortage in the future.
- The presence of feed impurities in the form of benzene coboilers will tend to accumulate in the liquid phase system all over time. These impurities are difficult to be separated from benzene by distillation because they have close boiling points [70].

3.7 Environmental, Safety and Health Concerns of the Process

In the alkylation process, light hydrocarbon benzene and ethylene react in the presence of zeolite catalyst to form a mixture of heavier hydrocarbon, ethylbenzene. It is important to consider the catalyst used so that it has minimal impact on the environment. EBZ-500 zeolite catalyst is one of the best choices for this reaction as it has longer catalyst life, which means simultaneously reducing the disposal amount of spent catalyst annually. Disposal of the hazardous waste directly to the river or nature could lead to a risk of environmental contamination due to the high toxicity. Generally, there are few methods to treat a spent catalyst such as reclamation of metals, rejuvenation and reuse, disposal in landfills and also preparation of useful materials, which could help in saving nature.

Moreover, the raw material and also products of this process are hazardous and may have insignificant effects to human health and other living things. Benzene is a flammable chemical which means that it cannot be exposed to heat or open flames and must be kept in a tightly closed container [71]. Long term exposure to benzene causes harmful effects on the bone, leads to decrease in red bloods and may cause cancer. For ethylene, it is determined that the chemical is extremely flammable, carcinogenic, and unstable explosive [72]. It is important to prevent entry into waterways or confined areas, as well as spreading of vapors through ventilation systems. Meanwhile, long term exposure to ethylbenzene could lead to respiratory problems. Therefore, it is important for the workers to wear suitable personal protective equipment (PPE) while handling the chemical. It is also crucial to have a well-prepared emergency plan for handling sudden or unexpected situations as stated in the OSHA standard (29 CFR 1910.38(a) and 29 CFR 1926.35). The objective is to prevent injuries and fatalities, and reduce fire damage while having a clear set of responsibilities.

3.7.1 Similar Plant in Malaysia (Plant Capacity and Capital Investment)

Petrochemical (Malaysia) Sdn Bhd is the first polystyrene (PS) in Malaysia and also ASEAN who is a subsidiary of a well-known company from Japan, called Idemitsu. This company is established in 1977 and landed at Pasir Gudang with its own exclusive chemical Jetty. The ethylbenzene monomer had been integrated after it achieves commercial production of styrene at 200,000 metric tons per year.

Idemitsu started the manufacturing of ethylbenzene around 215 KTA (in 1997) as a joint venture with Petronas. This plant had been expanded very quickly. Therefore, in 2017, the factory could be running with capacity, 270,000 tonnes/year, a full unit capacity [73]. The aim of ethylbenzene manufacture is to produce high impact polystyrene with various type of application. To build this plant, Idemitsu's company had invested close to RM116m in capital expenditure [73]. In terms of sustainability, this company focus to reduce the volume of industrial waste generation by reusing the raw material as well as utilizing the recycled raw material.

3.8 Demand and Supply of the Ethylbenzene

3.8.1 Current Supply and Demand of Ethylbenzene

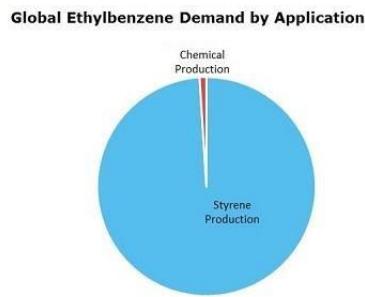


Figure 3.1 Global application of ethylbenzene [74].

Malaysia is accounted for only about 0.01% of world import share which valued USD 52,559 [75]. Though the wide application of ethylbenzene and almost exclusively used for styrene production in plastic industry, Malaysia still does not have the number of plants or production plant capacity to internationally supply ethylbenzene [74]. It is obvious that Malaysia does not produce much of Ethylbenzene locally since there is no registered global export value [75]. Therefore, creating and designing a new and efficient ethylbenzene production plant able to increase the production of ethylbenzene in Malaysia. Increase in ethylbenzene production may create the potential to globally export ethylbenzene from Malaysia and decrease the import value to Malaysia.

Current demand of ethylbenzene is unquestionably high as it is used almost fully by styrene production industry. Styrene monomer is versatile product that can be used in wide range of industry such as electronics, petrochemicals, and agriculture. Ethylbenzene demand can be extended to the huge gasoline industry. It is proven brings benefit to gasoline by

reducing the knocking of the internal combustion engines. Apart from that, ethylbenzene also currently used for packaging and inexpensive consumer product which is also an expanding market nowadays [76].

In Malaysia, related industries which creates demand for ethylbenzene is indeed increasing at a steady pace. Firstly, 12.6% of export growth recorded on the Q2 2021 for petroleum, chemical, rubber & plastic products [77]. The sales of manufacturing industry in Malaysia also grow 11.6% with petroleum, chemical, rubber & plastic industries leading the way with 29.2 increase compared to sales in August 2021 [78]. These increase in revenue of related industries will create more opportunities for ethylbenzene to grow its demand.

In global context, 7% growth rate of global electronics and IT industries production which based on USD 2,972.7 billion in 2020 to approximately USD 3,175.6 billion by 2021 also indirectly improve the demand of ethylbenzene due to its application in that industry. Not only that, but styrene monomer is also the precursor to industrial polymers such as polystyrene, acrylonitrile-butadiene-styrene, and styrene-acrylonitrile resins. Some of these polymers are used in construction industry. To relate, the US 12 trillion global construction industry in 2019 has the growth rate about 4%. Activity of construction industry already resumed after abruptly stopped due to COVID-19 [79].

Therefore, there is a lot of growing and existing huge industry for supply of ethylbenzene to grow. This ethylbenzene production plant will likely return a huge amount of its investment and sustain in long run.

3.8.2 Projected Demand / Supply for The Next 10 Years

Ethylbenzene (EB) is a highly flammable, colorless liquid that has a sweet aroma [80]. Ethylbenzene market is mainly used in applications (styrene, gasoline, diethylbenzene, natural gas, paint, and asphalt and naptha) and end-user industry (packaging, electronics, construction, agriculture, automotive, etc.) [81]. However, nearly all ethylbenzene produced in the world is used in the manufacture of styrene. Consumption of ethylbenzene for uses other than the production of styrene is estimated to be just around 2% [80]. The global market for ethylbenzene witnessed a strong growth over the recent few years owing to enhanced demand from the plastic industry. This phenomenon is believed to last for a few years due to the forecast styrene growing demand as shown below.

Global Styrene Market, By Region 2020-2026

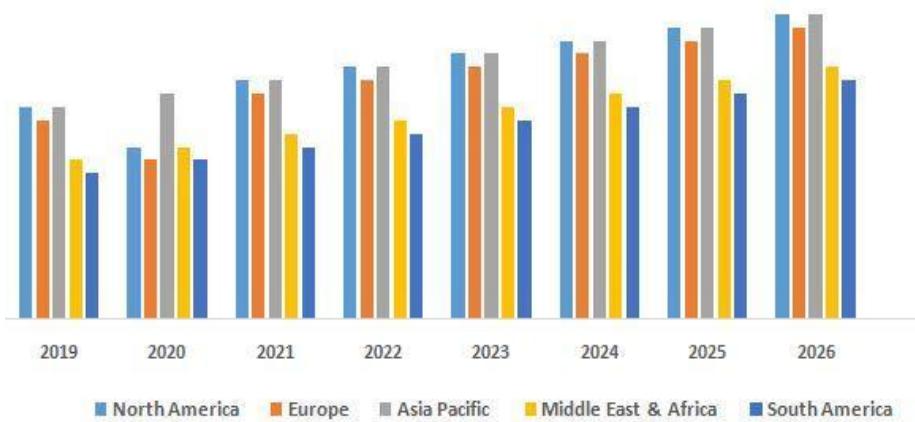


Figure 3.2 Global Styrene Market, By Region 2020-2026 [81].

As reported, the Global Ethylbenzene Market is projected to register a CAGR of over 4% during the forecast period (2021-2026) [9]. However, recently, the ethylbenzene market has been hit by outbreak of covid-19 pandemic. The pandemic negatively impacts the global ethylbenzene demand. This is because the construction and automotive manufacturing activities were stopped temporarily during the government-imposed lockdown, thus had decreased the demand for the ethylbenzene-based polymer and other products including automotive dashboard, exterior panels, styrene-acrylic emulsions, solvent and reagent for paints and coatings, and others [9]. However, the food and e-commerce packaging segment has increased the demand of ethylbenzene during the current situation, thereby stimulating the growth of ethylbenzene market [9]. Besides, there are more people getting vaccinated. Therefore, most of the countries and places have terminated the lockdown phase, this will also stimulate the growth of ethylbenzene market.

Other than that, nowadays, styrene is not only mainly used in the plastic industry but also industries like IT & electronics, construction, etc. For example, the global electronics and IT industries production was valued at USD 2,972.7 billion in 2020 and is estimated to reach USD 3,175.6 billion by 2021, with a growth rate of 7% year on year [9]. There was also another example in which the global construction industry was valued at about USD 12 trillion in 2019, with a growth rate of about 4% compared to the previous year [9]. Hence, it is believed that global demand on ethylbenzene will keep on increasing for the next ten years or even further.

According to a 2021 World Market Outlook, there is a forecast of the ethylbenzene market up to 2030. It says that most new capacity introductions are foreseen in Asia Pacific (mainly China) and this region's share in global output will increase. Besides, styrene production in Asia Pacific, Latin America and Middle East is expected to grow rapidly, while Europe and North America will lag [82]. However, the global ethylbenzene market growth is still forecast to be around 3-4% [82].

As mentioned above, the Asia-Pacific region dominated the global market share. The usage of ethylbenzene has been increasing in the region with the reason of growing construction and packaging industries as well as increasing application as solvent and reagents in paints and coatings, dyes, perfumes, inks, and synthetic rubber in countries, such as China, India, and Japan. Based on the report, by forecast, the global ethylbenzene market was valued at USD 19320 in 2020 and will reach USD 23620 million by the end of 2027, growing at a CAGR of 3.4% during 2021-2027. [83]

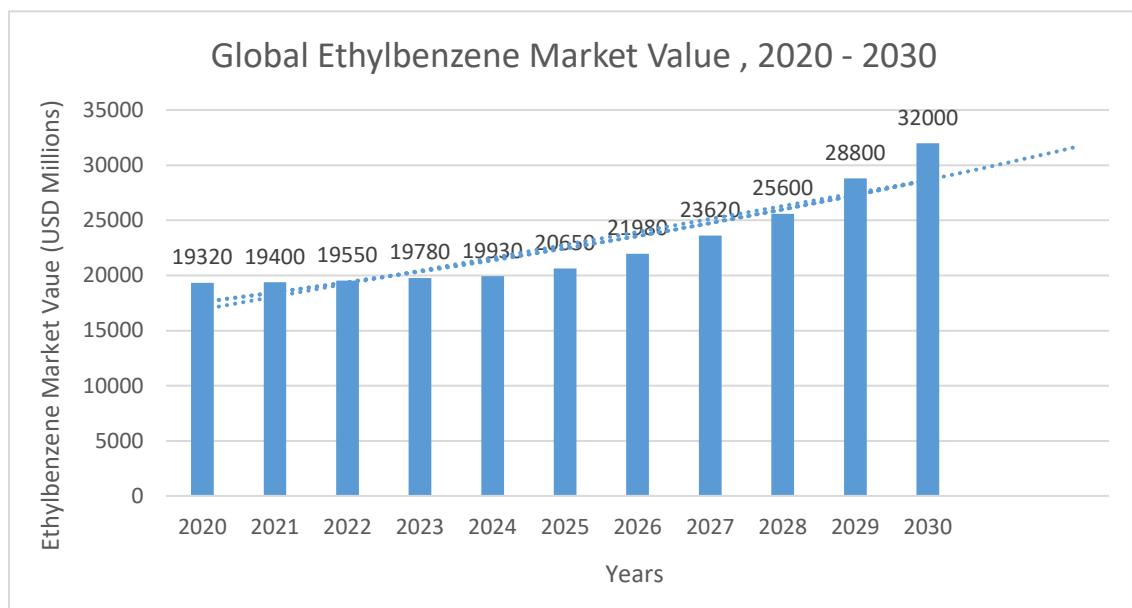


Figure 3.3 Projected global demand of ethylbenzene for next 10 years (forecast based on report [83])

Based on the forecast and trend analysis shown in Figure 3.4, we can justify that a new ethylbenzene plant built in Malaysia could not only make profit, but it is also able to ensure that there is sufficient supply of ethylbenzene in the global market to meet the global demand. Finally, by adding more ethylbenzene plants, we can reduce importation fees of ethylbenzene

from other countries as well. Therefore, this will ensure that the projected global demand and supply of ethylbenzene for the next ten years could be achieved.

Reporter	290260. Ethylbenzene			
	Exports		Imports	
	2020		2020	
	Value (US\$)	World Share (\$)	Value (US\$)	World Share (\$), %
Serbia			30.00	0.00
Romania			223.00	0.00
Qatar			168,650.00	0.05
Peru			83.00	0.00
Paraguay			1,006.00	0.00
Norway			139.00	0.00
New Zealand			606.00	0.00
Namibia			10.00	0.00
Morocco			1,557.00	0.00
Moldova			83.00	0.00
Mexico			67,430.00	0.02
Malaysia			52,559.00	0.01
Lithuania			105.00	0.00
Lebanon			16.00	0.00
Kenya			1,281.00	0.00
Italy			9,389,947.00	3.00
Israel			33,000.00	0.01
Ireland			3,376.00	0.00
Indonesia			307,817.00	0.09
Hungary			45,938.00	0.01
Hong Kong			58,788.00	0.01
Guatemala			287.00	0.00

Figure 3.4 Import of ethylbenzene to Malaysia in 2020 [75].

CHAPTER 4

PROCESS SYNTHESIS STRUCTURE AND ANALYSIS

4.1 Input-Output Structures

Packed Bed Reactor/ Alkylator with Fixed Bed of Zeolite Catalyst

Alkylation (Main & Side reaction)

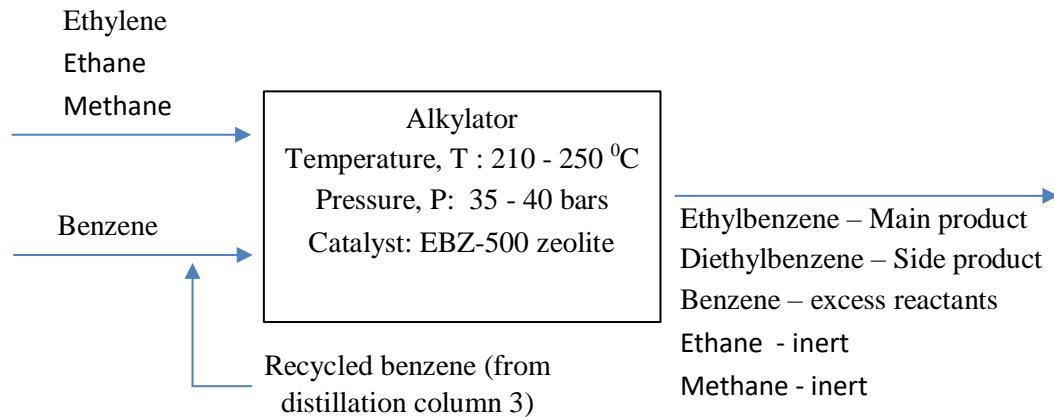


Figure 4.1 Alkylation process carried out in alkylator (*let ethylene be limiting reactant and 100% conversion).

Figure 4.1 shows the liquid zeolite-based process of benzene alkylation with ethylene which is being carried out in the alkylator. In this process, the reactants entering the reactor are benzene and ethylene. Both streams will pass together through the fixed bed of EBZ-500 zeolite catalyst in the reactor. To maintain the reaction undergoing in liquid phase at a reasonable reaction rate, the pressure and temperature of the alkylator is maintained at a pressure of 35 - 40 bars and temperature of 210 - 250 °C. Under this operating condition, the ethylene conversion is nearly 100%. Besides, the reaction is exothermic in an isothermal condition. Therefore, the heat generated can be used to generate heat in the distillation column for the purpose of saving energy.

Transalkylator with Fixed Bed of Zeolite Catalyst
Transalkylation

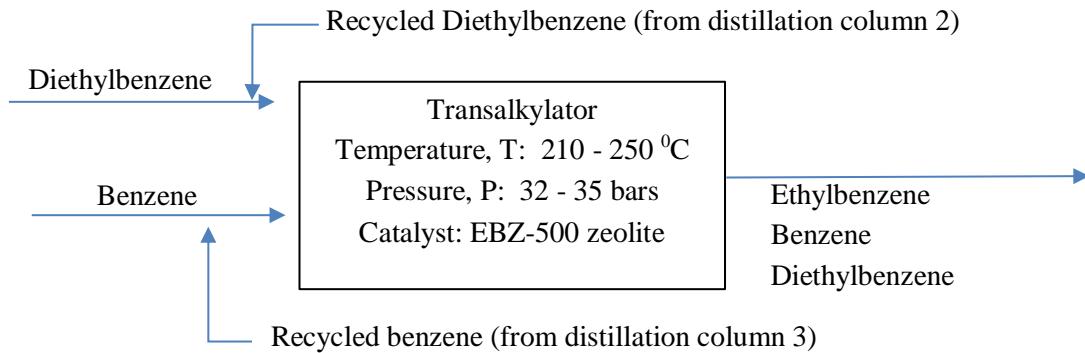


Figure 4.2 Transalkylation process carried out in transalkylator.

Figure 4.2 shows the process of transalkylation which is being carried out in transalkylator. The reactants of this process are diethylbenzene and benzene in liquid form. This process involves the recycled stream of diethylbenzene from the second distillation column as well as recycled benzene from the first distillation column. For optimizing the reaction rate, the reactor operates under the pressure of 32 - 35 bars and temperature 210 - 250 °C. The output products for this reactor are ethylbenzene and benzene. To separate them, they will be mixed with the effluent from alkylator and sent to the first distillation column. Then, the first distillation column or benzene distillation will separate the distillate as benzene and bottom product as mixture of diethyl benzene and ethylbenzene which will be sent to the second distillation column in the next step.

First Distillation/ Benzene Distillation

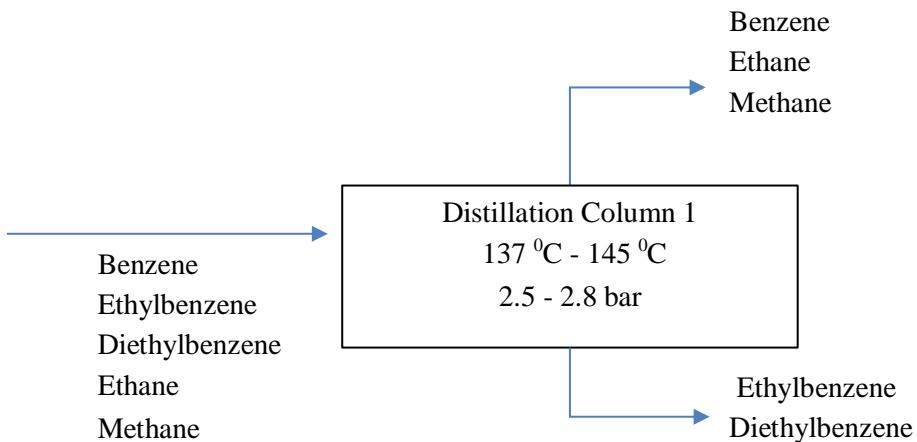


Figure 4.3 Benzene distillation.

The feed to the distillation column shown in Figure 4.3 is the effluent from alkylator and transalkylator. The feed is the mixture of benzene, ethylbenzene, diethylbenzene, ethane and methane. The distillation column operates under temperature which is between or equal to $137\text{ }^{\circ}\text{C}$ and $145\text{ }^{\circ}\text{C}$. This operating condition ensures the distillation column to separate the mixture based on their significant difference in volatility. After the separation, benzene, ethane, and methane will be separated as top product or distillate whereas ethylbenzene and diethylbenzene are separated as bottom product

Second Distillation/ Ethylbenzene Distillation

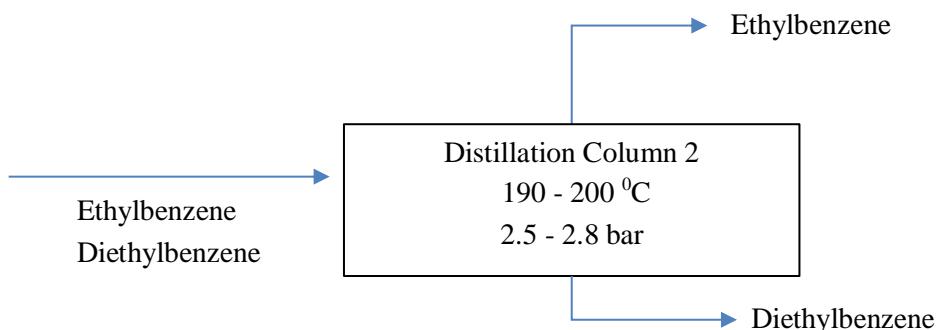
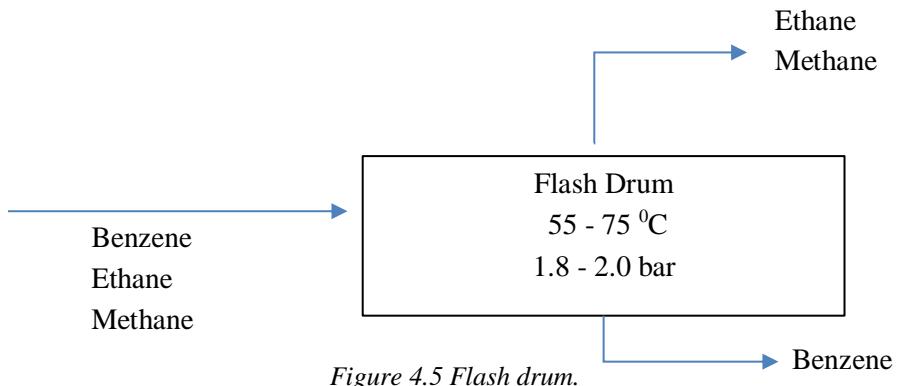


Figure 4.4 Ethylbenzene distillation.

The feed to the ethylbenzene distillation column shown in Figure 4.4 consists of ethylbenzene, and diethylbenzene in liquid form. The distillation column operates under temperature which is between or equal to $145\text{ }^{\circ}\text{C}$ and $170\text{ }^{\circ}\text{C}$. This operating condition

enables the distillation column to separate the mixture based on the difference of boiling point between ethylbenzene and diethylbenzene. After the separation, ethylbenzene will be separated as top product or distillate and recycled back to the alkylator whereas diethylbenzene are separated as bottom product in this process and recycled back to the transalkylator to produce ethylbenzene through the transalkylation process again.

Flash drum



The feed to the flash drum shown in Figure 4.5 consists of benzene in vapor form as well as ethane and methane in gaseous form. The distillation column operates under temperature of 55 - 75 °C and pressure of 1.8 - 2.0 bar. This operating condition enables the distillation column to separate the mixture based on the difference of boiling point between benzene, ethane, and methane. After the separation, ethane and methane will be separated as top product or distillate and removed as purge whereas benzene is separated as bottom product in this process and recycled back to the alkylator and transalkylator to produce ethylbenzene (main product).

Recycle Structure with Operating Condition

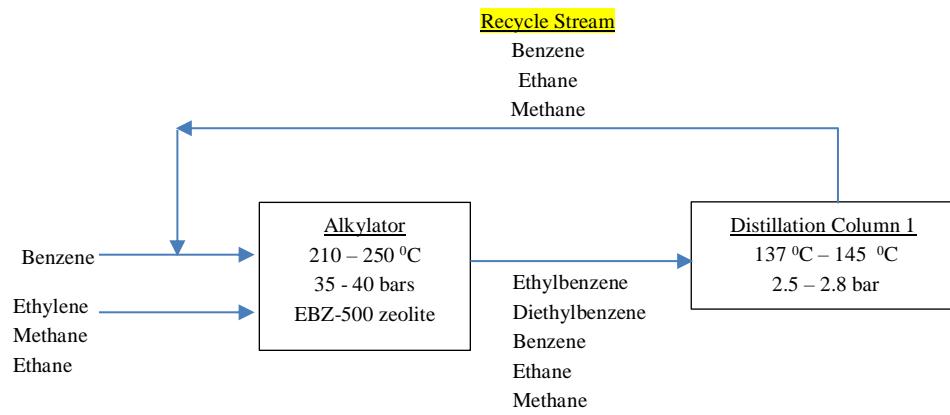


Figure 4.6 Recycle stream of benzene, ethane, and methane from distillation column 1 to fresh benzene feed.

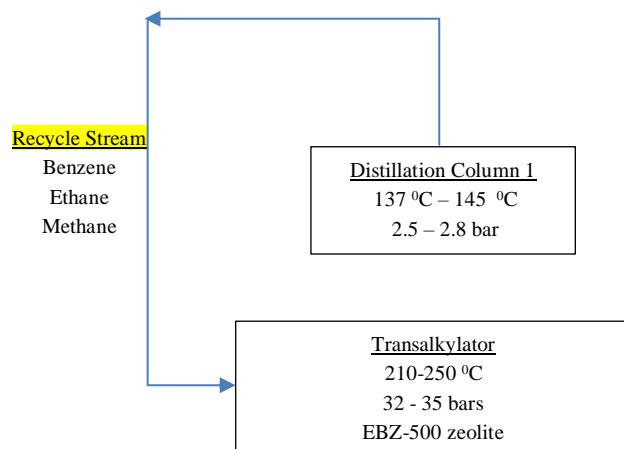


Figure 4.7 Recycle stream of benzene, ethane, and methane from distillation column 1 to transalkylator.

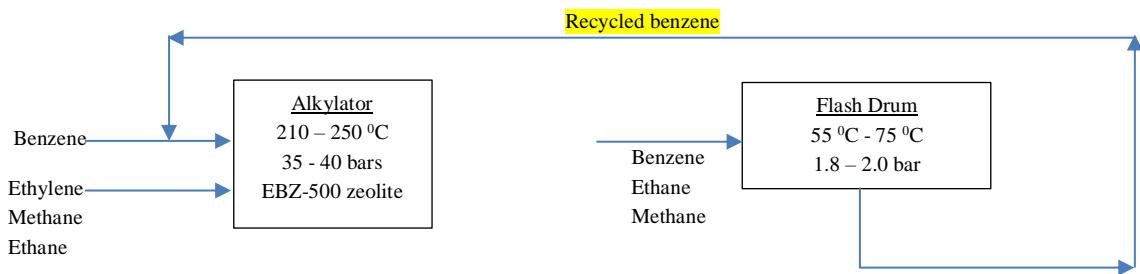


Figure 4.8 Recycle stream of benzene from flash drum to fresh benzene entering the alkylator.

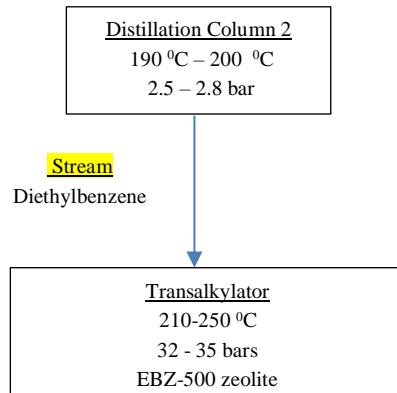


Figure 4.9 Stream of diethylbenzene from distillation column 2 to transalkylator.

To separate benzene from distillation column 1, we need to calculate vapor pressure first. For example, at temperature of 137 °C, the vapor pressure of benzene is 4.41 bar or maybe lower. Therefore, at a pressure below 4.41 bar or lower, the benzene including ethane and methane will exist only in the vapor phase, and we can separate it from other less volatile components which are ethylbenzene and diethylbenzene. Hence, before entering the distillation column, the liquid mixture that formed through the alkylation process will be cooled to temperature between 137 °C to 145 °C and pressure will be reduced to 2.5 – 2.8 bars. As a result, the benzene can separate from the mixture of benzene, ethylbenzene, and diethylbenzene. Then, the separated benzene, ethane, and methane will recycle back to the transalkylator (refer to Figure 4.7) to react with the stream of diethylbenzene (refer to figure 4.9) to produce more ethylbenzene. Besides, the separated benzene, ethane, and methane will also recycle back and join the fresh benzene feed entering alkylator (refer to Figure 4.6).

Whereas, for flash drum, the operating temperature and pressure is 55 – 75 °C and 1.8 – 2.0 bar respectively. This will ensure the gas stream of ethane and methane separated from benzene (bottom product) and thus, recycle back to the fresh benzene feed entering the alkylator (refer to Figure 4.8).

Process Flowsheet

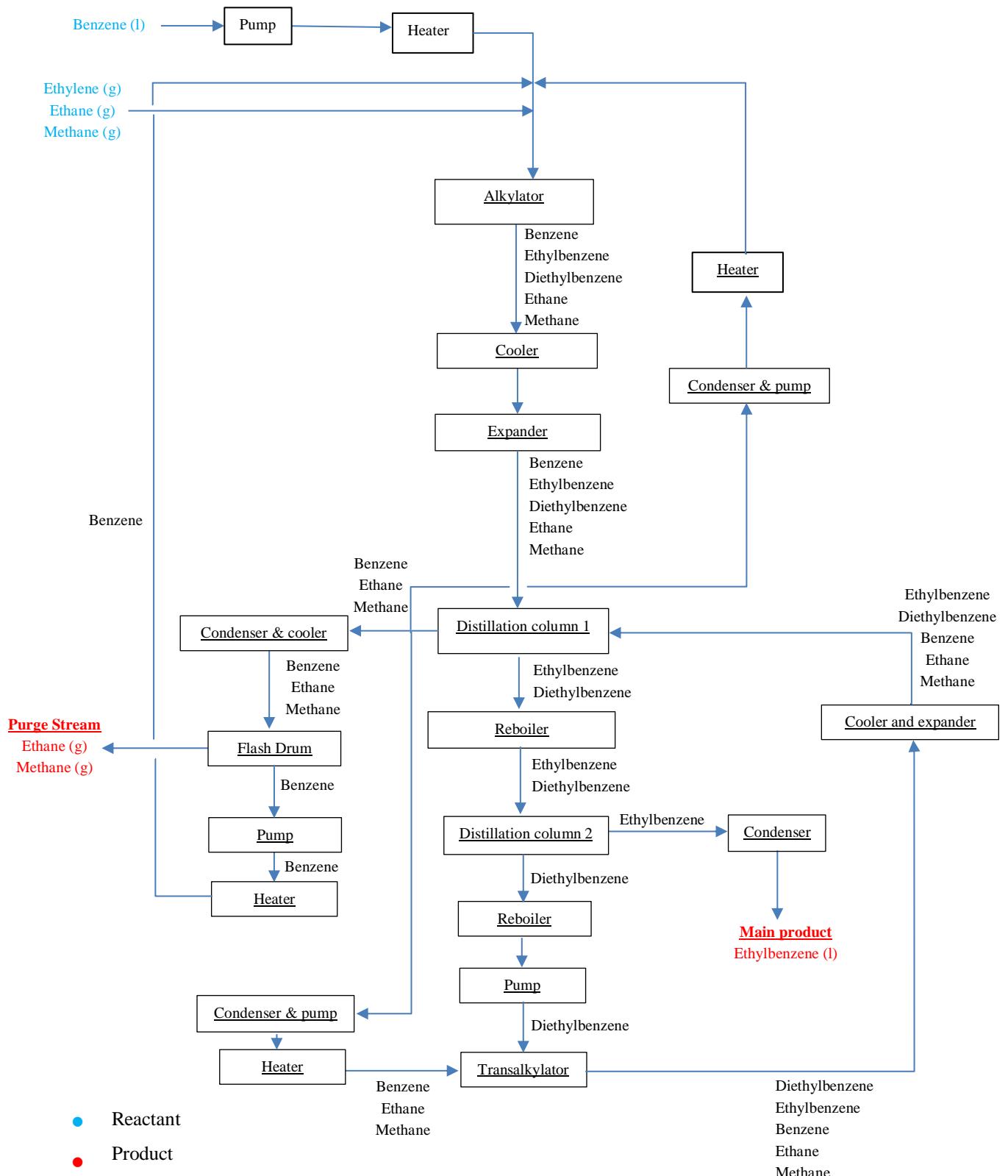


Figure 4.10 Process flowsheet of the production of ethylbenzene.

4.2 Feed and Product Specifications

The details of the components in feed and product specification are shown in table below.

Table 4.1 Feed and product specifications.

Chemical	Phase/State	Composition (wt%)
Feed		
Benzene	Liquid	>99.99
Ethylene	Gas	99.92
Ethane	Gas	0.053
Methane	Gas	0.027
Product		
Ethylbenzene	Liquid	99.97
Catalyst		
Zeolite EBZ-500™	Solid	-

4.3 Price of all Products, By-Products, and Raw Materials

The recorded price is based on the average market price of the chemical in year 2021.

Table 4.2 Price of raw materials, product, and by-product.

Chemical	Price (USD/kg)	Price (USD/ton)	Price (MYR/ton)
Feedstock			
Benzene [37]	0.88	883	3,690.06
Ethane [84]	6.00	6,000	25,073.99
Ethylene [36]	1.01	1,014	4,237.50
Methane [85]	6.00	6,000	25,073.99
Product			
Ethylbenzene [86]	1.20	1,200	5,016.00
Diethylbenzene [87]	2.50	2,500	10,447.50

Conversion of currency (17th November 2021)

USD 1 = MYR 4.18

4.3.1 Economic Potential

Economical potential is rough estimation of gross profit margin by calculating the difference between price and amount of feedstock used and price and amount of product produced in the plant correlate to that amount of feedstock based on the overall chemical reaction in the designated plant.

Overall chemical reaction:



Plant details:

Plant capacity (ton/yr)	50,000
Selectivity (%)	92
Yield (%wt.)	99.6

Basis of calculation: 50,000 ton/yr which equal to 470,987.189 kmol/yr.

Calculation of cost for the plant:

Table 4.3 Calculation of basis and cost for the designed plant.

Chemical	Stoichiometry	Molecular weight (kg/kmol)	Annual basis (kmol/yr)	Annual basis (ton/yr)	Price per ton (MYR/ton)	Total price (MYR/year)
Feedstock						
Benzene	1	78.11	470,987.189	36,789	3,690.06	135,753,617.30
Ethylene	1	29.05	470,987.189	13,682	4,237.50	57,977,475.00
Product						
Ethylbenzene	1	106.16	470,987.189	50,000	5,016.00	250,800,000.00

$$\begin{aligned} \text{Gross profit} &= \text{MYR } 250,800,000.00 - (\text{MYR } 135,753,617.30 \\ &\quad + \text{MYR } 57,977,475.00) \end{aligned}$$

$$\text{Gross profit} = \text{MYR } 57,068,907.70$$

$$\text{Gross profit margin} = \frac{\text{Gross profit}}{\text{Price of desired product}}$$

$$\text{Gross profit margin} = \frac{\text{MYR } 57,068,907.70}{\text{MYR } 250,800,000.00} \times 100\%$$

$$\text{Gross profit margin} = 22.75\%$$

4.5 Destination Codes and Component Classification

Table 4.4 Destination codes and component classification.

Components	Component Classification	Destination	Destination code
Benzene	Reactant	Alkylator Distillation column 1 Condenser Reflux Drum Flash Drum Transalkylator	R-101 T-201 E-201 V-201 V-501 R-301
Ethylene	Reactant	Alkylator	R-101
Ethylbenzene	Main Product	Alkylator Distillation Column 1 Reboiler Distillation Column 2 Condenser Reflux Drum Transalkylator	R-101 T-201 E-202 T-401 E-401 V-401 R-301
Diethylbenzene	By-Product	Distillation Column 1 Reboiler Distillation Column 2 Condenser Reflux Drum Reboiler Transalkylator	T-201 E-202 T-401 E-401 V-401 E-402 R-301
Methane	Inert	Alkylator Distillation column 1 Condenser Reflux Drum Flash Drum Transalkylator	R-101 T-201 E-201 V-201 V-501 R-301
Ethane	Inert	Alkylator Distillation column 1 Condenser Reflux Drum Flash Drum Transalkylator	R-101 T-201 E-201 V-201 V-501 R-301

4.6 Utilities

The basic and essential utilities in running and supporting the operation of the plant are shown in table below.

Table 4.5 Utilities of ethylbenzene production process.

Utilities	Specification
Electricity	<ul style="list-style-type: none">• As main power supply to all equipment including pump, expander, condenser, and control system.• Required for maintenance and system control of the process.• Used for both domestic and industrial supply.
Water	<ul style="list-style-type: none">• Used as coolant in heat exchangers to decrease the temperature of stream before entering the next unit operation.• Utilised in condenser to condense the vapour product partially or fully from the benzene and ethylbenzene distillation columns.• A suitable coolant due to low-cost, abundantly available, non-hazardous, and high heat capacity.
Steam	<ul style="list-style-type: none">• Used as energy supply for reboiler in distillation column.• Serves as heating element for heat exchanger to heat up recycled benzene stream.

CHAPTER 5

PROCESS FLOW DIAGRAM (PFD)

5.1 Block diagram of Process Structure

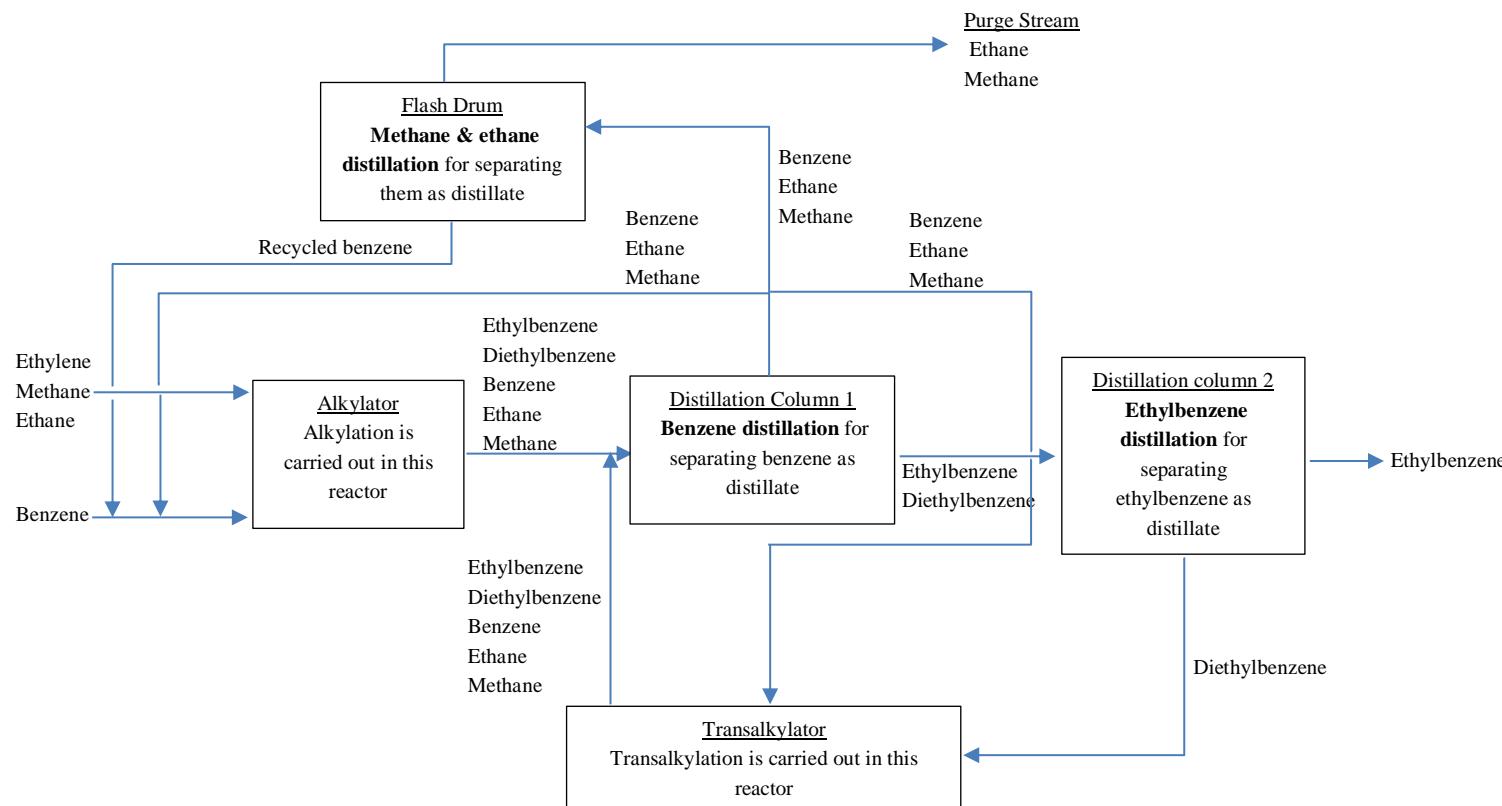
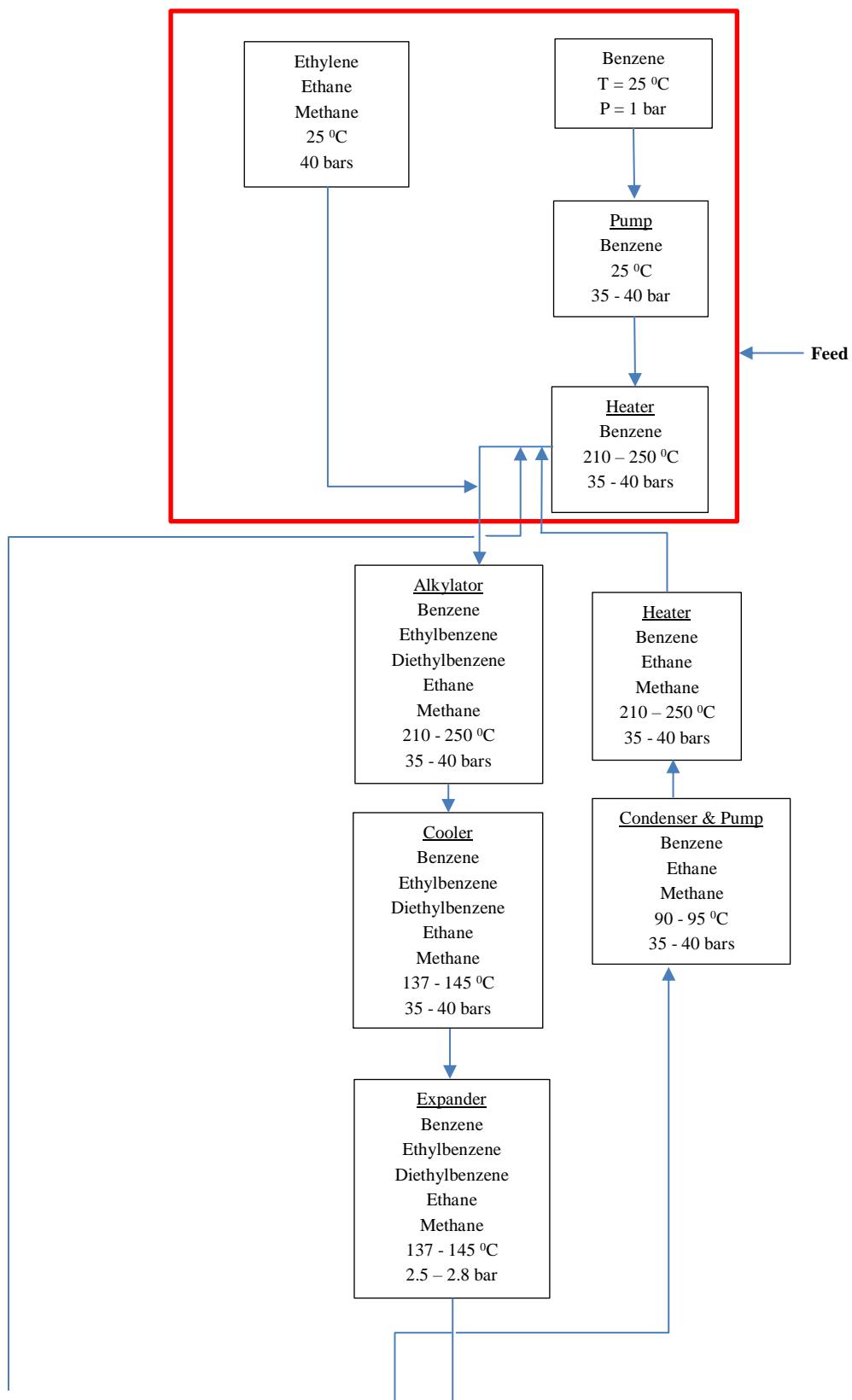


Figure 5.1 Block diagram to produce ethylbenzene.

5.2 Process Synthesis Flow Sheet



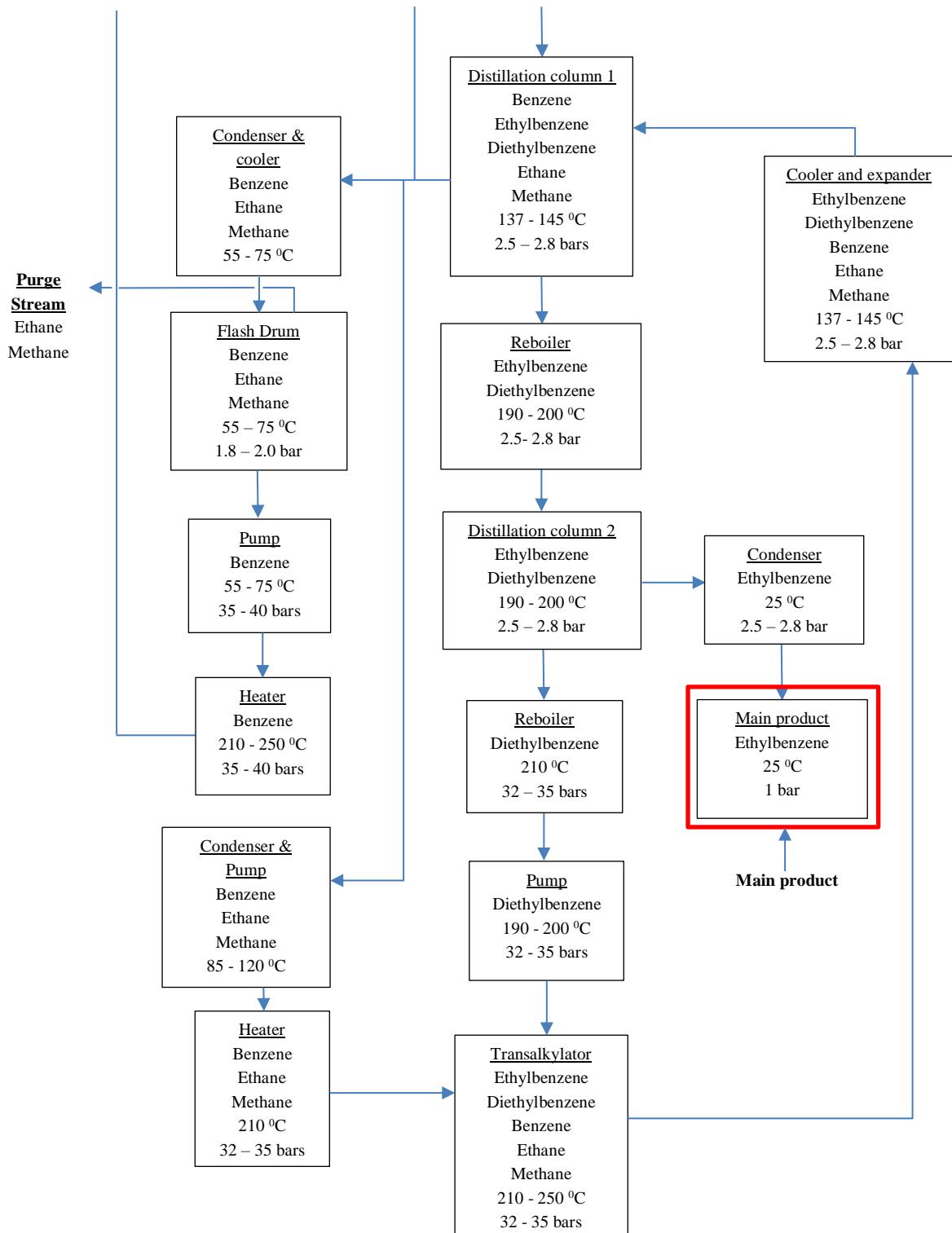


Figure 5.2 Process synthesis flow sheet to produce ethylbenzene.

5.3 Innovative Approach

Based on the plant we design, there are two innovative approaches implemented in the plant. First and foremost, as we know, the polymer grade ethylene consists of a small amount of ethane and methane. In our plant, ethane, and methane just act as inert and they are non-reactive. Hence, we need to remove these gases regularly as a purge stream. This is because without any purge, the ethane and methane will accumulate within the plant. This may cause the overload for the plant and the reaction rate will be significantly reduced and even stopped. To avoid this problem, we must remove them, but this will remove the benzene in vapor form together. Therefore, to minimize the loss of benzene through the purge stream, we implement a flash drum within our plant. The flash drum is used to separate the benzene from ethane and methane based on the significant difference of their volatility. Hence, the benzene will be condensed and recycled back to the alkylator and transalkylator. Other than that, this can also collect the highly purified ethane and methane and sell them as fuel in the global market. In short, this innovative approach can minimize the waste and make profit from the minor side or by product.

On the other hand, the innovative approach is implementing the concept of heat integration. As we know, benzene alkylation is a kind of exothermic reaction. This reaction will release a huge amount of heat during the reaction. The heat released will increase the temperature of all components within the reactor. This might cause the undesirable side reaction to occur as well. Therefore, we have to remove the heat released. Therefore, we apply the concept of heat integration by using the high temperature outlet stream from the reactor as heating fluid. When they pass through the heat exchanger, the heat will be transferred to the side of the low temperature stream. Then, the heat exchange will occur. Through this approach, the heat released from the reaction can be fully used for other parts. In addition, the heat could also be used to heat the reboiler of the distillation column to the desirable temperature for the desirable separation process to occur.

In conclusion, the main purpose of the innovative approach that we implement in our plant is used for recovering energy and making the best use of them to not only prevent the waste of energy but also make profit from them.

5.4 Process Flow Diagram

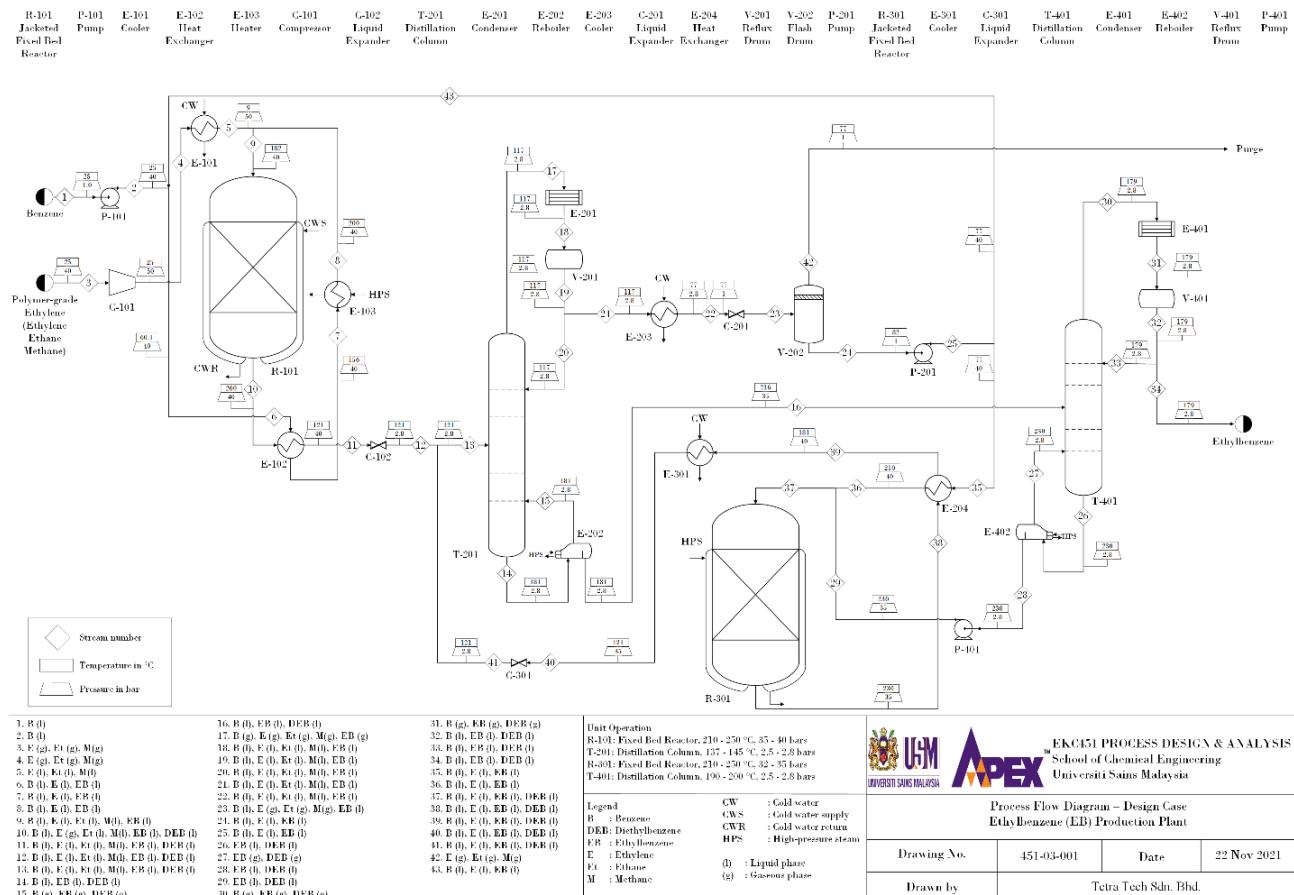


Figure 5.3 Process flow diagram of ethylbenzene production.

CHAPTER 6 PROCESS ANALYSIS

6.1 Material of Construction

The selection of construction materials for equipment in the plant is one of the most crucial parts in effective engineering design because it determines the reliability of the design in terms of industrial and economical aspects [90]. The important characteristics that need to be taken into account are the mechanical properties such as strength and stiffness, corrosion resistance, wear resistance, cost and availability [90]. The main constructional materials under metals and alloys include carbon steel, low alloy steels, stainless steels, nickel and its alloys, copper and its alloys, high alloy and heat-resisting steels, aluminium and its alloys [91]. Chemical compatibility of some common construction materials in production plant at 70°F (21°C) is shown in Table 6.1 below.

Table 6.1 Chemical compatibility of various construction materials [92].

Fluid	Metal				
	Aluminium	Carbon Steel	304 Stainless Steel	316 Stainless Steel	Hastelloy C
Benzene	B	A	B	B	B
Ethylene	A	-	A	A	-
Ethylbenzene	B	-	B	B	A
Diethylbenzene	-	-	-	-	-
Methane	A	-	A	A	A
Ethane	A	-	A	A	A
Water	B	D	A	A	A

*A = Excellent, B = Good, C = Fair to poor, D = Not recommended, - No data.

*The data is provided for the chemicals at 70°F (21°C).

Based on the Table 1.1 above, both Type 304 and Type 316 stainless steel are suitable for the construction of the equipment in the plant due to excellent chemical compatibility towards most of the chemicals in the plant. However, further justification needs to be made based on the cost of materials, temperature and corrosion resistance as well as the suitability of the materials.

Plain carbon steel as the most predominant material of construction for process equipment in chemical process industries has the lowest cost, easy availability, adequate thermal and mechanical properties, ease of fabrication, etc, although it has a limitation which is low corrosion resistance [73]. Plain carbon steel is satisfactorily used where strength and other property requirements are not severe and when high temperatures and corrosive environments are not a major factor in the selection of material [94].

When corrosive chemicals are involved in a chemical process plant or corrosion resistance becomes a factor to be concerned, for overall resistance to general uniform corrosion, it is more suitable to use the common austenitic stainless steel Type 304 [93]. However, Type 304 stainless steel has limitation with respect to uniform corrosion in reducing acids and to pitting corrosion, crevice corrosion and stress corrosion cracking in chloride containing media [93]. When comes to these cases, Type 316 stainless steels has better performance but it displays unsatisfactory corrosion behavior in strong reducing acids, in concentrated chloride solutions at elevated temperatures and in fluids flowing with high velocities [93].

Therefore, carbon steel is adequate to be used as the material of construction for all the equipment that operate under non-extreme and non-corrosive conditions. On the other hand, due to high operating temperature and acidic operating condition in the two fixed bed reactors which are alkylator and transalkylator, Type 304 stainless steel that is stronger with higher corrosion resistance than carbon steel will be used as the construction material.

Carbon Steel for All Mass Transfer, Heat Transfer and Auxiliary Equipment

Due to the characteristics of carbon steel mentioned previously, it will be used as the construction material for all the equipment in the chemical process plant except fixed bed reactors. Carbon steel is adequate to be the construction material for basic equipment such as pumps, heat exchangers, condensers, reflux drums, etc, as these unit operations are not operating at extreme condition and without any vigorous reaction involved.

The choice of carbon steel as the construction material instead of stainless steel that shows excellent chemical compatibility towards most of the chemicals in the plant is mainly because of its lower cost. Carbon steel contains relatively few alloying elements which are in low concentration, hence it is relatively inexpensive [95]. Moreover, pipes of carbon steel can be made much thinner than pipes made from other materials, resulting in greater carrying

capacity than pipes constructed by other materials with the same diameter. This allows more cost-saving.

Besides, carbon steel has high temperature resistance, where it is able to withstand heat to a temperature limit of 500°C [96]. This makes carbon steel a suitable material for most of the equipment in this plant as the operating temperature for all equipment in the plant are lower than 300°C. Moreover, carbon steel is extremely strong and more durable than stainless steel. However, this type of material may rust and corrode when exposed to moisture including moisture vapor in the air. It is also not prone to rotting as many metals are and safe to be used and work with. The price of carbon steels is about \$500/ton, relatively inexpensive. It is because the alloying elements of the carbon steel composition are low.

Stainless Steel for Fixed Bed Reactors

Stainless steel is particularly effective in acidic environments since it has good corrosion resistance, thus it will be used for the construction of alkylation and transalkylation reactors (fixed bed reactors) which operate in acidic condition with acidic catalyst, EBZ-500TM zeolite. The corrosion-resistant property of stainless steel is mainly due to the chromium alloy content. Stainless steel is about 200 times more resistant to corrosion compared to mild steel by having chromium content over 11%. The chromium content allows the formation of an invisible chromium oxide film on the surface of the steel, making it resistant to corrosion.

Type 304 stainless steel is chosen over Type 316 stainless steel because it has high corrosion resistance and yet with lower cost [97]. Type 304 stainless steel is more versatile and widely used compared to Type 316 stainless steel because of its lower cost results from minimum content of chromium and nickel [98]. The unique characteristic of stainless steel to resist corrosion with the addition of alloying elements such as nickel, molybdenum, copper and manganese makes it generally more expensive than carbon steels. However, stainless steel is chosen as the construction material for fixed bed reactors for long term perspective as the operating condition of the reactors is acidic which is inappropriate for the use of carbon steel. In terms price, stainless stain is more expensive compared to carbon steel as the concentration of alloying elements are high.

6.2 Justification of each equipment

6.2.1 Reaction Unit Operation

Equipment	Jacketed fixed bed reactor	
Code of equipment	R-101	
Material of construction	Reactor shell: Type 304 stainless steel Cooling jacket: 2205 duplex stainless alloy	
Orientation	Horizontal	
Operating conditions	Temperature	210 - 250°C
	Pressure	35 - 40 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	For alkylation reaction of benzene in the presence of EBZ-500™ zeolite catalyst to produce ethylbenzene as the main product and diethylbenzene as side product.	
Justification:	<p>Alkylation reaction of benzene with ethylene occurs in the reactor with the presence of acidic EBZ-500™ zeolite catalyst being distributed as beds. This exothermic reaction operates at temperature of 210 - 250°C and pressure of 35 - 40 bar. Due to acidic operating condition, the reactor is constructed from Type 304 stainless steel which has high corrosion resistance. Since catalyst is used, the type of reactor for alkylation process is fixed bed catalytic reactor. Cooling jacket is implemented to maintain the reactor temperature at 210 - 250°C. The cooling jacket of the reactor is constructed from 2205 duplex stainless alloy instead of 304 stainless steel because this material has greater strength which results in cheaper and thinner reactor wall, high thermal conductivity, good heat transfer between cooling jacket and reactor, and its lightweight characteristic eliminates the requirement of extra support and simplifies the overall reactor structural design [1].</p>	

Equipment	Jacketed fixed bed reactor
Code of equipment	R-301
Material of construction	Reactor shell: Type 304 stainless steel

	Cooling jacket: 2205 duplex stainless alloy	
Orientation	Horizontal	
Operating conditions	Temperature	210 - 250°C
	Pressure	32 - 35 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	For transalkylation reaction of benzene with diethylbenzene in the presence of EBZ-500™ zeolite catalyst to produce ethylbenzene.	
Justification:	<p>Transalkylation of benzene with diethylbenzene takes place in the fixed bed reactor with the presence of EBZ-500™ zeolite catalyst distributed as beds. This reaction is exothermic which operates at 210 - 250°C and 32 - 35 bar. Since it is a catalytic reaction under acidic condition, the type of reactor used for transalkylation process is a fixed bed catalytic reactor constructed with Type 304 stainless steel for corrosion resistance purpose. Cooling jacket made from 2205 duplex stainless alloy is applied to maintain the reactor at 210 - 250°C. The reasons 2205 duplex stainless alloy is used instead of Type 304 stainless steel are as mentioned previously.</p>	

6.2.2 Mass transfer unit operations

Equipment	Distillation column	
Code of equipment	T-201	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	137 - 145°C
	Pressure	2.5 – 2.8 bar
	Phase	Liquid and vapor
	Mode	Continuous
No. of unit required	1	
Purpose	To separate unreacted benzene, methane and ethane from ethylbenzene and diethylbenzene.	

Justification:

This distillation column is mainly designed to separate the unreacted benzene from the main product, ethylbenzene. The overhead products of this distillation column are benzene, methane and ethane in gaseous phase while the bottom products are ethylbenzene and diethylbenzene in liquid phase. Separated ethylbenzene and diethylbenzene are being sent to the second distillation column for further separation while the unreacted benzene together with the inert which are methane and ethane are recycled back to the first reactor which is the alkylator. Carbon steel is used as the casting materials as the operating temperature is below 500°C without any vigorous reaction. Besides, sieve tray which consists of metal plates with holes in them is used in this distillation column where vapor will pass straight upward through the liquid on the plate. The design parameters include the arrangement, size and number of the holes.

Equipment	Distillation column	
code of equipment	T-401	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	190 - 200°C
	Pressure	2.5 – 2.8 bar
	Phase	Liquid and vapor
	Mode	Continuous
No. of unit required	1	
Purpose	For separation of main product which is ethylbenzene from benzene and diethylbenzene.	

Justification:

This distillation column is designed to obtain ethylbenzene with a purity of > 99.5%. The overhead product of this distillation column is gaseous ethylbenzene which is the main product from this production plant with trace amount of gaseous benzene and diethylbenzene while the bottom products that contain liquid ethylbenzene and diethylbenzene are returned to the column for further separation. Carbon steel is used as the casting materials as the operating temperature is below 500°C without any vigorous reaction. Besides that, sieve tray which consists of metal plates with holes in them is used in this

distillation column where vapor will pass straight upward through the liquid on the plate. The design parameters include the arrangement, size and number of the holes.

Equipment	Flash drum	
Code of equipment	V-202	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	Inlet: 127°C (stream 23) Outlet: 77°C (stream 42), 82°C (stream 24)
	Pressure	1 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To separate out the trace components which are ethane and methane to be discharged as purge stream.	

Justification:

The flash column removes most of the trace components in gas phase which are ethane and methane by reducing the temperature of the inlet stream (S-23) from 122 to 77°C (S-42) while separates out most of the benzene in liquid phase to be recycled back to the mixing point of the feed stream by increasing the temperature of the inlet stream (S-23) from 77 to 82°C (S-24). Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Flash drum	
Code of equipment	V-202	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	Inlet: 127°C (stream 23) Outlet: 77°C (stream 42), 82°C (stream 24)
	Pressure	1 bar
	Phase	Liquid
	Mode	Continuous

No. of unit required	1
Purpose	To separate out the trace components which are ethane and methane to be discharged as purge stream.
Justification:	The flash column removes most of the trace components in gas phase which are ethane and methane by reducing the temperature of the inlet stream (S-23) from 122 to 77°C (S-42) while separates out most of the benzene in liquid phase to be recycled back to the mixing point of the feed stream by increasing the temperature of the inlet stream (S-23) from 77 to 82°C (S-24). Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

6.2.3 Heat transfer unit operations

Equipment	Heat exchanger (shell and tube)				
Code of equipment	E-102				
Material of construction	Carbon steel				
Orientation	Horizontal				
Operating conditions	Temperature	<u>Tube</u> Inlet: 200°C (stream 8) Outlet: 121°C (stream 9)	<u>Shell</u> Inlet: 60.1 °C (stream 6) Outlet: 156°C (stream 7)		
	Pressure	40 bar			
	Phase	Liquid			
	Mode	Continuous			
No. of unit required	1				
Purpose	To heat up the benzene in the inlet stream (S-6) before entering the alkylator which is a fixed bed reactor (R-101) while using outlet stream (S-10) of the alkylator as heating medium.				
Justification:	Shell and tube heat exchanger is chosen as it can support higher operating temperatures and pressures than other heat exchanger such as typical plate heat exchanger [99]. A shell and tube				

heat exchanger has a long service life [100]. Besides, it has higher resistance to scale formation, so cleaning needs to be done less frequently than with other heat exchangers [99]. It is also relatively cheap and can save more energy costs as the pressure drop from input to output is smaller [99]. This heat exchanger is designed by using outlet stream of fixed bed reactor as heat source for heating up feed to the same reactor. For the material of construction, carbon steel is chosen as the construction material for this heat exchanger as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Heat exchanger (shell and tube)				
Code of equipment	E-204				
Material of construction	Carbon steel				
Orientation	Horizontal				
Operating conditions	Temperature	<u>Tube</u> Inlet: 77°C (stream 35) Outlet: 210°C (stream 36)	<u>Shell</u> Inlet: 230°C (stream 38) Outlet: 181°C (stream 39)		
	Pressure	40 bar			
	Phase	Liquid			
	Mode	Continuous			
No. of unit required	1				
Purpose	To increase temperature of inlet stream (S-35) to the operating temperature for the transalkylation reaction before entering transalkylator which is a fixed bed reactor (R-301) while using outlet of R-301 (S-38) as heating medium.				
Justification:	The temperature of stream 35 is increased from 77°C to 210°C for stream 36 prior to entering benzene distillation column that operates at 210 - 250°C and 32 - 35 bar. Carbon steel is chosen as the construction material for this heat exchanger as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.				

Equipment	Condenser
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Code of equipment	E-101	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 25°C (stream 4) Outlet: 9°C (stream 5)
	Pressure	50 bar
	Phase	Vapor to liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To cool and liquefy vapor ethylene feed with trace components, ethane and methane before being transferred to alkylator R-101.	
Justification:	<p>The temperature of vapor ethylene feed with trace components, ethane and methane will be lowered before entering alkylator R-101. Carbon steel is chosen as the construction material for this condenser as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.</p>	

Equipment	Condenser	
Code of equipment	E-201	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	117°C
	Pressure	2.8 bar
	Phase	Vapor to liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To condense the vapor distillate from distillation column T-201 before returning to the distillation column or entering the flash drum.	
Justification:	<p>Vapor benzene, ethylbenzene, ethylbenzene, ethane and methane at the top of distillation column will be liquefied before some part of it being refluxed while the remainder being</p>	

transferred to the flash drum. Carbon steel is chosen as the construction material for this condenser as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Condenser	
Code of equipment	E-401	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	179°C
	Pressure	2.8 bar
	Phase	Vapor to liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To condense the vapor distillate from distillation column T-401 which are ethylbenzene benzene, and trace amount of diethylbenzene before returning part of it to the distillation column while discharging the remaining part with mainly ethylbenzene as the main product.	
Justification:	Vapor ethylbenzene and diethylbenzene at the top of distillation column will liquefied prior to being refluxed or discharged from the plant as the main product. Carbon steel is chosen as the construction material for this condenser as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.	

Equipment	Cooler	
Code of equipment	E-203	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 117°C Outlet: 77°C
	Pressure	2.8 bar
	Phase	Liquid
	Mode	Continuous

No. of unit required	1
Purpose	To lower the temperature of the liquid stream from reflux drum V-201 before being transferred to flash drum V-202.
Justification:	The temperature of liquid benzene, ethylene, ethylbenzene, ethane and methane coming out from reflux drum V-201 will be lowered before entering flash drum V-202. Carbon steel is chosen as the construction material for this cooler as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Cooler	
Code of equipment	E-301	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 181°C Outlet: 121°C
	Pressure	35 bar
	Phase	Vapor to liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To cool the products of transalkylator R-301 which consists of liquid benzene, ethylene, ethylbenzene and diethylbenzene before transferring to the distillation column T-201.	
Justification:	Cooler further cools down the products of transalkylator R-301 which consists of liquid benzene, ethylene, ethylbenzene and diethylbenzene to the operating temperature of the distillation column T-201 prior to entering the column. Carbon steel is chosen as the construction material for this cooler as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.	

Equipment	Heater
code of equipment	E-103
Material of construction	Carbon steel

Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 156°C Outlet: 200°C
	Pressure	40 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To heat up the products of alkylator R-101 mixed with recycled stream which consists of liquid benzene, ethylene and ethylbenzene before returning it to the same reactor.	
Justification:	<p>Heater heats up the liquid product from the alkylator R-101 mixed with the recycled stream to the operating temperature of the alkylator prior to returning to the same reactor. Carbon steel is chosen as the construction material for this heater as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.</p>	

Equipment	Reboiler	
code of equipment	E-202	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	181°C
	Pressure	2.8 bar
	Phase	Liquid to vapor
	Mode	Continuous
No. of unit required	1	
Purpose	To re-boil the bottom products of distillation column T-201 which are liquid benzene, ethylbenzene, ethylbenzene and diethylbenzene to vapor form before returning it to the distillation column T-201.	
Justification:	<p>Reboiler heats up the liquid bottom product to generate vapor which will be returned to the column to drive the separation process in the distillation column while the remaining liquid will enter distillation column T-401. Carbon steel is chosen as the construction material for</p>	

this reboiler as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Reboiler	
code of equipment	E-402	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	230°C
	Pressure	2.8 bar
	Phase	Liquid to vapor
	Mode	Continuous
No. of unit required	1	
Purpose	To re-boil the bottom products of distillation column T-401 which are liquid ethylbenzene and diethylbenzene to vapor form.	
Justification:	<p>Reboiler heats up the liquid ethylbenzene and diethylbenzene at the bottom of the distillation column T-401 to generate vapor which will be returned to the column to drive the separation process in the distillation column. Carbon steel is chosen as the construction material for this reboiler as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.</p>	

6.2.4 Auxiliary Units

Equipment	Pump	
Code of equipment	P-101	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	Inlet: 25°C Outlet: 25°C
	Pressure	1.0 bar to 40 bar
	Phase	Liquid

	Mode	Continuous
No. of unit required	1	
Purpose	To pump fresh liquid benzene (S-1) from storage tank to the operating pressure of the alkylator R-101.	
Justification: Centrifugal pump is used as this pump is suitable for lower viscosity liquids with high flow rates. The benzene feed enters the impeller at its axis and exits along the circumference between the vanes where the impeller is connected through a drive shaft to a motor and rotated at high speed. The rotational motion of the impeller accelerates the fluid benzene out through the impeller vanes into the pump casing. [101] Carbon steel is used as the construction material for this pump as it is able to withstand high temperature and pressure with excellent heat resistance and tensile strength.		

Equipment	Pump	
Code of equipment	P-201	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	Inlet: 82°C Outlet: 82°C
	Pressure	1 bar to 40 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To pump liquid benzene stream from the bottom of flash drum V-202 to the second fixed bed reactor which is the transalkylator R-301 and a part of it is being recycled back to the feed mixing point.	
Justification: Centrifugal pump is used to raise the pressure of the liquid benzene from 1 bar to 40 bar in order to meet the operating pressure requirement prior to enter the transalkylator R-301 while a part of it as recycled stream to the feed mixing point. Carbon steel is used as the construction material for this pump as it is able to withstand high temperature and pressure with excellent heat resistance and tensile strength.		

Equipment	Pump	
Code of equipment	P-401	
Material of construction	Carbon steel	
Orientation	Vertical	
Operating conditions	Temperature	Inlet: 230°C Outlet: 230°C
	Pressure	2.8 bar to 35 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To pump liquid stream from bottom product of the distillation column T-401 to the transalkylator R-301.	

Justification:

Centrifugal pump is used to raise the pressure of the recycle benzene from 2.8 bar to 35 bar in order to meet the operating pressure requirement prior to enter the transalkylator. Carbon steel is used as the construction material of the pump as it can withstand high pressure and temperature with excellent heat resistance and tensile strength.

Equipment	Compressor	
code of equipment	C-101	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 25°C Outlet: 25°C
	Pressure	40 bar to 50 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To increase pressure of the ethylene feed stream (S-3) prior to enter the alkylator R-101.	

Justification:

Compressor is used to increase the pressure the ethylene feed stream (S-3) from 40 to 50 bar (S-4) in order to meet the operating pressure of the alkylator (R-101). Carbon steel is used as

the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Liquid Expander	
Code of equipment	C-102	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 122°C Outlet: 122°C
	Pressure	40 bar to 2.8 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To reduce pressure of the liquid stream (S-11).	
Justification: Liquid expander is used to reduce the pressure the liquid stream (S-11) from 40 to 2.8 bar (S-12) in order to meet the operating pressure of the distillation column T-201. Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.		

Equipment	Liquid Expander	
Code of equipment	C-201	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 122°C Outlet: 122°C
	Pressure	2.8 bar to 1 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To reduce pressure of the liquid stream (S-22).	
Justification:		

Liquid expander is used to reduce the pressure the liquid stream (S-22) from 2.8 to 1 bar (S-23) prior to enter the flash drum V-202. Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Liquid Expander	
code of equipment	C-301	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 122°C Outlet: 122°C
	Pressure	35 bar to 2.8 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To reduce pressure of the liquid stream (S-26).	
Justification:	<p>Liquid expander is used to reduce the pressure the liquid stream (S-40) from 35 to 2.8 bar (S-41) in order to meet the operating pressure of the distillation column T-201. Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.</p>	

Equipment	Reflux drum	
code of equipment	V-201	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 117°C Outlet: 117°C
	Pressure	2.8 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	

Purpose	To hold the condensed vapor distillate from top of distillation column T-201 and allows part of it to return to the column as reflux while transfers part of it to the flash drum V-202.
Justification:	Horizontal configuration of reflux drum will be used due to larger amount of vapor space available compared to a vertical reflux drum [102]. Besides, liquid travels much slower in a horizontal vessel which allows easier control in a pre-determined position [102]. Reflux stream is returned to the distillation column for further separation while part of it is being transferred to the flash drum V-202 for further separation. Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.

Equipment	Reflux drum	
code of equipment	V-401	
Material of construction	Carbon steel	
Orientation	Horizontal	
Operating conditions	Temperature	Inlet: 179°C Outlet: 179°C
	Pressure	2.8 bar
	Phase	Liquid
	Mode	Continuous
No. of unit required	1	
Purpose	To hold condensed distillate from top of distillation column T-401 and returns part of it back to the column to yield higher purity of ethylbenzene product while discharge part of it as final product.	
Justification:	Reflux stream is returned to the distillation column for further separation while part of it with purity of >99.5% ethylbenzene product is discharged as the main product. Carbon steel is used as the construction material as the temperature and pressure are within the limitation of the material and there is no any vigorous reaction occurs.	

6.3 Economic Potential

The economic potential analysis is crucial to justify the economic feasibility of the production plant proposed. Besides, economic potential is an important factor in the evaluation of the possible revenue gained by the company in order to maintain steady operation of the company and its future growth. The economic potential of a plant is normally evaluated by determining the amount of profit gained from selling the product deducted by the cost of raw materials required. Moreover, it is important to evaluate whether the ratio of raw materials fed into the plant will be optimum or a waste.

In this ethylbenzene production plant, the benzene to ethylene molar ratio in the alkylation reaction is the sole design variable to be considered. B/E ratio of lowest 4.0 on molar basis is recommended by literature, however, it was found from mass balance analysis that a minimum B/E ratio of 4.11 is required in order to achieve desired ethylene conversion. A higher B/E ratio indicates a higher cost of raw materials needed; thus, an economic potential graph of gross profit margin versus B/E ratio of the reaction at input-output and recycle structure is plotted to forecast the economic potential of the proposed plant as well as to maximize the profits.

6.3.1 Economic Potential of Input-Output Structure

Level I Economic Potential: Input-Output Structure

Figure 6.1 Input-input structure for the production of ethylbenzene

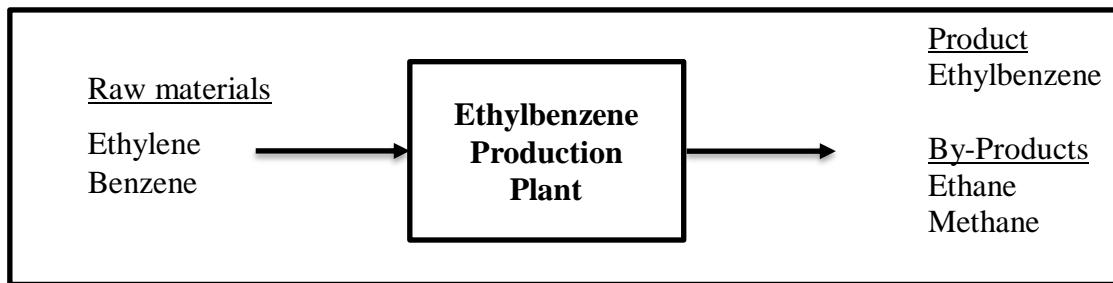


Table 6 2Price of feedstock and product

Chemical	Price (USD/kg)	Price (USD/ton)	Price (MYR/ton)
Feedstock			
Benzene [15]	0.88	883	3,690.06
Ethane [16]	6.00	6,000	25,073.99
Ethylene [17]	1.01	1,014	4,237.50
Methane [18]	6.00	6,000	25,073.99
Product			
Ethylbenzene [19]	1.20	1,200	5,016.00
Diethylbenzene [20]	2.50	2,500	10,447.50

Conversion of currency (17th November 2021)

USD 1 = MYR 4.18

The economic potential is calculated by using the formula shown below:

$$\mathbf{Gross\ profit = Economic\ Potential = Product\ cost - Raw\ material\ cost}$$

The gross profit margin is calculated by using the formula shown below:

$$\mathbf{Gross\ Profit\ Margin = \frac{Gross\ profit}{Value\ of\ Product} \times 100\%}$$

Calculation of cost for the plant:

Table 6 3 Calculation of basis and cost for the designed plant.

Chemical	Stoichiometry	Molecular weight (kg/kmol)	Annual basis (kmol/yr))	Annual basis (ton/yr)	Price per ton (MYR/ton)	Total price (MYR/year)
Feedstock						
Benzene	1	78.11	4,247,73 2.1600	331,790. 3590	3,690.06	1,224,326,332. 00
Ethylene	1	29.05	4,260,14 6.1680	119,497. 1000	4,237.50	506,368,961.3 0
Product						
Ethylbenzene	1	106.16	4,220,55 4.8000	448,096. 3031	5,016.00	2,247,651,056. 00
By-Product						
Ethane	-	30.07	2,257.92 15	67.8957	25,073.99	1,702,416.10
Methane	-	16.04	1,149.96 26	18.4454	25,073.99	462,499.78

**Benzene to ethylene molar ratio = 4.11

Gross profit = Economic Potential

$$\begin{aligned}
 &= \text{Product cost} - \text{Raw material cost} \\
 &= \text{MYR } 2,247,651,056.00 + \text{MYR } 1,702,416.10 + \text{MYR } 462,499.78 \\
 &\quad - (\text{MYR } 506,368,961.30 + \text{MYR } 1,224,326,332.00) \\
 &= \text{MYR } 519,120,634.80
 \end{aligned}$$

$$\begin{aligned}
 \text{Gross profit margin} &= \frac{\text{Gross profit}}{\text{Value of product}} \times 100\% \\
 &= \frac{\text{MYR } 519,120,634.80}{\text{MYR } 2,249,815,970.00} \times 100\% \\
 &= 23.0739\%
 \end{aligned}$$

6.3.2 Economic Potential of Recycle Structure

Level I Economic Potential: Input-Output Structure

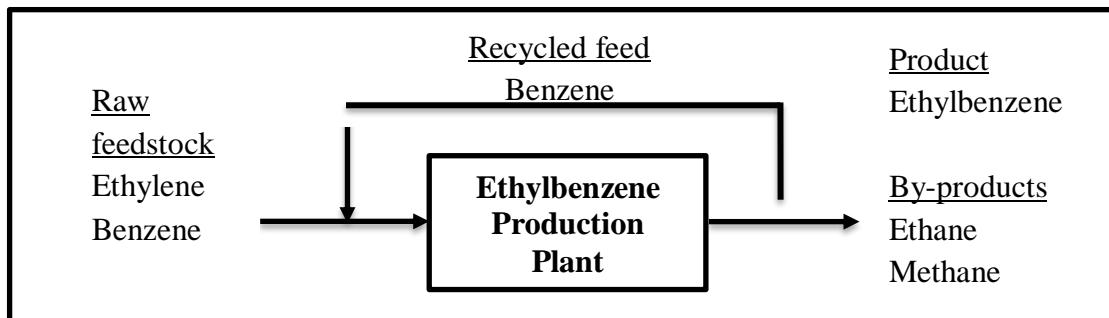


Figure 6 2Recycle structure for production of ethylbenzene

Table 6 4Economic potential for input-output and recycle structure of ethylbenzene production by varying B/E ratio.

B/E Ratio	Mass flowrate (ton/year)						Cost (MYR/year)						Economic Potential (MYR/year)	Gross Profit Margin (%)		
	Reactants		Recycled Benzene & ethylene	Product	By-Products		Reactant	Product	Recycled Benzene	By-Products						
	Benzene	Ethylene			Ethane	Methane				Ethane	Methane					
4.11	1369484.977	119497.11	1037694.62	53344.7980	67895.65	18445.3584	5053481735	506369003.1	3829155403	267577506.7	1702414959	462498732.1	701795862.9	11.20785		
4.20	1397620.503	119497.11	1065830.14	53344.7980	67895.65	18445.3584	5157303513	506369003.1	3932977180	267577506.7	1702414959	462498732.1	701795862.9	11.02505		
4.30	1430897.181	119497.11	1099106.82	53344.7980	67895.65	18445.3584	5280096453	506369003.1	4055770121	267577506.7	1702414959	462498732.1	701795862.9	10.81639		
4.40	1464173.86	119497.11	1132383.50	53344.7980	67895.65	18445.3584	5402889394	506369003.1	4178563062	267577506.7	1702414959	462498732.1	701795862.9	10.61549		
4.50	1497450.539	119497.11	1165660.18	53344.7980	67895.65	18445.3584	5525682335	506369003.1	4301356003	267577506.7	1702414959	462498732.1	701795862.9	10.42192		

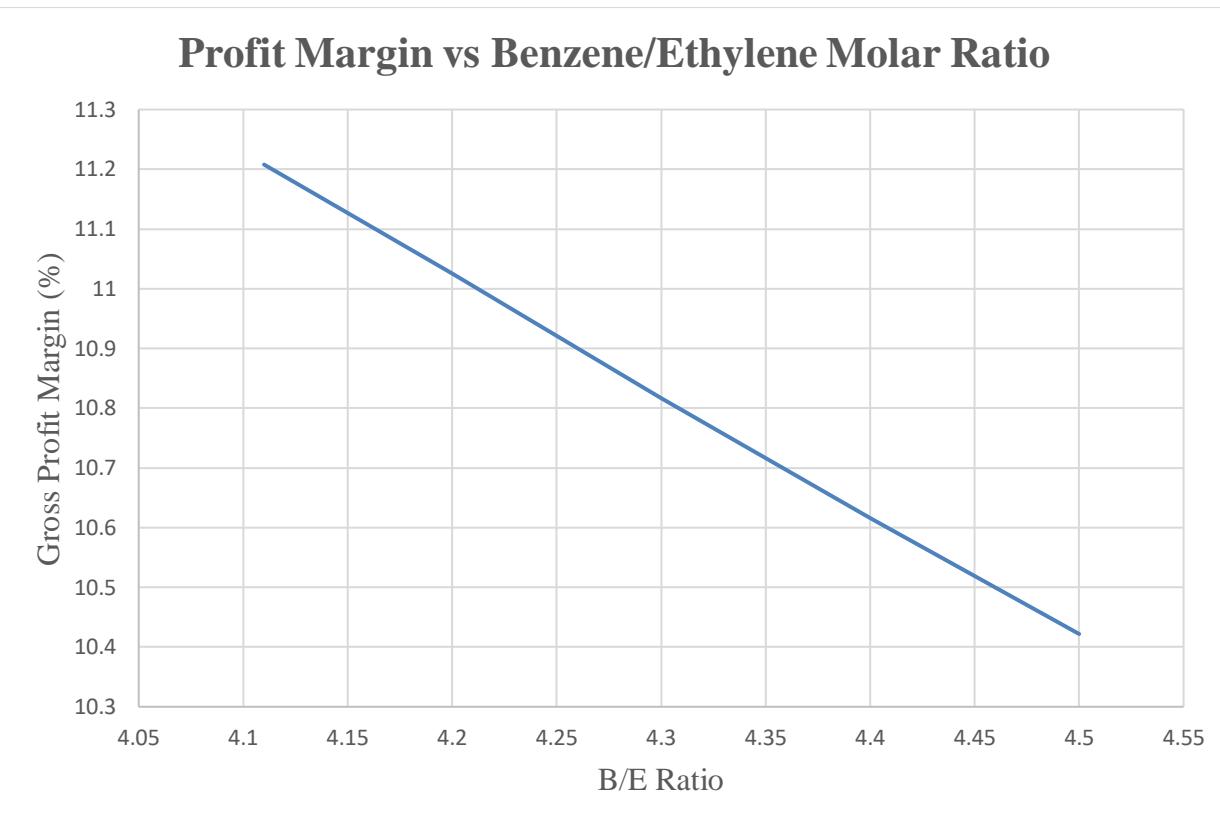


Figure 6 3Graph of profit margin vs B/E ratio for production of ethylbenzen

Economic potential of the production plant is analysed based on gross profit margin by varying the benzene to ethylene ratio in the alkylator. Benzene to ethylene (B/E) ratio for the alkylation reaction is set between 4.11 and 4.5. A higher B/E ratio can increase the selectivity of benzene, reduce coke formation and absorb the heat of reaction. However, a high B/E ratio might result in lower benzene conversion and higher recycle costs. Based on Figure 1.4 above, the gross profit margin of plant decreases when B/E ratio increases. For the input-output with recycle structure, the production plant shows the highest gross profit margin of 11.20785% at B/E ratio of 4.11. This indicates that the plant is able to generate the highest profit with minimum B/E ratio. The highest revenue for input-output structure is attainable at the B/E ratio of 4.11 around RM 701.8 million per year. Therefore, B/E ratio of 4.11 is set instead of a higher ratio in order to achieve trades off between economics potential and higher cost incurred by implementing more fresh benzene feed into the reactor to push the reaction towards full conversion.

6.4 Separation Operations in the Process

Table 6 5Separation equipment selected in ethylbenzene plant

Separation Equipment	Distillation column	
Quantity	2	
Code	T-201	T-401
Type of Phase	Liquid & vapor	Liquid & vapor
Operation Temperature	137 – 145 °C	190 – 200 °C
Operation Pressure	2.5 - 2.8 bar	2.5 - 2.8 bar
Justification	<p>The distillation column T-201 is used to separate the unreacted benzene from the main product, ethylbenzene since there is a significant difference on the volatility of benzene and ethylbenzene. The liquid mixture travels down the column over the plates and vapor bubbles up through the liquid via holes in the plates. The vapor and liquid are brought into contact as the energy released from the conversion of the component of higher boiling point from vapor to liquid phase is utilized by another component of lower boiling material in order to convert from liquid to vapor phase [20]. The bottom products are heated up by a reboiler and components in gaseous form is returned back to the distillation column for further separation while components in liquid form is being transferred to the second distillation column T-401. The distillate in gas phase is condensed by a condenser and part of it is returned back to the column as reflux while the remainder is transferred to a flash drum. On the other hand, the second distillation column T-401 is used to separate the main product, ethylbenzene from benzene and diethylbenzene. The distillate contains ethylbenzene with purity of >99.5wt%, together with trace amount of benzene and diethylbenzene whereas the bottom products contain liquid diethylbenzene together with small amount are being transferred to the transalkylator for transalkylation process.</p>	
Separation Equipment	Flash drum	

Quantity	2
Code	V-202
Type of Phase	Liquid & vapor
Operation Temperature	77 °C
Operation Pressure	1 bar
Justification	<p>Flash drum is one of the simplest separation processes where it is used to separate the liquid and vapor phase components. It is called ‘flash’ due to the process of vaporization occurs at extremely swift. As the inlet stream enters the flash drum, the components with higher volatility are heading to the overhead product and come out in vapor phase while the components with less volatility are coming out as bottom product in liquid phase. Flash drum V-202 is used to separate out the trace components which are methane and ethane from the mixture where the trace components are discharged as purge stream. The remaining components which consist of liquid benzene and trace amount ethylene are recycled back to the mixing point of feed stream while the remaining liquid benzene together with trace amount of liquid ethylene and ethylbenzene are being transferred to the transalkylation section.</p>

CHAPTER 7 MASS AND ENERGY BALANCE

7.1 Mass Balance of the Process Plant

Mass balance is conducted for the continuous system of ethylbenzene production plant. Mass balance or material balance is an application of conservation of the mass to the analysis of physical system by accounting for the material entering and leaving a process system. Mass balance is calculated based on the Law of Conservation of Mass which states that mass can neither be created nor destroyed in a process. The general equation for mass balance is shown as below:

$$\text{Accumulation} = \text{In} - \text{Out} + \text{Generation} - \text{Consumption}$$

According to the equation above, generation and consumption terms refer to generation of product and consumption of reactants in the chemical reaction. These terms will appear zero as no chemical reaction occurs.

Since the production of ethylbenzene is a continuous process, no accumulation is involved in the mass balance. Therefore,

$$\text{In} + \text{Generation} = \text{Out} + \text{Consumption}$$

For non-reactive process, the mass balance equation reduces to the following:

$$\text{In} = \text{Out}$$

Table 7 1Molecular weight of each component in process plant. [108]1092]

Components	Formula	Molecular weight (kg/kmol)	Molecular weight (ton/kmol)
Benzene	C ₆ H ₆	78.1	0.0781
Ethylene	C ₂ H ₄	28.05	0.0281
Ethylbenzene	C ₈ H ₁₀	106.17	0.1062
Diethylbenzene	C ₆ H ₄ (C ₂ H ₅) ₂	134.22	0.1342
Methane	CH ₄	16.04	0.0160
Ethane	C ₂ H ₆	30.07	0.0301

Mass balance involved in the production plant is calculated using Microsoft Excel Spreadsheet based on molar and mass basis. The calculations are done based on targeted ethylbenzene of 24.4379 kg/hr and 0.6909 kmol/hr as exact amount of benzene required with scale up/down ratio of 0.000329016.

Some assumptions made for the mass balance of ethylbenzene production plant are as shown below:

- 1) The production line will stop for maintenance for 2 days each month
- 2) The production line will run for 24 hours each working day

Mass balance calculation for each unit and stream table are presented in this section. Kindly refer to the Microsoft Spreadsheet file for detailed calculation.

7.2 Steam Table

Table 7 2 Simulated result from Aspen Plus

Stream Properties																	
Stream Number		1	2	3	4	5	6	7	8	9	10	11	12	13	16	21	
From		P-101		C-101	E-101	M-1	E-102	E-103	M-2	R-101	E-102	C-102	M-3	T-101	T-101		
To		P-101	M-1	C-101	E-101	M-2	E-102	E-103	M-2	R-101	E-102	C-102	M-3	T-101	T-401	E-203	
Phase		Liquid	Liquid	Vapor	Vapor	Vapor	Liquid										
Temperature	C	25	30.92056	25	42.90806	9	62.3356	162.6415	200	177.9917	200	120.6244	119.3261	119.479	181.0014	116.2214	
Pressure	bar	1	40	40	50	50	40	40	40	40	40	40	40	2.8	2.8	2.8	
Molar Vapor Fraction		0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	
Molar Liquid Fraction		1	1	0	0	0	1	1	1	1	1	1	1	1	1	1	
Molar Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mass Vapor Fraction		0	0	1	1	1	0	0	0	0.161214	0	0	0	0	0	0	
Mass Liquid Fraction		1	1	0	0	0	1	1	1	0.838786	1	1	1	1	1	1	
Mass Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Molar Enthalpy	cal/mol	11705.52	11901.51	12541.8	12729.28	12380.63	12990.41	17151.03	19042.85	17378.33	14978.24	10817.61	10756.58	10655.89	4496.169	15084.99	
Mass Enthalpy	cal/gm	149.8524	152.3615	447.063	453.7459	441.3181	166.3092	219.5754	243.7953	264.8985	171.271	123.6957	122.9978	121.5372	41.5466	193.1396	
Molar Entropy	cal/mol-K	-60.4277	-59.7816	-20.0608	-19.8934	-21.0594	-56.404	-45.9945	-42.1018	-36.0749	-53.7363	-62.9155	-63.0664	-63.3632	-86.6757	-50.7684	
Mass Entropy	cal/gm-K	-0.77359	-0.76532	-0.71508	-0.70912	-0.75068	-0.72211	-0.58884	-0.53901	-0.54989	-0.61446	-0.71942	-0.72114	-0.7227	-0.80092	-0.65001	
Molar Density	mol/cc	0.011164	0.011088	0.001614	0.001903	0.002131	0.010672	0.009135	0.00842	0.00301	0.007655	0.008781	0.008797	0.008773	0.006587	0.009897	
Mass Density	gm/cc	0.872073	0.866143	0.045268	0.053379	0.059793	0.833625	0.713552	0.657647	0.197487	0.669419	0.767889	0.769323	0.769193	0.712887	0.772994	
Enthalpy Flow	cal/sec	374664	380937.3	400981.8	406975.9	395829.1	1247013	1646411	1828015	2223844	1437834	1038436	1032577	1159383	155482.9	1119621	
Average MW		78.11364	78.11364	28.05376	28.05376	28.05376	78.10999	78.10999	65.60375	87.45343	87.45343	87.45343	87.67596	108.2199	78.10406		
Molar flow rate																	
Benzene	kmol/hr	115.2269	115.2269	0	0	0	345.4664	345.4664	345.4664	239.5764	239.5764	239.5764	267.2045	0.104097	267.1004		
Ethylene	kmol/hr	0	0	115.0979	115.0979	115.0979	0.0575	0.0575	0.0575	115.1554	0.0576	0.0576	0.0576	0.0668	2.51E-23	0.0668	
Ethylbenzene	kmol/hr	0	0	0	0	0	0.0576	0.0576	0.0576	0.0576	96.7398	96.7398	96.7398	115.2038	115.1758	0.027997	
Diethylbenzene	kmol/hr	0	0	0	0	0	0	0	0	0	9.2078	9.2078	9.2078	9.2124	9.2124	7.66E-12	
Total	kmol/hr	115.2269	115.2269	115.0979	115.0979	115.0979	345.5815	345.5815	345.5815	460.6794	345.5816	345.5816	345.5816	391.6875	124.4923	2.67E+02	
Mole fraction																	
Benzene		1	1	0	0	0	0.999667	0.999667	0.999667	0.749906	0.693256	0.693256	0.693256	0.682188	0.000836	0.999645	
Ethylene		0	0	1	1	1	0.000166	0.000166	0.000166	0.249969	0.000167	0.000167	0.000167	0.000171	2.02E-25	0.00025	
Ethylbenzene		0	0	0	0	0	0.000167	0.000167	0.000167	0.000125	0.279933	0.279933	0.279933	0.294122	0.925164	0.000105	
Diethylbenzene		0	0	0	0	0	0	0	0	0	0.026644	0.026644	0.026644	0.02352	0.074	2.87E-14	
Total		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
Mass flow rate																	
Benzene	kg/hr	9000.793	9000.793	0	0	0	26985.64	26985.64	26985.64	26985.64	18714.18	18714.18	18714.18	20872.32	8.131427	20864.18	
Ethylene	kg/hr	0	0	3228.929	3228.929	3228.929	1.613091	1.613091	1.613091	3230.542	1.615897	1.615897	1.615897	1.873991	7.05E-22	1.873991	
Ethylbenzene	kg/hr	0	0	0	0	0	6.115242	6.115242	6.115242	6.115242	10270.61	10270.61	10270.61	12230.89	12227.92	2.972411	
Diethylbenzene	kg/hr	0	0	0	0	0	0	0	0	0	1235.882	1235.882	1235.882	1236.499	1236.499	1.03E-09	
Total	kg/hr	9000.793	9000.793	3228.929	3228.929	3228.929	26993.37	26993.37	26993.37	30222.3	30222.3	30222.3	30222.3	34341.58	13472.55	2.09E+04	
Mass fraction																	
Benzene		1	1	0	0	0	0.999714	0.999714	0.999714	0.892905	0.619218	0.619218	0.619218	0.607786	0.000604	0.999768	
Ethylene		0	0	1	1	1	5.98E-05	5.98E-05	5.98E-05	0.106893	5.35E-05	5.35E-05	5.35E-05	5.46E-05	5.23E-26	8.98E-05	
Ethylbenzene		0	0	0	0	0	0.000227	0.000227	0.000227	0.000202	0.339836	0.339836	0.339836	0.356154	0.907617	0.000142	
Diethylbenzene		0	0	0	0	0	0	0	0	0.040893	0.040893	0.040893	0.040893	0.036006	0.091779	4.93E-14	
Total		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	

Table 7 3Simulated result from Aspen Plus (cont.)

Stream Properties																			
Stream Number		22	23	24	25	28	29	34	35	36	37	38	39	40	41	41-Recycle	43	43-Recycle	
From		E-203	C-201	V-202	P-201	T-401	P-401	T-401	S-1	E-204	M-4	R-301	E-204	E-301	C-301	M-3	M-3	S-1	
To		C-201	V-202	P-201	S-1	P-401	M-4		E-204	M-4	R-301	E-204	E-301	C-301	M-3	M-3	M-1		
Phase		Liquid	Liquid	Liquid	Liquid	Liquid													
Temperature	C	77.1381	77.07841	77.1381	81.41254	229.2201	235.0288	178.5645	81.41256	210	216.9805	229.5292	148.4464	120.6244	120.6244	120.6244	77.1381	81.412557	
Pressure	bar	2.8	1.0133	1.0133		40	2.8	35	2.8	40	40	35	35	35	40	2.8	2.8	40	40
Molar Vapor Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Molar Liquid Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
Molar Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mass Vapor Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mass Liquid Fraction		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
Mass Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Molar Enthalpy	cal/mol	13537.13	13534.89	13537.13	13698.73	-2351.67	-1832.9	5221.133	13698.73	19595.56	15290.06	15993.88	11281.87	9901.265	9901.166	9901.1659	13535.09	13698.729	
Mass Enthalpy	cal/gm	173.3217	173.293	173.3217	175.3907	-17.5441	-13.6739	49.18942	175.3907	250.8904	171.1376	179.0153	126.275	110.8222	110.8208	110.82081	173.2865	175.39073	
Molar Entropy	cal/mol-K	-54.8358	-54.842	-54.8358	-54.3872	-118.428	-117.429	-84.3393	-54.3872	-41.029	-55.4024	-52.7526	-62.4083	-65.6892	-65.68923	-54.8396	-54.38721		
Mass Entropy	cal/gm-K	-0.70209	-0.70217	-0.70209	-0.69634	-0.8835	-0.87605	-0.79458	-0.69634	-0.52531	-0.6201	-0.59045	-0.69852	-0.73524	-0.73524	-0.73524	-0.7021	-0.696343	
Molar Density	mol/cc	0.010469	0.010469	0.010469	0.010409	0.005014	0.004968	0.006731	0.010409	0.008204	0.007257	0.007021	0.008248	0.0086	0.0086	0.0085995	0.010468	0.0104085	
Mass Density	gm/cc	0.817644	0.817709	0.817644	0.812947	0.672137	0.665934	0.714426	0.812947	0.640772	0.648381	0.627299	0.73688	0.768316	0.768316	0.7683161	0.817641	0.8129475	
Enthalpy Flow	cal/sec	1004738	1004571	1004738	1016732	-6052.55	-4717.38	167115.3	140215.9	200574	195856.6	204872.2	144514.1	126829.3	126806.2	126806.16	866075.2	876515.97	
Average MW		78.10406	78.10406	78.10406	78.10406	134.0436	134.0436	106.1434	78.10406	78.10406	89.34368	89.34368	89.34368	89.34392	89.34392	78.10816	78.104064		
Molar flow rate																			
Benzene	kmol/hr	267.1004	267.1004	267.1004	267.1004	1.29E-09	1.29E-09	0.104076	36.83539	36.8354	36.8354	27.6322	27.6322	27.6322	27.6281	27.6281	230.2395	230.26501	
Ethylene	kmol/hr	0.0668	0.0668	0.0668	0.0668	0	0	0	0.009212	0.009212	0.009212	0.009212	0.009212	0.009212	0.0092	0.0092	0.0575	0.0575877	
Ethylbenzene	kmol/hr	0.027976	0.027976	0.027976	0.027997	0.058639	0.058639	115.1172	0.003861	0.003858	0.062497	18.4689	18.4689	18.4689	18.464	18.464	0.0576	0.0241363	
Diethylbenzene	kmol/hr	7.66E-12	7.66E-12	7.66E-12	7.66E-12	9.21E+00	9.21E+00	5.64E-03	1.06E-12	1.06E-12	9.21E+00	3.56E-03	3.56E-03	3.56E-03	0.0046	0.0046	0	6.61E-12	
Total	kmol/hr	2.67E+02	2.67E+02	2.67E+02	2.67E+02	9.27E+00	9.27E+00	1.15E+02	3.68E+01	3.68E+01	4.61E+01	4.61E+01	4.61E+01	4.61E+01	46.1059	46.1059	230.3546	230.34673	
Mole fraction																			
Benzene		0.999645	0.999645	0.999645	0.999645	1.39E-10	1.39E-10	0.000903	0.999645	0.999645	0.798792	0.599217	0.599217	0.599217	0.599231	0.599231	0.9995	0.9996452	
Ethylene		0.00025	0.00025	0.00025	0.00025	0	0	0	0.00025	0.00025	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.00025	0.00025	
Ethylbenzene		0.000105	0.000105	0.000105	0.000105	0.006329	0.006329	0.999048	0.000105	0.000105	0.001355	0.400506	0.400506	0.400506	0.400469	0.400469	0.00025	0.0001048	
Diethylbenzene		2.87E-14	2.87E-14	2.87E-14	2.87E-14	9.94E-01	9.94E-01	4.89E-05	2.87E-14	2.87E-14	2.00E-01	7.72E-05	7.72E-05	9.98E-05	9.98E-05	0	2.87E-14		
Total		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
Mass flow rate																			
Benzene	kg/hr	20864.19	20864.19	20864.19	20864.18	1.01E-07	1.01E-07	8.129728	2877.347	2877.347	2877.347	2158.451	2158.451	2158.451	2158.131	2158.131	17984.85	17986.838	
Ethylene	kg/hr	1.873991	1.873991	1.873991	1.873991	0	0	0	0.258439	0.258439	0.258439	0.258439	0.258439	0.258439	0.258095	0.2580946	1.613091	1.615552	
Ethylbenzene	kg/hr	2.970103	2.970103	2.970103	2.972411	6.22552	6.22552	12221.69	0.409921	0.409602	6.635122	1960.795	1960.795	1960.795	1960.275	1960.2749	6.115242	2.5624908	
Diethylbenzene	kg/hr	1.03E-09	1.03E-09	1.03E-09	1.03E-09	1.24E+03	1.24E+03	7.57E-01	1.42E-10	1.42E-10	1.24E+03	4.78E-01	4.78E-01	4.78E-01	0.617417	0.617417	0	8.87E-10	
Total	kg/hr	2.09E+04	2.09E+04	2.09E+04	2.09E+04	1.24E+03	1.24E+03	1.22E+04	2.88E+03	2.88E+03	4.12E+03	4.12E+03	4.12E+03	4.119.282	4119.2818	17992.57	17991.016		
Mass fraction																			
Benzene		0.999768	0.999768	0.999768	0.999768	8.12E-11	8.12E-11	0.000665	0.999768	0.999768	0.698388	0.523898	0.523898	0.523898	0.52391	0.5239096	0.9995	0.9997678	
Ethylene		8.98E-05	8.98E-05	8.98E-05	8.98E-05	0.00E+00	0.00E+00	0.00E+00	8.98E-05	8.98E-05	6.27E-05	6.27E-05	6.27E-05	6.27E-05	6.27E-05	8.97E-05	8.98E-05		
Ethylbenzene		0.000142	0.000142	0.000142	0.000142	0.005013	0.005013	0.999273	0.000142	0.000142	0.00161	0.475923	0.475923	0.475923	0.475878	0.4758778	0.00034	0.0001424	
Diethylbenzene		4.92E-14	4.92E-14	4.92E-14	4.93E-14	9.95E-01	9.95E-01	6.19E-05	4.93E-14	4.92E-14	3.00E-01	1.16E-04	1.16E-04	1.16E-04	0.00015	0.0001499	0	4.93E-14	
Total		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	

7.3 Energy Balance of the Process Plant

The Law of Conservation of Energy which states that energy is neither be created nor destroyed in a process, but it can be transformed from one form of energy to another is applied for energy balance calculation for ethylbenzene production plant. Energy balances are carried out to determine the energy demand of a process for instance the heat duty (heating and cooling). The general energy balance for a continuous system in which the accumulation term can be neglected is as follows:

$$\Delta\dot{H} + \Delta\dot{E}_k + \Delta\dot{E}_p = \dot{Q} + \dot{W}_s$$

where $\Delta\dot{H}$ is the rate of change in the stream enthalpy, $\Delta\dot{E}_k$ is the rate of change in kinetic energy, $\Delta\dot{E}_p$ is the rate of change of potential energy, \dot{Q} is the heat supplied or removed per time and \dot{W}_s is the shaft work provided to the system. With the coupling of wide range of temperatures and pressures for all units in ethylbenzene production, the heat requirement, power requirement and enthalpy change of each stream is more significant and thus, assumption is made by neglecting $\Delta\dot{E}_k$ and $\Delta\dot{E}_p$ in current energy balance calculation by assuming there is no significant change in the pipe diameters and no change in height of the equipment respectively.

Three main categories in the process plant comprises of heat requiring unit, power requiring unit and constant enthalpy unit in which the energy balance equation governing each of them is summarized as below.

- Heat requiring units: Reactor and heat exchanger ($\dot{Q} = \Delta\dot{H}$)
- Power requiring units: Pump ($\dot{W}_s = \Delta\dot{H}$)
- Constant enthalpy units: Mixing and splitting points ($\Delta\dot{H} = 0$)

For reactor and heat exchangers, the temperatures are set and thus the difference in enthalpies between inlet and outlet stream will represent the heating or cooling required for the system.

$$\dot{Q} = \Delta\dot{H} = \dot{n}(\hat{H}_{out} - \hat{H}_{in})$$

All the enthalpies are calculated for each stream with reference to a reference state (25°C, 1atm) with the following equation:

$$\dot{Q} = \Delta\dot{H} = \dot{n} \times \left\{ \int_{T_{ref}}^T C_p dT + \hat{H}_f + \hat{H}_v + \hat{v}\Delta P \right\}$$

where C_p is specific heat capacity, \hat{H}_f is heat of formation, \hat{H}_v is heat of vaporization while $\hat{v}\Delta P$ term does not apply in gaseous components.

For pumps, the mechanical energy balance equation, $\frac{\Delta P}{\rho} + \frac{\Delta u^2}{2} + g\Delta z + \hat{F} = -\frac{W_s}{m}$ is applied with the assumption of negligible changes in velocity and height and no friction, pump work is simplified to $W_s = \frac{\dot{P}}{\rho} \times \dot{m}$.

These are some assumptions made during the execution of energy balance calculation:

- Energy balance is based on ideal condition.
- There is no heat loss through pipeline, pump, heater and etc.
- No component interactions during the mixing of streams.
- Total condenser and reboiler condenses and evaporates all vapours and liquids into liquids and vapours respectively.
- Heat of solution is negligible with the gaseous components dissolve in liquid components due to the infinitesimal amount of those gases. 100% heat and power efficiency in calculations.

The simulation of the ethylbenzene production process in Aspen Plus is carried out in order to compare the mass and energy balance calculation in Microsoft Excel for validation. The process flow diagram (PFD) and simulated results from Aspen Plus are shown and discussed in this section.

The thermodynamic model applied for the prediction of the behaviour of each component is important in order to acquire an accurate simulation of all the process streams in the plant. We used ASPEN Plus V10 to further analyse and verify the value we obtained by our own calculation. This is important as ASPEN Plus V10 able to model and simulate the whole plant in a more realistic behaviour and with specified equation of state. In the simulation of ethylbenzene production plant, non-random two liquids model (NRTL) was selected as the thermodynamics model in ASPEN Plus V10 simulation. The multi-component liquid-liquid and liquid-vapor equilibrium cannot be reliably predicted from binary interaction parameters which fitted to binary data only. Therefore, the liquid-liquid and liquid vapor equilibria is predicted by using the activity coefficient models, NRTL and more accurate results can be obtained.

7.4 Comparison of Mass and Energy Balance by using Aspem Plus

7.4.1 Process flow diagram (PFD)

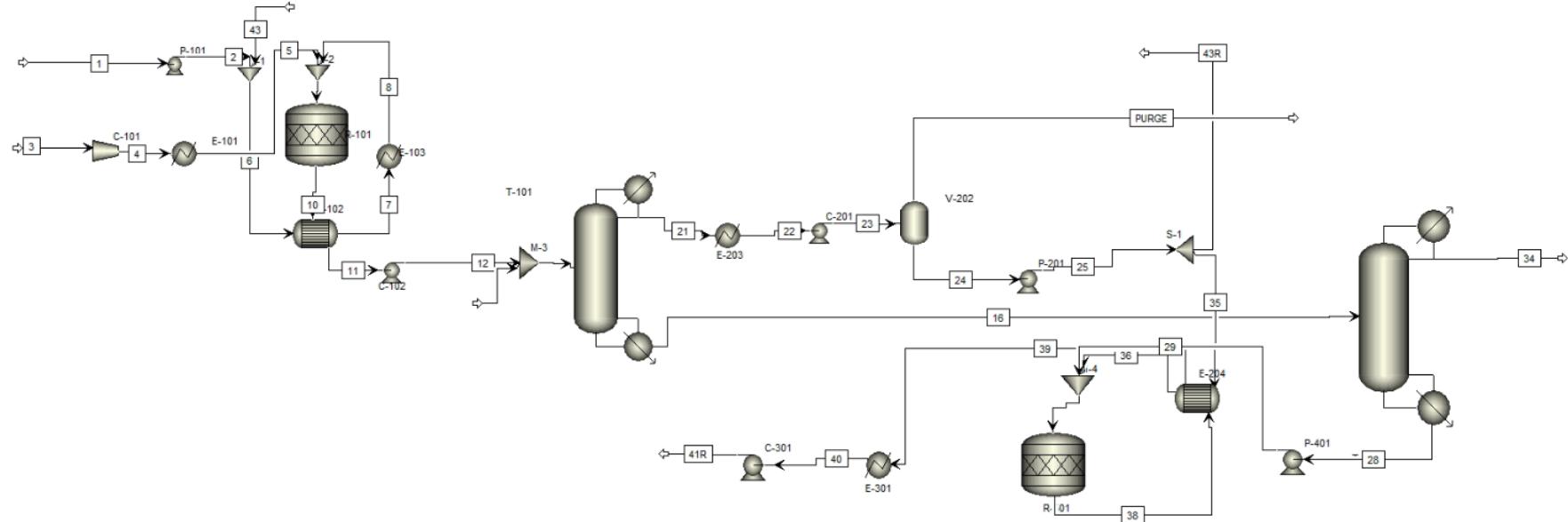


Table 7.4 Aspen Plus process flow sheet for production of ethylbenzene.

7.4.2 Justification of Simulated Result

Table 7.5 Stream properties comparison

Temperature

Comparing our own calculation in Excel spreadsheet and simulation results using ASPEN Plus V10, there are differences in some values between both software. Firstly, by comparing temperature obtained from Excel and Aspen Plus, there are some streams that showed deviation. Stream 6, 7, 9, 12, 13, 16, 21, 23, 25, 28, 29, 37, 41, and 43 showed minor deviation in terms of temperature. This resulting deviation might be due to the assumption of no heat loss in manual calculation using Excel but this assumption was not made in Aspen Plus simulation. The streams that showed most significant deviation in terms of temperature are stream 2, 4 and stream 39. Temperature of stream 2 which is after pump P-101 showed deviation of 19.148%. Besides, there is a significant deviation in the temperature of the outlet stream of compressor C-101 which is stream 4 simulated in Aspen Plus from the calculated value in Excel. Temperature of stream 4 simulated in Aspen Plus showed percentage of deviation of 41.736% from the value calculated in Excel. This deviation in temperature of

stream 2 and 4 might be due to the assumption of ideal isentropic operating condition of pump or compressor in Excel calculation whereby the work transfer of the system is frictionless and there is no transfer of heat; however, in the Aspen Plus simulation, the non-ideal state of the gases was being taken into consideration in the calculation. Moreover, temperature of stream 39 simulated in Aspen Plus also showed large deviation from the calculated value in Excel with percentage of deviation of 21.691% from the value calculated in Excel. This resulting deviation might be due to the assumption of no heat loss in manual calculation using Excel, but this assumption was not made in ASPEN Plus simulation.

Molar Flowrate and Mass Flowrate

When comparing molar flowrate from both Aspen Plus and Excel, there is only minor deviation occurs in stream 3, 4, 5, 10, 11, 12, 13, 16, 21, 22, 23 and 34 which is less than 0.05%. This is contributed by the calculation by the software that may cause the minor deviation however, value of crucial operating condition set in each equipment able to keep the margin of error to a small value. Meanwhile, mass flowrate has minor deviation in every stream simulated in Aspen Plus due to the difference in molecular weight of components set in ASPEN Plus and Excel. Holistically, different approach of calculation for our Excel and ASPEN Plus software resulted in slightly different for molar flowrate, which is our basis and consequently affect the mass flowrate.

7.5 Justification of equipment

Distillation column

In addition, we calculated the properties of both distillation column using RadFrac model available in ASPEN Plus V10 to get better accuracy of calculation comparing with DSTWU model. In advance, we determined the important variable using the parameter that we calculated to be input into RadFrac model.

For distillation column, T-201, the feed position simulated by Excel is at stream 22 while the feed position simulated by Aspen Plus is at stream 15 above-stage. For the second distillation column, T-401, Excel simulation acquired the feed position at stream 26 whereas Aspen Plus simulation acquired the feed position at stream 22 above-stage. The feed position of both distillation columns entered in Aspen Plus is different from the calculated value by using Excel because the calculated feed stage produced far different composition of both bottom and

distillate from the value we calculated in Excel. Thus, we improvised by manually change the feed position until we get the closest composition to our desired value.

This may be influenced by different temperature at the condenser and reboiler of the distillation column. Temperature of condenser and reboiler for both distillation column slightly deviates from value obtained in Excel calculation. Moreover, resulted heat duty of condenser and reboiler for both distillation column also has slightly deviated value under 5%. Only reboiler of second distillation column, T-401, has large deviation with 96.657% from value calculated in Excel.

- Pump and compressor

Table 7 6Table 3.10 Work required for pump and compressor

Unit operation	Work required (kW)		
	Excel	Aspen	Deviation (%)
P-101	11.17118367	26.2653728	57.468
C-101	17.69870892	25.0957944	29.475
P-201	0.353435187	50.2169801	99.296
P-401	0.014966601	5.59006403	99.732

Table 3.10 shows the deviation percentage of pumps and compressor used in our plant.

In average, all of the unit operation resulted in considerably high deviation percentage. This may be caused by the assumption made during calculation of work required for each equipment. Also note that, outlet temperature of the equipment used are assumed to be constant in our Excel calculation. However, outlet temperature of the equipment in ASPEN Plus simulation will deviates from the input temperature. Therefore, it will influence the work required to operate the equipment.

- Heat exchanger

Table 7 7Heat duty for heat exchanger

Unit operation	Heat duty (MJ/hr)		
	Excel	Aspen	Deviation (%)
E-101	-2322.4151	-168.0098	1282.3091
E-103	2666.5898	2736.9838	2.5720
E-201	-12333.5600	-12148.5048	1.5233
E-202	3255.0978	3318.2184	1.9022
E-203	-1620.6382	-1731.5804	6.4070
E-301	-127.8110	-266.5525	52.0504
E-401	-7029.6040	-6653.5277	5.6523
E-402	225.2096	6737.6301	96.6574

Table 3.11 shows the deviation of heat duty for each heat exchanger including the condenser and reboiler of distillation column. It can be seen that most of the heat exchanger exhibit only minor error from ASPEN Plus simulation. However, for E-101, the value of deviation percentage of Excel calculation is quite high comparing to the value obtained in ASPEN Plus simulation. This also contributed by the assumptions made in our Excel calculation for the chemical properties such as calculation involving changing of phase for the chemical used. Value of specific enthalpy for the process may varies between the calculation and simulation.

- Reactor

Table 7 8Heat duty for reactor

Unit operation	Heat duty (MJ/hr)		
	Excel	Aspen	Deviation (%)
R-101	-7028.0137	-11847.1199	40.6774
R-301	533.3798	135.8868	292.5178

From Table 3.12, the alkylator, R-101 exhibit highly exothermic reaction which is agreed by the ASPEN Plus simulation. The difference in value of heat duty may be due to different approach of calculation for our own calculation and ASPEN Plus simulation. Similarly, for transalkylator, R-301 both value shows that the reactor is endothermic with quite large difference of heat duty.

Conclusion

Overall, we are able to run ASPEN Plus simulation without any major error occurred and acquired quite similar values. On a side note, big difference in heat duty or work required from comparing our own Excel calculation and ASPEN Plus simulation may be due to the fact that we set several assumptions that may neglect some aspect of calculation. Nevertheless, the deviation we obtained is only magnitude of the value due to approach of calculation and no conflict of heat released with heat absorbed. Ultimately, the calculations using Excel were in good accordance with Aspen simulation where there are only minor deviations for some values which might be due to difference in molecular weight except the temperature of the a few intermediate streams that have large deviation.

CHAPTER 8 UTILITIES AND WASTE

8.1 Overview of Utilities

Utilities such as water, natural gas, electricity and also power are essential services that play a vital role in economic development of any industrial plant. The usage of the utilities needs to be calculated in order to provide the generation, supply and control, as well as estimate the overall amount needed to operate the plant. In the ethylbenzene production plant, natural gas is used as a fuel to generate heat that is adsorbed by the reboiler. Superheated stream at high temperature also being supplied for the reboiler while water is used as a cooling and heating media for some equipment such as cooler heater, reactor and also condenser. Another utility is the electricity where should be calculated based on the usage power of equipment. For sustainable approach, the designated plant will recycle water to decrease the use of source material.

8.2 Utilities

The utilities of superheated steam, cooling water and electricity are calculated as shown in Table 4.1, 4.2 and 4.3. The unit price of each component is:

- 1 unit price of water is RM 1.38 per cubic meter
- 1 unit price of natural gas is RM 36.43 per mmBTU
- 1 unit price of electricity is RM 0.388 per kWh

Table 8.1 Utilities for unit operations using superheated steam

Unit	Code	Temperature of superheated steam (°C)		Heat Duty, Q		Required Flow Rate				Price of Water (RM/yr)	Unit Price of Natural Gas (RM/yr)	
						Natural Gas	Molar Flow Rate of Superheated Steam		Mass Flow Rate of Superheated Steam			
		In	Out	MJ/hr	MJ/yr	mmbtu/yr	kmol/hr	kmol/yr	ton/hr	ton/yr		
Reboiler	E-202	450.00	250.30	3255.10	26639720.29	25307.73	4446.27	36388277.77	80.03	654989.25	1024101.51	921960.76
Reboiler	E-402	450.00	250.30	225.21	1843115.56	1750.96	307.62	2517586.63	5.54	45316.44	70854.25	63787.46
Heater	E-103	450.00	250.30	2666.59	21823371.23	20732.20	3642.40	29809431.06	65.56	536570.05	838948.27	755274.14
Jacketed fixed bed reactor	R-301	450.00	250.30	533.38	4365180.21	4146.92	728.57	5962577.60	13.11	107326.61	167809.11	151072.34
Total (RM/yr)										2101713.14	1892094.70	

Table 8 2 Utilities for unit operations using cooling water

Unit	Code	Temperature of water stream (°C)		Heat duty, Q		Required flow rate				Price (RM/yr)
		In	Out	MI/hr	MI/yr	kmol/hr	kmol/yr	ton/hr	ton/yr	
Cooler	E-101	30	45	2322.41512	19006645.37311	18056.31310	147772866.44683	325.01364	2659911.59604	4158878.18
Jacketed fixed bed reactor	R-101	30	45	7028.01371	57517264.17368	54641.40096	447185225.49753	983.54522	8049334.05896	12585455.77
Condenser	E-201	30	45	12333.56003	100937855.27703	95890.96251	784771637.20788	1726.03733	14125889.46974	22086393.22
Cooler	E-203	30	45	1620.63819	13263302.96966	12600.13782	103119527.92849	226.80248	1856151.50271	2902167.12
Condenser	E-401	30	45	7029.60396	57530278.80895	54653.76487	447286411.68383	983.76777	8051155.41031	12588303.53
Cooler	E-301	30	45	127.81099	1046005.14908	993.70489	8132480.83305	17.88669	146384.65499	228878.26
total (RM/yr)										54550076.09

Table 8 3 Utilities for unit operations using electricity

Unit	Code	Power requirement (kW)	Total electrical energy consumption (kW/yr)	Price (RM/yr)
Pump	P-101	11.1712	91424.9672	35472.89
Compressor	C-101	17.6987	144846.2338	56200.34
Pump	P-201	0.3534	2892.5136	1122.30
Pump	P-401	0.0150	122.4867	47.52
total (RM/yr)				92843.05

8.3 Waste Generated in Ethylbenzene Production Plant

- PURGE GAS**

Ethane and methane produced at the purge stream could be harmful to human and environment. Because of its high volatility, the product is unlikely to cause ground or water pollution rapidly or completely vaporize at atmospheric pressure and normal ambient temperature. The amount of methane produced is 0.0225kmol/hr while ethane is 0.0442kmol/hr. In order to avoid any environmental problem, the compounds will be stored and sold to the third party. It can be used as burning fuel, where surely be profitable.

- SPENT ZEOLITE CATALYST**

The lifetime of zeolite catalyst varies based on its properties and other combinations. Zeolite catalyst used in the ethylbenzene plant, EBZ-500 could be used up to 5 years which will be greatly reduce the formation of waste. After 5 years, the catalyst will be replaced with the new one to ensure the reaction take place at high efficiency. The spent catalyst should undergo pre-treatment process and then dispose to the landfill to avoid increase of operation cost. The disposal of spent catalyst to the landfill should not be a big problem as the gap of time is quite far.

- WASTEWATER**

Water used for heat transfer equipment is quite high, which leads to higher disposal of liquid waste. However, it is not a big problem as the water can be reused and recycled as cooling media.

CHAPTER 9 MASS TRANSFER EQUIPMENT DESIGN

9.1 Distillation Column (T-201)

Design basis

Parameter	Inlet			Outlet		Distillate	Bottom
	Feed	Reflux	Boilup	Top	Bottom		
Molar Flow Rate (kmol/hr)	391.79	157.48	92.16	424.77	216.66	267.29	124.50
Mass Flow Rate (kg/hr)	34346.74	12298.65	9973.02	33172.55	23445.87	20873.89	13472.85

Component distribution		
Component	Boiling point (°C)	Key component
Benzene	80.1	Light key
Ethylene	-103.9	Light non-key
Ethylbenzene	136.2	Heavy key
Diethylbenzene	180	Heavy non-key
Methane	-161.4	Light non-key
Ethane	-88.8	Light non-key

Design Parameters

Component Distribution	Column Sizing	Plate Hydraulic Design	Mechanical Design
Number of Stages	Tray Spacing	Active Area	Design Pressure
Reflux Ratio	Flooding Velocity	Hole Area	Design Temperature
Number of Actual Stages	Net Area	Tray Thickness	Material of Construction
Tray Efficiency	Downcomer Area	Hole Diameter	Column Wall Thickness
Location of Feed Stage	Column Diameter	Liquid Flow Arrangement	Column Head Design
	Column Height	Column Pressure Drop	Insulation
		Weeping checking	Stress Analysis
		Downcomer Liquid Backup	Column Support
		Residence Time	Nozzle Size
		Entrainment checking	
		Number of holes	

Design Criteria

Operating Pressure	: 2.80 bar	Benzene recovery	: 99.95%
Type of Column	: Tray Column	Ethylbenzene purity	: 99.95 wt%
Type of Tray	: Sieve tray		

Design Method

Fenske-Underwood-Gilliland shortcut method is utilized for component distribution calculation. The, the reflux ratio is determined by using Underwood equation and proceed to calculation of boil-up ratio. These values are used to find the theoretical number of stages. Then, actual number of stages for design is calculated by multiplying the theoretical number of stages to O'Connell efficiency together with feed location for the actual number of stages. Afterwards, the details for designing the adequate distillation column are done guided mainly by Coulson and Richardson's Chemical Engineering Design Volume 6 4th edition book. Overall design of T-201 distillation column can be referred from Table 9.

Type of column and construction material justification

The selected construction material for T-201 distillation column is stainless steel 304 mainly due to the corrosion resistance in high temperature and its considerably high tensile strength compared to other common distillation column construction material based on Table 13.2 in Coulson and Richardson book. The designated tensile strength of the selected material is 510 N/mm² and the design stress is 117.7 N/mm² at T-201 operating temperature, 191°C. Thus, the material is appropriate for such operating condition. Besides, the type of T-201 is plate distillation column to provide high ratio of liquid-vapor flow rate. While sieve tray is utilized as it has versatile contactor and economically better than bubble cap or valve.

Table 9 1 Specification sheet of distillation column T-201

T-401			
Item	Distillation column	Date:	2nd February 2022
Item no	T-401	By:	Muhammad Ariffin
No. required	1		
General			
Function: To separate Diethylbenzene from Ethylbenzene			
Operation: Continuous		Material of Construction : Stainless steel (304)	
Type : Plate Distillation Column		Orientation : Vertical	
Operating Data			
Stream	IN	OUT	
	S-16	S-34	S-28
Pressure (bar)	2.80	2.80	2.80
Temperature (°C)	180.91	178.59	229.53
Quantity (kg/h)	13472.85	12230.86	1241.99
Vapor Fraction	0	0	0
Composition (kg/h)			
Benzene	10.44	10.44	0.00
Ethylene	0.00	0.00	0.00
Ethylbenzene	12225.92	12219.81	6.11
Diethylbenzene	1236.49	0.62	1235.87
Methane	0.00	0.00	0.00
Ethane	0.00	0.00	0.00
Operational Design			
Maximum liquid flowrate (kg/s)	7.92	No. of trays (minus reboiler)	51
Maximum vapor flowrate (m³/s)	0.84	Feed point (from bottom)	35
Column Height (m)	35.47	Reflux ratio	0.76
Column Diameter (m)	1.37	Tray spacing (m)	0.60
Ratio of column height to diameter	25.83	Overall tray efficiency (%)	56.79
Plate Hydraulic Design			
Active area (m²)	1.58	Plate material:	Stainless steel (304)
Type of Tray	Seive Tray	Plate thickness (mm):	3.00
Hole size (mm)	0.005	Weir length (m):	1.49
Active holes	8043	Weir height (m):	0.05
Flow Rate Turndown (%)	70	Plate pressure drop (mm liquid):	120.04
Flooding (%)	8.00	Entrainment	0.02
Calming Zone Width (mm)	50.00	Unperforated strip round plate edge(mm)	50
		Liquid flow arrangement:	Cross flow, single pass
Mechanical Design			
Design pressure (bar):	3.08	Vessel support:	Conical skirt

Design temperature (°C):	191.00	Insulation:	Fibreglass
Type of Head	Torusperical head	Insulation thickness (mm):	75
Wall thickness (mm):	10.733	Head Thickness (mm)	10.246
Welding joint factor :	0.85	Skirt thickness (mm) :	16
Corrosion allowance (mm):	1	Feed nozzle diameter (in):	4.00
Top nozzle diameter (in):	18.00	Reflux nozzle diameter (in):	3.00
Bottom nozzle diameter (in):	4.00	Boilup nozzle diameter (in):	2

The designed distillation column is within acceptable range with height to diameter (HC/DC) ratio is below 30, no occurrence of weeping as actual minimum vapor velocity exceeds weeping velocity, and satisfactory stress difference. The obtained values will then be compared with the simulated value from AspenPlus to further validate the design.

Comparison of calculated and simulated design values

Table 9 2Comparison of parameters between calculated values in Excel and simulated values in AspenPlus for T-401.

Parameter	Calculated value (Excel)	Simulated value (Radfrac)	Relative error (%)
Column diameter (m)	1.373	1.373	0.00
Column height (m)	31.924	29.4	8.59
Tray Spacing (m)	0.6	0.6	0.00
Hole diameter (m)	0.005	0.005	0.00
Hole area / Active area	0.1	0.1	0.00
Cross-sectional area (m ²)	1.481	1.481	0.00
Active area (m ²)	0.948	0.97	2.27
Net area (m ²)	1.214	1.225	0.90
Downcomer clearance (m)	0.04	0.04	0.00
Weir height (m)	0.05	0.05	0.00
Weir length (m)	1.15339	1.15339	0.00
Trays with weeping	None	None	
Flooding (%)	80	71.97	11.16
Condenser performance			
Temperature (°C)	178.5856	178.676	0.05
Heat duty (MJ/hr)	-7029.6	-6719.89	4.61
Distillate rate (kmol/hr)	115.235	115.235	0.00
Reflux rate (kmol/hr)	88.136	88.1316	0.00
Reflux ratio	0.7648	0.7648	0.00
Reboiler Performance			
Temperature (°C)	229.529	229.397	0.06
Heat duty (MJ/hr)	225.21	6801.69	96.69
Bottoms rate (kmol/hr)	9.2654	9.2654	0.00
Boilup rate (kmol/hr)	1.3148	183.239	99.28
Boilup ratio	0.1419	19.7767	99.28

The comparison values are summarized above in Table_. Radfrac model in AspenPlus also used in validating the calculated parameters of distillation column T-401. By comparing the values using relative error of calculated values to simulated values, sizing parameters of distillation column is consistently comparable for most of the parameters. The most significant difference of the distillation column sizing is only the column height with 8.59% which is still acceptable. This is due to in our own calculation, the column height considered additional height to accommodate the operating condition. Meanwhile, Radfrac model in AspenPlus calculated the column height based on the dimension sets to the tray such as tray spacing and weir length. The flooding level from simulation also lower than the calculated values. This also may be influenced by the resulted shorter column height.

Furthermore, the value for related areas such as cross-sectional area, active area, and net area can be observed to slightly deviate from the simulated values with only active area has 2.27% relative error and net area 0.90% relative area. This may be influenced by the usage of K1 in determining the flooding velocity. K1 is approximated based on graph which will likely cause minor error to the calculation. As for the reboiler performance, the overall relative error is low with only 4.61% error on the heat duty which is considered minor. This proved the calculation for the reboiler is considered accurate. However, major errors are observed for the boiler performance for the heat duty, boilup rate, and boilup ratio. The heat duty difference is resulted from the wide difference of boilup ratio which will increase the boilup rate in the distillation column. This probably caused by the design specification at the bottom of the column to obtain high purity product.

Engineering drawing of T-201

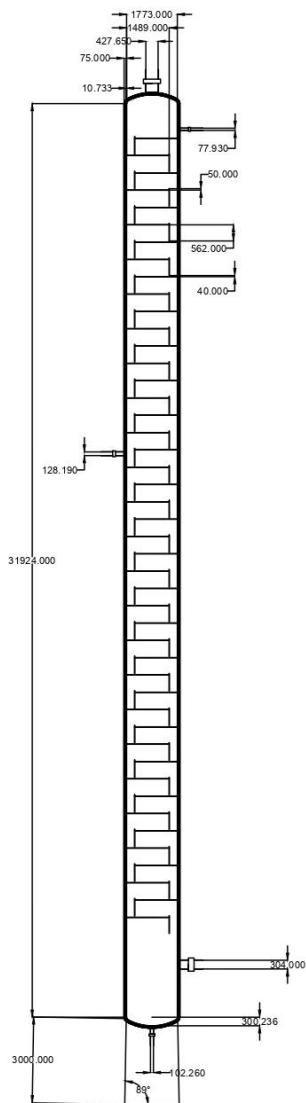


Figure 9 1Autocad engineering deisgn distillation column T-201

9.2 Distillation Column (T-401)

Design basis

Parameter	Inlet			Outlet		Distillate	Bottom
	Feed	Reflux	Boilup	Top	Bottom		
Molar Flow Rate (kmol/hr)	124.500	88.136	1.315	203.370	10.580	115.235	9.265
Mass Flow Rate (kg/hr)	13472.850	9354.592	176.239	21585.45 ₄	1418.227	12230.862	1241.988

Component distribution		
Component	Boiling point (°C)	Key component
Benzene	80.1	Light key
Ethylbenzene	136.2	Light key
Diethylbenzene	180	Heavy key

Design Parameters

Component Distribution	Column Sizing	Plate Hydraulic Design	Mechanical Design
Number of Stages	Tray Spacing	Active Area	Design Pressure
Reflux Ratio	Flooding Velocity	Hole Area	Design Temperature
Number of Actual Stages	Net Area	Tray Thickness	Material of Construction
Tray Efficiency	Downcomer Area	Hole Diameter	Column Wall Thickness
Location of Feed Stage	Column Diameter	Liquid Flow Arrangement	Column Head Design
	Column Height	Column Pressure Drop	Insulation
		Weeping checking	Stress Analysis
		Downcomer Liquid Backup	Column Support
		Residence Time	Nozzle Size
		Entrainment checking	
		Number of holes	

Design Criteria

Operating Pressure	: 2.80 bar	Ethylbenzene recovery	: 99.95%
Type of Column	: Tray Column	Ethylbenzene purity	: 99.88 wt%
Type of Tray	: Sieve tray		

Design Method

Fenske-Underwood-Gilliland shortcut method is utilized for component distribution calculation. The, the reflux ratio is determined by using Underwood equation and proceed to calculation of boil-up ratio. These values are used to find the theoretical number of stages. Then, actual number of stages for design is calculated by multiplying the theoretical number

of stages to O'Connell efficiency together with feed location for the actual number of stages. Afterwards, the details for designing the adequate distillation column are done guided mainly by Coulson and Richardson's Chemical Engineering Design Volume 6 4th edition book. Overall design of T-401 distillation column can be referred from Table 9.4.

Type of column and construction material justification

The selected construction material for T-401 distillation column is stainless steel 304 mainly due to the corrosion resistance in high temperature and its considerably high tensile strength compared to other common distillation column construction material based on Table 13.2 in Coulson and Richardson book. The designated tensile strength of the selected material is 510 N/mm² and the design stress is 111 N/mm² at T-401 operating temperature, 240°C. Thus, the material is appropriate for such operating condition. Besides, the type of T-401 is plate distillation column to provide high ratio of liquid-vapor flow rate. While sieve tray is utilized as it has versatile contactor and economically better than bubble cap or valve.

Table 9.3 Specification sheet of distillation column T-401

T-401					
Item	Distillation column	Date:	2nd February 2022		
Item no	T-401	By:	Muhammad Ariffin		
No. required	1				
General					
Function: To separate Diethylbenzene from Ethylbenzene					
Operation: Continuous		Material of Construction : Stainless steel (304)			
Type : Plate Distillation Column		Orientation : Vertical			
Operating Data					
Stream	IN		OUT		
	S-16	S-34	S-28		
Pressure (bar)	2.80	2.80	2.80		
Temperature (°C)	180.91	178.59	229.53		
Quantity (kg/h)	13472.85	12230.86	1241.99		
Vapor Fraction	0	0	0		
Composition (kg/h)					
Benzene	10.44	10.44	0.00		
Ethylene	0.00	0.00	0.00		
Ethylbenzene	12225.92	12219.81	6.11		
Diethylbenzene	1236.49	0.62	1235.87		
Methane	0.00	0.00	0.00		
Ethane	0.00	0.00	0.00		
Operational Design					
Maximum liquid flowrate (kg/s)	7.92	No. of trays (minus reboiler)	51		
Maximum vapor flowrate (m³/s)	0.84	Feed point (from bottom)	35		
Column Height (m)	35.47	Reflux ratio	0.76		
Column Diameter (m)	1.37	Tray spacing (m)	0.60		
Ratio of column height to diameter	25.83	Overall tray efficiency (%)	56.79		
Plate Hydraulic Design					
Active area (m²)	0.95	Plate material:	Stainless steel (304)		
Type of Tray	Seive Tray	Plate thickness (mm):	3.00		
Hole size (mm)	0.005	Weir length (m):	1.15		
Active holes	4827	Weir height (m):	0.05		
Flow Rate Turndown (%)	70	Plate pressure drop (mm liquid):	112.80		
Flooding (%)	80.00	Entrainment	0.02		
Calming Zone Width (mm)	50.00	Unperforated strip round plate edge(mm)	50		
		Liquid flow arrangement:	Cross flow, single pass		
Mechanical Design					
Design pressure (bar):	3.08	Vessel support:	Conical skirt		
Design temperature (°C):	240.00	Insulation:	Fibreglass		

Type of Head	Torispherical head	Insulation thickness (mm):	75
Wall thickness (mm):	10.246	Head Thickness (mm)	10.246
Welding joint factor:	0.85	Skirt thickness (mm) :	16
Corrosion allowance (mm):	1	Feed nozzle diameter (in):	4.00
Top nozzle diameter (in):	16.00	Reflux nozzle diameter (in):	3.00
Bottom nozzle diameter (in):	1.50	Boilup nozzle diameter (in):	2.00

The designed distillation column is within acceptable range with height to diameter (HC/DC) ratio is below 30, no occurrence of weeping as actual minimum vapor velocity exceeds weeping velocity, and satisfactory stress difference. The obtained values will then be compared with the simulated value from AspenPlus to further validate the design.

Comparison of calculated and simulated design values

Table 9 4Comparison of parameters between calculated values in Excel and simulated values in AspenPlus for T-401.

Parameter	Calculated value (Excel)	Simulated value (Radfrac)	Relative error (%)
Column diameter (m)	1.373	1.373	0.00
Column height (m)	31.924	29.4	8.59
Tray Spacing (m)	0.6	0.6	0.00
Hole diameter (m)	0.005	0.005	0.00
Hole area / Active area	0.1	0.1	0.00
Cross-sectional area (m ²)	1.481	1.481	0.00
Active area (m ²)	0.948	0.97	2.27
Net area (m ²)	1.214	1.225	0.90
Downcomer clearance (m)	0.04	0.04	0.00
Weir height (m)	0.05	0.05	0.00
Weir length (m)	1.15339	1.15339	0.00
Trays with weeping	None	None	
Flooding (%)	80	71.97	11.16
Condenser performance			
Temperature (°C)	178.5856	178.676	0.05
Heat duty (MJ/hr)	-7029.6	-6719.89	4.61
Distillate rate (kmol/hr)	115.235	115.235	0.00
Reflux rate (kmol/hr)	88.136	88.1316	0.00
Reflux ratio	0.7648	0.7648	0.00
Reboiler Performance			
Temperature (°C)	229.529	229.397	0.06
Heat duty (MJ/hr)	225.21	6801.69	96.69
Bottoms rate (kmol/hr)	9.2654	9.2654	0.00

Boilup rate (kmol/hr)	1.3148	183.239	99.28
Boilup ratio	0.1419	19.7767	99.28

The comparison values are summarized above in Table_. Radfrac model in AspenPlus also used in validating the calculated parameters of distillation column T-401. By comparing the values using relative error of calculated values to simulated values, sizing parameters of distillation column is consistently comparable for most of the parameters. The most significant difference of the distillation column sizing is only the column height with 8.59% which is still acceptable. This is due to in our own calculation, the column height considered additional height to accommodate the operating condition. Meanwhile, Radfrac model in AspenPlus calculated the column height based on the dimension sets to the tray such as tray spacing and weir length. The flooding level from simulation also lower than the calculated values. This also may be influenced by the resulted shorter column height.

Furthermore, the value for related areas such as cross-sectional area, active area, and net area can be observed to slightly deviate from the simulated values with only active area has 2.27% relative error and net area 0.90% relative area. This may be influenced by the usage of K1 in determining the flooding velocity. K1 is approximated based on graph which will likely cause minor error to the calculation. As for the reboiler performance, the overall relative error is low with only 4.61% error on the heat duty which is considered minor. This proved the calculation for the reboiler is considered accurate. However, major errors are observed for the boiler performance for the heat duty, boilup rate, and boilup ratio. The heat duty difference is resulted from the wide difference of boilup ratio which will increase the boilup rate in the distillation column. This probably caused by the design specification at the bottom of the column to obtain high purity product.

Engineering drawing of T-401

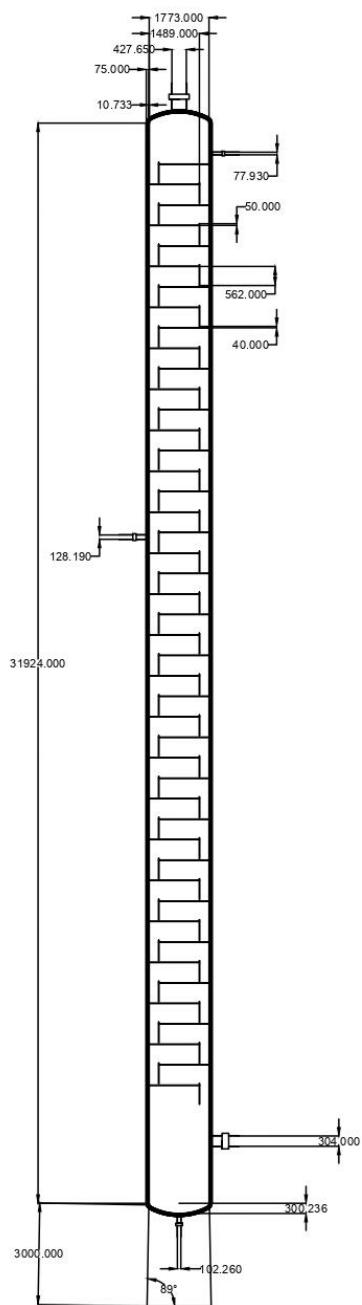


Figure 9 2Autocad engineering deisgn distillation column T-201

CHAPTER 10 HEAT TRANSFER EQUIPMENT

Design basis

The are few types of heat exchanger used for the ethylbenzene production, with the aids to increase or decrease the temperature of fluid process. Cooler is used to decrease the temperature of process fluid and transfer it to the service media such as water. Besides, condenser unit equipment is used to condense the vapor component to liquid by using cooling water. Reboiler also being used to vaporize process fluid by proving heat to the bottom of a distillation. Meanwhile, normal heat exchanger is being used to transfer heat between two process fluid.

Design calculation and assumption

The calculation of heat exchanger had been done by referring to Coulson and Richardson's Chemical Engineering Design Vol 6 Chemical Engineering Third Edition. The example of calculation steps are written in appendix.

Types of heat exchanger	Code/labelling	Design criteria
Heat exchanger (shell and tube)	E-102	To heat up the benzene in the inlet stream (S-6) before entering the alkylator which is a fixed bed reactor (R-101) while using outlet stream (S-10) of the alkylator as heating medium
	E-204	To increase temperature of inlet stream (S-35) to the operating temperature for the transalkylation reaction before entering transalkylator which is a fixed bed reactor (R-301) while using outlet of R-301 (S-38) as heating medium.
Condenser	E-101	To cool and liquefy vapor ethylene feed with trace components, ethane and methane before being transferred to alkylator R-101
	E-201	To condense the vapor distillate from distillation column T201 before returning to the distillation column or entering the flash drum.
	E-401	To condense the vapor distillate from distillation column T401 which are ethylbenzene benzene, and trace amount of diethylbenzene before returning part of it to the distillation column while discharging the remaining part with mainly ethylbenzene as the main product
Cooler	E-203	To cool down liquid coming from distillate T-201
	E-301	To cool the products of transalkylator R-301 which consists of liquid benzene, ethylene, ethylbenzene and diethylbenzene before transferring to the distillation column T-201.
Heater	E-103	To heat up the products of alkylator R-101 mixed with recycled stream which consists of liquid benzene, ethylene and ethylbenzene before returning it to the same reactor.
Reboiler	E-202	To re-boil the bottom products of distillation column T-201 which are liquid benzene, ethylbenzene, ethylbenzene and diethylbenzene to vapor form before returning it to the distillation column T-201.

	E-402	To re-boil the bottom products of distillation column T-401 which are liquid ethylbenzene and diethylbenzene to vapor form
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Design parameter

1. Heat transfer area
2. Shell and tube diameter
3. Tube wall thickness
4. Nominal length
5. Pitch arrangement
6. Number of shells
7. Number of tubes and number of passes
8. Baffle spacing
9. Overall heat transfer coefficient
10. Shell and tube side pressure drop
11. Mechanical design (including vessel support and nozzle diameter)

All physical properties such as density, specific heat capacity, viscosity and thermal conductivity are taken from ASPEN plus.

Material of construction

Carbon steel is adequate to be the construction material for basic equipment such as pumps, heat exchangers, condensers, reflux drums, etc, as these unit operations are not operating at extreme condition and without any vigorous reaction involved. Besides, carbon steel has high temperature resistance and also makes carbon steel a suitable material for most of the equipment in this plant as the operating temperature for all equipment in the plant are lower than 300°C. Moreover, carbon steel is extremely strong and more durable than stainless steel.

10.1 E-102 HEAT EXCHANGER (SHELL AND TUBE)

Table 10 1 Specification sheet of HEX E-104

HEAT EXCHANGER					
Item	:	heat exchanger	Date	:	15/1/2022
Item Code	:	E102	By	:	Tetra Tech Sdn Bhd
Function	:	To heat up process			
Type	:	shell and tube (2 shell passes; 2 tube passes), torispherical head			
Material of construction	:	Carbon Steel	Operation	:	Continuous
Orientation	:	Horizontal	Utility	:	-
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	8.40	7.50	
	Liquid	kg/s	8.40	7.50	
Temperature (In/Out)		K	473.15	393.77	333.27
Inlet pressure		bar	40	40	
Density, ρ		kg/m ³	745.0564244	782.6291524	
Specific heat capacity, C_p		kJ/kg.K	0.8186279	2.1874022	
Viscosity, μ		kg/m.s	0.0001000	0.0002435	
Thermal conductivity, k_f		W/m.K	0.0893697	0.1179484	
Fouling factor		W/m ² .°C	5000	5000	
Heat exchanged	J/s	:	140827.7778		
LMTD	K	:	44.23		
Total heat transfer area	m ²	:	31.84		
Overall heat transfer coefficient	W/m ² .K	:	91.89		
Construction Design					
			Shell Side	Tube Side	
Fluid Allocation					
Design pressure		bar	44.0000	44.0000	
Design temperature		K	498.1500	453.7500	
No. of shell pass			2.0000	-	
No. of tube pass			-	4.0000	
Number of tubes			-	69.0000	
Number of tubes/pass				17.0000	
Inner diameter	m		0.3637	0.0260	
Outer diameter	m		0.3770	0.0306	
Wall thickness	m		0.0067	0.0023	
Length	m		4.8800	4.8800	
Arrangement			-	Triangular	
Pitch	m		-	0.0375	
Baffle cut	%		25.0000	-	
Baffle spacing	m		0.1818	-	
Pressure drop	bar		20.3281	0.5899	
MAWP	bar		110.6647	499.8247	
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
	MAWP	bar	3824.1714		
	Thickness	m	0.4119		
	Corrosion allowance	m	0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t_2	m
	C	m	0.55	t_1	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	3347.12		
	Filled with water	N	4972.26		
	Bundle	N	5773.87		
	Insulation	N	382.33		
	TOTAL	N	14475.57		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
			Shell Side	Tube Side	
Nozzle size (Inlet/Outlet)		m	0.2645	0.2555	0.2073
					0.2230

10.2 E-204 HEAT EXCHANGER (SHELL AND TUBE)

Table 10 2: Specification HEX E-204

HEAT EXCHANGER					
Item	:	Heater	Date	:	15/1/2022
Item Code	:	E204	By	:	Tetra TechSdn.Bhd
Function	:	To heat up process			
Type	:	Shell and tube (2 shell passes; 4 tube passes), torispherical head			
Material of construction	:	Carbon Steel	Operation	:	Continuous
Orientation	:	Horizontal	Utility	:	-
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	1.14	0.80	
	Vapor	kg/s			
	Liquid	kg/s	1.14	0.80	
	Steam	kg/s			
Temperature (In/Out)		K	502.6792	454.15	350.2881
Inlet pressure		bar	35	40	
Density, ρ		kg/m ³	664.5604567	739.1970213	
Specific heat capacity, C_p		kJ/kg.K	0.6874492	2.4112646	
Viscosity, μ		kg/m.s	0.0000947	0.0001774	
Thermal conductivity, k_f		W/m.K	0.0872752	0.1070225	
Fouling factor		W/m ² .°C	5000	5000	
Heat exchanged	J/s	:	22296.11111		
LMTD	K	:	45.92		
Total heat transfer area	m ²	:	4.86		
Overall heat transfer coefficient	W/m ² .K	:	117.76		
Construction Design					
			Shell Side	Tube Side	
Fluid Allocation					
Design pressure		bar	38.5000	44.0000	
Design temperature		K	527.6792	508.1500	
No. of shell pass			2.0000	-	
No. of tube pass			-	4.0000	
Number of tubes			-	20.0000	
Number of tubes/pass				5.0000	
Inner diameter	m		0.2300	0.0136	
Outer diameter	m		0.2395	0.0180	
Wall thickness	m		0.0047	0.0022	
Length	m		4.8800	4.8800	
Arrangement			-	Triangular	
Pitch	m		-	0.0200	
Baffle cut	%		25.0000	-	
Baffle spacing	m		0.0460	-	
Pressure drop	bar		79.3827	1.9100	
MAWP	bar		123.3438	845.0359	
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
MAWP	bar		3829.2185		
Thickness	m		0.2613		
	m		0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t_2	m
	C	m	0.55	t_1	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	1467.22		
	Filled with water	N	1989.00		
	Bundle	N	877.02		
	Insulation	N	239.61		
	TOTAL	N	4572.84		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
			Shell Side	Tube Side	
Nozzle size (Inlet/Outlet)		m	0.11	0.10	0.06
					0.07

10.3 E201 CONDENSER HEAT EXCHANGER (SHELL AND TUBE)

Table 10 3 Specification sheet of condenser E-201

HEAT EXCHANGER					
Item	:	condenser	Date	:	15/1/2022
Item Code	:	E201	By	:	Tetra Sdn.Bhd
Function	:	To heat up process			
Type	:	BFM, Shell and tube (1 shell passes; 1 tube passes)			
Material of construction	:	Carbon Steel	Operation	:	Continuous
Orientation	:	Horizontal	Utility	:	-
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	0.03	479.45	
	Vapor	kg/s	0.03		
	Liquid	kg/s		479.45	
	Steam	kg/s			
Temperature (In/Out)	K		390.3962	390.3962	303.15 318.15
Inlet pressure	bar		2.8	1	
Density, ρ	kg/m ³		389.3143734	989.7802221	
Specific heat capacity, C_p	kJ/kg.K		1.8282001	1.8282001	
Viscosity, μ	kg/m.s		0.0001164	0.0007156	
Thermal conductivity, k_f	W/m.K		0.0668555	0.6225055	
Fouling factor	W/m ² .°C		5000	12000	
Heat exchanged	J/s	:	342598.8889		
LMTD	K	:	79.51		
Total heat transfer area	m ²	:	21.54		
Overall heat transfer coefficient	W/m ² .K	:	96.36		
Construction Design					
			Shell Side	Tube Side	
Fluid Allocation					
Design pressure	bar		3.0800	1.1000	
Design temperature	K		415.3962	343.1500	
No. of shell pass			2.0000	-	
No. of tube pass			-	1.0000	
Number of tubes			-	75.0000	
Number of tubes/pass				75.0000	
Inner diameter	m		0.7027	0.0460	
Outer diameter	m		0.7078	0.0500	
Wall thickness	m		0.0026	0.0020	
Length	m		1.8300	1.8300	
Arrangement			-	Triangular	
Pitch	m		-	0.0625	
Baffle cut	%		25.0000	-	
Baffle spacing	m		0.0703	-	
Pressure drop	bar		0.0006	0.7436	
MAWP	bar		22.1285	256.4196	
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
	MAWP	bar	3819.2827		
	Thickness	m	0.7939		
	Corrosion allowance	m	0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t_2	m
	C	m	0.55	t_1	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	1122.73		
	Filled with water	N	6963.11		
	Bundle	N	3528.55		
	Insulation	N	309.31		
	TOTAL	N	11923.71		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
			Shell Side	Tube Side	
Nozzle size (Inlet/Outlet)		m	0.1705	0.0159	0.0796 0.0798

10.4 E401 CONDENSER HEAT EXCHANGER (SHELL AND TUBE)

Table 10 4 Specification sheet of condenser E-401

HEAT EXCHANGER					
Item	:	Condenser	Date	:	15/1/2022
Item Code	:	E401	By	:	Tetra Sdn.Bhd
Function	:	To heat up process			
Type	:	Shell and tube (1 shell passes; 1 tube passes), torispherical head			
Material of construction	:	Carbon Steel	Operation	:	Continuous
Orientation	:	Horizontal	Utility	:	-
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	6.00	273.27	
	Vapor	kg/s	6.00		
Temperature (In/Out)		K	451.7356	451.7356	303.15 318.15
Inlet pressure		bar	2.8	1	
Density, ρ		kg/m ³	393.9003820	989.7802221	
Specific heat capacity, C_p		kJ/kg.K	1.9715546	1.9715546	
Viscosity, μ		kg/m.s	0.0001403	0.0007156	
Thermal conductivity, k_f		W/m.K	0.0658075	0.6225055	
Fouling factor		W/m ² .°C	5000	6000	
Heat exchanged	J/s	:	195275		
LMTD	K	:	0.00		
Total heat transfer area		m ²	12.05		
Overall heat transfer coefficient		W/m ² .K	129.31		
Construction Design					
			Shell Side	Tube Side	
Fluid Allocation					
Design pressure		bar	3.0800	1.1000	
Design temperature		K	476.7356	343.1500	
No. of shell pass			2.0000	-	
No. of tube pass			-	1.0000	
Number of tubes			-	42.0000	
Number of tubes/pass				42.0000	
Inner diameter		m	0.5460	0.0460	
Outer diameter		m	0.5510	0.0500	
Wall thickness		m	0.0025	0.0020	
Length		m	1.8300	1.8300	
Arrangement			-	Triangular	
Pitch		m	-	0.0625	
Baffle cut	%		25.0000	-	
Baffle spacing	m		0.1092	-	
Pressure drop	bar		15.8228	0.7854	
MAWP	bar		27.5576	256.4196	
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
MAWP	bar		3820.6443		
Thickness	m		0.6173		
Corrosion allowance	m		0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t_2	m
	C	m	0.55	t_1	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	801.33		
	Filled with water	N	4203.81		
	Bundle	N	1975.99		
	Insulation	N	232.11		
	TOTAL	N	7213.24		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
			Shell Side	Tube Side	
Nozzle size (Inlet/Outlet)		m	1.7393	0.1751	0.5953 0.5972

10.5 E-203 COOLER

Table 10.5 Specification sheet for cooler E-203.

COOLER						
Item	:	Cooler		Date	: 18th January 2022	
Item Code	:	E-203		By	: How Mun Cheng	
No. of unit	:	1				
General						
Function	:	To lower the temperature of the liquid stream before being transferred to flash drum V-202.				
Type	:	BEM, Shell and tube (1 shell pass; 8 tube passes)				
Material of construction	:	Carbon Steel		Operation	: Continuous	
Orientation	:	Horizontal		Utility	: Process Fluid	
Performance of One Unit						
Fluid Allocation			Shell Side	Tube Side		
Fluid name			Process Fluid	Process Fluid		
Fluid quantity	Total	kg/s	96.92	5.80		
Vapor						
Liquid			96.92	5.80		
Steam						
Water						
Temperature (In/Out)		K	303.15	313.15	390.40	350.29
Inlet pressure		bar	1		2.8	
Density, ρ		kg/m ³	999.80		772.87	
Specific heat capacity, C_p		kJ/kg.K	4.22		1.96	
Viscosity, μ		kg/m.s	0.58		0.00	
Thermal conductivity, k_f		W/m.K	0.57		0.12	
Fouling factor		W/m ² .°C	3000.00		5000.00	
Heat exchanged	MJ/hr	1620.64				
LMTD	K	59.83				
Total heat transfer area	m ²	10.03				
Overall heat transfer coefficient	W/m ² .K	864.47				
Construction Design						
Fluid Allocation			Shell Side	Tube Side		
Design pressure		bar	3.08	3.08		
Design temperature		K	323.15	400.40		
No. of shell pass			1	-		
No. of tube pass			-	8		
Number of tubes			-	58		
Number of tubes/pass				7		
Inner diameter	mm	529.35		26.00		
Outer diameter	mm	534.78		30.00		
Wall thickness	mm	0.71		0.04		
Length	mm	1830.00		1830.00		
Arrangement			-	Triangular		
Pitch	mm	-		37.5		
Baffle cut	%	25.00		-		
Baffle spacing	m	0.26		-		
Pressure drop	bar	4.61		0.66		
MAWP	bar	31.19		445.61		
Mechanical Design						
Material	Carbon steel					
Type of head	Torospherical head					
MAWP	bar	41.50				
Thickness	mm	3.07				
Corrosion allowance	mm	2				
Vessel support	Saddle					
V	mm	580	G	mm	95	
Y	mm	150	t_2	mm	8	
C	mm	700	t_1	mm	5	
E	mm	290	Bolt diameter	mm	20	
J	mm	225	Bolt holes	mm	25	
Weight	Shell	N	848.45			
	Filled with water	N	3950.95			
	Bundle	N	1603.80			
	Insulation	N	252.75			
Insulation	Calcium silicate board		Insulation thickness	mm	50	
			Shell Side	Tube Side		
Nozzle size (Inlet/Outlet)		mm	308.36	308.36	94.07	94.00

10.6 E-301 COOLER

Table 10 6 Specification sheet for cooler E-301.

COOLER									
Item	Cooler		Date	: 3rd February 2022					
Item Code	E-301		By	: How Mun Cheng					
No. of unit	1								
General									
Function	To lower the temperature of the liquid stream before being transferred to flash drum V-202.								
Type	BEM, Shell and tube (1 shell pass; 8 tube passes)								
Material of construction	Carbon Steel		Operation	: Continuous					
Orientation	Horizontal		Utility	: Process Fluid					
Performance of One Unit									
Fluid Allocation				Shell Side	Tube Side				
Fluid name				Process Fluid	Process Fluid				
Fluid quantity	Total	kg/s		7.64	1.14				
Vapor									
Liquid				7.64	1.14				
Steam									
Water									
Temperature (In/Out)	K		303.15	318.15	453.80	393.77			
Inlet pressure	bar			1	35				
Density, ρ	kg/m ³			999.80	701.86				
Specific heat capacity, C_p	kJ/kg.K			4.21	2.28				
Viscosity, μ	kg/m.s			1.07	0.00				
Thermal conductivity, k_f	W/m.K			0.57	0.09				
Fouling factor	W/m ² .°C			6000.00	5000.00				
Heat exchanged	MJ/hr		127.81						
LMTD	K		110.26						
Total heat transfer area	m ²		0.64						
Overall heat transfer coefficient	W/m ² .K		538.33						
Construction Design									
Fluid Allocation				Shell Side	Tube Side				
Design pressure	bar			1.10	38.50				
Design temperature	K			328.15	463.80				
No. of shell pass				1	-				
No. of tube pass				-	4				
Number of tubes				-	4				
Number of tubes/pass					1				
Inner diameter	mm			376.23	26.00				
Outer diameter	mm			380.56	30.00				
Wall thickness	mm			0.16	0.86				
Length	mm			1830.00	1830.00				
Arrangement				-	Triangular				
Pitch	mm			-	37.5				
Baffle cut	%			25.00	-				
Baffle spacing	m			0.19	-				
Pressure drop	bar			0.11	0.69				
MAWP	bar			34.96	605.62				
Mechanical Design									
Material	Carbon steel								
Type of head	Ellipsoidal head								
	MAWP	bar		43.27					
	Thickness	mm		2.27					
	Corrosion allowance	mm		2					
Vessel support	Saddle								
	V	mm	480	G	mm	95			
	Y	mm	150	t_2	mm	6			
	C	mm	550	t_1	mm	5			
	E	mm	240	Bolt diameter	mm	20			
	J	mm	190	Bolt holes	mm	25			
Weight	Shell	N	454.85						
	Filled with water	N	1995.83						
	Bundle	N	159.23						
	Insulation	N	168.19						
Insulation	Calcium silicate board		Insulation thickness	mm	50				
				Shell Side	Tube Side				
Nozzle size (Inlet/Outlet)	mm		98.32	98.32	46.74	46.63			

10.7 E-103 HEATER

Table 10.7 Specification sheet for cooler E-301

HEAT EXCHANGER					
Item	:	Heater		Date	:
Item Code	:	E-103		By	:
Function	:	To heat up process			
Type	:	Shell and tube (1 shell passes; 1 tube passes), torispherical head			
Material of construction	:	Carbon Steel		Operation	:
Orientation	:	Horizontal		Utility	:
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	7.50	18.21	
	Vapor	kg/s	7.50		
	Liquid	kg/s		18.21	
Temperature (In/Out)	K		428.7498	473.15	723.15 523.45
Inlet pressure	bar		40	40	
Density, ρ	kg/m ³		450.6995610	14.2718129	
Specific heat capacity, C_p	kJ/kg.K		2.6986830	2.6986830	
Viscosity, μ	kg/m.s		0.0001375	0.0000223	
Thermal conductivity, k_f	W/m.K		0.0668556	0.0573635	
Fouling factor	W/m ² .°C		5000	5000	
Heat exchanged	J/s	:	74071.94444		
LMTD	K	:	143.98		
Total heat transfer area	m ²	:	8.57		
Overall heat transfer coefficient	W/m ² .K	:	71.97		
Construction Design					
Fluid Allocation			Shell Side	Tube Side	
Design pressure	bar		44.0000	44.0000	
Design temperature	K		453.7498	548.4500	
No. of shell pass			2.0000	-	
No. of tube pass			-	1.0000	
Number of tubes			-	30.0000	
Number of tubes/pass			-	30.0000	
Inner diameter	m		0.4741	0.0460	
Outer diameter	m		0.4895	0.0513	
Wall thickness	m		0.0077	0.0026	
Length	m		1.8300	1.8300	
Arrangement			-	Triangular	
Pitch	m		-	0.0625	
Baffle cut	%		25.0000	-	
Baffle spacing	m		0.2370	-	
Pressure drop	bar		2.3860	61.5229	
MAWP	bar		97.7386	333.3081	
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
	MAWP	bar	3822.1391		
	Thickness	m	0.5364		
	Corrosion allowance	m	0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t_2	m
	C	m	0.55	t_1	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	2141.12		
	Filled with water	N	3169.02		
	Bundle	N	1884.23		
	Insulation	N	202.68		
	TOTAL	N	7397.06		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
			Shell Side	Tube Side	
Nozzle size (Inlet/Outlet)		m	0.4597	0.2802	0.5499 0.4678

10.8 E-202 REBOILER

Table 10.8 Specification sheet for cooler E-301

HEAT EXCHANGER					
Item	:	reboiler	Date	:	15/1/2022
Item Code	:	E202	By	:	Tetra tech Sdn.Bhd
Function	:	To heat up process			
Type	:	Fixed and utube (1 shell passes; 1 tube passes), torispherical head			
Material of construction	:	Carbon Steel	Operation	:	Continuous
Orientation	:	Horizontal	Utility	:	-
Performance of One Unit					
			Shell Side	Tube Side	
Fluid name			Process Fluid (hot fluid)	Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	6.51	22.23	
	Liquid	kg/s		22.23	
	Steam	kg/s	6.51		
Temperature (In/Out)	K		454.063	454.063	723.15 523.45
Inlet pressure	bar		2.8		40
Density, ρ	kg/m ³		718.4156293		14.2718129
Specific heat capacity, C_p	kJ/kg.K		3.4202332		2.5128550
Viscosity, μ	kg/m.s		0.0001939		0.0000223
Thermal conductivity, k_f	W/m.K		0.1050421		0.0573635
Fouling factor	W/m ² .°C		5000		5000
Heat exchanged	J/s	:	90419.44444		
LMTD	K	:	147.34		
Total heat transfer area	m ²	:	10.23		
Overall heat transfer coefficient	W/m ² .K	:	69.83		
Construction Design					
Fluid Allocation			Shell Side	Tube Side	
Design pressure	bar		3.0800		44.0000
Design temperature	K		479.0630		548.4500
No. of shell pass			2.0000		-
No. of tube pass			-		1.0000
Number of tubes			-		36.0000
Number of tubes/pass					36.0000
Inner diameter	m		0.4671		0.0460
Outer diameter	m		0.4719		0.0513
Wall thickness	m		0.0024		0.0026
Length	m		1.8300		1.8300
Arrangement			-		Triangular
Pitch	m		-		0.0625
Baffle cut	%		25.0000		-
Baffle spacing	m		0.2336		-
Pressure drop	bar		1.2477		63.6634
MAWP	bar		31.3264		333.3081
Mechanical Design					
Material	Carbon steel 5%				
Type of head	Torispherical head				
MAWP	bar		3821.6275		
Thickness	m		0.5284		
Corrosion allowance	m		0.0020		
Vessel support	Saddle				
	V	m	0.48	G	m
	Y	m	0.15	t ₂	m
	C	m	0.55	t ₁	m
	E	m	0.24	Bolt diameter	m
	J	m	0.19	Bolt holes	m
Weight	Shell	N	648.96		
	Filled with water	N	3076.87		
	Bundle	N	2261.08		
	Insulation	N	195.10		
	TOTAL	N	6182.01		
Insulation	Calcium silicate board		Insulation thickness	m	0.05
Nozzle size (Inlet/Outlet)			Shell Side	Tube Side	
	inlet	outlet 1	outlet 2		
	m	0.03343111	0.315405936	0.006388041	0.0602 0.0512

10.9 E-402 REBOILER

Table 10.9 Specification sheet for cooler E-301

HEAT EXCHANGER						
Item	:	reboiler	Date	:	15/1/2022	
Item Code	:	E402	By	:	Tetra tech Sdn.Bhd	
Function	:	To heat up process				
Type	:	Fixed and utube (1 shell passes; 2 tube passes)				
Material of construction	:	Carbon Steel	Operation	:	Continuous	
Orientation	:	Horizontal	Utility	:	-	
Performance of One Unit						
			Shell Side		Tube Side	
Fluid name			Process Fluid (hot fluid)		Process Fluid (cold fluid)	
Fluid quantity	Total	kg/s	0.39		1.54	
	Liquid	kg/s			1.54	
	Steam	kg/s	0.39			
Temperature (In/Out)		K	502.6792	502.6792	723.15	523.45
Inlet pressure		bar	2.8		40	
Density, ρ		kg/m ³	693.2019754		14.2718129	
Specific heat capacity, C_p		kJ/kg.K	3.8635301		2.8788050	
Viscosity, μ		kg/m.s	0.0001742		0.0000223	
Thermal conductivity, k_f		W/m.K	0.1050421		0.0573635	
Fouling factor		W/m ² .°C	5000		5000	
Heat exchanged	J/s	:	90419.44444			
LMTD	K	:	84.54			
Total heat transfer area	m ²	:	21.39			
Overall heat transfer coefficient	W/m ² .K	:	59.58			
Construction Design						
			Shell Side		Tube Side	
Fluid Allocation						
Design pressure		bar	3.0800		44.0000	
Design temperature		K	527.6792		548.4500	
No. of shell pass			2.0000		-	
No. of tube pass			-		2.0000	
Number of tubes			-		31.0000	
Number of tubes/pass					16.0000	
Inner diameter		m	0.2775		0.0260	
Outer diameter		m	0.2820		0.0307	
Wall thickness		m	0.0023		0.0024	
Length		m	7.3200		7.3200	
Arrangement			-		Triangular	
Pitch		m	-		0.0375	
Baffle cut	%		25.0000		-	
Baffle spacing		m	0.0555		-	
Pressure drop		bar	4.7523		79.9933	
MAWP		bar	49.4494		510.6932	
Mechanical Design						
Material	Carbon steel 5%					
Type of head	Torispherical head					
MAWP	bar		3826.3126			
Thickness	m		0.3147			
Corrosion allowance	m		0.0020			
Vessel support	Saddle					
	V	m	0.48	G	m	0.095
	Y	m	0.15	t ₂	m	0.006
	C	m	0.55	t ₁	m	0.005
	E	m	0.24	Bolt diameter	m	0.02
	J	m	0.19	Bolt holes	m	0.025
Weight	Shell	N	1243.42			
	Filled with water	N	4341.83			
	Bundle	N	3984.99			
	Insulation	N	421.32			
	TOTAL	N	9991.57			
Insulation	Calcium silicate board		Insulation thickness	m	0.05	
Nozzle size (Inlet/Outlet)			Shell Side		Tube Side	
		inlet	outlet 1	outlet 2		
		m	0.1256399	1.100247907	0.18916158	0.2270 0.1931

Drawing of heat exchanger

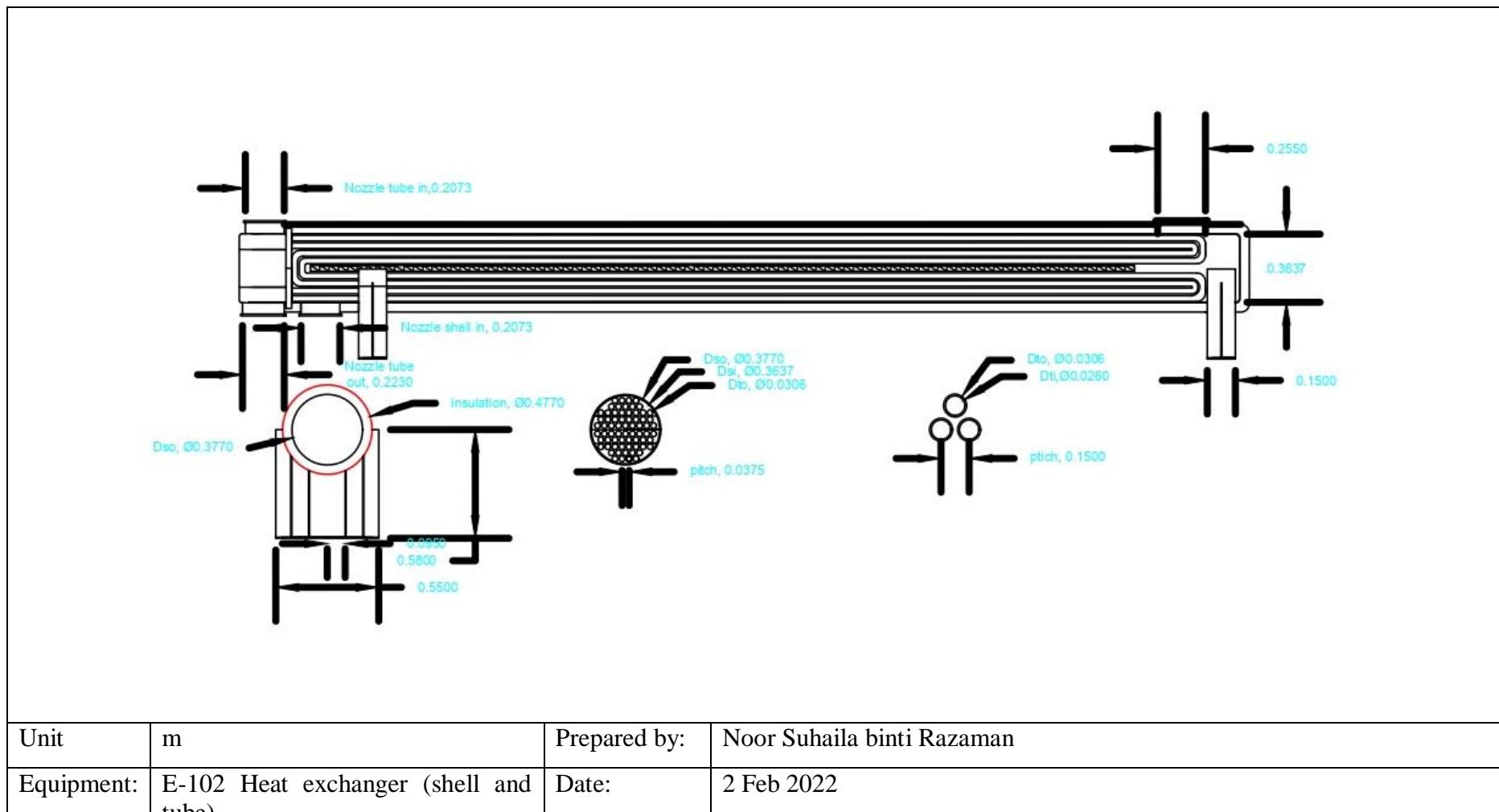


Figure 10 1Autocade engineering drawing E102 heat exchanger

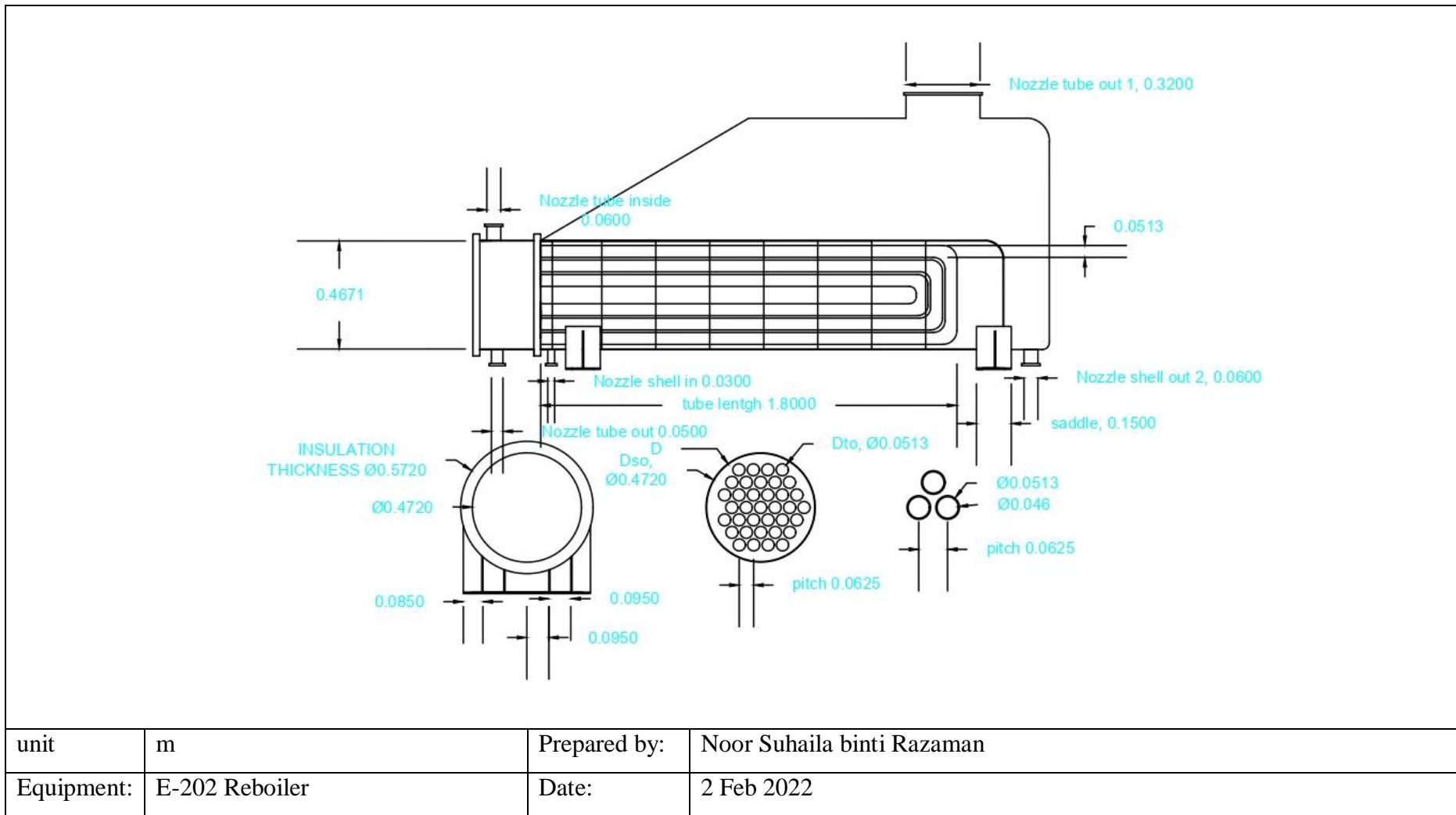


Figure 10 2 Autocade engineering drawing E202 reboiler

Comparison of Manual Calculation with ASPEN Plus simulation

Table 10.10 Comparison table of manual calculation and Aspen Plus simulation for cooler E-203.

Parameters	E-203	
	Aspen	Excel
Location of hot fluid	Tube	Tube
Tube outer diameter, Do (m)	0.3	0.3
Tube pattern	Triangular	Triangular
Shell inside diameter, Ds (m)	0.5294	0.5294
Shell outside diameter, Dso (m)	0.5348	0.5348
Nominal length, L (m)	1.83	1.83
Baffle spacing, lb (single segmental) (m)	0.26	0.26
Number of tubes, Nt	58	58
Number of passes	8	8
Tube side pressure drop (bar)	0.1551	0.6554
Shell side pressure drop (bar)	0.0038	4.6056
Shell side temperature (In/Out) (°C)	30/34.1521	30/40
Tube side temperature (In/Out) (°C)	117.25/77.14	117.25/77.14
Heat duty, Q (MJ/hr)	6007.6800	1260.2400
Heat transfer area, Ao (m ²)	8.1350	10.0300
Percent excess surface area (%)	69.1308	-
Overall heat transfer coefficient (W/m ² . °C)	415.6390	846.4700
LMTD (corrected) (K)	83.4739	59.8300
Vibration indication	No	-

In Aspen simulation, the allocation of hot fluid of either being in shell side or tube side is run with trial until there is no vibration indication which poses high risks for the heat exchanger damage whereby the results are then followed in manual calculation. As shown in Table 10.10, the Aspen simulation result for cooler E-203 and manual calculation using Excel shows large difference in value in terms of pressure drop, heat duty, heat transfer area and overall heat transfer coefficient, U. As both the U and heat transfer area larger than that simulated in Aspen, the design and sizing done in manual calculation is assured in its design as the percent excess surface area for those design will always be positive value. The deviation of manual calculation for cooler E-203 from Aspen simulation might be due to the trade-off in manual calculation in which the pressure drop parameters at the shell and tube side must be considered in adjusting the manipulated parameters and at the same time, the initial and calculated U value must be meet accordingly. With the different approach being utilized in heat exchanger sizing in manual calculation in which the manipulated parameters are evaluated based on some recommended range and estimation of data extracted from graph, some inaccurate sizing and justification will occur.

Comparison of Manual Calculation with ASPEN Plus simulation

Table 10.11 Comparison table of manual calculation and Aspen Plus simulation for cooler E-301.

Parameters	E-301	
	Aspen	Excel
Location of hot fluid	Tube	Tube
Tube outer diameter, Do (m)	0.3	0.3
Tube pattern	Triangular	Triangular
Shell inside diameter, Ds (m)	0.37623	0.37623
Shell outside diameter, Dso (m)	0.39528	0.38056
Nominal length, L (m)	1.83	1.83
Baffle spacing, lb (single segmental) (m)	0.19	0.19
Number of tubes, Nt	62	4
Number of passes	4	4
Tube side pressure drop (bar)	0.2926	0.6900
Shell side pressure drop (bar)	0.0038	0.1100
Shell side temperature (In/Out) (°C)	30/35.2587	30/45
Tube side temperature (In/Out) (°C)	180.65/120.62	180.65/120.62
Heat duty, Q (MJ/hr)	600.3850	127.8100
Heat transfer area, Ao (m ²)	0.6526	0.6400
Percent excess surface area (%)	45.1658	-
Overall heat transfer coefficient (W/m ² .°C)	1206.0456	538.3300
LMTD (corrected) (K)	116.1980	110.2600
Vibration indication	No	-

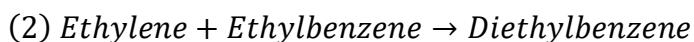
As shown in Table 10.11, large difference in value of pressure drop, heat duty, heat transfer area and overall heat transfer coefficient, U occur between the Aspen simulation and manual calculation using Excel. The design and sizing done in manual calculation for E-301 is assured as the percent excess surface area for those design will always be positive value. The deviation of manual calculation for cooler E-301 from Aspen simulation might be due to the trade-off in manual calculation in which the pressure drop parameters at the shell and tube side must be considered in adjusting the manipulated parameters and at the same time, the initial and calculated U value must be meet accordingly. With the different approach being utilized in heat exchanger sizing in manual calculation in which the manipulated parameters are evaluated based on some recommended range and estimation of data extracted from graph, it is likely to have some inaccurate sizing and justification.

CHAPTER 11 REACTION DESIGN

11.1 R-101, Packed-Bed Reactor

Design Basis

Benzene is alkylated with ethylene in the presence of zeolite catalyst by introducing a mixture of fresh and recycle benzene into a packed bed reactor having at least 2 beds [109] to produce ethylbenzene where ethylene in its liquid phase goes through almost a complete reaction accompanied by the excess benzene being introduced [110]. Design criteria with 99.95% of ethylene conversion is being considered during reactor design. Exothermic nature of the reaction requires the cooling jacket design with the flow of cooling water around the reactor to maintain the reactor temperature. MWW MCM-22 zeolite catalyst with high selectivity toward monoalkylated products and a high stability lead to the only dominant side product of 1,4-diethylbenzene formation [111]. Co-current gas-liquid downflow is applied to the reactor configuration as for gas-limited reactions, it facilitates the transport of the gaseous reactant to the catalyst and the liquid flow approaches plug-flow behaviour which can lead to higher conversion [112]. The reaction kinetics applied in determining the weight of catalyst are taken from Luyben (2010) as shown as below [113]:



$$r_1 = 1.528E + 06 \exp \frac{-7.113E+04}{RT} [a][b]$$

$$k_1 = 1.528E + 06 \exp \frac{-7.113E + 04}{RT}$$

$$r_2 = 2.778E + 07 \exp \frac{-8.368E+04}{RT} [c][b]$$

$$k_2 = 2.778E + 07 \exp \frac{-8.368E + 04}{RT}$$

$$R = 8.314 \text{J/mol. K}; T (\text{K})$$

Design Parameters

Reactor design is crucial to ensure that the reactor vessel able to carry out the desired reaction rate and the production capacity whilst mechanical design of the reactor must be

performed to ensure that the reactor vessel able to withstand the stresses to ensure a safe operation.

Reactor Design

1. Reactor sizing (Reactor inner and outer diameter, Height of reactor, Reactor wall thickness)
2. Volume and mass of catalyst
3. Cooling jacket (Jacket thickness, Jacket length, Heat transfer area, Cooling water mass flow rate)

Mechanical design

1. Design temperature and pressure for both reactor and cooling jacket
2. Maximum allowable working pressure (MAWP) for both reactor and cooling jacket
3. Reactor vessel head design (Head type, Head thickness, MAWP)
4. Weight load
5. Stress Analysis
6. Vessel support
7. Base ring and anchor bolt design
8. Nozzle dimensions

Design Criteria

Type of reactor: Fixed bed reactor with cooling jacket

Orientation: Vertical

Material of construction: Stainless steel 304

Operating temperature: 182.4655°C

Operating pressure: 40 bar

Benzene/Ethylene feed ratio: 4.11

Ethylene conversion: 0.9995

Selectivity towards ethylbenzene production: 0.92 [109]

Selectivity towards diethylbenzene production: 0.08

Catalyst type: MWW MCM-22 zeolite

Bulk density: 892.89kg/m³ [113]

Effective particle size of the catalyst, D_p: 0.005m [113]

Void fraction, ε: 0.48 [113]

Design method

The mass of catalyst is determined by applying fixed bed reactor design equation coupled with the reaction kinetics using POLYMATH. The design of the reactor with its mechanical design reference is based on Coulson and Richardson's Chemical Engineering Design and the cooling jacket design guideline is based on J. P. Holman's Heat transfer.

Material of construction

The exothermic alkylation of benzene with ethylene in the presence of acidic MCM-22 zeolite catalyst distributed as beds is carried out at 170°C and 35 bar. To prevent temperature rise across reactor beds, the reactor is jacketed with cooling water flow to maintain the reaction temperature at 170°C. Stainless steel alloy is chosen for the construction of reactor to prevent the formation of carbonyls which will cause catalyst poisoning. Besides, the reactor cooling jacket is erected from 2205 duplex stainless alloy rather than 304 stainless steel as it has greater strength (cheaper and thinner reactor wall), high thermal conductivity, good heat transfers between cooling jacket and reactor as well as its lightweight characteristic which do not require support that simplifies the overall reactor structural design [114].

Table 11 1 Specification Sheet of Packed Bed Reactor R-101.

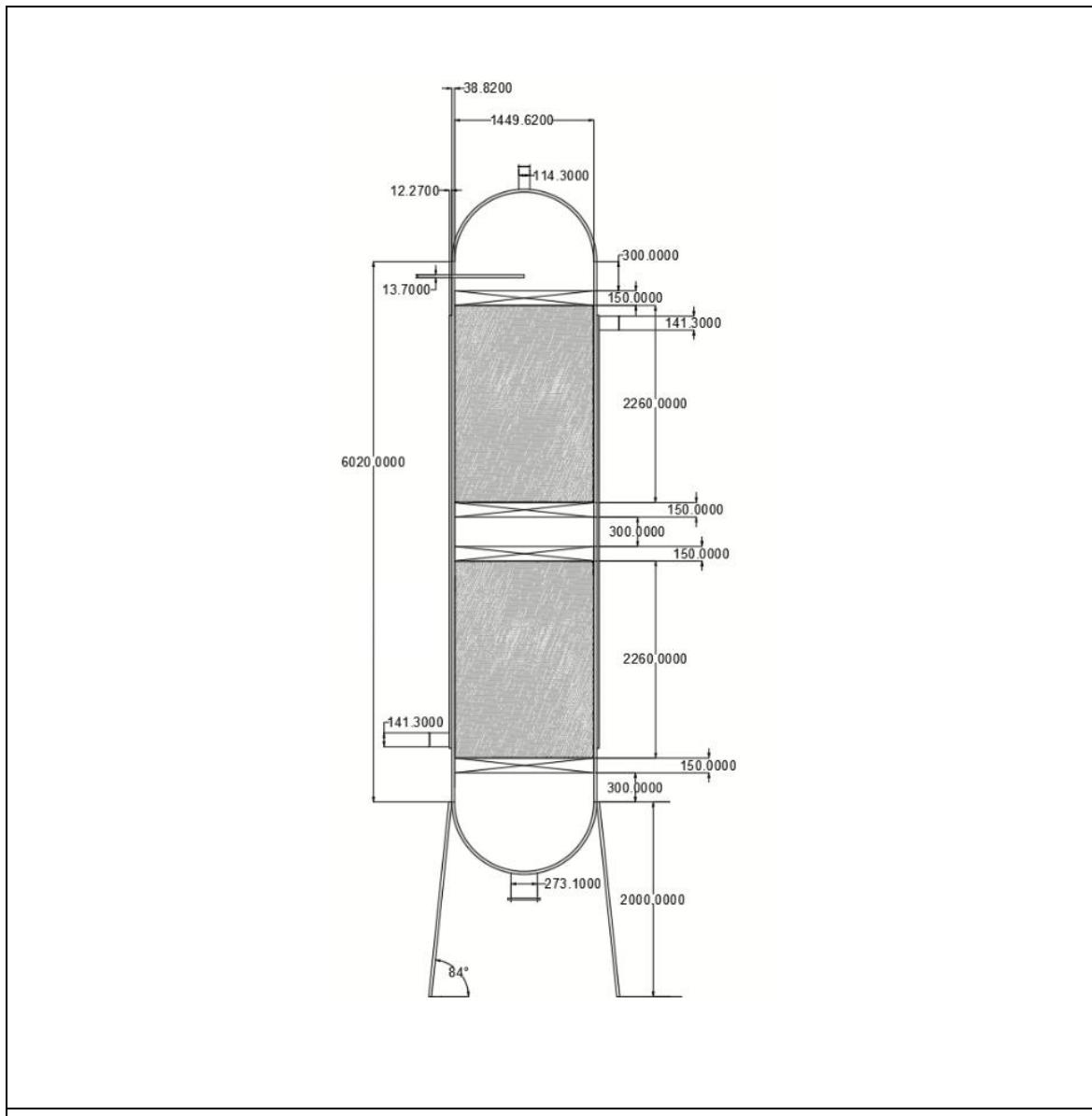
REACTOR					
Item	:	Fixed bed reactor		Date	: 18th January 2022
Item Code	:	R-101		By	: How Mun Cheng
No. of unit	:	1			
General					
Function	:	Alkylation of benzene to product ethylbenzene as main product and diethylbenzene as by-product with the presence of zeolite catalyst.			
Operation	:	Continuous			
Type	:	Catalytic, fixed bed reactor with cooling jacket (Isothermal)			
Orientation	:	Vertical			
Reaction Bed					
COMPONENT		INLET (kg/hr)		OUTLET (kg/hr)	
Benzene		26987.8326		18715.7021	
Ethylene		3230.1105		1.6151	
Ethylbenzene		6.1160		10270.8671	
Diethylbenzene		0.0000		1235.8750	
Methane		0.4987		0.4987	
Ethane		1.8352		1.8352	
Cooling Jacket (Cooling Medium: Cooling Water)					
Cooling duty:	MJ/hr	7028.01	Design pressure	bar	1.10
Mass flow rate:	ton/hr	46.7	Design temperature	K	328.15
Total heat transfer area	m ²	7.94	Corrosion allowance	mm	2
Jacket thickness:	mm	17.3	Inner diameter	m	1.45
Cooling jacket length:	m	4.81	MAWP	bar	15.4
Reactor Construction Data					
Material of Construction:		Stainless steel type	Catalyst density:	kg/m ³	892.89 kg/m ³
Functional height:	m	6.015 m	Catalyst support:		Support grid
Diameter (internal):	m	1.38 m	Mass of catalyst:		3008.46 kg
Diameter (external):	m	1.45 m	Bed volume:		6.48 m ³
Catalyst:		Zeolite	Bed Void fraction:		0.48
Catalyst diameter:	m	0.005 m	Pressure drop:		0.04 bar
Mechanical Design					
Design Pressure:	bar	44.00 bar	Design Temperature:	K	483.15
Type of head:		Hemispherical head	Type of support:		Conical skirt
Vessel wall thickness:	mm	33.82	Skirt thickness:	mm	33.82
Head thickness:	mm	20.29	MAWP (Reactor/Head):	bar	207.1
Nozzle size (B/E/Effluent):	in	5/0.25/4	Nozzle size CW (In/Out):		10/10
Bolt:		M24	Number of bolts:		8
Base ring width:	mm	159.82	Min. Base ring thickness:	mm	6.27
ASPEN Simulation					
Cooling duty:	MJ/hr	12190.30			

* The detailed design calculation steps are shown in Appendix.

Comparison of Manual Calculation with ASPEN Plus simulation

The cooling duty obtained from ASPEN simulation is 12190.30 MJ/hr which is higher than the cooling duty that is obtained from manual energy balance calculation (7028.01 MJ/hr). On the other hand, the product molar flow rates of each component are compared between manual calculation and ASPEN simulation in which for manual calculation, the generation and consumption of each component is calculated based on the selectivity and conversion data extracted from literature while ASPEN simulates the reaction based on reaction kinetics. In Aspen simulation, the ethylbenzene shows no difference in

molar flowrate between inlet and outlet streams while there is no ethylene occurs at the outlet stream. The negative deviation from ASPEN result might be due to the different correlation used in determining the thermodynamic data of the components for instance specific heat capacity, specific molar volume, heat of vaporization and others. In energy balance calculation, the component properties are taken from various sources of handbooks in which the data are mostly taken at 1 atm but not at the reactor operating pressure of 40 bar. Acceptable assumption is made for ease calculation in which the properties do not alter significantly with pressure whilst the calculation from ASPEN able to predict the properties more accurately at the specified temperature and pressure.



*Unit of measurement in millimeters, mm.

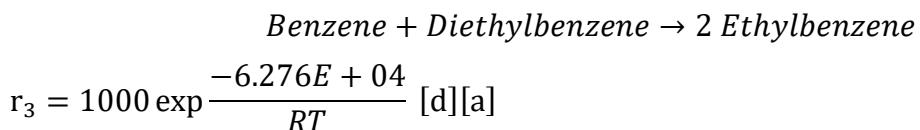
UNIT CODE:	R-101	DATE:	2.2.2022
EQUIPMENT:	PACKED BED REACTOR	DRAWN BY:	HOW MUN CHENG

Figure 11 IAUOCAD engineering drawing of packed-bed reactor, R-101.

11.2 R-301, Packed-Bed Reactor

Design Basis

Transalkylation of benzene with diethylbenzene occurs in the presence of zeolite catalyst in a packed bed reactor having at least 2 beds [109] to produce more ethylbenzene where diethylbenzene in its liquid phase goes through almost a complete reaction with benzene. Design criteria with 99.95% of diethylbenzene conversion is being considered during reactor design. Exothermic nature of the reaction requires the cooling jacket design with the flow of cooling water around the reactor to maintain the reactor temperature. MWW MCM-22 zeolite catalyst with high selectivity toward monoalkylated products and a high stability lead to the only dominant side product of 1,4-diethylbenzene formation [111]. The reaction kinetics applied in determining the weight of catalyst are shown as follows []:



$$R = 8.314 \text{ J/mol.K}; T (\text{K})$$

Design Parameters

Reactor design is crucial to ensure that the reactor vessel able to carry out the desired reaction rate and the production capacity whilst mechanical design of the reactor must be performed to ensure that the reactor vessel able to withstand the stresses to ensure a safe operation.

Reactor Design

1. Reactor sizing (Reactor inner and outer diameter, Height of reactor, Reactor wall thickness)
2. Volume and mass of catalyst
3. Cooling jacket (Jacket thickness, Jacket length, Heat transfer area, Cooling water mass flow rate)

Mechanical design

1. Design temperature and pressure for both reactor and cooling jacket
2. Maximum allowable working pressure (MAWP) for both reactor and cooling jacket
3. Reactor vessel head design (Head type, Head thickness, MAWP)
4. Weight load
5. Stress Analysis
6. Vessel support
7. Base ring and anchor bolt design
8. Nozzle dimensions

Design Criteria

Type of reactor: Fixed bed reactor with cooling jacket

Orientation: Vertical

Material of construction: Stainless steel 304

Operating temperature: 229.5292°C

Operating pressure: 35 bar

Diethylbenzene conversion: 0.9995

Selectivity towards ethylbenzene production: 1

Catalyst type: MWW MCM-22 zeolite

Bulk density: 720.00 kg/m³ [Ali, A. (2012). Liquid Phase Alkylation of Benzene with Ethylene. Retrieved from <https://ar.scribd.com/doc/106876722/Liquid-Phase-Alkylation-of-Benzene-with-Ethylene.>]

Effective particle size of the catalyst, D_p: 0.005m [21]

Void fraction, ε: 0.48 [21]

Design method

The mass of catalyst is determined by applying fixed bed reactor design equation coupled with the reaction kinetics using POLYMATH. The design of the reactor with its mechanical design reference is based on Coulson and Richardson's Chemical Engineering Design and the cooling jacket design guideline is based on J. P. Holman's Heat transfer.

Material of construction

The exothermic transalkylation of benzene with ethylene in the presence of acidic MCM-22 zeolite catalyst distributed as beds is carried out at 229.5292°C and 35 bar. In order to maintain the operating temperature of the reactor R-301, the reactor is jacketed with high pressure stream flow to provide heat to the reactor. Stainless steel alloy is chosen for the construction of reactor to prevent the formation of carbonyls which will cause catalyst poisoning. Besides, the reactor cooling jacket is erected from 2205 duplex stainless alloy rather than 304 stainless steel as it has greater strength (cheaper and thinner reactor wall), high thermal conductivity, good heat transfers between cooling jacket and reactor as well as its lightweight characteristic which do not require support that simplifies the overall reactor structural design.

Table 1 Specification Sheet of Packed Bed Reactor R-301.

REACTOR					
Item	:	Fixed bed reactor		Date	: 4th February 2022
Item Code	:	R-301		By	: How Mun Cheng
No. of unit	:	1			
General					
Function	:	Transalkylation of diethylbenzene with benzene to produce ethylbenzene with the presence of zeolite catalyst.			
Operation	:	Continuous			
Type	:	Catalytic, fixed bed reactor with cooling jacket (Isothermal)			
Orientation	:	Vertical			
Reaction Bed					
COMPONENT		INLET (kg/hr)		OUTLET (kg/hr)	
Benzene		2877.2621		2158.3062	
Ethylene		0.2582		0.2582	
Ethylbenzene		6.9564		1961.1690	
Diethylbenzene		1235.8747		0.6179	
Methane		0.0000		0.0000	
Ethane		0.0000		0.0000	
Heating Jacket (Heating Medium: High Pressure Steam)					
Heat duty:	MJ/hr	533.38	Design pressure	bar	4.40
Mass flow rate:	ton/hr	0.37	Design temperature	K	533.45
Total heat transfer area	m ²	8.33	Corrosion allowance	mm	2
Jacket thickness:	mm	0.000606	Inner diameter	m	1.44
Heating jacket length:	m	5.09	MAWP	bar	22.51
Reactor Construction Data					
Material of Construction:		Stainless steel type 304		Catalyst density: kg/m ³ 720.00	
Functional height:	m	6.36	Catalyst support:	Support grid	
Diameter (internal):	m	1.38	Mass of catalyst:	kg	2897.944
Diameter (external):	m	1.44	Bed volume:	m ³	7.74
Catalyst:	Zeolite		Bed Void fraction:	0.48	
Catalyst diameter:	m	0.005			
Mechanical Design					
Design Pressure:	bar	38.50	Design Temperature:	K	512.69
Type of head:	Hemispherical head		Type of support:	Conical skirt	
Vessel wall thickness:	mm	31.05	Skirt thickness:	mm	31.05
Head thickness:	mm	18.63	MAWP (Reactor/Head):	bar	190.50 127.50
Nozzle size (B/E/Effluent):	in	2/0.125/2	Nozzle size steam (In/Out)	inch	12/12
Bolt:	M24		Number of bolts:	8	
Base ring width:	mm	157.05	Min. Base ring thickness:	mm	7.34
ASPEN Simulation					
Heat duty:	MJ/hr		147.78		

* The detailed design calculation steps are shown in Appendix.

Comparison of Manual Calculation with ASPEN Plus simulation

The heat duty obtained from ASPEN simulation is 147.78 MJ/hr which is higher than the cooling duty that is obtained from manual energy balance calculation (533.38 MJ/hr). The large difference from ASPEN result Besides, might be due to the different correlation used in determining the thermodynamic data of the components for instance

specific heat capacity, specific molar volume, heat of vaporization and others. In energy balance calculation, the component properties are taken from various sources of handbooks in which the data are mostly taken at 1 atm but not at the reactor operating pressure of 35 bar. Acceptable assumption is made for ease calculation in which the properties do not alter significantly with pressure whilst the calculation from ASPEN able to predict the properties more accurately at the specified temperature and pressure. On the other hand, the product molar flow rates of each component are compared between manual calculation and ASPEN simulation in which for manual calculation, the generation and consumption of each component is calculated based on the selectivity and conversion data extracted from literature while ASPEN simulates the reaction based on reaction kinetics. Since RStoic was only used in ASPEN, the conversion and selectivity are same, which result in similar molar flow and mass flow.



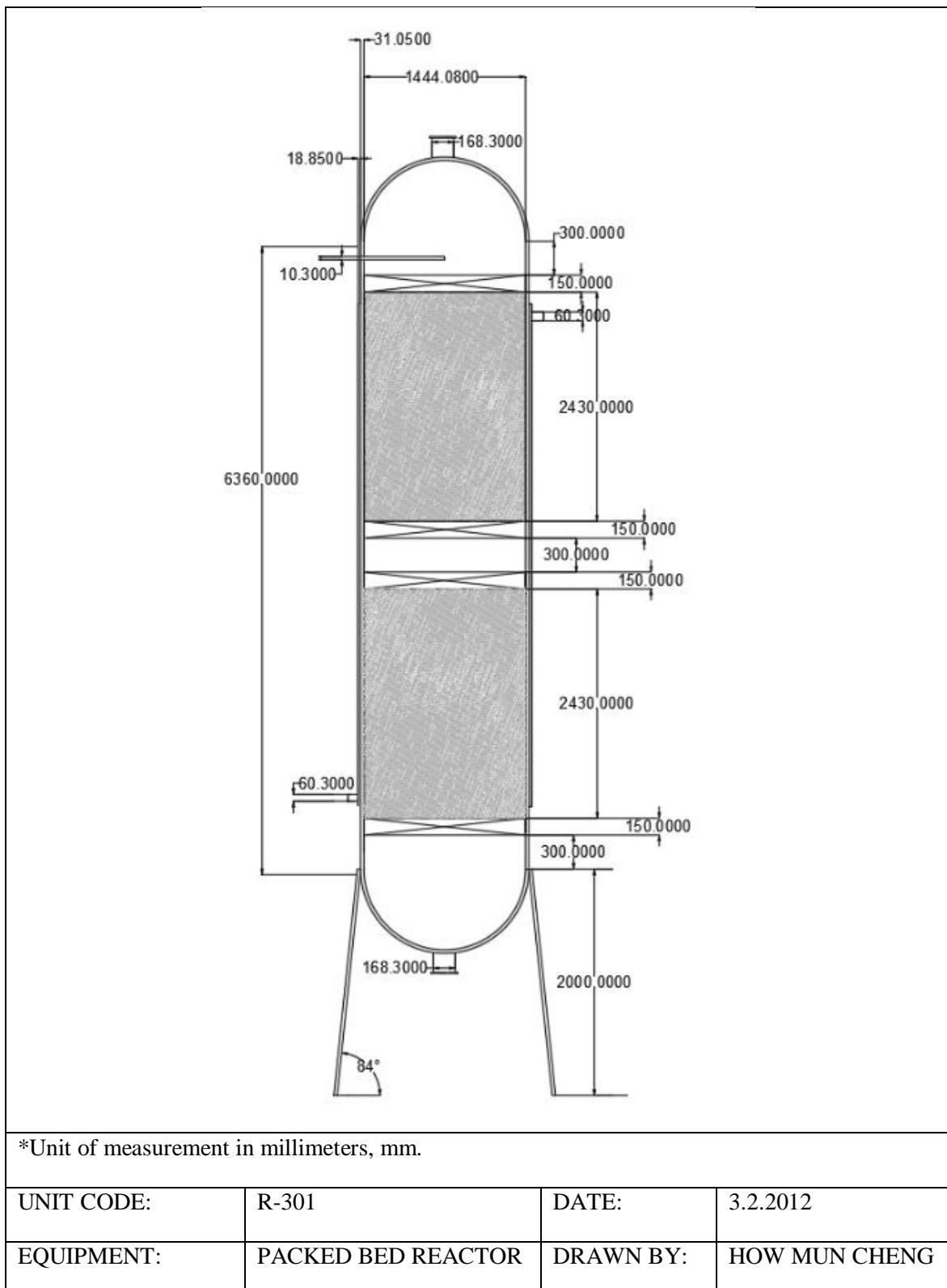


Figure 11 2AUTOCAD engineering drawing of packed-bed reactor, R-301.

CHAPTER 12 AUXILARY

12.1 PUMP P-101

Design Basis

Stream	S-1 (Input)	S-2 (Output)
Molar Flowrate (kmol/hr)	115.2269	115.2269
Mass Flowrate (kg/s)	2.5004	2.5004

Design Parameters

Pump Design	
Operating temperature	
Operating pressure	
Friction loss	
Net positive suction head, NPSH	
Nozzle size	
Motor power	

Design Criteria

Type of pump: Positive Displacement Piston Pump

Operating Temperature (°C)	25.00
Operating Pressure – Inlet (bar)	1.0
Operating Pressure – Outlet (bar)	40.0

Design Method

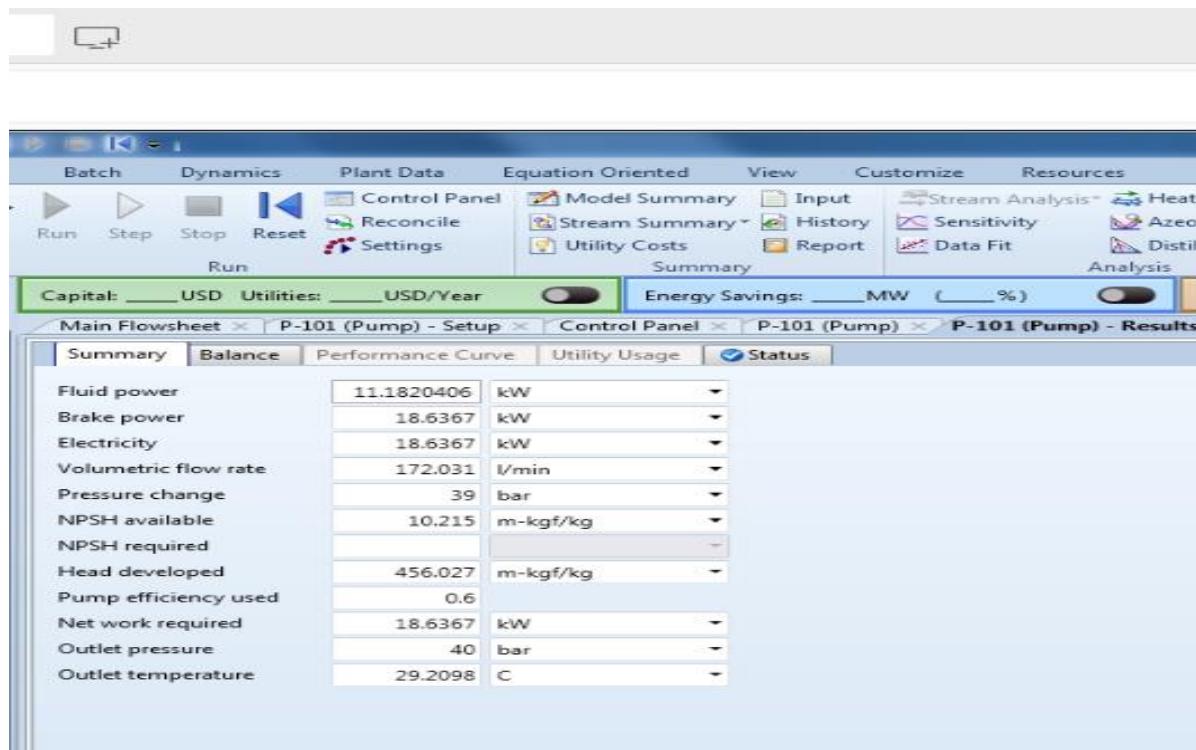
The pump designed is calculated by using Coulson and Richardson's Chemical Engineering Design. Hence, the pump design is based on Bernoulli's Equation which is:

$$\frac{P_1}{\rho g} + z_1 + \frac{v_1^2}{2g} + h_p = \frac{P_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_f$$

*The detailed calculation can refer in Appendix H.

Table 12.1 Specification Data Sheet for Mixture Feed Pump (P-101)

P-101		
Identification:	Item: Pump	Date: 18-1-2022
	Item No: P-101	By: NG KAH HOE
	No. Required: 2	
Function:	Used to pump fluid	
Operation:	Continuous	
Type:	Positive Displacement Piston Pump	
Construction Material:	Stainless Steels Type 316 (L)	
FLOW STREAM CONDITION		
Stream	INLET	OUTLET
Temperature (°C)	25	25
Pressure (bar)	1	40
COMPONENTS		Mass Flow Rate (kg/s)
Benzene	2.5004	2.5004
Ethylene	0.00	0.00
Ethylbenzene	0.00	0.00
Diethylbenzene	0.00	0.00
Methane	0.00	0.00
Ethane	0.00	0.00
GENERAL DESIGN DATA		
Pipe diameter:	2.5	inch
Total Pump Head:	461.9338	m
NPSHA:	8.9694	m
Pump Efficiency:	60	%
Power required:	11.2478	kW
Motor Power:	18.7464	kW



The specifications for pump, P-101 obtained from both Aspen simulation and manual calculation are relatively similar with insignificant difference. Through aspen calculation, the work required for the pump to generate a pressure up to 39 bar is 18.6367 kW with a total head of approximately 456.027m for a defined pump efficiency of 60%. On the other hand, through manual calculation, the work required is 18.7464 kW with a total head of 461.9338m under the same pump efficiency. By analysing this, we can conclude that the power calculated for the P-101 is considered accurate with little deviation.

12.2 PUMP (P-201)

Design Basis

Stream	S-24 (Input)	S-25 (Output)
Molar Flowrate (kmol/hr)	267.1952	267.1952
Mass Flowrate (kg/s)	5.7977	5.7977

Design Parameters

Pump Design
Operating temperature
Operating pressure
Friction loss
Net positive suction head, NPSH
Nozzle size
Motor power

Design Criteria

Type of pump: Positive Displacement Screw Pump

Operating Temperature (°C)	77.1381
Operating Pressure – Inlet (bar)	1.0
Operating Pressure – Outlet (bar)	40.0

Design Method

The pump designed is calculated by using Coulson and Richardson's Chemical Engineering Design. Hence, the pump design is based on Bernoulli's Equation which is:

$$\frac{P_1}{\rho g} + z_1 + \frac{v_1^2}{2g} + h_p = \frac{P_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_f$$

Table 12.2 Specification Data Sheet for Mixture Feed Pump (P-201)

P-201			
Identification:	Item: Pump	Date: 18-1-2022	
	Item No: P-201	By: NG KAH HOE	
	No. Required: 2		
Function:	Used to pump fluid		
Operation:	Continuous		
Type:	Positive Displacement Screw Pump		
Construction Material:	Stainless Steels Type 316 (L)		
FLOW STREAM CONDITION			
Stream	INLET	OUTLET	
Temperature (°C)	77.1381	77.1381	
Pressure (bar)	1	40	
COMPONENTS			
Mass Flow Rate (kg/s)			
Benzene	5.7954	5.7954	
Ethylene	0.0005	0.0005	
Ethylbenzene	0.0017	0.0017	
Diethylbenzene	0.00	0.00	
Methane	0.00	0.00	
Ethane	0.00	0.00	
GENERAL DESIGN DATA			
Pipe diameter:	3.5	inch	
Total Pump Head:	497.4909	m	
NPSHA:	9.0218	m	
Pump Efficiency:	60	%	
Power required:	28.2948	kW	
Motor Power:	47.1580	kW	

	Main Flowsheet	P-101 (Pump) - Setup	Control Panel	Results Summary	P-101 (Pump) - Res
	Summary	Balance	Performance Curve	Utility Usage	Status
Fluid power	27.6538521	kW			
Brake power	46.0898	kW			
Electricity	46.0898	kW			
Volumetric flow rate	425.444	l/min			
Pressure change	39	bar			
NPSH available	0.467711	m-kgf/kg			
NPSH required					
Head developed	486.384	m-kgf/kg			
Pump efficiency used	0.6				
Net work required	46.0898	kW			
Outlet pressure	40	bar			
Outlet temperature	81.0625	C			

This is same as the specifications for pump, P-201 obtained from both Aspen simulation and manual calculation are relatively similar with insignificant difference. Through aspen calculation, the work required for the pump to generate a pressure up to 39 bar is 46.0898 kW with a total head of approximately 486.384m for a defined pump efficiency of 60%. On the other hand, through manual calculation, the work required is 47.1580 kW with a total head of 497.4909 m under the same pump efficiency. By analysing this, we can conclude that the power calculated for the P-201 is considered accurate with little deviation.

12.3 PUMP (P-401)

Design Basis

Stream	S-28 (Input)	S-29 (Output)
Molar Flowrate (kmol/hr)	267.1952	267.1952
Mass Flowrate (kg/s)	5.7977	5.7977

Design Parameters

Pump Design
Operating temperature
Operating pressure
Friction loss
Net positive suction head, NPSH
Nozzle size
Motor power

Design Criteria

Type of pump: Centrifugal pump

Operating Temperature (°C)	77.1381
Operating Pressure – Inlet (bar)	1.0
Operating Pressure – Outlet (bar)	40.0

Design Method

The pump designed is calculated by using Coulson and Richardson's Chemical Engineering Design. Hence, the pump design is based on Bernoulli's Equation which is:

$$\frac{P_1}{\rho g} + z_1 + \frac{v_1^2}{2g} + h_p = \frac{P_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_f$$

Table 12.3 Specification Data Sheet for Mixture Feed Pump (P-401)

P-201			
Identification:	Item: Pump	Date: 18-1-2022	
	Item No: P-401	By: NG KAH HOE	
	No. Required: 2		
Function:	Used to pump fluid		
Operation:	Continuous		
Type:	Centrifugal Pump		
Construction Material:	Stainless Steels Type 316 (L)		
FLOW STREAM CONDITION			
Stream	INLET	OUTLET	
Temperature (°C)	229.5292	229.5292	
Pressure (bar)	2.8	35	
COMPONENTS	Mass Flow Rate (kg/s)		
Benzene	5.7954	5.7954	
Ethylene	0.0005	0.0005	

Ethylbenzene	0.0017	0.0017
Diethylbenzene	0.00	0.00
Methane	0.00	0.00
Ethane	0.00	0.00
GENERAL DESIGN DATA		
Pipe diameter:	1	inch
Total Pump Head:	382.0101	m
NPSHA:	4.8909	m
Pump Efficiency:	60	%
Power required:	1.2929	kW
Motor Power:	2.1548	kW

	Summary	Balance	Performance Curve	Utility Usage	S
Fluid power	1.54061295	kW			
Brake power	2.56769	kW			
Electricity	2.56769	kW			
Volumetric flow rate	30.8123	l/min			
Pressure change	30	bar			
NPSH available	33.1386	m-kgf/kg			
NPSH required					
Head developed	455.359	m-kgf/kg			
Pump efficiency used	0.6				
Net work required	2.56769	kW			
Outlet pressure	35	bar			
Outlet temperature	232.204	C			

However, the specifications for pump, P-401 obtained from both Aspen simulation and manual calculation have a remarkable difference. Through aspen calculation, the work required for the pump to generate a pressure up to 30 bar is 2.56769 kW with a total head of approximately 455.359m for a defined pump efficiency of 60%. On the other hand, through manual calculation, the work required is 2.1548 kW with a total head of 382.0101m under the same pump efficiency. By analysing this, we can make hypothesis that there might be vapor phase existed when entering or passing by the pump, so this will significantly affect the calculation and even the result obtained through the calculation.

12.4 C-101, Compressor

Design Basis and Criteria

Ethylene feed consisting trace amount of methane and ethane inert, which is one of the raw materials for ethylbenzene production is compressed from its storage tank at 40 bar to 50 bar using a compressor. The molar flow rate of the compressor inlet is 115.196 kmol/hr consisting of 0.9990 of ethylene, 0.0003 of ethylbenzene, 0.0002 of methane and 0.0006 of ethane. The inlet process stream temperature to the compressor is 25 °C whilst the outlet temperature after compression is to be determined.

Design Parameters

The design parameters for the compressor are number of compression stages, motor efficiency and power requirement and compressor outlet temperature.

Design Method

The compressor design is based on Coulson and Richardson's Chemical Engineering Design while the properties of the process stream are evaluated at the average value based on the mole fraction of each component as the process stream is a mixture. Besides, the ratio of specific heats, is calculated at the average inlet and outlet temperature of the process stream for a more accurate calculation as the outlet temperature will increase significantly after compression in which the outlet temperature is approximated by isentropic compression relation.

Material of Construction & Type of Compressor

The type of compressor used is centrifugal compressor as the application is a high-pressure lift whereby the feed is compressed from 40 bar to 50 bar and hence, centrifugal compressor which is made up of one or more stages is more suitable for the application. The material of construction for the compressor is carbon steel. This is because it is cheaper than stainless steel and has a good corrosion resistance for water. The use of a carbon steel is adequate for the operating conditions of the compressor.

Table 12.4 Specification Sheet of Compressor C-101.

Compressor		
Identification:	Item: Compressor Item No: C-101 No. Required: 1	Date: 22nd January 2022 By: How Mun Cheng
Function:	To increase pressure of the ethylene feed stream (S-3) from 40 bar to 50 bar.	
Operation:	Continuous	
Type:	Centrifugal compressor	
FLOW STREAM CONDITION		
COMPONENTS	INLET (kg/hr)	OUTLET (kg/hr)
Benzene	0	0
Ethylene	3228.4964	3228.4964
Ethylbenzene	0.8435	0.8435
Diethylbenzene	0	0
Methane	0.4987	0.4987
Ethane	1.8352	1.8352
GENERAL DESIGN DATA		
Inlet Pressure (bar) :	40	Outlet Pressure (bar) : 50
Inlet Temperature (°C) :	25	Outlet Temperature (°C) : 26.12
Number of stages:	1 stage	Power required (kW) : 15.498
Compressor efficiency (%) :	85	
ASPEN Simulation		
Power required (kW) :	27.91742	

Comparison of Manual Calculation with ASPEN Plus Simulation

ASPEN is run with the operating conditions from manual calculation. As shown from Table 54, the power required for the compressor simulated using ASPEN Plus is higher than of manual calculation. Besides, the stream outlet temperature simulated from ASPEN is also higher than that from manual calculation. These differences in value might be due to the different approach in evaluating the thermodynamic properties such as the specific heat capacity values and the compressibility factor of the non-ideal gases. In manual calculation, these properties were obtained from handbooks or correlation diagram whereas in ASPEN Plus, all the thermodynamic properties are evaluated under chosen model.

Table 12.5 Compressor design parameters obtained through manual calculation and ASPEN Plus.

	Manual Calculation	Aspen Simulation	Difference
Power Required (kW)	15.49795752	27.9174222	12.42
Stream Outlet Temperature (°C)	25	44.8559565	19.86

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APPENDIX A: MATERIAL SAFETY DATA SHEET (MSDS) BENZENE

A.1 BENZENE

MSDS of benzene [63].

Product identifier	
Chemical Name	Benzene
CAS-No.	71-43-2
Formula	C ₆ H ₆
Other names	benzene, purebenzol; cyclohexatriene; phenyl hydride; phene; coal naphtha; pyrobenzol
Product type	Liquid
Use of the substance/mixture	Synthetic/Analytical chemistry.
Hazard identification	
OSHA/HCS status	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Classification of the substance or mixture	
FLAMMABLE LIQUIDS	Category 2
SKIN IRRITATION	Category 2
EYE IRRITATION	Category 2A
GERM CELL MUTAGENICITY	Category 1
CARCINOGENICITY	Category 1
SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE)	Category 1
GHS-US Label elements	
Hazard pictograms (GHS-US)	  
Signal word (GHS-US)	Danger
Hazard statements	<p>Highly flammable liquid and vapor. Causes skin irritation. Causes serious eye irritation. May cause genetic defects. May cause cancer. May form explosive mixtures with air.</p>
Precautionary statements	
General	Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand.
Prevention	Obtain special instructions before use. Wear protective gloves. Wear protective clothing. Wear eye or face protection. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use explosion-proof electrical, ventilating or lighting

	equipment. Use non-sparking tools. Take action to prevent static discharges. Keep container tightly closed. Do not breathe vapor. Do not eat, drink or smoke when using this product. Wash thoroughly after handling.
Response	IF exposed or concerned: Get medical advice or attention. Take off contaminated clothing and wash it before reuse. IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice or attention.
Storage	Store locked up. Store in a well-ventilated place. Keep cool.
Disposal	Dispose of contents and container in accordance with all local, regional, national, and international regulations.

First aid measures

Description	
Eye contact	Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention.
Inhalation	Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
Skin contact	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
Ingestion	Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt, or waistband.

Potential acute health effects

Eye contact	Causes serious eye irritation.
Inhalation	No known significant effects or critical hazards.
Skin contact	Causes skin irritation.
Frostbite	Try to warm up the frozen tissues and seek medical attention.
Ingestion	No known significant effects or critical hazards.

Over-exposure signs/symptoms

Eye contact	Adverse symptoms may include the following: pain or irritation, watering, redness
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Inhalation	No specific data.
Skin contact	Adverse symptoms may include the following: irritation, redness
Ingestion	No specific data.
Indication of immediate medical attention and special treatment needed, if necessary	
Notes to physician	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
Specific treatments	No specific treatment.
Protection of first aiders	No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.
Fire-fighting measures	
Suitable extinguishing media	Use dry chemical, CO ₂ , water spray (fog) or foam.
Unsuitable extinguishing media	Do not use water jet.
Special hazards arising from the substance or mixture	Highly flammable liquid and vapor. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back.
Hazardous thermal decomposition products	Decomposition products may include the following materials: carbon dioxide carbon monoxide
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. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
Special protective equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
Accidental release measures	
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 unnecessary and unprotected personnel from entering. Do not touch or walk-through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
For emergency responders	If specialized clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For nonemergency personnel".
Environmental precautions	Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the

	product has caused environmental pollution (sewers, waterways, soil, or air).
Methods and materials for containment and cleaning up	
Small spill	Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.
Large spill	Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Approach release from upwind. Prevent entry into sewers, water courses, basements, or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g., sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see Section 13). Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see Section 1 for emergency contact information and Section 13 for waste disposal.
Handling and storage	
Precautions for safe handling	
Protective measures	Put on appropriate personal protective equipment. Do not get in eyes or on skin or clothing. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Do not ingest. Empty containers retain product residue and can be hazardous. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Do not reuse container. Store and use away from heat, sparks, open flame, or any other ignition source. Use explosion-proof electrical (ventilating, lighting, and material handling) equipment. Do not breathe vapor or mist. Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood.
Advice on general occupational hygiene	Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.
Safe storage conditions	Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Store locked up. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate

	containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.
Exposure controls/personal protection	
Control parameters	
Exposure limits	<p>ACGIH TLV (United States, 3/2019).</p> <p>Absorbed through skin.</p> <p>STEL: 8 mg/m³ 15 minutes.</p> <p>STEL: 2.5 ppm 15 minutes.</p> <p>TWA: 1.6 mg/m³ 8 hours.</p> <p>TWA: 0.5 ppm 8 hours.</p> <p>NIOSH REL (United States, 10/2016).</p> <p>STEL: 1 ppm 15 minutes.</p> <p>TWA: 0.1 ppm 10 hours.</p> <p>OSHA PEL (United States, 5/2018).</p> <p>STEL: 5 ppm 15 minutes.</p> <p>TWA: 1 ppm 8 hours.</p> <p>OSHA PEL 1989 (United States, 3/1989).</p> <p>STEL: 5 ppm 15 minutes.</p> <p>TWA: 1 ppm 8 hours.</p> <p>OSHA PEL Z2 (United States, 2/2013).</p> <p>AMP: 50 ppm 10 minutes.</p> <p>CEIL: 25 ppm</p> <p>TWA: 10 ppm 8 hours.</p>
Exposure controls	
Appropriate engineering controls	Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
Environmental exposure controls	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.
Individual protection measures	
Hygiene measures	Wash hands, forearms, and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.
Eye/face protection	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.
Skin protection	

Hand protection	Chemical-resistant, impervious gloves complying with an approved standard should be always worn when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.
Body protection	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear antistatic protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.
Other skin protection	Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory protection	Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use.
Stability and reactivity	
Reactivity	No specific test data related to reactivity available for this product or its ingredients.
Chemical stability	The product is stable.
Possibility of hazardous reactions	Under normal conditions of storage and use, hazardous reactions will not occur.
Conditions to avoid	Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition. Do not allow vapor to accumulate in low or confined areas.
Incompatible materials	Reactive or incompatible with the following materials: oxidizing materials
Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	Under normal conditions of storage and use, hazardous polymerization will not occur.
Toxicological information	
Acute toxicity	Not classified
Skin corrosion/irritation	Not classified
Serious eye damage/irritation	Not classified
Respiratory or skin sensitization	Not classified

Germ cell mutagenicity	Not classified	
Carcinogenicity	Not classified	
IARC group	1 - Known to be a human carcinogen.	
Reproductive toxicity	Not classified	
Specific target organ toxicity – single exposure	May cause drowsiness or dizziness.	
Specific target organ toxicity – repeated exposure	Category 1	
Aspiration hazard	Not classified	
Information on the likely routes of exposure	Not available.	
Potential acute health effects		
Eye contact	Causes serious eye irritation	
Inhalation	No known significant effects or critical hazards.	
Skin contact	Causes skin irritation.	
Ingestion	No known significant effects or critical hazards.	
Symptoms related to the physical, chemical, and toxicological characteristics		
Eye contact	Adverse symptoms may include the following:, pain or irritation, watering, redness	
Inhalation	No specific data.	
Skin contact	Adverse symptoms may include the following:, irritation, redness	
Ingestion	No specific data.	
Potential chronic health effects		
General	Causes damage to organs through prolonged or repeated exposure.	
Carcinogenicity	May cause cancer. Risk of cancer depends on duration and level of exposure.	
Mutagenicity	May cause genetic defects.	
Teratogenicity	No known significant effects or critical hazards.	
Developmental effects	No known significant effects or critical hazards.	
Fertility effects	No known significant effects or critical hazards.	
Ecological information		
Result	Species	Exposure
Acute EC50 29000 µg/l Fresh water	Algae - Pseudokirchneriella subcapitata	72 hours
Acute EC50 1600000 µg/l Fresh water	Algae - Selenastrum sp.	96 hours
Acute EC50 9.23 mg/l Fresh water	Daphnia - Daphnia magna - Neonate	48 hours
Acute LC50 21 mg/l Marine water	Crustaceans - Artemia salina	48 hours
Acute LC50 5.28 µL/L Fresh water	Fish - Oncorhynchus gorbuscha - Fry	96 hours

Chronic EC10 >1360 mg/l Fresh water	Algae – Scenedesmus subspicatus	96 hours												
Chronic NOEC 98 mg/l Fresh water	Daphnia - Daphnia magna	21 days												
Chronic NOEC 1.5 to 5.4 ul/L Marine water	Fish - Morone saxatilis - Juvenile (Fledgling, Hatchling, Weanling)	4 weeks												
Bioaccumulative potential														
Potential	Low													
Disposal considerations														
Product/Packaging disposal recommendations	<p>The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapor from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.</p>													
Hazard Rating														
NFPA		 <table style="margin-left: auto; margin-right: auto;"> <tr> <td>Health</td> <td>3</td> <td>Flammability</td> </tr> <tr> <td></td> <td>2</td> <td>Instability/Reactivity</td> </tr> <tr> <td></td> <td>0</td> <td></td> </tr> <tr> <td></td> <td></td> <td>Special</td> </tr> </table>	Health	3	Flammability		2	Instability/Reactivity		0				Special
Health	3	Flammability												
	2	Instability/Reactivity												
	0													
		Special												

A.2 ETHYLENE

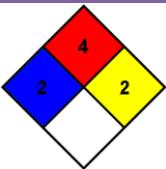
MSDS of ethylene [64].

Product identifier	
Chemical Name	Ethylene
CAS-No.	74-85-1
Formula	C ₂ H ₄
Other names	Ethene, Acetene, Olefiant Gas, refrigerant gas R1150
Use of the substance/mixture	Industrial use; Use as directed.
Hazard identification	
GHS-US Classification of the substance or mixture	
Flam. Gas 1	H220
Press. Gas (Liq.)	H280
STOT SE 3	H336
GHS-US Label elements	
Hazard pictograms (GHS-US)	  
Signal word (GHS-US)	Danger
Hazard statements (GHS-US)	H220 - Extremely flammable gas H280 - Contains gas under pressure; may explode if heated H336 - May cause drowsiness or dizziness OSHA-H01 - May displace oxygen and cause rapid suffocation. CGA-HG04 - May form explosive mixtures with air CGA-HG01 - May cause frostbite.
Precautionary statements (GHS-US)	P202 - Do not handle until all safety precautions have been read and understood. P210 - Keep away from Heat, Open flames, Sparks, Hot surfaces. - No smoking P261 - Avoid breathing gas P262 - Do not get in eyes, on skin, or on clothing. P271+P403 - Use and store only outdoors or in a well-ventilated place. P377 - Leaking gas fire: Do not extinguish unless leak can be stopped safely. P381 - Eliminate all ignition sources if safe to do so. CGA-PG05 - Use a back flow preventive device in the piping. CGA-PG06 - Close valve after each use and when empty. CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles. CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).
Other hazards	

Other hazards not contributing to the classification	Contact with liquid may cause cold burns/frostbite.
First aid measures	
First-aid measures after inhalation	Remove to fresh air and keep at rest in a position comfortable for breathing. If not breathing, give artificial respiration. If breathing is difficult, trained personnel should give oxygen. Call a physician.
First-aid measures after skin contact	The liquid may cause frostbite. For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible
First-aid measures after eye contact	Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.
First-aid measures after ingestion	Ingestion is not considered a potential route of exposure.
Firefighting measures	
Suitable extinguishing media	Carbon dioxide, Dry chemical, Water spray or fog
Special hazards arising from the substance or mixture	
Fire hazard	Extremely Flammable Gas. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device
Explosion hazard	Extremely Flammable Gas. Forms explosive mixtures with air and oxidizing agents
Reactivity	No reactivity hazard other than the effects described in sub-sections below
Firefighting instructions	Danger: Flammable liquid and vapor. Evacuate all personnel from danger area. Use self-contained breathing apparatus. Immediately cool surrounding containers with water spray from maximum distance, taking care not to extinguish flames. Avoid spreading burning liquid with water. Remove ignition sources if safe to do so. If flames are accidentally extinguished, explosive reignition may occur. Reduce vapors with water spray or fog. Stop flow of liquid if safe to do so, while continuing cooling water spray. Remove all containers from area of fire if safe to do so. Allow fire to burn out. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1919 Subpart L - Fire Protection.
Accidental release measures	

General measures	Danger: Flammable, liquefied gas. Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.
Handling and storage	
Precautions for safe handling	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment. Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g, wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.
Storage conditions	<p>Store only where temperature will not exceed 125°F (52°C). Post “No Smoking/No Open Flames” signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g, NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.</p> <p>Other Precautions for Handling, Storage, And Use: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national,</p>

	state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.			
Exposure controls/personal protection				
Control paremeters				
ACGIH	ACGIH TLV-TWA (ppm)	200 ppm		
ACGIH	Remark (ACGIH)	Asphyxia		
Exposure controls				
Appropriate engineering controls	Use an explosion-proof local exhaust system. Local exhaust and general ventilation must be adequate to meet exposure standards. Mechanical (General): Inadequate - Use only in a closed system. Use explosion proof equipment and lighting			
Eye protection	Wear safety glasses when handling cylinders; vapor-proof goggles and a face shield during cylinder changeout or whenever contact with product is possible. Select eye protection in accordance with OSHA 29 CFR 1910.133.			
Skin and body protection	Wear metatarsal shoes and work gloves for cylinder handling, and protective clothing where needed. Wear appropriate chemical gloves during cylinder changeout or wherever contact with product is possible. Select per OSHA 29 CFR 1910.132, 1910.136, and 1910.138.			
Respiratory protection	When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure. For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA). Self-contained breathing apparatus (SCBA) or positive pressure airline with mask are to be used in oxygen-deficient atmospheres.			
Thermal hazard protection	Wear cold insulating gloves when transfilling or breaking transfer connections			
Stability and reactivity				
Reactivity	No reactivity hazard other than the effects described in sub-sections below			
Chemical stability	Stable under normal conditions.			
Possibility of hazardous reactions	May occur			
Conditions to avoid	May decompose violently at high temperature and/or pressure or in the presence of a catalyst.			
Incompatible materials	Oxidizing agents. Halogens. Halogenated compounds. Chlorine. Acids. Aluminum chloride.			
Hazardous decomposition products	Thermal decomposition may produce: Carbon dioxide. Carbon monoxide.			
Toxicological information				
Acute toxicity	Not classified			

Skin corrosion/irritation	Not classified
Serious eye damage/irritation	Not classified
Respiratory or skin sensitization	Not classified
Germ cell mutagenicity	Not classified
Carcinogenicity	Not classified
IARC group	3 - Not classifiable
Reproductive toxicity	Not classified
Specific target organ toxicity – single exposure	May cause drowsiness or dizziness.
Specific target organ toxicity – repeated exposure	Not classified
Aspiration hazard	Not classified
Ecological information	
Ecological information	No known ecological damage caused by this product.
Persistence and degradability	The substance is biodegradable. Unlikely to persist
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.
Mobility in soil	No data available
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution
Effect on ozone layer	None.
Effect on the global warming	No known effects from this product
Disposal considerations	
Product/Packaging disposal recommendations	Do not attempt to dispose of residual or unused quantities. Return container to supplier
Hazard Rating	
NFPA	
NFPA health hazard	2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury
NFPA fire hazard	4 - Materials that rapidly or completely vaporize at atmospheric pressure and normal ambient temperature or that are readily dispersed in air and burn readily.

NFPA fire hazard	2 - Materials that readily undergo violent chemical change at elevated temperatures and pressures.
Health	1 Slight Hazard - Irritation or minor reversible injury possible
Flammability	4 Severe Hazard
Physical	3 Serious Hazard

A3 ETHYLBENZENE

MSDS of ethylbenzene [65].

Product identifier	
Chemical Name	Ethylbenzene
CAS-No.	71-43-2
Formula	C ₈ H ₁₀
Use of the substance/mixture	Laboratory chemical Laboratory and analytical use
Hazard identification	
Classification of the substance or mixture	
FLAMMABLE LIQUIDS	Category 3
ACUTE TOXICITY (INHAL.)	Category 4
ASPIRATION HAZARD	Category 1
SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE)	Category 2
GHS-US Label elements	
Hazard pictograms (GHS-US)	  
Signal word (GHS-US)	Danger
Hazard statements	Highly flammable liquid and vapor. May be fatal if swallowed and enters airways Harmful if inhaled May cause damage to organs through prolonged or repeated exposure
Precautionary statements	
Prevention	<ul style="list-style-type: none"> Keep away from heat/sparks/open flames/hot surfaces. - No smoking Do not breathe dust/fume/gas/mist/vapours/spray
Response	<ul style="list-style-type: none"> If swallowed: Immediately call a Poison Center or doctor/physician In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction Do not induce vomiting
Storage	Store in a well-ventilated place. Keep cool
First aid measures	
Description	
Eye contact	Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.
Inhalation	Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Skin contact	Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.
Ingestion	Call a physician immediately. Observe aspiration hazard if vomiting occurs.
Most important symptoms and effects, both acute and delayed	Irritant effects, Vertigo, Headache, Dizziness, Spasms, Nausea, Vomiting, Aspiration hazard
Fire-fighting measures	
Suitable extinguishing media	co-ordinate firefighting measures to the fire surroundings water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO ₂)
Unsuitable extinguishing media	Do not use water jet.
Special hazards arising from the substance or mixture	Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g., unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.
Hazardous combustion products	In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO ₂)
Advice for fire-fighters	In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.
Accidental release measures	
Personal precautions, protective equipment, and emergency procedures	
For non-emergency personnel	Use personal protective equipment as required. Avoid contact with skin, eyes, and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.
Environmental precautions	Keep away from drains, surface, and ground water. Danger of explosion.
Methods and materials for containment and cleaning up	
Advice on how to contain a spill	Covering of drains.
Advice on how to clean up a spill	Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).
Other information relating to spills and releases	Place in appropriate containers for disposal. Ventilate affected area.
Handling and storage	
Precautions for safe handling	Provision of sufficient ventilation.
Measures to prevent fire as well as aerosol and dust generation	Keep away from sources of ignition - No smoking. Take precautionary measures against static discharge.
Advice on general occupational hygiene	Wash hands before breaks and after work. Keep away from food, drink and animal feeding stuffs. When using do not smoke.
Safe storage conditions	Keep container tightly closed.

Incompatible substances or mixtures	Observe hints for combined storage.		
Consideration of other advice:	Ground/bond container and receiving equipment.		
Ventilation requirements	Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation.		
Specific designs for storage rooms or vessels	Recommended storage temperature: 15 – 25 °C		
Exposure controls/personal protection			
Control parameters			
Exposure limits	<ul style="list-style-type: none"> • TWA [ppm] – 100 • TWA [mg/m³] – 434 • STEL [ppm] – 125 • STEL [mg/m³] – 543 		
Relevant DNELs threshold levels to human health values			
Route of exposure	Threshold level	Exposure time	
human, inhalatory	77 mg/m ³	chronic - systemic effects	
human, inhalatory	293 mg/m ³	acute - local effects	
human, dermal	180 mg/kg bw/day	chronic - systemic effects	
Relevant DNELs threshold levels to aquatic organism			
Organism	Environmental compartment	Threshold level	Exposure time
aquatic organisms	freshwater	0.1 mg/l	short-term (single instance)
aquatic organisms	marine water	0.01 mg/l	short-term (single instance)
aquatic organisms	sewage treatment plant (STP)	9.6 mg/l	short-term (single instance)
aquatic organisms	freshwater sediment	13.7 mg/kg	short-term (single instance)
aquatic organisms	Marine sediment	1.37 mg/kg	short-term (single instance)
terrestrial organisms	soil	2.68 mg/kg	short-term (single instance)
Individual exposure controls (personal protective equipment)			
Eye/face protection	Use safety goggles with side protection.		
Skin protection	<p>• hand protection</p> <p>For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable</p>		

	<p>reduction of the breakthrough time. If in doubt, contact manufacturer.</p> <p>At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.</p> <ul style="list-style-type: none"> • type of material FKM: fluoro-elastomer • material thickness 0,4 mm • breakthrough times of the glove material >480 minutes (permeation: level 6) • Splash protection - Protective gloves <ul style="list-style-type: none"> • type of material: NBR (Nitrile rubber) • material thickness: 0,4 mm • breakthrough times of the glove material: >10 minutes (permeation: level 1) • other protection measures Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.
Respiratory protection	Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C, colour code: Brown).
Environmental exposure controls	Keep away from drains, surface, and ground water.
Stability and reactivity	
Reactivity	It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.
If heated	Risk of ignition.
Chemical stability	The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.
Possibility of hazardous reactions	Violent reaction with strong oxidiser
Conditions to avoid	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Incompatible materials	Rubber articles, different plastics
Hazardous decomposition products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Toxicological information	
Acute toxicity	Harmful if inhaled.

Skin corrosion/irritation	Shall not be classified as corrosive/irritant to skin.	
Serious eye damage/irritation	Shall not be classified as seriously damaging to the eye or eye irritant.	
Respiratory or skin sensitization	Shall not be classified as a respiratory or skin sensitisier.	
Germ cell mutagenicity	Shall not be classified as germ cell mutagenic.	
Carcinogenicity	Shall not be classified as carcinogenic.	
Reproductive toxicity	Shall not be classified as a reproductive toxicant.	
Specific target organ toxicity – single exposure	Shall not be classified as a specific target organ toxicant (single exposure).	
Specific target organ toxicity – repeated exposure	May cause damage to organs through prolonged or repeated exposure.	
Aspiration hazard	May be fatal if swallowed and enters airways.	
Symptoms related to the physical, chemical, and toxicological characteristics		
Eye contact	Causes serious eye irritation	
Inhalation	No known significant effects or critical hazards.	
Skin contact	Data are not available.	
Ingestion	No known significant effects or critical hazards.	
Other adverse effects	Headache, Spasms, Nausea, Vertigo, Dizziness	
Ecological information		
Result	Species	Exposure
LC50 5.1 mg/l	Fish	96 hours
EC50 2.4 mg/l	Aquatic invertebrates	48 hours
LC50 3.6 mg/l	Aquatic invertebrates	7 d
Process of degradability		
Theoretical Oxygen Demand	3.167 mg/mg	
Theoretical Carbon Dioxide	3.318 mg/mg	
Bioctic/abiotic	Degradation rate: 79%	Time: 28 d
Bioaccumulative potential		
Potential	Does not significantly accumulate in organisms.	
Disposal considerations		
Waste treatment methods	This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.	
Sewage disposal-relevant information	Do not empty into drains.	
Waste treatment of containers/packagings	Only packagings which are approved (e.g., acc. to the Dangerous Goods Regulations) may be used.	

A.4 1,4-DIETHYLBENZENE

MSDS of 1,4-Diethylbenzene [66].

Product identifier	
Chemical Name	1,4-Diethylbenzene
CAS-No.	105-05-5
Formula	C ₁₀ H ₁₄
Other names	benzene, purebenzol; cyclohexatriene; phenyl hydride; phene; coal naphtha; pyrobenzol
Product type	Liquid
Use of the substance/mixture	Laboratory chemicals
Hazard identification	
OSHA/HCS status	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Classification of the substance or mixture	
FLAMMABLE LIQUIDS	Category 3
SKIN IRRITATION	Category 2
EYE IRRITATION	Category 2
ASPIRATION TOXICITY	Category 1
GHS-US Label elements	
Hazard pictograms (GHS-US)	  
Signal word (GHS-US)	Danger
Hazard statements	Flammable liquid and vapor May be fatal if swallowed and enters airways Causes skin irritation Causes serious eye irritation
Precautionary statements	
General	Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand.
Prevention	Wash face, hands, and any exposed skin thoroughly after handling Wear protective gloves/protective clothing/eye protection/face protection Keep away from heat/sparks/open flames/hot surfaces. - No smoking Keep container tightly closed Ground/bond container and receiving equipment Use explosion-proof electrical/ventilating/lighting/equipment Use only non-sparking tools Take precautionary measures against static discharge
Skin	If skin irritation occurs: Get medical advice/attention

	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower Wash contaminated clothing before reuse
Eyes	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing If eye irritation persists: Get medical advice/attention
Ingestion	If swallowed: Immediately call a Poison Center or doctor/physician Do NOT induce vomiting
Fire	In case of fire: Use CO ₂ , dry chemical, or foam for extinction
Storage	Store locked up Store in a well-ventilated place. Keep cool
Disposal	Dispose of contents/container to an approved waste disposal

First aid measures

Description

General Advice	If symptoms persist, call a physician.
Eye contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).
Skin contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Do not induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
Most important symptoms and effects	None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

Fire-fighting measures

Suitable extinguishing media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Chemical foam. Water mist may be used to cool closed, contain
Unsuitable extinguishing media	No information available
Special hazards arising from the substance or mixture	Combustible material. Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.
Hazardous thermal decomposition products	Carbon monoxide (CO). Carbon dioxide (CO ₂).
Special protective equipment and precautions for fire-fighters	As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

Accidental release measures

Personal Precautions	Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharge
Environmental Precautions	Do not flush into surface water or sanitary sewer system.
Methods for Containment and Clean Up	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment
Handling and storage	
Precautions for safe handling	
Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.
Safe storage conditions	Keep in a dry, cool, and well-ventilated place. Refer product specification and/or product label for specific storage temperature requirement. Keep container tightly closed. Keep away from heat, sparks, and flame. Keep container tightly closed in a dry and well-ventilated place.
Exposure controls/personal protection	
Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limits established by the region-specific regulatory bodies.
Engineering Measures	Measures Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.
Personal Protective Equipment	
Hygiene measures	Handle in accordance with good industrial hygiene and safety practice
Eye/face protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory protection	No protective equipment is needed under normal use conditions.
Stability and reactivity	
Reactivity	None known, based on information available
Chemical stability	Stable under normal conditions
Possibility of hazardous reactions	Under normal conditions of storage and use, hazardous reactions will not occur.
Conditions to avoid	Keep away from open flames, hot surfaces, and sources of ignition. Excess heat. Exposure to light. Incompatible products

Incompatible materials	Strong oxidizing agents	
Hazardous decomposition products	Carbon monoxide (CO), Carbon dioxide (CO2)	
Hazardous polymerization	Hazardous polymerization does not occur.	
Hazardous reactions	None under normal processing	
Toxicological information		
Toxicologically Synergistic Products	Not classified	
Irritation	Irritating to eyes and skin	
Sensitization	Sensitization	
Carcinogenicity	Not classified	
Reproductive Effect	Not classified	
Developmental Effects	Not classified	
Teratogenicity	Not classified	
Specific target organ toxicity – single exposure	None known	
Specific target organ toxicity – repeated exposure	None known	
Aspiration hazard	Category 1	
Symptoms / effects, both acute and delayed	Symptoms of overexposure may be headache, dizziness, tiredness, nausea, and vomiting	
Endocrine Disruptor Information	No information	
Other Adverse Effect	The toxicological properties have not been fully investigated	
Ecological information		
Ecotoxicity	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous	
Result	Species	Exposure
EC50 = 1.9 mg/L Freshwater Algae	Pseudokirchnerella Subcapitata	72 hours
LC50 = 1.8 mg/L Freshwater Fish	Oryzias Latipes	96 hours
EC50 = 250 mg/L Microtox	-	-
LC50 = 32 mg/L Water Flea	Daphnia Magna	24 hours
Persistence and Degradability	May persist based on information available	
Bioaccumulative potential		
Potential	No information available	
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.
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A.5 ETHANE

MSDS of ethane [67].

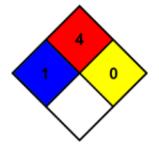
Product identifier	
Chemical Name	Ethane
CAS-No.	74-84-0
Formula	C_2H_6
Use of the substance/mixture	Industrial use; Use as directed.
Hazard identification	
Classification of the substance or mixture	
FLAMMABLE LIQUIDS	H220
SIMPLE ASPHYXIANT	SIAS
PRESS. GAS (LIQ.)	H280
AQUATIC ACUTE 3	H402
GHS-US Label elements	
Hazard pictograms (GHS-US)	  <small>GHS02 GHS04</small>
Signal word (GHS-US)	Danger
Hazard statements	<ul style="list-style-type: none"> • H220 - Extremely flammable gas • H280 - Contains gas under pressure; may explode if heated • OSHA-H01 - May displace oxygen and cause rapid suffocation. • CGA-HG04 - May form explosive mixtures with air • CGA-HG01 - May cause frostbite.
Precautionary statements	<ul style="list-style-type: none"> • P202 - Do not handle until all safety precautions have been read and understood. • P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Heat, Open flames, Sparks, Hot surfaces • P262 - Do not get in eyes, on skin, or on clothing. • P271+P403 - Use and store only outdoors or in a well-ventilated place. • P280 - Wear protective gloves/protective clothing/eye protection/face protection. • P377 - Leaking gas fire: Do not extinguish unless leak can be stopped safely.

	<ul style="list-style-type: none"> • P381 - Eliminate all ignition sources if safe to do so. • P302, P336, P315 - If on skin: Thaw frosted parts with lukewarm water. Do not rub affected area. Get immediate medical advice/attention. • CGA-PG05 - Use a back flow preventive device in the piping. • CGA-PG12 - Do not open valve until connected to equipment prepared for use. • CGA-PG06 - Close valve after each use and when empty. • CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles. • CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).
Other hazards which do not result in classification	Contact with liquid may cause cold burns/frostbite.
First aid measures	
Description	
Eye contact	The liquid may cause frostbite. Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.
Inhalation	Remove victim to uncontaminated area wearing self-contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
Skin contact	The liquid may cause frostbite. For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.
Ingestion	Ingestion is not considered a potential route of exposure.
Fire-fighting measures	
Suitable extinguishing media	Carbon dioxide, Dry chemical, Water spray or fog.
Special hazards arising from the substance or mixture	Highly flammable liquid and vapor. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back.
Hazardous thermal decomposition products	Decomposition products may include the following materials: carbon dioxide carbon monoxide
Special protective actions for fire-fighters	Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-

	site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.
Protection during firefighting	Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.
Special protective equipment for fire-fighters	Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.
Specific methods	<ul style="list-style-type: none"> • Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems. • Stop flow of product if safe to do so. • Use water spray or fog to knock down fire fumes if possible. • Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive reignition may occur. Extinguish any other fire
Other information	Containers are equipped with a pressure relief device. (Exceptions may exist where authorized by DOT.).
Accidental release measures	
Personal precautions, protective equipment, and emergency procedures	
General measures	Danger: Flammable, liquefied gas. FORMS EXPLOSIVE MIXTURES WITH AIR. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.
For non-emergency personnel	No additional information available
For emergency responders	No additional information available
Environmental precautions	Try to stop release. Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.
Methods and materials for containment and cleaning up	No additional information available
Handling and storage	
Precautions for safe handling	
Protective measures	<ul style="list-style-type: none"> • Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

	<ul style="list-style-type: none"> • Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. • All piped systems and associated equipment must be grounded. • Leak-check system with soapy water; never use a flame. • May cause anaesthetic effects. • Avoid breathing gas.
Safe storage conditions	<ul style="list-style-type: none"> • Store only where temperature will not exceed 125°F (52°C). Post “No Smoking/No Open Flames” signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. • OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.
Exposure controls/personal protection	
Control parameters	
ACGIH	Not established
USA OSHA	Not established
Exposure controls	

Appropriate engineering controls	Use an explosion-proof local exhaust system. Local exhaust and general ventilation must be adequate to meet exposure standards. Mechanical (General): Inadequate - Use only in a closed system. Use explosion proof equipment and lighting.
Environmental exposure controls	Refer to local regulations for restriction of emissions to the atmosphere.
Eye protection	Wear safety glasses with side shields. Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections.
Hand protection	Wear working gloves when handling gas containers.
Respiratory protection	When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure. For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA). Self-contained breathing apparatus (SCBA) or positive pressure airline with masks are to be used in oxygen-deficient atmospheres.
Thermal hazard protection	Wear cold insulating gloves when transfilling or breaking transfer connections.
Other information	Consider the use of flame resistant anti-static safety clothing. Wear safety shoes while handling containers.
Stability and reactivity	
Reactivity	No reactivity hazard other than the effects described in sub-sections below.
Chemical stability	Stable under normal conditions.
Possibility of hazardous reactions	May occur.
Conditions to avoid	Keep away from heat/sparks/open flames/hot surfaces. – No smoking.
Incompatible materials	Oxidizing agents. Chlorine dioxide. Chlorine. Chlorine dioxide and ethane explode spontaneously; chlorine and ethane mixtures have been known to explode.
Hazardous decomposition products	At high temperature and low pressure, ethane decomposes to form hydrogen. Thermal decomposition may produce: Carbon dioxide. Carbon monoxide.
Toxicological information	
Acute toxicity	Not classified
Skin corrosion/irritation	Not classified
Serious eye damage/irritation	Not classified
Respiratory or skin sensitization	Not classified
Germ cell mutagenicity	Not classified
Carcinogenicity	Not classified
Reproductive toxicity	Not classified

Specific target organ toxicity – single exposure	Not classified
Specific target organ toxicity – repeated exposure	Not classified
Aspiration hazard	Not classified
Ecological information	
Ecology - general	No ecological damage caused by this product.
Persistence and degradability	The substance is biodegradable. Unlikely to persist.
Bioaccumulative potential	
Partition coefficient n-octanol/water (Log Pow)	1.81
Partition coefficient n-octanol/water (Log Kow)	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4).
Mobility in soil	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.
Disposal considerations	
Product/Packaging disposal recommendations	Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.
Hazard Rating	
NFPA	
NFPA health hazard	1 - Materials that, under emergency conditions, can cause significant irritation.
NFPA fire hazard	4 - Materials that rapidly or completely vaporize at atmospheric pressure and normal ambient temperature or that are readily dispersed in air and burn readily.
NFPA instability	0 - Material that in themselves are normally stable, even under fire conditions.
Health	1 Slight Hazard - Irritation or minor reversible injury possible
Flammability	4 Severe Hazard
Physical	3 Serious Hazard

A.6 METHANE

MSDS of methane [68].

Product identifier	
Chemical Name	Methane
CAS-No.	74-82-8
Formula	C ₂ H ₄
Other names	Methane or natural gas; Marsh gas; Methyl hydride; CH4; Fire Damp
Product type	Gas
Use of the substance/mixture	Synthetic/Analytical chemistry.
Hazard identification	
OSHA/HCS status	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Classification of the substance or mixture	
FLAMMABLE GASES	Category 1
GASES UNDER PRESSURE	Compressed gas
GHS-US Label elements	
Hazard pictograms (GHS-US)	 
Signal word (GHS-US)	Danger
Hazard statements	<ul style="list-style-type: none"> Extremely flammable gas. May form explosive mixtures with air. Contains gas under pressure; may explode if heated. May displace oxygen and cause rapid suffocation.
Precautionary statements	
General	Read and follow all Safety Data Sheets (SDS'S) before use. Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use. Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction. Approach suspected leak area with caution.
Prevention	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Response	Leaking gas fire: Do not extinguish, unless leak can be stopped safely. Eliminate all ignition sources if safe to do so.
Storage	Protect from sunlight. Store in a well-ventilated place.
Disposal	Not applicable.
Hazards not otherwise classified	In addition to any other important health or physical hazards, this product may displace oxygen and cause rapid suffocation.
First aid measures	
Description	

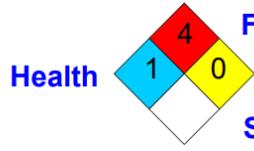
Eye contact	Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.
Inhalation	Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
Skin contact	Wash contaminated skin with soap and water. Remove contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.
Ingestion	As this product is a gas, refer to the inhalation section.
Potential acute health effects	
Eye contact	Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation	No known significant effects or critical hazards
Skin contact	Contact with rapidly expanding gas may cause burns or frostbite
Frostbite	Try to warm up the frozen tissues and seek medical attention.
Ingestion	As this product is a gas, refer to the inhalation section.
Over-exposure signs/symptoms	
Eye contact	No specific data.
Inhalation	No specific data.
Skin contact	No specific data.
Ingestion	No specific data.
Indication of immediate medical attention and special treatment needed, if necessary	
Notes to physician	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
Specific treatments	No specific treatment.
Protection of first aiders	No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
Fire-fighting measures	
Suitable extinguishing media	Use an extinguishing agent suitable for the surrounding fire.
Unsuitable extinguishing media	None known
Special hazards arising from the substance or mixture	Contains gas under pressure. Extremely flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Hazardous thermal decomposition products	Decomposition products may include the following materials: carbon dioxide carbon monoxide
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. No action shall be taken involving any personal risk or without suitable training. Contact supplier immediately for specialist advice. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. If involved in fire, shut off flow immediately if it can be done without risk. If this is impossible, withdraw from area and allow fire to burn. Fight fire from protected location or maximum possible distance. Eliminate all ignition sources if safe to do so
Special equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
Accidental release measures	
Personal precautions, protective equipment, and emergency procedures	
For non-emergency personnel	Accidental releases pose a serious fire or explosion hazard. No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing gas. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
For emergency responders	If specialized clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".
Environmental precautions	Ensure emergency procedures to deal with accidental gas releases are in place to avoid contamination of the environment. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).
Methods and materials for containment and cleaning up	
Small spill	Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment.
Large spill	Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment.
Handling and storage	
Precautions for safe handling	
Protective measures	<ul style="list-style-type: none"> Put on appropriate personal protective equipment (see Section 8). Contains gas under pressure. Avoid breathing gas. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Use only non-sparking tools. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue and can be hazardous. Store and use away from heat, sparks, open flame, or any

	other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment.
Advice on general occupational hygiene	Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking, and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.
Safe storage conditions	Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Eliminate all ignition sources. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). Keep container tightly closed and sealed until ready for use. See Section 10 for incompatible materials before handling or use.
Exposure controls/personal protection	
Control parameters	
Exposure limits	None
Exposure controls	
Appropriate engineering controls	Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Eliminate all ignition sources. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). Keep container tightly closed and sealed until ready for use. See Section 10 for incompatible materials before handling or use.
Environmental exposure controls	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.
Individual protection measures	
Hygiene measures	Wash hands, forearms, and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.
Eye/face protection	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with side-shields.
Skin protection	
Hand protection	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that

	the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.
Body protection	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.
Other skin protection	Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Respiratory protection	Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
Stability and reactivity	
Reactivity	No specific test data related to reactivity available for this product or its ingredients.
Chemical stability	The product is stable.
Possibility of hazardous reactions	Under normal conditions of storage and use, hazardous reactions will not occur.
Conditions to avoid	Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
Incompatible materials	Oxidizers
Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	Under normal conditions of storage and use, hazardous polymerization will not occur.
Toxicological information	
Acute toxicity	Not available
Skin corrosion/irritation	Not available
Serious eye damage/irritation	Not available
Respiratory or skin sensitization	Not available
Germ cell mutagenicity	Not available
Carcinogenicity	Not available
Reproductive toxicity	Not available

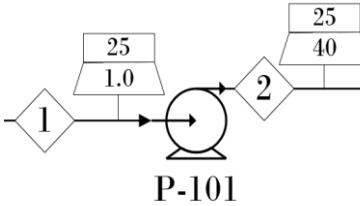
Tetatogenicity	Not available
Specific target organ toxicity – single exposure	Not available
Specific target organ toxicity – repeated exposure	Not available
Aspiration hazard	Not available
Information on the likely routes of exposure	Not available.
Potential acute health effects	
Eye contact	Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation	No known significant effects or critical hazards.
Skin contact	Contact with rapidly expanding gas may cause burns or frostbite.
Ingestion	As this product is a gas, refer to the inhalation section.
Symptoms related to the physical, chemical, and toxicological characteristics	
Eye contact	No specific data.
Inhalation	No specific data.
Skin contact	No specific data.
Ingestion	No specific data.
Potential chronic health effects	
General	No known significant effects or critical hazards.
Carcinogenicity	No known significant effects or critical hazards.
Mutagenicity	No known significant effects or critical hazards.
Teratogenicity	No known significant effects or critical hazards.
Developmental effects	No known significant effects or critical hazards.
Fertility effects	No known significant effects or critical hazards.
Ecological information	
Toxicity	Not available
Persistence and degradability	Not available
Bioaccumulative potential	
Potential	Low
Mobility in soil	Not available
Disposal considerations	
Product/Packaging disposal recommendations	<ul style="list-style-type: none"> The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should always comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Empty Airgas-owned pressure vessels should be returned to Airgas. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and

	its container must be disposed of in a safe way. Empty containers or liners may retain some product residues. Do not puncture or incinerate container.
Hazard Rating	
NFPA	 <p>The diamond hazard rating consists of four colored quadrants. The top-right quadrant is red with the number '4' and the word 'Flammability'. The bottom-right quadrant is yellow with the number '0' and the words 'Instability/Reactivity'. The bottom-left quadrant is white with the number '1' and the word 'Special'. The top-left quadrant is blue with the word 'Health'.</p>

APPENDIX B

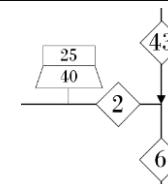
MASS BALANCE

Benzene Feed Pump, P-101

P-101		 P-101							
Stream		In			Out				
		S-1	S-2						
Vapor fraction		0.0000					0.0000		
Pressure (bar)		1.0000					40.0000		
Temperature (°C)		25.0000					25.0000		
Components		Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene		115.2269	1.0000	9001.5234	1.0000	115.2269	1.0000	9001.5234	1.0000
Ethylene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Diethylbenzene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total		115.2269	1.0000	9001.5234	1.0000	115.2269	1.0000	9001.5234	1.0000
Total mass flow rate (kg/hr)			9001.52				9001.52		
Remark		MASS BALANCED							

Benzene Feed Mixing Point

Fresh Benzene Feed & Recycle Stream mixing point, S-6													
Stream	In				In				Out				
	S-2				S-43				S-6				
Vapor fraction	0.0000				0.0000				0.0000				
Pressure (bar)	40.0000				40.0000				40.0000				
Temperature (°C)	25.0000				77.1381				60.1156				
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	
Benzene	115.2269	1.0000	9001.5234	1.0000	230.2395	0.9995	17986.3092	0.9996	345.4664	0.9997	26987.8326	0.9997	
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0575	0.0002	1.6141	0.0001	0.0575	0.0002	1.6141	0.0001	
Ethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0497	0.0002	5.2726	0.0003	0.0497	0.0001	5.2726	0.0002	
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Total	115.2269	1.0000	9001.5234	1.0000	230.3467	1.0000	17993.1959	1.0000	345.5736	1.0000	26994.7193	1.0000	
Total mass flow rate (kg/hr)	26994.72								26994.72				
Remark	MASS BALANCED												



Compressor, C-101

C-101

Stream	In				Out			
	S-3				S-4			
Vapor fraction	1.0000				1.0000			
Pressure (bar)	40.0000				50.0000			
Temperature (°C)	25.0000				25.0000			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	115.0979	0.9991	3228.4964	0.9990	115.0979	0.9991	3228.4964	0.9990
Ethylbenzene	0.0079	0.0001	0.8435	0.0003	0.0079	0.0001	0.8435	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0311	0.0003	0.4987	0.0002	0.0311	0.0003	0.4987	0.0002
Ethane	0.0610	0.0005	1.8352	0.0006	0.0610	0.0005	1.8352	0.0006
Total	115.1980	1.0000	3231.6738	1.0000	115.1980	1.0000	3231.6738	1.0000
Total mass flow rate (kg/hr)	3231.67				3231.67			
Remark	MASS BALANCED							

Condenser, E-101

E-101

Stream	In				Out			
	S-4				S-5			
Vapor fraction	1.0000				0.0000			
Pressure (bar)	50.0000				50.0000			
Temperature (°C)	25.0000				9.0000			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	115.0979	0.9991	3228.4964	0.9990	115.0979	0.9991	3228.4964	0.9990
Ethylbenzene	0.0079	0.0001	0.8435	0.0003	0.0079	0.0001	0.8435	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0311	0.0003	0.4987	0.0002	0.0311	0.0003	0.4987	0.0002
Ethane	0.0610	0.0005	1.8352	0.0006	0.0610	0.0005	1.8352	0.0006
Total	115.1980	1.0000	3231.6738	1.0000	115.1980	1.0000	3231.6738	1.0000
Total mass flow rate (kg/hr)	3231.67				3231.67			
Remark	MASS BALANCED							

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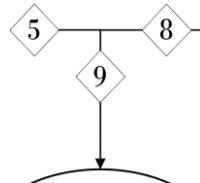
Heat Exchanger, E-102

E-102 (Cooling Fluid)							
Stream	In			Out			
Vapor fraction	S-6			S-7			
Pressure (bar)	0.0000			0.0000			
Temperature (°C)	40.0000			40.0000			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)
Benzene	345.4664	0.9997	26987.8326	0.9997	345.4664	0.9997	26987.8326
Ethylene	0.0575	0.0002	1.6141	0.0001	0.0575	0.0002	1.6141
Ethylbenzene	0.0497	0.0001	5.2726	0.0002	0.0497	0.0001	5.2726
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	345.5736	1.0000	26994.7193	1.0000	345.5736	1.0000	26994.7193
Total mass flow rate (kg/hr)	26994.72						
Remark	MASS BALANCED						

Heater, E-103

E-103 Heater								
Stream	In	Out						
	S-7	S-8						
Vapor fraction	0.0000	0.0000						
Pressure (bar)	40.0000	40.0000						
Temperature (°C)	155.5964	200.0000						
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	345.4664	0.9997	26987.8326	0.9997	345.4664	0.9997	26987.8326	0.9997
Ethylene	0.0575	0.0002	1.6141	0.0001	0.0575	0.0002	1.6141	0.0001
Ethylbenzene	0.0497	0.0001	5.2726	0.0002	0.0497	0.0001	5.2726	0.0002
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	345.5736	1.0000	26994.7193	1.0000	345.5736	1.0000	26994.7193	1.0000
Total mass flow rate (kg/hr)	26994.72			26994.72				
Remark	MASS BALANCED							

Reactor Input Mixing point

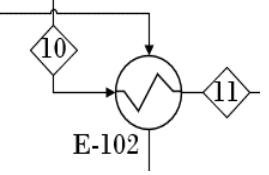


Stream	In				In				Out			
	S-8				S-5				S-9			
Vapor fraction	0.0000				0.0000				0.0000			
Pressure (bar)	40.0000				50.0000				40.0000			
Temperature (°C)	155.5964				9.0000				182.4714			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	345.4664	0.9997	26987.8326	0.9997	0.0000	0.0000	0.0000	0.0000	345.4664	0.7498	26987.8326	0.8929
Ethylene	0.0575	0.0002	1.6141	0.0001	115.0979	0.9991	3228.4964	0.9990	115.1555	0.2499	3230.1105	0.1069
Ethylbenzene	0.0497	0.0001	5.2726	0.0002	0.0079	0.0001	0.8435	0.0003	0.0576	0.0001	6.1160	0.0002
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0311	0.0003	0.4987	0.0002	0.0311	0.0001	0.4987	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0610	0.0005	1.8352	0.0006	0.0610	0.0001	1.8352	0.0001
Total	345.5736	1.0000	26994.7193	1.0000	115.1980	1.0000	3231.6738	1.0000	460.7716	1.0000	30226.3931	1.0000
Total mass flow rate (kg/hr)	30226.39				MASS BALANCED				30226.39			
Remark												

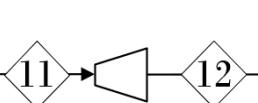
Alkylator, R-101

R-101		Temperature = 473.15 K; Pressure: 40 bars						
		Selectivity (Desirable)	0.9200					
		Selectivity (Undesirable)	0.0800					
		Conversion of Ethylene (Limiting Reactant)	0.9995					
Stream	In	Out						
	S-9	S-10						
Vapor fraction	0.0000	0.0000						
Pressure (bar)	40.0000	40.0000						
Temperature (°C)	182.4714	200.0000						
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	345.4664	0.7498	26987.8326	0.8929	239.5763	0.6931	18715.7021	0.6192
Ethylene	115.1555	0.2499	3230.1105	0.1069	0.0576	0.0002	1.6151	0.0001
Ethylbenzene	0.0576	0.0001	6.1160	0.0002	96.7398	0.2799	10270.8671	0.3398
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	9.2078	0.0266	1235.8750	0.0409
Methane	0.0311	0.0001	0.4987	0.0000	0.0311	0.0001	0.4987	0.0000
Ethane	0.0610	0.0001	1.8352	0.0001	0.0610	0.0002	1.8352	0.0001
Total	460.7716	1.0000	30226.3931	1.0000	345.6737	1.0000	30226.3931	1.0000
Total mass flow rate (kg/hr)	3.02E+04		3.02E+04					
Remark	MASS BALANCED							

Heat Exchanger, E-102

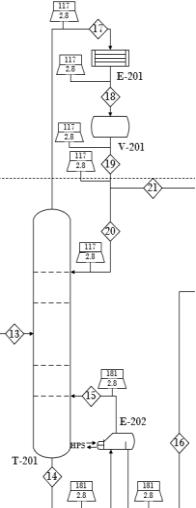
E-102 (Process Fluid)								
Stream	In				Out			
Vapor fraction	S-10				S-11			
Pressure (bar)	40.0000				40.0000			
Temperature (Degree Celsius)	200.0000				120.6244			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	239.5763	0.6931	18715.7021	0.6192	239.5763	0.6931	18715.7021	0.6192
Ethylene	0.0576	0.0002	1.6151	0.0001	0.0576	0.0002	1.6151	0.0001
Ethylbenzene	96.7398	0.2799	10270.8671	0.3398	96.7398	0.2799	10270.8671	0.3398
Diethylbenzene	9.2078	0.0266	1235.8750	0.0409	9.2078	0.0266	1235.8750	0.0409
Methane	0.0311	0.0001	0.4987	0.0000	0.0311	0.0001	0.4987	0.0000
Ethane	0.0610	0.0002	1.8352	0.0001	0.0610	0.0002	1.8352	0.0001
Total	345.6737	1.0000	30226.3931	1.0000	345.6737	1.0000	30226.3931	1.0000
Total mass flow rate (kg/hr)	30226.39				30226.39			
Remark	MASS BALANCED							

Liquid Expander, C-102

C-102	 <p style="text-align: center;">C-102</p>							
Stream	In				Out			
Vapor fraction	S-11				S-12			
Pressure (bar)	40.0000				2.8000			
Temperature (°C)	120.6244				120.6244			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	239.5763	0.6931	18715.7021	0.6192	239.5763	0.6931	18715.7021	0.6192
Ethylene	0.0576	0.0002	1.6151	0.0001	0.0576	0.0002	1.6151	0.0001
Ethylbenzene	96.7398	0.2799	10270.8671	0.3398	96.7398	0.2799	10270.8671	0.3398
Diethylbenzene	9.2078	0.0266	1235.8750	0.0409	9.2078	0.0266	1235.8750	0.0409
Methane	0.0311	0.0001	0.4987	0.0000	0.0311	0.0001	0.4987	0.0000
Ethane	0.0610	0.0002	1.8352	0.0001	0.0610	0.0002	1.8352	0.0001
Total	345.6737	1.0000	30226.3931	1.0000	345.6737	1.0000	30226.3931	1.0000
Total mass flow rate (kg/hr)	30226.39				30226.39			
Remark	MASS BALANCED							

Overall Boundary for T-201

Overall boundary for T-201



Stream	In				Out				Out			
	S-13				S-21				S-16			
Vapor fraction	0.0000				0.0000				0.0000			
Pressure (bar)	2.8000				2.8000				2.8000			
Temperature (°C)	120.6244				117.2462				180.9130			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	267.2044	0.6820	20874.0083	0.6077	267.0708	0.9992	20863.5713	0.9995	0.1336	0.0011	10.4370	0.0008
Ethylene	0.0668	0.0002	1.8733	0.0001	0.0668	0.0002	1.8733	0.0001	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	115.2118	0.2941	12232.0360	0.3561	0.0576	0.0002	6.1160	0.0003	115.1542	0.9249	12225.9200	0.9074
Diethylbenzene	9.2124	0.0235	1236.4929	0.0360	0.0000	0.0000	0.0000	0.0000	9.2124	0.0740	1236.4929	0.0918
Methane	0.0311	0.0001	0.4987	0.0000	0.0311	0.0001	0.4987	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0610	0.0002	1.8352	0.0001	0.0610	0.0002	1.8352	0.0001	0.0000	0.0000	0.0000	0.0000
Total	391.7875	1.0000	34346.7445	1.0000	267.2873	1.0000	20873.8945	1.0000	124.5002	1.0000	34346.74	1.0000
Total mass flow rate (kg/hr)	34346.74				MASS BALANCED				34346.74			
Remark												

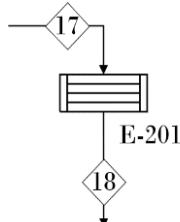
Distillation Column, T-201

T-201

Stream	In				In				M
	S-13		S-15						
Vapor fraction		0.0000				1.0000			
Pressure (bar)		2.8000				2.8000			
Temperature (°C)		120.6244				180.9130			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	M
Benzene	267.2044	0.6820	20874.0083	0.6077	0.0989	0.0011	7.7258	0.0008	
Ethylene	0.0668	0.0002	1.8733	0.0001	0.0000	0.0000	0.0000	0.0000	
Ethylbenzene	115.2118	0.2941	12232.0360	0.3561	85.2407	0.9249	9050.0022	0.9074	
Diethylbenzene	9.2124	0.0235	1236.4929	0.0360	6.8193	0.0740	915.2901	0.0918	
Methane	0.0311	0.0001	0.4987	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane	0.0610	0.0002	1.8352	0.0001	0.0000	0.0000	0.0000	0.0000	
Total	391.7875	1.0000	34346.7445	1.0000	92.1589	1.0000	9973.0181	1.0000	
Total mass flow rate (kg/hr)					56618.42				
Remark									

In				Out				Out			
S-20				S-14				S-17			
0.0000				0.0000				1.0000			
2.8000				2.8000				2.8000			
117.2462				180.9130				117.2462			
Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
157.3550	0.9992	12292.5721	0.9995	0.2325	0.0011	18.1628	0.0008	424.4258	0.9992	33156.1434	0.9995
0.0393	0.0002	1.1037	0.0001	0.0000	0.0000	0.0000	0.0000	0.1061	0.0002	2.9770	0.0001
0.0339	0.0002	3.6035	0.0003	200.3949	0.9249	21275.9223	0.9074	0.0915	0.0002	9.7195	0.0003
0.0000	0.0000	0.0000	0.0000	16.0318	0.0740	2151.7830	0.0918	0.0000	0.0000	0.0000	0.0000
0.0183	0.0001	0.2938	0.0000	0.0000	0.0000	0.0000	0.0000	0.0494	0.0001	0.7926	0.0000
0.0360	0.0002	1.0813	0.0001	0.0000	0.0000	0.0000	0.0000	0.0970	0.0002	2.9165	0.0001
157.4826	1.0000	12298.6545	1.0000	216.6591	1.0000	23445.8681	1.0000	424.7699	1.0000	33172.5490	1.0000
MASS BALANCED											

Condenser, E-201

E-201								
Stream	In				Out			
	S-17				S-18			
Vapor fraction		1.0000				0.0000		
Pressure (bar)		2.8000				2.8000		
Temperature (°C)		117.2462				117.2462		
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	424.4258	0.9992	33156.1434	0.9995	424.4258	0.9992	33156.1434	0.9995
Ethylene	0.1061	0.0002	2.9770	0.0001	0.1061	0.0002	2.9770	0.0001
Ethylbenzene	0.0915	0.0002	9.7195	0.0003	0.0915	0.0002	9.7195	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0494	0.0001	0.7926	0.0000	0.0494	0.0001	0.7926	0.0000
Ethane	0.0970	0.0002	2.9165	0.0001	0.0970	0.0002	2.9165	0.0001
Total	424.7699	1.0000	33172.5490	1.0000	424.7699	1.0000	33172.5490	1.0000
Total mass flow rate (kg/hr)	33172.55				33172.55			
Remark	MASS BALANCED							

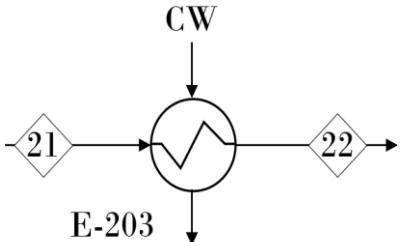
Reflux Drum, V-201

Stream	In				Out				Out			
	S-18		S-20		S-21							
Vapor fraction	0.0000		0.0000		0.0000				0.0000			
Pressure (bar)	2.8000		2.8000		2.8000				2.8000			
Temperature (°C)	117.2462		117.2462		117.2462				117.2462			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	424.4258	0.9992	33156.1434	0.9995	157.3550	0.9992	12292.5721	0.9995	267.0708	0.9992	20863.5713	0.9995
Ethylene	0.1061	0.0002	2.9770	0.0001	0.0393	0.0002	1.1037	0.0001	0.0668	0.0002	1.8733	0.0001
Ethylbenzene	0.0915	0.0002	9.7195	0.0003	0.0339	0.0002	3.6035	0.0003	0.0576	0.0002	6.1160	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0494	0.0001	0.7926	0.0000	0.0183	0.0001	0.2938	0.0000	0.0311	0.0001	0.4987	0.0000
Ethane	0.0970	0.0002	2.9165	0.0001	0.0360	0.0002	1.0813	0.0001	0.0610	0.0002	1.8352	0.0001
Total	424.7699	1.0000	33172.5490	1.0000	157.4826	1.0000	12298.6545	1.0000	267.2873	1.0000	20873.8945	1.0000
Total mass flow rate (kg/hr)			33172.55					33172.55				
Remark	MASS BALANCED											

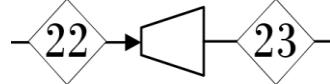
Reboiler, E-202

Stream	In				Out				Out			
	S-14		S-15		S-16							
Vapor fraction	0.0000		1.0000		0.0000				0.0000			
Pressure (bar)	2.8000		2.8000		2.8000				2.8000			
Temperature (°C)	180.9130		180.9130		180.9130				180.9130			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.2325	0.0011	18.1628	0.0008	0.0989	0.0011	7.7258	0.0008	0.1336	0.0011	10.4370	0.0008
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	200.3949	0.9249	21275.9223	0.9074	85.2407	0.9249	9050.0022	0.9074	115.1542	0.9249	12225.9200	0.9074
Diethylbenzene	16.0318	0.0740	2151.7830	0.0918	6.8193	0.0740	915.2901	0.0918	9.2124	0.0740	1236.4929	0.0918
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	216.6591	1.0000	23445.8681	1.0000	92.1589	1.0000	9973.0181	1.0000	124.5002	1.0000	13472.8499	1.0000
Total mass flow rate (kg/hr)			23445.87				9973.0181		124.5002			
Remark	MASS BALANCED											

Cooler, E-203

E-203	 <p style="text-align: center;">E-203</p>								
Stream	In				Out				
	S-21				S-22				
Vapor fraction	0.0000				0.0000				
Pressure (bar)	2.8000				2.8000				
Temperature (°C)	117.2462				77.1381				
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	
Benzene	267.0708	0.9992	20863.5713	0.9995	267.0708	0.9992	20863.5713	0.9995	
Ethylene	0.0668	0.0002	1.8733	0.0001	0.0668	0.0002	1.8733	0.0001	
Ethylbenzene	0.0576	0.0002	6.1160	0.0003	0.0576	0.0002	6.1160	0.0003	
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Methane	0.0311	0.0001	0.4987	0.0000	0.0311	0.0001	0.4987	0.0000	
Ethane	0.0610	0.0002	1.8352	0.0001	0.0610	0.0002	1.8352	0.0001	
Total	267.2873	1.0000	20873.8945	1.0000	267.2873	1.0000	20873.8945	1.0000	
Total mass flow rate (kg/hr)	20873.89				20873.89				
Remark	MASS BALANCED								

Liquid Expander, C-201

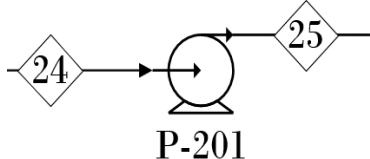
C-201	 <p style="text-align: center;">C-201</p>													
Stream	In				Out									
	S-22				S-23									
Vapor fraction	0.0000				0.0003									
Pressure (bar)	2.8000				1.0133									
Temperature (°C)	77.1381				77.1381									
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction						
Benzene	267.0708	0.9992	20863.5713	0.9995	267.0708	0.9992	20863.5713	0.9995						
Ethylene (liquid)	0.0668	0.0002	1.8733	0.0001	0.0667	0.0002	1.8723	0.0001						
Ethylbenzene	0.0576	0.0002	6.1160	0.0003	0.0576	0.0002	6.1160	0.0003						
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000						
Methane (liquid)	0.0311	0.0001	0.4987	0.0000	0.0000	0.0000	0.0000	0.0000						
Ethane (liquid)	0.0610	0.0002	1.8352	0.0001	0.0000	0.0000	0.0000	0.0000						
Ethylene (vapor)					0.0000	0.0000	0.0009	0.0000						
Methane (vapor)					0.0311	0.0001	0.4987	0.0000						
Ethane (vapor)					0.0610	0.0002	1.8352	0.0001						
Total	267.2873	1.0000	20873.8945	1.0000	267.2873	1.0000	20873.8945	1.0000						
Total mass flow rate (kg/hr)	20873.89				20873.89									
Remark	MASS BALANCED													

Flash Drum, V-202

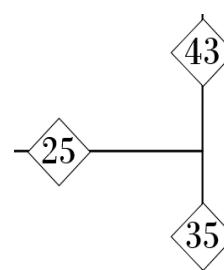
V-202

Stream	In				Out				Out			
	S-23				S-24				S-42			
Vapor fraction		0.0003				0.0000				1.0000		
Pressure (bar)		1.0133				1.0133				1.0133		
Temperature (°C)		77.1381				77.1381				77.1381		
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	267.0708	0.9992	20863.5713	0.9995	267.0708	0.9995	20863.5713	0.9996	0.0000	0.0000	0.0000	0.0000
Ethylene (liquid)	0.0667	0.0002	1.8723	0.0001	0.0667	0.0002	1.8723	0.0001	0.0000	0.0004	0.0009	0.0004
Ethylbenzene	0.0576	0.0002	6.1160	0.0003	0.0576	0.0002	6.1160	0.0003	0.0000	0.0000	0.0000	0.0000
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane (liquid)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0311	0.3374	0.4987	0.2136
Ethane (liquid)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0610	0.6623	1.8352	0.7860
Ethylene (vapor)	0.0000	0.0000	0.0009	0.0000								
Methane (vapor)	0.0311	0.0001	0.4987	0.0000								
Ethane (vapor)	0.0610	0.0002	1.8352	0.0001								
Total	267.2873	1.0000	20873.8945	1.0000	267.1952	1.0000	20871.5596	1.0000	0.0922	1.0000	2.3349	1.0000
Total mass flow rate (kg/hr)			20873.89						20873.89			
Remark	MASS BALANCED											

Pump, P-201

P-201	 <p>P-201</p>							
Stream	In				Out			
	S-24				S-25			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	1.0133				40.0000			
Temperature (°C)	77.1381				77.1381			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	267.0708	0.9995	20863.5713	0.9996	267.0708	0.9995	20863.5713	0.9996
Ethylenne	0.0667	0.0002	1.8723	0.0001	0.0667	0.0002	1.8723	0.0001
Ethylbenzene	0.0576	0.0002	6.1160	0.0003	0.0576	0.0002	6.1160	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	267.1952	1.0000	20871.5596	1.0000	267.1952	1.0000	20871.5596	1.0000
Total mass flow rate (kg/hr)	20871.56				20871.56			
Remark	MASS BALANCED							

Separating Point after P-201



Separating point P-201

Stream	In				Out				Out			
	S-25				S-35				S-43			
Vapor fraction		0.0000				0.0000				0.0000		
Pressure (bar)		40.0000				40.0000				40.0000		
Temperature (°C)		77.1381				77.1381				77.1381		
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	267.0708	0.9995	20863.5713	0.9996	36.8313	0.9995	2877.2621	0.9996	230.2395	0.9995	17986.3092	0.9996
Ethylene	0.0667	0.0002	1.8723	0.0001	0.0092	0.0002	0.2582	0.0001	0.0575	0.0002	1.6141	0.0001
Ethylbenzene	0.0576	0.0002	6.1160	0.0003	0.0079	0.0002	0.8435	0.0003	0.0497	0.0002	5.2726	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	267.1952	1.0000	20871.5596	1.0000	36.8485	1.0000	2878.3637	1.0000	230.3467	1.0000	17993.1959	1.0000
Total mass flow rate (kg/hr)	20871.56				20871.56				20871.56			
Remark	MASS BALANCED											

Overall Boundary for T-401

Overall Boundary System for T-401

Stream	In				Out				Out			
	S-16				S-34				S-28			
Vapor fraction	0.000				0.000				0.000			
Pressure (bar)	2.8000				2.8000				2.8000			
Temperature (°C)	180.9130				178.5856				229.5292			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.1336	0.0011	10.4370	0.0008	0.1336	0.0012	10.4370	0.0009	0.0000	0.0000	0.0000	0.0000
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	115.1542	0.9249	12225.9200	0.9074	115.0966	0.9988	12219.8071	0.9991	0.0576	0.0062	6.1130	0.0049
Diethylbenzene	9.2124	0.0740	1236.4929	0.0918	0.0046	0.0000	0.6182	0.0001	9.2078	0.9938	1235.8747	0.9951
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	124.5002	1.0000	13472.8499	1.0000	115.2348	1.0000	12230.8623	1.0000	9.2654	1.0000	1241.9876	1.0000
Total mass flow rate (kg/hr)	13472.85				13472.85				MASS BALANCED			
Remark												

Distillation Column, T-401

Stream	In				In			
	S-16				S-33			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	2.8000				2.8000			
Temperature (°C)	180.9130				178.5856			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.1336	0.0011	10.4370	0.0008	0.1022	0.0012	7.9826	0.0009
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	115.1542	0.9249	12225.9200	0.9074	88.0299	0.9988	9346.1366	0.9991
Diethylbenzene	9.2124	0.0740	1236.4929	0.0918	0.0035	0.0000	0.4729	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	124.5002	1.0000	13472.8499	1.0000	88.1356	1.0000	9354.5920	1.0000
Total mass flow rate (kg/hr)	23003.68							
Remark								

In	Out				Out				
S-27	S-30	S-26							
1.0000	1.0000	0.0000							
2.8000	2.8000	2.8000							
229.5292	178.5856	229.5292							
n	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	
0.0000	0.0000	0.0000	0.0000	0.2358	0.0012	18.4196	0.0009	0.0000	
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
0.0082	0.0062	0.8674	0.0049	203.1265	0.9988	21565.9437	0.9991	0.0657	
1.3066	0.9938	175.3716	0.9951	0.0081	0.0000	1.0911	0.0001	10.5144	
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
1.3148	1.0000	176.2390	1.0000	203.3704	1.0000	21585.4544	1.0000	10.5802	
23003.68									
MASS BALANCED									

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Condenser, E-401

E-401

E-401

Stream	In				Out			
	S-30				S-31			
Vapor fraction	1.0000				0.0000			
Pressure (bar)	2.8000				2.8000			
Temperature (°C)	178.5856				178.5856			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.2358	0.0012	18.4196	0.0009	0.2358	0.0012	18.4196	0.0009
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	203.1265	0.9988	21565.9437	0.9991	203.1265	0.9988	21565.9437	0.9991
Diethylbenzene	0.0081	0.0000	1.0911	0.0001	0.0081	0.0000	1.0911	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	203.3704	1.0000	21585.4544	1.0000	203.3704	1.0000	21585.4544	1.0000
Total mass flow rate (kg/hr)	21585.45				21585.45			
Remark	MASS BALANCED							

Reflux Drum, V-401

V-401

Stream	In				Out			
	S-31				S-33			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	2.8000				2.8000			
Temperature (°C)	178.5856				178.5856			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.2358	0.0012	18.4196	0.0009	0.1022	0.0012	7.9826	0.0009
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	203.1265	0.9988	21565.9437	0.9991	88.0299	0.9988	9346.1366	0.9991
Diethylbenzene	0.0081	0.0000	1.0911	0.0001	0.0035	0.0000	0.4729	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	203.3704	1.0000	21585.4544	1.0000	88.1356	1.0000	9354.5920	1.0000
Total mass flow rate (kg/hr)	21585.45							
Remark	MASS BALANCED							

Out			
S-34			
0.0000			
2.8000			
178.5856			
Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
0.1336	0.0012	10.4370	0.0009
0.0000	0.0000	0.0000	0.0000
115.0966	0.9988	12219.8071	0.9991
0.0046	0.0000	0.6182	0.0001
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
115.2348	1.0000	12230.8623	1.0000
21585.45			

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Reboiler, E-402

Stream	In			Out				
	S-26			S-27				
Vapor fraction	0.0000			1.0000				
Pressure (bar)	2.8000			2.8000				
Temperature (°C)	229.5292			229.5292				
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	0.0657	0.0062	6.9804	0.0049	0.0082	0.0062	0.8674	0.0049
Diethylbenzene	10.5144	0.9938	1411.2463	0.9951	1.3066	0.9938	175.3716	0.9951
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	10.5802	1.0000	1418.2266	1.0000	1.3148	1.0000	176.2390	1.0000
Total mass flow rate (kg/hr)	1418.23							
Remark	MASS BALANCED							

Out			
S-28			
0.0000			
2.8000			
229.5292			
Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0576	0.0062	6.1130	0.0049
9.2078	0.9938	1235.8747	0.9951
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
9.2654	1.0000	1241.9876	1.0000
1418.23			

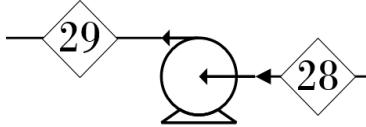
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Heat Exchanger, E-204

E-204 (Process Fluid)								
Stream	In				Out			
	S-35		S-36		S-35		S-36	
Vapor fraction		0.0000				0.0000		
Pressure (bar)		40.0000				40.0000		
Temperature (°C)		77.1381				210.0000		
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	36.8313	0.9995	2877.2621	0.9996	36.8313	0.9995	2877.2621	0.9996
Ethylene	0.0092	0.0002	0.2582	0.0001	0.0092	0.0002	0.2582	0.0001
Ethylbenzene	0.0079	0.0002	0.8435	0.0003	0.0079	0.0002	0.8435	0.0003
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	36.8485	1.0000	2878.3637	1.0000	36.8485	1.0000	2878.3637	1.0000
Total mass flow rate (kg/hr)	2878.36				2878.36			
Remark	MASS BALANCED							

Pump, P-401

P-401

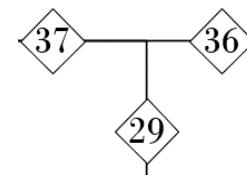


P-401

Stream	In				Out			
	S-28				S-29			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	2.8000				35.0000			
Temperature (°C)	229.5292				229.5292			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylbenzene	0.0576	0.0062	6.1130	0.0049	0.0576	0.0062	6.1130	0.0049
Diethylbenzene	9.2078	0.9938	1235.8747	0.9951	9.2078	0.9938	1235.8747	0.9951
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	9.2654	1.0000	1241.9876	1.0000	9.2654	1.0000	1241.9876	1.0000
Total mass flow rate (kg/hr)	1241.99				1241.99			
Remark	MASS BALANCED							

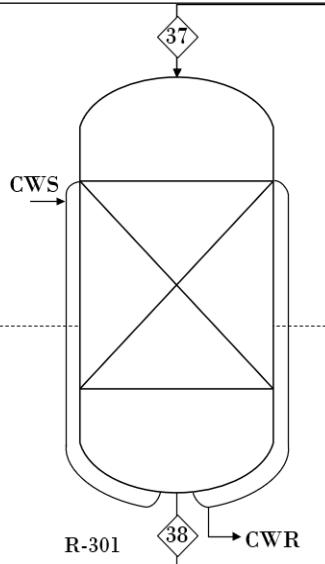
Mixing Point before R-301

Mixing Stream, S-36 (different)



Stream	In	In	Out									
	S-36	S-29	S-37									
Vapor fraction	0.0000	0.0000	0.0000									
Pressure (bar)	40.0000	35.0000	35.0000									
Temperature (°C)	210.0000	229.5292	216.0149									
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	36.8313	0.9995	2877.2621	0.9996	0.0000	0.0000	0.0000	0.0000	36.8313	0.7987	2877.262073	0.698305029
Ethylene	0.0092	0.0002	0.2582	0.0001	0.0000	0.0000	0.0000	0.0000	0.0092	0.0002	0.258209857	6.2667E-05
Ethylbenzene	0.0079	0.0002	0.8435	0.0003	0.0576	0.0062	6.1130	0.0049	0.0655	0.0014	6.956410376	0.001688305
Diethylbenzene	0.0000	0.0000	0.0000	0.0000	9.2078	0.9988	1235.8747	0.9951	9.2078	0.1997	1235.874665	0.299943999
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0	0
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0	0
Total	36.8485	1.0000	2878.3637	1.0000	9.2654	1.0000	1241.9876	1.0000	46.1139	1.0000	4120.3514	1.0000
Total mass flow rate (kg/hr)			4120.35								4120.35	
Remark	MASS BALANCED											

Transalkylator, R-301

R-301		Selectivity (desirable)	1.0000					
		Selectivity (undesirable)	0.0000					
		Conversion of Diethylbenzene	0.9995					
Stream	In			Out				
	S-37			S-38				
Vapor fraction	0.0000			0.0000				
Pressure (bar)	35.0000			35.0000				
Temperature (°C)	216.0149			229.5292				
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	36.8313	0.7987	2877.2621	0.6983	27.6281	0.5991	2158.3062	0.5238
Ethylene	0.0092	0.0002	0.2582	0.0001	0.0092	0.0002	0.2582	0.0001
Ethylbenzene	0.0655	0.0014	6.9564	0.0017	18.4720	0.4006	1961.1690	0.4760
Diethylbenzene	9.2078	0.1997	1235.8747	0.2999	0.0046	0.0001	0.6179	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	46.1139	1.0000	4120.3514	1.0000	46.1139	1.0000	4120.3514	1.0000
Total mass flow rate (kg/hr)	4120.35			4120.35				
Remark	MASS BALANCED							

Heat Exchanger, E-204

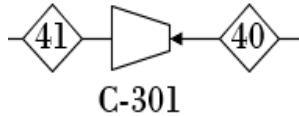
E-204 (Heating Fluid)

Stream	In				Out			
	S-38				S-39			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	35.0000				35.0000			
Temperature (°C)	229.5292				180.6455			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	27.6281	0.5991	2158.3062	0.5238	27.6281	0.5991	2158.3062	0.5238
Ethylene	0.0092	0.0002	0.2582	0.0001	0.0092	0.0002	0.2582	0.0001
Ethylbenzene	18.4720	0.4006	1961.1690	0.4760	18.4720	0.4006	1961.1690	0.4760
Diethylbenzene	0.0046	0.0001	0.6179	0.0001	0.0046	0.0001	0.6179	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	46.1139	1.0000	4120.3514	1.0000	46.1139	1.0000	4120.3514	1.0000
Total mass flow rate (kg/hr)	4120.35				4120.35			
Remark	MASS BALANCED							

Cooler, E-301

E-301 Cooler								
Stream	In				Out			
	S-39				S-40			
Vapor fraction	0.0000				0.0000			
Pressure (bar)	40.0000				40.0000			
Temperature (°C)	180.6455				120.6244			
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene	27.6281	0.5991	2158.3062	0.5238	27.6281	0.5991	2158.3062	0.5238
Ethylenne	0.0092	0.0002	0.2582	0.0001	0.0092	0.0002	0.2582	0.0001
Ethylbenzene	18.4720	0.4006	1961.1690	0.4760	18.4720	0.4006	1961.1690	0.4760
Diethylbenzene	0.0046	0.0001	0.6179	0.0001	0.0046	0.0001	0.6179	0.0001
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	46.1139	1.0000	4120.3514	1.0000	46.1139	1.0000	4120.3514	1.0000
Total mass flow rate (kg/hr)	4120.35				4120.35			
Remark	MASS BALANCED							

Liquid Expander, C-301

C-301									
									
Stream		In			Out				
		S-40			S-41				
Vapor fraction		0.0000			0.0000				
Pressure (bar)		35.0000			2.8000				
Temperature (°C)		120.6244			120.6244				
Components		Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction
Benzene		27.6281	0.5991	2158.3062	0.5238	27.6281	0.5991	2158.3062	0.5238
Ethylenne		0.0092	0.0002	0.2582	0.0001	0.0092	0.0002	0.2582	0.0001
Ethylbenzene		18.4720	0.4006	1961.1690	0.4760	18.4720	0.4006	1961.1690	0.4760
Diethylbenzene		0.0046	0.0001	0.6179	0.0001	0.0046	0.0001	0.6179	0.0001
Methane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total		46.1139	1.0000	4120.3514	1.0000	46.1139	1.0000	4120.3514	1.0000
Total mass flow rate (kg/hr)		4120.35			4120.35				
Remark		MASS BALANCED							

Mixing Input Stream before Distillation Column, T-201

Mixing Input Stream, S-11

Stream	In	In							
	S-41	S-12							
Vapor fraction	0.0000	0.0000							
Pressure (bar)	2.8000	2.8000							
Temperature (°C)	120.6244	120.6244							
Components	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	Molar Flow rate (kmol/hr)	Mole fraction	Mass Flow Rate (kg/hr)	Mass fraction	N
Benzene	27.6281	0.5991	2158.3062	0.5238	239.5763	0.6931	18715.7021	0.6192	
Ethylene	0.0092	0.0002	0.2582	0.0001	0.0576	0.0002	1.6151	0.0001	
Ethylbenzene	18.4720	0.4006	1961.1690	0.4760	96.7398	0.2799	10270.8671	0.3398	
Diethylbenzene	0.0046	0.0001	0.6179	0.0001	9.2078	0.0266	1235.8750	0.0409	
Methane	0.0000	0.0000	0.0000	0.0000	0.0311	0.0001	0.4987	0.0000	
Ethane	0.0000	0.0000	0.0000	0.0000	0.0610	0.0002	1.8352	0.0001	
Total	46.1139	1.0000	4120.3514	1.0000	345.6737	1.0000	30226.3931	1.0000	
Total mass flow rate (kg/hr)			34346.74						MASS BALANCED
Remark									

	Out
	S-13
	0.0000
	2.8000
	120.6244
Molar Flow rate (kmol/hr)	Mole fraction
267.2044	0.6820
0.0668	0.0002
115.2118	0.2941
9.2124	0.0235
0.0311	0.0001
0.0610	0.0002
391.7875	1.0000
	34346.74

A.1 Stream table

Stream number	1	2	3	4	5	6	7
Vapor Pressure	0.000	0.000	1.000	1.000	0.000	0.000	0.000
Pressure (bar)	1.000	40.000	40.000	50.000	50.000	40.000	40.000
Temperature (°C)	25.000	25.000	25.000	25.000	9.000	60.116	200.000
Molar flow rate (kmol/hr)							
Benzene	115.227	115.227	0.000	0.000	0.000	345.466	345.466
Ethylene	0.000	0.000	115.098	115.098	115.098	0.058	0.058
Ethylbenzene	0.000	0.000	0.000	0.000	0.000	0.058	0.058
Diethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.031	0.031	0.031	0.000	0.000
Ethane	0.000	0.000	0.061	0.061	0.061	0.000	0.000
Total	115.227	115.227	115.190	115.190	115.190	345.582	345.582
Mole fraction							
Benzene	1.000	1.000	0.000	0.000	0.000	1.000	1.000
Ethylene	0.000	0.000	0.999	0.999	0.999	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Diethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.001	0.001	0.001	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)							
Benzene	9001.523	9001.523	0.000	0.000	0.000	26987.833	26987.833
Ethylene	0.000	0.000	3228.496	3228.496	3228.496	1.614	1.614
Ethylbenzene	0.000	0.000	0.000	0.000	0.000	6.115	6.115

Diethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.499	0.499	0.499	0.000	0.000
Ethane	0.000	0.000	1.835	1.835	1.835	0.000	0.000
Total	9001.523	9001.523	3230.831	3230.831	3230.831	26995.562	26995.562
Mass fraction							
Benzene	1.000	1.000	0.000	0.000	0.000	1.000	1.000
Ethylene	0.000	0.000	0.999	0.999	0.999	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Diethylbenzene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.001	0.001	0.001	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream number	7	8	9	10	11	12	13	14
Vapor Pressure	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Pressure (bar)	40.000	40.000	40.000	40.000	40.000	2.800	2.800	2.800
Temperature (°C)	200.000	200.000	182.471	200.000	120.624	120.624	120.624	180.913
Molar flow rate (kmol/hr)								
Benzene	345.466	345.466	345.466	239.576	239.576	239.576	267.204	0.232
Ethylene	0.058	0.058	115.155	0.058	0.058	0.058	0.067	0.000
Ethylbenzene	0.058	0.058	0.058	96.740	96.740	96.740	115.204	200.375
Diethylbenzene	0.000	0.000	0.000	9.208	9.208	9.208	9.212	16.031
Methane	0.000	0.000	0.031	0.031	0.031	0.031	0.031	0.000
Ethane	0.000	0.000	0.061	0.061	0.061	0.061	0.061	0.000
Total	345.582	345.582	460.772	345.674	345.674	345.674	391.780	216.639

Mole fraction								
Benzene	1.000	1.000	0.750	0.693	0.693	0.693	0.682	0.001
Ethylene	0.000	0.000	0.250	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.280	0.280	0.280	0.294	0.925
Diethylbenzene	0.000	0.000	0.000	0.027	0.027	0.027	0.024	0.074
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)								
Benzene	26987.833	26987.833	26987.833	18715.702	18715.702	18715.702	20874.008	18.162
Ethylene	1.614	1.614	3230.111	1.615	1.615	1.615	1.873	0.000
Ethylbenzene	6.115	6.115	6.116	10270.867	10270.867	10270.867	12231.192	21273.807
Diethylbenzene	0.000	0.000	0.000	1235.875	1235.875	1235.875	1236.493	2151.718
Methane	0.000	0.000	0.499	0.499	0.499	0.499	0.499	0.000
Ethane	0.000	0.000	1.835	1.835	1.835	1.835	1.835	0.000
Total	26995.562	26995.562	30226.393	30226.393	30226.393	30226.393	34345.900	23443.687
Mass fraction								
Benzene	1.000	1.000	0.893	0.619	0.619	0.619	0.608	0.001
Ethylene	0.000	0.000	0.107	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.340	0.340	0.340	0.356	0.907
Diethylbenzene	0.000	0.000	0.000	0.041	0.041	0.041	0.036	0.092
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream number	15	16	17	18	19	20	21
Vapor Pressure	1.000	0.000	1.000	0.000	0.000	0.000	0.000
Pressure (bar)	2.800	2.800	2.800	2.800	2.800	2.800	2.800
Temperature (°C)	180.913	180.913	117.246	117.246	117.246	117.246	117.246
Molar flow rate (kmol/hr)							
Benzene	0.099	0.134	424.423	424.423	424.423	157.352	267.071
Ethylene	0.000	0.000	0.106	0.106	0.106	0.039	0.067
Ethylbenzene	85.229	115.146	0.092	0.092	0.092	0.034	0.058
Diethylbenzene	6.819	9.212	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.049	0.049	0.049	0.018	0.031
Ethane	0.000	0.000	0.097	0.097	0.097	0.036	0.061
Total	92.146	124.492	424.767	424.767	424.767	157.479	267.287
Mole fraction							
Benzene	0.001	0.001	0.999	0.999	0.999	0.999	0.999
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.925	0.925	0.000	0.000	0.000	0.000	0.000
Diethylbenzene	0.074	0.074	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)							
Benzene	7.725	10.437	33155.888	33155.888	33155.888	12292.316	20863.571
Ethylene	0.000	0.000	2.977	2.977	2.977	1.104	1.873
Ethylbenzene	9048.731	12225.076	9.719	9.719	9.719	3.603	6.116
Diethylbenzene	915.225	1236.493	0.000	0.000	0.000	0.000	0.000

Methane	0.000	0.000	0.793	0.793	0.793	0.294	0.499
Ethane	0.000	0.000	2.917	2.917	2.917	1.081	1.835
Total	9971.680	13472.006	33172.292	33172.292	33172.292	12298.398	20873.894

Mass fraction

Benzene	0.001	0.001	1.000	1.000	1.000	1.000	1.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.907	0.907	0.000	0.000	0.000	0.000	0.000
Diethylbenzene	0.092	0.092	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream number	22	23	24	25	26	27	28
Vapor Pressure	0.000	0.000	0.000	0.000	0.000	1.000	0.000
Pressure (bar)	2.800	1.013	1.013	40.000	2.800	2.800	2.800
Temperature (°C)	77.138	77.138	77.138	77.138	229.529	229.529	229.529

Molar flow rate (kmol/hr)

Benzene	267.071	267.071	267.071	267.071	0.000	0.000	0.000
Ethylene	0.067	0.067	0.067	0.067	0.000	0.000	0.000
Ethylbenzene	0.058	0.058	0.058	0.058	0.066	0.008	0.058
Diethylbenzene	0.000	0.000	0.000	0.000	10.515	1.307	9.208
Methane	0.031	0.031	0.000	0.000	0.000	0.000	0.000
Ethane	0.061	0.061	0.000	0.000	0.000	0.000	0.000
Total	267.287	267.287	267.195	267.195	10.580	1.315	9.265

Mole fraction

Benzene	0.999	0.999	1.000	1.000	0.000	0.000	0.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.000	0.006	0.006	0.006
Diethylbenzene	0.000	0.000	0.000	0.000	0.994	0.994	0.994
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)							
Benzene	20863.571	20863.571	20863.571	20863.571	0.000	0.000	0.000
Ethylene	1.873	1.872	1.872	1.872	0.000	0.000	0.000
Ethylbenzene	6.116	6.116	6.116	6.116	6.980	0.867	6.113
Diethylbenzene	0.000	0.000	0.000	0.000	1411.259	175.384	1235.875
Methane	0.499	0.499	0.000	0.000	0.000	0.000	0.000
Ethane	1.835	1.835	0.000	0.000	0.000	0.000	0.000
Total	20873.894	20873.893	20871.559	20871.559	1418.239	176.251	1241.987
Mass fraction							
Benzene	1.000	1.000	1.000	1.000	0.000	0.000	0.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.000	0.000	0.000	0.005	0.005	0.005
Diethylbenzene	0.000	0.000	0.000	0.000	0.995	0.995	0.995
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream number	29	30	31	32	33	34	35
Vapor Pressure	0.000	1.000	0.000	0.000	0.000	0.000	0.000

Pressure (bar)	35.000	2.800	2.800	2.800	2.800	2.800	40.000
Temperature (°C)	229.529	178.586	178.586	178.586	178.586	178.586	77.138
Molar flow rate (kmol/hr)							
Benzene	0.000	0.236	0.236	0.236	0.102	0.134	36.831
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.009
Ethylbenzene	0.058	203.113	203.113	203.113	88.024	115.089	0.000
Diethylbenzene	9.208	0.008	0.008	0.008	0.004	0.005	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	9.265	203.357	203.357	203.357	88.130	115.227	36.841
Mole fraction							
Benzene	0.000	0.001	0.001	0.001	0.001	0.001	1.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.006	0.999	0.999	0.999	0.999	0.999	0.000
Diethylbenzene	0.994	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)							
Benzene	0.000	18.420	18.420	18.420	7.983	10.437	2877.262
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.258
Ethylbenzene	6.113	21564.503	21564.503	21564.503	9345.539	12218.964	0.000
Diethylbenzene	1235.875	1.091	1.091	1.091	0.473	0.618	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1241.987	21584.013	21584.013	21584.013	9353.994	12230.019	2877.520

Mass fraction							
Benzene	0.000	0.001	0.001	0.001	0.001	0.001	1.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.005	0.999	0.999	0.999	0.999	0.999	0.000
Diethylbenzene	0.995	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream number	36	37	38	39	40	41	42	43
Vapor Pressure	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000
Pressure (bar)	40.000	35.000	35.000	35.000	40.000	2.800	1.013	40.000
Temperature (°C)	210.000	216.016	229.529	180.644	120.624	120.624	77.138	77.138
Molar flow rate (kmol/hr)								
Benzene	36.831	36.831	27.628	27.628	27.628	27.628	0.000	230.239
Ethylene	0.009	0.009	0.009	0.009	0.009	0.009	0.000	0.058
Ethylbenzene	0.000	0.058	18.464	18.464	18.464	18.464	0.000	0.058
Diethylbenzene	0.000	9.208	0.005	0.005	0.005	0.005	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.031	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.061	0.000
Total	36.841	46.106	46.106	46.106	46.106	46.106	0.092	230.355
Mole fraction								
Benzene	1.000	0.799	0.599	0.599	0.599	0.599	0.000	1.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.001	0.400	0.400	0.400	0.400	0.000	0.000

Diethylbenzene	0.000	0.200	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.337	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.662	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Mass flow rate (kg/hr)								
Benzene	2877.262	2877.262	2158.306	2158.306	2158.306	2158.306	0.000	17986.309
Ethylene	0.258	0.258	0.258	0.258	0.258	0.258	0.001	1.614
Ethylbenzene	0.000	6.113	1960.325	1960.325	1960.325	1960.325	0.000	6.115
Diethylbenzene	0.000	1235.875	0.618	0.618	0.618	0.618	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.499	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	1.835	0.000
Total	2877.520	4119.508	4119.508	4119.508	4119.508	4119.508	2.335	17994.039
Mass fraction								
Benzene	1.000	0.698	0.524	0.524	0.524	0.524	0.000	1.000
Ethylene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethylbenzene	0.000	0.001	0.476	0.476	0.476	0.476	0.000	0.000
Diethylbenzene	0.000	0.300	0.000	0.000	0.000	0.000	0.000	0.000
Methane	0.000	0.000	0.000	0.000	0.000	0.000	0.214	0.000
Ethane	0.000	0.000	0.000	0.000	0.000	0.000	0.786	0.000
Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

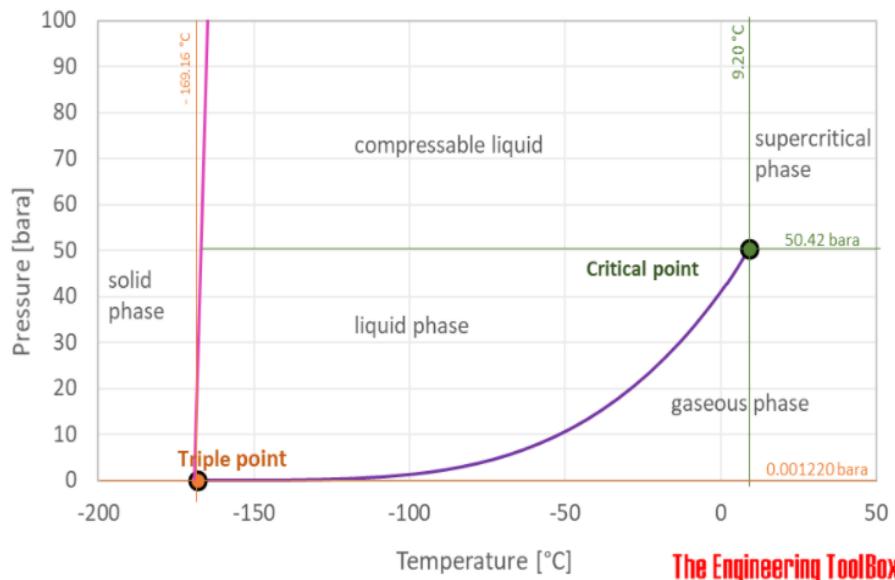
APPENDIX C: THERMODYNAMIC DATA

Calculation Formula
Heat capacity, $C_p [J/(kmol.K)] = C1 + C2 \times T + C3 \times T^2 + C4 \times T^3 + C5 \times T^4$
Heat capacity, $C_p [J/(mol.K)] = A + BT + CT^2 + DT^3$
Heat capacity, $C_p [J/(mol.K)] = R + (a0 + a1T + a2T^2 + a3T^3 + a4T^4), \quad R=8.3143 J/(mol.K)$
Density, $\rho (g/ml) = A * B^{-(1 - \frac{T}{T_c})^n}, T(K)$

Density of gas:

$$W_{A \rightarrow B} = - \int_{V_A}^{V_B} p dV = - \int_{V_A}^{V_B} \frac{nRT}{V} dV = -nRT \int_{V_A}^{V_B} \frac{1}{V} dV = -nRT \ln \frac{V_B}{V_A}$$

Ethylene phase diagram



The Engineering ToolBox

Figure C.1 Equation and diagram used for thermodynamic calculation

Table C 1 Liquid state heat capacity of components.

Components	Liquid State Heat Capacity (J/K.mol)				
	A	B	C	D	E
Benzene	-31.662	1.30E+00	-3.61E-03	3.82E-06	0
Ethylene	25.597	5.71E-01	-3.36E-03	8.41E-06	0
Ethylbenzene	102.111	5.60E-01	-1.56E-03	2.01E-06	0
Diethylbenzene	104.866	1.04E+00	-2.68E-03	2.95E-06	0
Methane	-0.018	1.20E+00	-9.87E-03	3.17E-05	0
Ethane	38.332	4.10E-01	-2.30E-03	5.93E-06	0

Table C 2 Gaseous state heat capacity of components

Components	Gaseous State Heat Capacity (J/K.mol)				
	C1	C2	C3	C4	C5
Benzene	-31.368	4.75E-01	-3.11E-04	8.52E-08	-5.05E-12
Ethylene	32.083	-1.48E-02	2.48E-04	-2.38E-07	6.83E-11
Ethylbenzene	-20.527	5.96E-01	-3.08E-04	3.56E-08	1.24E-11
Diethylbenzene	28.958	5.22E-01	4.43E-05	-2.79E-07	1.00E-10
Methane	34.942	-4.00E-02	1.92E-04	-1.53E-07	3.93E-11
Ethane	28.146	4.34E-02	1.89E-04	-1.91E-07	5.33E-11

Table C 3Latent heat of vaporization of components.

Latent Heat of Vaporization		
Components	Hv (J/kmol)	Normal boiling point
Benzene	3.08E+07	8.0100E+01
Ethylene	1.35E+07	-1.0390E+02
Ethylbenzene	3.60E+07	1.3620E+02
Diethylbenzene	4.58E+07	1.8000E+02
Methane	9.40E+05	-1.6140E+02
Ethane	2.86E+06	-8.8800E+01

Table C 4Specific heat of formation of components

Specific Heat of Formation at 25°C	
Components	Hf (J/kmol)
Benzene	4.87E+07
Ethylene	5.29E+07
Ethylbenzene	1.25E+07
Diethylbenzene	-7.28E+07
Methane	-7.49E+07
Ethane	-8.47E+07

Table C 5Physical properties of components

Physical Properties		
Components	Molecular Weight, kg/kmol	Specific Gravity
Benzene	7.81E+01	8.79E-01
Ethylene	2.91E+01	1.05E+00
Ethylbenzene	1.06E+02	8.67E-01
Diethylbenzene	1.34E+02	8.60E-01
Methane	1.60E+01	5.54E-01
Ethane	3.01E+01	5.46E-01

Table C 6Density of components.

Density of Pure Components Liquid (g/ml)					
Components	A	B	n	T _c	T _{range, K}
Benzene	3.01E-01	2.68E-01	2.82E-01	5.62E+02	278.68-562.16
Ethylbenzene	2.89E-01	2.64E-01	2.92E-01	6.17E+02	178.2-617.17
1,4 Diethylbenzene	2.71E-01	2.54E-01	2.86E-01	6.58E+02	230.32-657.96

Table C 7Reference state of components.

Reference State			
Components	Temperature, T (K)	Pressure, P (bar)	State
Benzene	298.15	1	Liquid
Ethylene	298.15	1	Gas
Ethylbenzene	298.15	1	Liquid
Diethylbenzene	298.15	1	Liquid
Methane	298.15	1	Gas
Ethane	298.15	1	Gas
Water	298.15	1	Liquid

Table C 8Reference condition for each component (excluding utilities)

Reference Condition			
Components	Temperature (°C)	Pressure (bar)	State
Benzene	25	1	Liquid
Ethylene	25	1	Gas
Ethylbenzene	25	1	Liquid
Diethylbenzene	25	1	Liquid
Methane	25	1	Gas
Ethane	25	1	Gas

Table C 9Reference condition for utilities:

Reference Condition			
Utilities	Temperature (°C)	Pressure (bar)	State
High Pressure Steam	250.3	1	Gas
Cooling Water	25	1	Liquid

APPENDIX D ENERGY BALANCE OF EACH INDIVIDUAL UNIT OPERATION

Benzene Feed Pump, P-101

Benzene Feed Mixing Point

Compressor, C-101

Condenser, E-101

E-101	In													Out											
Stream	S-4							S-5						Vapor fraction	0.0000	0.0000	Pressure (bar)	50.0000	50.0000	Temperature (°C)	25.0000	9.0000	0.0000	0.0000	0.0000
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)							
Benzene	0.0000	1876784.9149	30765000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-2183366.6040	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	441086.0148	0.0000	0.0000	0.0000	0.0000		
Ethylene	115.0979	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	115.0979	-675726.3331	-13540000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	137722.5263	0.0000	0.0000	-2320316782.4627			
Ethylbenzene	0.0079	12434707.7905	35980000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0079	-2916645.1393	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	607781.3057	0.0000	0.0000	-18342.3946			
Diethylbenzene	0.0000	15604765.3051	45800000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-4062088.9654	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	774693.5047	0.0000	0.0000	0.0000	0.0000		
Methane	0.0311	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0311	-41086349.5431	-940000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	143714.3466	0.0000	0.0000	-1302213.7644			
Ethane	0.0610	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0610	-3856231.1946	-2859000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	273367.1410	0.0000	0.0000	-39162.3691			
Total	115.1980	0.0000	112545000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	384622.8003	115.1980	-60861307.7795	-17339000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2378354.8390	0.0000	0.0000	-2322030500.9908			
Final Enthalpy Flow Rate (Ml/hr)									0.3846										-2322.42						
Heat Duty (Mj/hr)																									

Heat Exchanger, E-102

E-102	Out													Out												
Stream	S-6							S-7						Vapor fraction	0.0000	0.0000	Pressure (bar)	40.0000	40.0000	Temperature (°C)	60.1156	155.5998	0.0000	0.0000	0.0000	0.0000
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)								
Benzene	345.4664	4946452.6214	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	1830115363.0391	345.4664	1.96E+07	0.00E+00	0	0	3.51E+05	0	0	0	0	6.90E+09	0	0	0	0		
Ethylene	0.0575	-4655768.0519	-13540000.0000	0.0000	0.0000	109615.8883	0.0000	0.0000	-1040755.6228	0.0575	8.94E+05	-1.35E+07	0	0	1.10E+05	0	0	0	0	-7.21E+05	0	0	0	0		
Ethylbenzene	0.0497	6553953.5222	0.0000	0.0000	0.0000	483744.3045	0.0000	0.0000	349503.6021	0.0497	2.57E+07	0.00E+00	0	0	4.84E+05	0	0	0	0	1.30E+06	0	0	0	0		
Diethylbenzene	0.0000	9123057.0491	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	9.00E+07	0.00E+00	0	0	0	0	6.17E+05	0	0	0	0	0.00E+00	0	0	0	0		
Methane	0.0000	-3957982.5260	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	-3.44E+07	-9.40E+05	0	0	0	0	1.14E+05	0	0	0	0	0.00E+00	0	0	0	0		
Ethane	0.0000	-1319327.4069	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	-3.08E+07	-9.40E+05	0	0	0	0	2.18E+05	0	0	0	0	0.00E+00	0	0	0	0		
Total	345.5736	-2493154.9320	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	182942410.4784	345.5736	52084572.0697	-17339000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	68992273.7204				
Final Enthalpy Flow Rate (Ml/hr)									1829.4241																	
Heat Duty (Mj/hr)										5069.80																

Heater, E-103

E-103 Heater	In													Out												
Stream	S-7							S-8						Vapor fraction	0.0000	0.0000	Pressure (bar)	40.0000	40.0000	Temperature (°C)	155.5998	200.0000	0.0000	0.0000	0.0000	0.0000
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)								
Benzene	345.4664	19618003.6329	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	6898642791.0614	345.4664	2.73E+07	0.00E+00	0	0	3.51E+05	0	0	0	0	9.56E+09	0	0	0	0		
Ethylene	0.0575	893530.0892	-13540000.0000	0.0000	0.0000	109615.8883	0.0000	0.0000	-721424.9443	0.0575	3.92E+06	-1.35E+07	0	0	1.10E+05	0	0	0	0	-5.47E+05	0	0	0	0		
Ethylbenzene	0.0497	25721023.3823	0.0000	0.0000	0.0000	483744.3045	0.0000	0.0000	1301369.6032	0.0497	3.56E+07	0.00E+00	0	0	4.84E+05	0	0	0	0	1.79E+06	0	0	0	0		
Diethylbenzene	0.0000	35548482.1761	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	0	0.0000	4.89E+07	0.00E+00	0	0	6.17E+05	0	0	0	0	0.00E+00	0	0	0	0		
Methane	0.0000	-34386137.2941	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	0	0.0000	0.0000	-3.08E+07	-9.40E+05	0	0	1.14E+05	0	0	0	0	0.00E+00	0	0	0	0	
Ethane	0.0000	4689670.0833	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	0	0.0000	7.88E+06	-2.86E+06	0	0	2.18E+05	0	0	0	0	0.00E+00	0	0	0	0		
Total	345.5736	52084572.0697	-17339000.0000	0.0000	0.0000	1892976.3024	0.0000	0.0000	689922735.7204	345.5736	92791062.0830	-17339000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	9565.812574				
Total Enthalpy Flow Rate (Ml/hr)									6899.22736																	
Heat Duty (Mj/hr)										2666.59																

Reactor Input Mixing point

Reactor/Inlet	In												Out																	
Stream																														
Vapor fraction	0.0000						0.0000						0.0000						0.0000											
Pressure (bar)	40.0000						50.0000						0.0000						40.0000											
Temperature (°C)	200.0000						182.4635						182.4635						182.4635											
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Enthalpy Change, ΔH (J/hr)				
Benzene	345.4664	27334993.4879	0.0000	0.0000	351068.4608	0.0000	0.0000	965643694.7720	0.0000	-2183306.6040	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	345.4664	2419543.9694	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	84806568.1484			
Ethylene	0.0575	89353.9138	13540000.0000	0.0000	109615.8883	0.0000	547006.6980	115.0979	457522.3331	13540000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	109615.8883	109615.8883	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	123738934.6449			
Ethylbenzene	0.1497	3557802.2791	0.0000	0.0000	483744.3045	0.0000	0.0000	1790346.5138	0.0000	-2958648.3567	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	483744.3045	18842.3946	0.0576	3150451.7533	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1847020.5722	
Diethylbenzene	0.0100	1523.0723	0.0000	0.0000	52932.0253	0.0000	0.0000	1790346.5138	0.0000	-2958648.3567	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	52932.0253	18842.3946	0.0576	3150451.7533	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	107470.8163	
Methane	0.0000	3862684.3119	9460000.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	114384.8881	145714.3466	0.0311	3340415.1575	9460000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	105318.8105
Ethane	0.0000	7884469.7909	-2859000.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	217577.9286	27334993.4879	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	240715.3879			
Total	345.5736	52084572.0697	-17339000.0000	0.0000	892976.3004	0.0000	0.0000	1892976.3004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	892976.3004	4087136	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	124760313.6250				
Heat Duty (Mj/hr)		9650.8126																									7243.7621			

Alkylator, R-101

R-101	In												Out																
Stream																													
Vapor fraction	0.0000						0.0000						0.0000						0.0000										
Pressure (bar)	40.0000						40.0000						200.0000						200.0000										
Temperature (°C)	182.4635						182.4635						182.4635						182.4635										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Enthalpy Change, ΔH (J/hr)			
Benzene	345.4664	19618003.6329	0.0000	0.0000	351068.4608	0.0000	0.0000	689642791.0614	239.5763	2.73E+07	0.00E+00	4.87E+07	0	0.00E+00	0	0.00E+00	0	3.51E+05	0	0.00E+00	6.63E+09								
Ethylene	115.1555	893530.6892	-1354000.0000	0.0000	109615.8883	0.0000	483744.3045	0.0000	-721424.9443	0.0576	3.92E+06	-1.35E+07	5.29E+07	0	0.00E+00	0	1.10E+05	0	0.00E+00	-5.47E+05									
Ethylbenzene	0.0576	25721023.3823	0.0000	0.0000	483744.3045	0.0000	1301369.6032	96.7398	3.56E+07	0.00E+00	1.29E+07	0	0.00E+00	0	4.84E+05	0	0.00E+00	0	3.49E+09										
Diethylbenzene	0.0000	35548482.1761	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	9.2078	4.89E+07	0.00E+00	-7.28E+07	0	0.00E+00	0	6.17E+05	0	0.00E+00	0	4.56E+08									
Methane	0.0311	-34386137.2941	-946000.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	0.0311	-3.08E+07	-9.40E+05	-7.49E+07	0	1.14E+05	0	0.00E+00	0	2.18E+05	0	0.00E+00	-9.84E+05								
Ethane	0.0610	4689670.0833	-2859000.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	0.0610	7.88E+06	-2.86E+06	-2.86E+06	0	0.00E+00	0	2.18E+05	0	0.00E+00	0	0.00E+00	-1.74E+04								
Total	345.5736	52084572.0697	-17339000.0000	0.0000	892976.3004	0.0000	0.0000	1892976.3004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00E+00	1.89E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.51E+03			
Heat Duty (Mj/hr)		6899.2227																											
		-7028.01																											

Heat Exchanger, E-102

E-102 (Process Fluid to heat S-6)	In												Out											
Stream																								
Vapor fraction	0.0000						0.0000						0.0000						0.0000					
Pressure (bar)	40.0000						40.0000						40.0000						40.0000					
Temperature (°C)	120.6244						120.6244						120.6244						120.6244					
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporation, Hv (J/kmol)	Specific Heat of Formation, Hf (J		

Liquid Expander, C-102

C-102																		
Stream	In							Out										
Vapor fraction	S-11							S-12										
Pressure (bar)	0.0000							0.0000										
Temperature (°C)	40.0000							2.8000										
	120.6244							120.6244										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	239.5763	13998650.2682	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	3437852797.2781	239.5763	13998650.2682	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	335762700.9696
Ethylene	0.0576	-1291470.6074	-13540000.0000	0.0000	0.0000	105915.8883	0.0000	0.0000	-847650.9445	0.0576	-1291470.6074	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	-853671.0814
Ethybenzene	96.7398	1842873.6811	0.0000	0.0000	0.0000	483744.3045	0.0000	0.0000	1829603323.9583	96.7398	1842873.6811	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	1784965862.5359
Diethylbenzene	9.2078	25558364.9851	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	241014494.3998	9.2078	25558364.9851	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	235599120.1913
Methane	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	-1161052.2183	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	-116444.5262
Ethane	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	217487.9286	0.0000	0.0000	-17368.2050	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	-3034.6155
Total	345.6737	22534375.0344	-17339000.0000	0.0000	0.0000	182976.3004	0.0000	0.0000	550644544.2684	345.6737	22534375.0344	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	537614383.4737
Total Enthalpy Flow Rate (MJ/hr)	5506.4445							5376.1438										
Heat Duty (MJ/hr)	-130.30																	

Overall Boundary for T-201

Overall boundary for T-201																			
Stream	In								Out										
Vapor fraction	S-13								S-16										
Pressure (bar)	0.0000								0.0000										
Temperature (°C)	120.6244								180.9130										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	267.9944	13998650.2681	0.0000	0.0000	0.0000	3437852797.2781	0.0000	0.0000	3437852797.2781	267.9944	13998650.2681	0.0000	0.0000	0.0000	20201.1597	0.0000	0.0000	310443.3854	
Ethylene	0.0658	-1291470.6074	-13540000.0000	0.0000	0.0000	105915.8883	0.0000	0.0000	-847650.9445	0.0658	-1291470.6074	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	360397764.0096	
Ethybenzene	115.2118	1842873.6811	0.0000	0.0000	0.0000	22126.6602	0.0000	0.0000	21579872.0200	0.0576	17743074.9737	0.0000	0.0000	0.0000	115.1542	0.0000	0.0000	22326.6602	
Diethylbenzene	9.2124	25558364.9851	0.0000	0.0000	0.0000	26474.8324	0.0000	0.0000	241014494.3998	9.2124	25558364.9851	0.0000	0.0000	0.0000	21347.5713	0.0000	0.0000	235599120.1913	
Methane	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	-1161052.2183	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	-116444.5262	
Ethane	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	303934.6355	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	6473034.3211	0.0000	0.0000	10042.0582	
Total	399.7809	22534375.0344	-17339000.0000	0.0000	0.0000	69349679.0863	267.2673	303934.6355	-17339000.0000	0.0000	399.7809	22534375.0344	-17339000.0000	0.0000	124.5002	24949602.9809	27339000.0000	0.0000	87368.1369
Total Enthalpy Flow Rate (MJ/hr)	6504.1598							5622.4139							4001.0546				
Heat Duty (MJ/hr)	1509.29																		

Distillation Column, T-201

T-201																				
Stream	In							Out												
	S-13		S-15		S-16		S-17		S-18		S-19									
Vapor fraction	0.0000							1.0000												
Pressure (bar)	2.8000							2.8000												
Temperature (°C)	120.6244							180.9130												
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	M	
Benzene	267.2044	13998650.2682	0.0000	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0989	3744830600.8605	19426760.2799	30765000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	4963787.5393	
Ethylene	0.0668	-1291470.6074	-13540000.0000	0.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	-900153.2764	0.0000	7849883.8950	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethylbenzene	115.2118	18428873.6811	0.0000	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	212579582.0000	85.2407	29788699.5462	35980000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	5606168122.1719
Diethylbenzene	9.2124	2558364.9851	0.0000	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	235716919.7219	6.8193	43012286.0693	45800000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	60564003.5424
Methane	0.0311	-36516891.8026	-9400000.0000	0.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	-1164444.5262	0.0000	6205773.2365	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	0.0000	1042.0582	0.0000	0.0000	-30034.6155	0.0000	970943.3577	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Total	391.7875	22534375.0344	0.0000	0.0000	0.0000	0.0000	8768.1369	0.0000	0.0000	6104158760.1663	92.1589	115987345.3846	112545000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	621671953.2536
Total Enthalpy Flow Rate (Mj/hr)							6104.1588												6216.7720	
Heat Duty (Mj/hr)																				

Condenser, E-201

E-201																			
Stream	In							Out											
	S-17		S-18		S-19		S-20		S-21		S-22		S-23						
Vapor fraction	1.0000							0.0000											
Pressure (bar)	2.8000							2.8000											
Temperature (°C)	117.2462							117.2462											
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	M
Benzene	424.4258	11806051.2138	30765000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1806825413.4927	424.4258	13472949.6742	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	572514465.4991
Ethylene	0.1061	439406.7565	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	466382.2303	0.1061	42017193.7103	-13540000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	302284.3974
Ethylbenzene	0.0915	1839066.6823	35980000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	4977468.8914	0.0915	17743074.9737	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1626362.4138	
Diethylbenzene	0.0000	2777232.0341	45800000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	24614285.3279	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Methane	0.0494	350759.4742	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	174458.3557	0.0494	17625672.9416	-940000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	8662783.5390
Ethane	0.0970	5400224.4777	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	523778.3706	0.0970	2736603.1639	-2859000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2378014.5284
Total	424.7699	7129504.6387	112545000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	18074394501.3407	424.7699	30146779.7916	-17339000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	5740834472.3777
Total Enthalpy Flow Rate (Mj/hr)																		5.74E+03	
Heat Duty (Mj/hr)																			18074.3945
																			-12333.56

Reflux Drum, V-201

V-201	In	Out																			
Stream	In	Out																			
	5.18	5.20																			
Vapor fraction	0.0000	0.0000																			
Pressure [bar]	2.8000	2.8000																			
Temperature (°C)	117.2462	117.2462																			
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)			
Benzene	424.4258	13472949.6742	0.0000	0.0000	16203.1597	0.0000	5725144465.4991	157.3550	13472949.6742	361203.1597	2127585560.7269	267.0708	13472949.6742	0.0000	0.0000	16203.1597	0.0000	0.0000	360253894.7721		
Ethane	0.0668	42017193.7103	-13540000.0000	0.0000	5059.1948	0.0000	1902132.2994	0.0000	1902132.2994	0.0668	24838728.3382	-13540000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	5059.1948	0.0000		
Ethylene	0.0576	17743074.9737	0.0000	0.0000	22326.6602	0.0000	10482642.4138	0.0339	17743074.9737	0.0000	602075.5271	0.0576	0.0000	0.0000	0.0000	0.0000	0.0000	22326.6602	0.0000		
Diethylbenzene	0.0000	24614285.3279	0.0000	0.0000	28457.7614	0.0000	0.0000	0.0000	0.0000	361203.1597	267.0708	2127585560.7269	267.0708	13472949.6742	0.0000	0.0000	13472949.6742	0.0000	0.0000		
Dimethylbenzene	0.0000	24614285.3279	0.0000	0.0000	279.0251	0.0000	80250.0000	0.0000	80250.0000	0.0000	22326.6602	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	22326.6602	0.0000		
Methane	0.0311	176255672.9416	-940000.0000	0.0000	5279.3025	0.0000	0.0000	0.0000	0.0000	5451074.3208	0.0311	111583811.4026	-940000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	5279.3025	0.0000	
Ethane	0.0610	27366603.1639	-285900.0000	0.0000	10042.0582	0.0000	0.0000	1496370.5225	0.0610	15245821.0692	-285900.0000	0.0000	0.0000	0.0000	0.0000	0.0000	10042.0582	0.0000	0.0000		
Total	424.4258	301469779.7916	-17390000.0000	0.0000	87368.1369	0.0000	0.0000	0.0000	0.0000	3612431873.8015	267.0708	182553599.4476	-17390000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	87368.1369	0.0000	
Total Enthalpy Flow Rate (M/hr)					3612.4319														1991.7937		
Heat Duty (M/hr)																				-1620.64	

Reboiler, E-202

E-202	In	Out																						
Stream	In	Out																						
	5.14	5.15																						
Vapor fraction	0.00	0.00																						
Pressure [bar]	2.8000	2.8000																						
Temperature (°C)	180.9130	180.9130																						
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)						
Benzene	0.0315	31018464.4832	0.0000	0.0000	16203.1597	0.0000	0.0000	566019.6077	0.0895	194260.7199	302500.0000	0.0000	0.0000	0.0000	4963870.5300	0.1136	21018464.4832	0.0000	0.0000	16203.1597	0.0000	0.0000	31018464.4832	
Ethylene	0.0000	8253926.9172	-13540000.0000	0.0000	5059.1948	0.0000	0.0000	0.0000	0.0000	794983.8950	0.0000	0.0000	0.0000	0.0000	0.0000	257680.3254	-13540000.0000	0.0000	5059.1948	0.0000	0.0000	0.0000		
Ethylene	200.3940	3124792.0871	0.0000	0.0000	22326.6602	0.0000	0.0000	626939129.7266	85.2407	2978898.5462	3998000.0000	0.0000	0.0000	0.0000	560616812.3219	115.1542	3124792.0871	0.0000	0.0000	22326.6602	0.0000	0.0000	360297768.0096	
Dimethylbenzene	0.0000	24614285.3279	0.0000	0.0000	279.0251	0.0000	0.0000	0.0000	0.0000	428250.0000	0.0000	0.0000	0.0000	0.0000	0.0000	428250.0000	0.0000	0.0000	279.0251	0.0000	0.0000	0.0000		
Methane	0.0000	33831534.6779	-940000.0000	0.0000	5279.3025	0.0000	0.0000	0.0000	0.0000	620573.2865	0.0000	0.0000	0.0000	0.0000	0.0000	3253154.7279	-940000.0000	0.0000	5279.3025	0.0000	0.0000	0.0000		
Ethane	0.0000	5597380.2098	-285900.0000	0.0000	10042.0582	0.0000	0.0000	0.0000	0.0000	9703943.3277	0.0000	0.0000	0.0000	0.0000	0.0000	6473038.3291	-285900.0000	0.0000	10042.0582	0.0000	0.0000	0.0000		
Total	256.6591	965340285.9562	-17390000.0000	0.0000	87368.1369	0.0000	0.0000	0.0000	0.0000	626939129.7266	224.3602	428250.0000	0.0000	0.0000	0.0000	428250.0000	224.3602	7449802.0869	-17390000.0000	0.0000	87368.1369	0.0000	0.0000	40029484.9701
Total Enthalpy Flow Rate (M/hr)					6962.6888														4.00e+03					
Heat Duty (M/hr)																				525.30				

Cooler, E-203

E-203	In	Out																				
Stream	In	Out																				
	S-21	S-22																				
Vapor fraction	0.0000	0.0000																				
Pressure [bar]	2.8000	2.8000																				
Temperature (°C)	117.2462	77.1381																				
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/hr)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)				
Benzene	267.0708	13472949.6742	0.0000	0.0000	16203.1597	0.0000	0.0000	3602558904.7721	267.0708	7421057.7551	0.0000	0.0000	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	13472949.6742			
Ethylene	0.0668	42017193.7103	-13540000.0000	0.0000	5059.1948	0.0000	0.0000	1902132.2994	0.0668	24838728.3382	-13540000.0000	0.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	754901.6380	0.0000	0.0000	0.0000	
Ethylene	0.0576	17743074.9737	0.0000	0.0000	22326.6602	0.0000	0.0000	1023391.8867	0.0576	9813585.2052	0.0000	0.0000	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	56606.5203	0.0000	0.0000	0.0000
Diethylbenzene	0.0000	24614285.3279	0.0000	0.0000	28457.7614	0.0000	0.0000	13650595.6573	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	0.0000	
Methane	0.0311	176255672.9416	-940000.0000	0.0000	5279.3025	0.0000	0.0000	5451074.3208	0.0311	111583811.4026	-940000.0000	0.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	3402938.5452	0.0000	0.0000	0.0000	
Ethane	0.0610	27366603.1639	-285900.0000	0.0000	10042.0582	0.0000	0.0000	1496370.5225	0.0610	15245821.0692	-285900.0000	0.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	756610.2041	0.0000	0.0000	0.0000	
Total	267.2873	301469779.7916	-17390000.0000	0.0000	87368.1369	0.0000	0.0000	3612431873.8015	267.0708	182553599.4476	-17390000.0000	0.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	199179361.0281	0.0000	0.0000	0.0000	
Total Enthalpy Flow Rate (M/hr)					3612.4319														1991.7937			
Heat Duty (M/hr)																				-1620.64		

Liquid Expander, C-201

C-201																			
Stream	In							Out											
	S-23							S-23											
Vapor fraction			0.0000							0.0003									
Pressure (bar)			2.8000							1.0133									
Temperature (°C)			77.1381							77.1381									
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	267.0708	7421057.7751	0.0000	0.0000	16203.1597	0.0000	0.0000	1986275264.1204	267.0708	7421057.7751	0.0000	0.0000	0.0000	119.7233	0.0000	0.0000	1981979847.8208		
Ethylene (liquid)	0.0668	24838728.3382	-13540000.0000	0.0000	5059.1948	0.0000	0.0000	754901.6380	0.0667	24838728.3382	-13540000.0000	0.0000	37.3818	0.0000	0.0000	754188.9828			
Ethy(benzene	0.0576	9813585.2052	0.0000	0.0000	23236.6602	0.0000	0.0000	566606.5203	0.0576	9813585.2052	0.0000	0.0000	0.0000	164.9692	0.0000	0.0000	56320.8762		
Diethylbenzene	0.0000	1365095.6573	0.0000	0.0000	28457.7614	0.0000	0.0000	0.0000	0.0000	1365095.6573	0.0000	0.0000	0.0000	210.2712	0.0000	0.0000	0.0000		
Methane (liquid)	0.0311	111583811.4026	-940000.0000	0.0000	5279.3025	0.0000	0.0000	3440298.5452	0.0000	111583811.4026	-940000.0000	0.0000	39.0082	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane (liquid)	0.0610	15245821.0692	-2859000.0000	0.0000	10042.0582	0.0000	0.0000	756610.2041	0.0000	15245821.0692	-2859000.0000	0.0000	74.1997	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethylene (vapor)										0.0000	2397552.7256	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	80.0580
Methane (vapor)										0.0311	1949310.2662	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	60607.9022
Ethane (vapor)										0.0610	2932267.1877	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	178963.2791
Total	267.2873	182553599.4476	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	1991793681.0281	267.2873	189832729.6272	-17339000.0000	0.0000	645.5535	0.0000	0.0000	1983539017.9191		
Total Enthalpy Flow Rate (MJ/hr)						1991.7937								1983.5390					
Heat Duty (MJ/hr)																			

Flash Drum, V-202

V-202																		
Stream	In							Out										
	S-23							S-24										
Vapor fraction			0.0003							0.0000								
Pressure (bar)			1.0133							1.0133								
Temperature (°C)			77.1381							77.1381								
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	267.0708	7421057.7751	0.0000	0.0000	119.7233	0.0000	0.0000	1981979847.8208	267.0708	7421057.7751	0.0000	0.0000	0.0000	119.7233	0.0000	0.0000	1981979847.8208	
Ethylene (liquid)	0.0667	24838728.3382	-13540000.0000	0.0000	37.3818	0.0000	0.0000	754901.6380	0.0667	24838728.3382	-13540000.0000	0.0000	37.3818	0.0000	0.0000	754188.9828		
Ethy(benzene	0.0576	9813585.2052	0.0000	0.0000	164.9692	0.0000	0.0000	56320.8762	0.0576	9813585.2052	0.0000	0.0000	0.0000	164.9692	0.0000	0.0000	56320.8762	
Diethylbenzene	0.0000	1365095.6573	0.0000	0.0000	210.2712	0.0000	0.0000	0.0000	0.0000	1365095.6573	0.0000	0.0000	0.0000	210.2712	0.0000	0.0000	0.0000	
Methane (liquid)	0.0000	111583811.4026	-940000.0000	0.0000	31.0062	0.0000	0.0000	0.0000	0.0000	111583811.4026	-940000.0000	0.0000	39.0082	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane (liquid)	0.0610	15245821.0692	-2859000.0000	0.0000	74.1997	0.0000	0.0000	0.0000	0.0000	15245821.0692	-2859000.0000	0.0000	74.1997	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene (vapor)										80.0580								
Methane (vapor)	0.0311	1949310.2662	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	60607.9022								
Ethane (vapor)	0.0610	2932267.1877	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	178963.2791								
Total	267.2873	189832729.6272	-17339000.0000	0.0000	645.5535	0.0000	0.0000	1983539017.9191	267.1952	182553599.4476	-17339000.0000	0.0000	645.5535	0.0000	0.0000	1983299366.7978		
Total Enthalpy Flow Rate (MJ/hr)						1983.5390								1986.03				
Heat Duty (MJ/hr)																		

	Out							
	S-42							
	1.0000							
Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
0.0000	7.56E+06	30760000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	2.40E+07	85.0000	0.0000	0.0000	0.0000	0.0000	0.0000	85.0000
0.0000	1.20E+07	35900000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0000	1.91E+07	45800000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0311	1.95E+06	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	60607.9022
0.0610	2.93E+06	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	178963.2791
	0.0922	4056938.8233	112545000.0000	0.0000	0.0000	0.0000	0.0000	238651.2393
				2.40E-01				

Pump, P-201

P-201																		
Stream	In							Out										
	S-24	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	S-25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000				
Vapor fraction								Pressure (bar)							40.0000			
Temperature (°C)								77.1381							77.1381			
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	267.0708	7421057.7751	0.0000	0.0000	0.0000	119.7233	0.0000	0.0000	1981979847.8208	267.0708	7421057.7751	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	207570809.5979
Ethylene	0.0667	24839728.3382	-13540000.0000	0.0000	0.0000	37.3818	0.0000	0.0000	754188.9828	0.0667	24839728.3382	-13540000.0000	0.0000	109615.8883	0.0000	0.0000	761503.3129	
Ethybenzene	0.0576	9813585.2052	0.0000	0.0000	0.0000	164.9692	0.0000	0.0000	565329.8762	0.0576	9813585.2052	0.0000	0.0000	483744.3045	0.0000	0.0000	593186.8973	
Diethylbenzene	0.0000	1365095.6573	0.0000	0.0000	0.0000	210.2712	0.0000	0.0000	0.0000	0.0000	1365095.6573	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	
Methane	0.0000	111583811.4026	-940000.0000	0.0000	0.0000	39.0082	0.0000	0.0000	0.0000	0.0000	111583811.4026	-940000.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	
Ethane	0.0000	15245821.0692	-2859000.0000	0.0000	0.0000	74.1997	0.0000	0.0000	0.0000	0.0000	15245821.0692	-2859000.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	
Total	267.1952	182553599.4476	-17339000.0000	0.0000	0.0000	645.5535	0.0000	0.0000	1983299346.6798	267.1952	182553599.4476	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	2077062699.8081
Total Enthalpy Flow Rate (MJ/hr)				1983.2994										2077.0627				
Heat Duty (MJ/hr)								93.76										

Separating Point after P-201

Separating point																		
Stream	In							Out										
	S-25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	S-35	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000				
Vapor fraction								40.0000										
Pressure (bar)								77.1381										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	267.0708	7421057.7751	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	207570809.5979	36.8313	7421057.7751	0.0000	0.0000	351068.4608	0.0000	0.0000	286257604.2669	
Ethylene	0.0667	24839728.3382	-13540000.0000	0.0000	0.0000	109615.8883	0.0000	0.0000	24939728.3382	0.0667	109615.8883	-13540000.0000	0.0000	109615.8883	0.0000	0.0000	109317.7159	
Ethybenzene	0.0576	9813585.2052	0.0000	0.0000	0.0000	483744.3045	0.0000	0.0000	593186.8973	0.0576	9813585.2052	0.0000	0.0000	483744.3045	0.0000	0.0000	81895.4656	
Diethylbenzene	0.0000	1365095.6573	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	0.0000	1365095.6573	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	
Methane	0.0000	111583811.4026	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	0.0000	111583811.4026	-940000.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	
Ethane	0.0000	15245821.0692	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	0.0000	15245821.0692	-2859000.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	
Total	267.1952	182553599.4476	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	2077062699.8081	36.8485	182553599.4476	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	28644427.4683
Total Enthalpy Flow Rate (MJ/hr)				2077.0627											286.4444			0.00
Heat Duty (MJ/hr)																		

Stream	In							Out										
	S-43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	S-51	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000				
Vapor fraction								40.0000										
Pressure (bar)								77.1381										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	230.7395	7421057.7751	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000	179450405.3111									
Ethylene	0.0575	24839728.3382	-13540000.0000	0.0000	0.0000	109615.8883	0.0000	0.0000	650485.5970									
Ethybenzene	0.0497	9813585.2052	0.0000	0.0000	0.0000	483744.3045	0.0000	0.0000	511381.4317									
Diethylbenzene	0.0000	1365095.6573	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000									
Methane	0.0000	111583811.4026	-940000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	0.0000									
Ethane	0.0000	15245821.0692	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	0.0000									
Total	230.7395	182553599.4476	-17339000.0000	0.0000	0.0000	17906183	0.0000	0.0000	179061827.3398									

Overall Boundary for T-401

Overall Boundary System for T-401																		
Stream	In							Out										
	S-16							S-34										
	Vapor fraction	0.0000							0.0000									
	Pressure (bar)	2.8000							2.8000									
Temperature (°C)	180.9130							178.3856										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
Benzene	0.1336	23923846.4832	0.0000	0.0000	16203.1597	0.0000	0.0000	3198443.3854	0.1336	23518185.2068	0.0000	0.0000	16203.1597	0.0000	0.0000	3144246.1450		
Ethylene	0.0000	2578683.3254	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	80721476.1397	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	0.0000		
Ethylbenzene	115.1542	31247902.0871	0.0000	0.0000	22326.6602	0.0000	0.0000	360089768.0096	115.0966	30729920.2215	0.0000	0.0000	22326.6602	0.0000	0.0000	353479362.4171		
Diethylbenzene	9.2124	43056619.1041	0.0000	0.0000	28457.7614	0.0000	0.0000	396918433.5751	0.0046	42355380.0089	0.0000	0.0000	28457.7614	0.0000	0.0000	19529.1573		
Methane	0.0000	-32531054.7479	-940000.0000	0.0000	5279.3025	0.0000	0.0000	0.0000	0.0000	32197143.8805	-940000.0000	0.0000	5279.3025	0.0000	0.0000	0.0000		
Ethane	0.0000	6473034.3291	-2859000.0000	0.0000	10042.0582	0.0000	0.0000	0.0000	0.0000	54674822.0320	-2859000.0000	0.0000	10042.0582	0.0000	0.0000	0.0000		
Total	124.5002	74749030.5809	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	4001014644.9701	115.2348	553971527.4895	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	354281837.7194
Total Enthalpy Flow Rate (MJ/hr)	4001.0146							3542.8188							81.28			
Heat Duty (MJ/hr)																		
	Out																	
	S-28																	
	0.0000																	
	2.8000																	
	229.5292																	
#	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)									
1	0.0000	32951335.7295	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	0.0000									
	0.0000	127400797.4229	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	0.0000									
	0.0576	42596938.0973	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	2453893.3914									
9.2078	58294342.9134	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	537026313.3207										
0.0000	497717161.0285	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	0.0000										
	87609299.9927	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	0.0000										
9.2654	846569866.1842	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	539480206.7121										
	539.4802																	

Distillation Column, T-401

T-401																			
Stream	In							Out											
Vapor fraction	S-16							S-33											
Pressure (bar)	0.0000							0.0000											
Temperature (°C)	2.8000							2.8000											
Components	180.9120							180.9120											
	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Mo
Benzene	0.1336	23923846.4832	0.0000	0.0000	16203.1597	0.0000	0.0000	3198443.3854	0.1022	23518185.2068	0.0000	0.0000	16203.1597	0.0000	0.0000	2404829.6194	0.0000	0.0000	
Ethylene	0.0000	2578683.3254	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	80721476.1397	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	23236.6602	0.0000	0.0000	270717832.1948
Ethylibenzene	115.1542	31247902.0871	0.0000	0.0000	23236.6602	0.0000	0.0000	3600897768.0096	88.0299	30729920.2215	0.0000	0.0000	23236.6602	0.0000	0.0000	28457.7614	0.0000	0.0000	149318.0999
Diethylbenzene	9.2124	4305619.1041	0.0000	0.0000	28457.7614	0.0000	0.0000	396918433.5751	0.0335	42355380.0089	0.0000	0.0000	28457.7614	0.0000	0.0000	5279.3025	0.0000	0.0000	0.0000
Methane	0.0000	-3251054.7479	-9400000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	321971743.8905	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	10042.0562	0.0000	0.0000	0.0000
Ethane	0.0000	647304.3291	-2859000.0000	0.0000	0.0000	1.0042.0562	0.0000	0.0000	54674822.0320	-2859000.0000	0.0000	0.0000	54674822.0320	0.0000	0.0000	87368.1369	0.0000	0.0000	2709671979.5141
Total	124.5002	74749030.589	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	4001014644.9701	63.7629	553971527.4895	-17339000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2709671979.5141
Total Enthalpy Flow Rate (Mj/hr)	4001.0146									2709.6720									
Heat Duty (Mj/hr)																			

In	Out							In	Out							Out		
	5.30	5.30	5.30	5.30	5.30	5.30	5.30		5.30	5.30	5.30	5.30	5.30	5.30	5.30	5.30	5.30	5.30
Molar Flow Rate (kmol/hr)	229.5292							178.5856								229.5292		
Sensible Heat, H(T) (J/kmol)	8070000.0000							8070000.0000								8070000.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							1932015.3067								0.2358		
Molar Flow Rate (kmol/hr)	1072998.5028							717278.5247								1072998.5028		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							1932015.3067								0.2358		
Molar Flow Rate (kmol/hr)	5059.1948							5059.1948								5059.1948		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							1932015.3067								0.2358		
Molar Flow Rate (kmol/hr)	133053.2533							133053.2533								133053.2533		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							133053.2533								0.2358		
Molar Flow Rate (kmol/hr)	133053.2533							133053.2533								133053.2533		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							133053.2533								0.2358		
Molar Flow Rate (kmol/hr)	13282.0948							13282.0948								13282.0948		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							13282.0948								0.2358		
Molar Flow Rate (kmol/hr)	13282.0948							13282.0948								13282.0948		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							13282.0948								0.2358		
Molar Flow Rate (kmol/hr)	13282.0948							13282.0948								13282.0948		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Mixing/Solution, Hm (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Pressure Change (J/kmol)	0.0000							0.0000								0.0000		
Enthalpy Change, ΔH (J/hr)	0.2358							13282.0948								0.2358		
Molar Flow Rate (kmol/hr)	13282.0948							13282.0948								13282.0948		
Sensible Heat, H(T) (J/kmol)	0.0000							0.0000								0.0000		
Specific Latent Heat of Vaporization, Hv (J/kmol)	0.0000							0.0000								0.0000		
Specific Heat of Formation, Hf (J/kmol)	0.0000		</															

Reflux Drum, V-401

V-401																					
Stream		In																			
Vapor fraction		5.31																			
Pressure (bar)		0.0000																			
Temperature (°C)		20.00																			
	178.5856																				
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)			
Benzene	0.7358	235185.2068	0.0000	0.0000	16203.1597	0.0000	5260575.7644	0.0022	235185.2068	0.0000	0.0000	2804529.6294	0.1336	235185.2068	0.0000	0.0000	16203.1597	0.0000	314026.1450		
Ethene	0.0000	8072146.1397	-13540000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000			
Ethybenzene	203.1205	3072950.2215	-13540000.0000	0.0000	0.0000	23236.6602	0.0000	624697194.6318	88.0299	3072950.2215	0.0000	0.0000	270711783.2948	115.0956	3072950.2215	0.0000	0.0000	22326.6602	0.0000	35947932.4171	
Diethylbenzene	0.0081	4235380.0289	0.0000	0.0000	28457.7624	0.0000	3464547.2572	0.0053	4235380.0289	0.0000	0.0000	28457.7624	0.0000	4235380.0289	0.0000	0.0000	28457.7624	0.0000	195229.1573		
Methane	0.0000	312771743.8803	-9400000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
Ethane	0.0000	5457482.0220	-2859000.0000	0.0000	0.0000	50042.0523	0.0000	0.0000	0.0000	0.0000	0.0000	5467482.0320	0.0000	0.0000	0.0000	0.0000	2859000.0000	0.0000	10942.0582	0.0000	
Total	203.3704	864.6862	-17339000.0000	0.0000	0.0000	6252409817.4334	88.1356	53971527.4895	17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	2709671697.8481	115.2348	53971527.4895	-17339000.0000	0.0000	87368.1369	0.0000
Heat Duty (Mj/hr)																			35426.8817 7194		
Heat Duty (Mj/hr)																			35426.8817		

Reboiler, E-402

E-402																						
Stream		In																				
Vapor fraction		5.31																				
Pressure (bar)		0.0000																				
Temperature (°C)		20.00																				
	229.5292																					
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)				
Benzene	0.0000	235185.2068	0.0000	0.0000	16203.1597	0.0000	0.0000	0.0000	0.0000	20916091.8434	3076000.0000	0.0000	0.0000	0.0000	0.0000	3295135.7226	0.0000	0.0000	16203.1597	0.0000	0.0000	
Ethylene	0.0000	8072146.1397	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000			
Ethybenzene	0.0081	4235380.0289	0.0000	0.0000	23236.6602	0.0000	3464547.2572	0.0053	4235380.0289	0.0000	0.0000	28457.7624	0.0000	4235380.0289	0.0000	0.0000	28457.7624	0.0000	35947932.4171			
Diethylbenzene	0.0144	4235380.0289	0.0000	0.0000	28457.7624	0.0000	44644574.2437	1.3956	5380299.4772	4500000.0000	0.0000	0.0000	0.0000	0.0000	13277684.2428	0.2078	5629432.9134	0.0000	0.0000	28457.7624	0.0000	53702311.3267
Methane	0.0000	312771743.8803	-9400000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	4971716.0285	940000.0000	0.0000	5279.3025	0.0000	0.0000	
Ethane	0.0000	5457482.0220	-2859000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	6766716.0277	250000.0000	0.0000	0.0000	0.0000	0.0000	
Total	203.3704	864.6862	-17339000.0000	0.0000	0.0000	44644574.2437	1.3948	5380299.4772	11254500.0000	0.0000	0.0000	0.0000	0.0000	13339303.4883	0.8304	4856898.1842	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	5380299.4772
Heat Duty (Mj/hr)																			35426.8817			
Heat Duty (Mj/hr)																			35426.8817			

Heat Exchanger, E-204

E-204 (Process Fluid)																			
Stream		In																	
Vapor fraction		5.35																	
Pressure (bar)		0.0000																	
Temperature (°C)		40.0000																	
	77.1381																		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/ Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	36.8313	7421057.7751	0.0000	0.0000	351068.4608	0.0000	0.0000	0.0000	0.0000	28625.7604.2869	36.8313	29187176.2879	0.0000	0.0000	0.0000	0.0000	351068.4608	0.0000	0.0000
Ethylene	0.0092	24638728.3382	-13540000.0000	0.0000	0.0000	109615.9883	0.0000	0.0000	0.0000	105017.1759	0.0092	107728716.0903	-13540000.0000	0.0000	0.0000	109615.9883	0.0000	0.0000	24638728.3382
Ethybenzene	0.0079	9813585.2052	0.0000	0.0000	483744.3045	0.0000	0.0000	0.0000	0.0000	81805.4656	0.0079	37908369.9609	0.0000	0.0000	483744.3045	0.0000	0.0000	350504.6968	
Diethylbenzene	0.0000	13650595.6573	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	0.0000	52029173.0342	0.0000	0.0000	0.0000	0.0000	616584.8302	0.0000	0.0000	0.0000	
Methane	0.0000	11158311.4026	-9400000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	0.0000	0.0000	4235290.8806	0.0000	-9400000.0000	0.0000	0.0000	114384.8881	0.0000	0.0000	0.0000
Ethane	0.0000	15245821.0692	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	0.0000	0.0000	15521948.4284	0.0000	-2859000.0000	0.0000	0.0000	217577.9286	0.0000	0.0000	15245821.0692
Total	36.8485	182553599.4476	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	0.0000	28644427.4683	36.8485	805719334.6824	-17339000.0000	0.0000	0.0000	1892976.3004	0.0000	0.0000	108910535.7697
Total Enthalpy Flow Rate (Mj/hr)						286.4444												10891054	
Heat Duty (Mj/hr)																			802.66

Pump, P-401

P-401																			
Stream	In								Out										
Vapor fraction	S-28								S-29										
Pressure (bar)	0.0000								0.0000										
Temperature (°C)	229.5292								35.0000										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	0.0000	32951335.7295	0.0000	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	32951335.7295	0.0000	0.0000	0.0000	0.0000	0.0000	306059.6837	0.0000	0.0000	
Ethylene	0.0000	127400797.4229	-135400000.0000	0.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	127400797.4229	-135400000.0000	0.0000	0.0000	95562.5692	0.0000	0.0000	0.0000	0.0000	
Ethylbenzene	0.0576	42596938.0973	0.0000	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	2453893.3914	0.0576	42596938.0973	0.0000	0.0000	0.0000	0.0000	421725.8039	0.0000	0.0000
Diethylbenzene	9.2078	5829432.9134	0.0000	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	537026313.3207	9.2078	5829432.9134	0.0000	0.0000	0.0000	0.0000	53735.4930	0.0000	0.0000
Methane	0.0000	497717161.0285	-940000.0000	0.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	497717161.0285	0.0000	0.0000	0.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	
Ethane	0.0000	87609290.9927	-285900.0000	0.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	87609290.9927	-285900.0000	0.0000	0.0000	0.0000	0.0000	18963.3233	0.0000	0.0000	
Total	9.2654	846569866.1842	-17339000.0000	0.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	539480206.7121	9.2654	846569866.1842	-17339000.0000	0.0000	0.0000	1650287.0311	0.0000	0.0000	
Total Enthalpy Flow Rate (MJ/hr)	539.4802								544.1907										
Heat Duty (MJ/hr)	4.71																		

Mixing Point before R-301

Mixing Stream, S-30 (referencing)																			
In	H ₂								H ₂										
Vapor fraction	0.0000								0.0000										
Pressure (bar)	40.0000								35.0000										
Temperature (°C)	229.5292								235.0349										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	36.8313	29487176.2879	0.0000	0.0000	0.0000	0.0000	351068.4680	0.0000	0.0000	32951335.7295	0.0000	0.0000	0.0000	36.8313	303095.6837	0.0000	0.0000	312380754.6448	
Ethylene	0.0092	107728716.0963	125400000.0000	0.0000	0.0000	0.0000	869048.4424	0.0000	0.0000	127400797.4229	125400000.0000	0.0000	0.0000	91350740.1607	-135400000.0000	0.0000	0.0000	914415436	
Ethylbenzene	0.0000	40.0000	0.0000	0.0000	0.0000	0.0000	40.0000	0.0000	0.0000	40.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Diethylbenzene	0.0000	52029173.9342	0.0000	0.0000	0.0000	0.0000	63584.8320	0.0000	0.0000	52029173.9342	0.0000	0.0000	0.0000	54717161.4993	9.2078	5393671.5341	0.0000	0.0000	537524.4930
Methane	0.0000	42652520.8866	-940000.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	946000.0000	0.0000	0.0000	0.0000	44653841.2154	946000.0000	0.0000	0.0000	50158128.9038	
Ethane	0.0000	15512540.4204	-285900.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	87609290.9927	-285900.0000	0.0000	0.0000	7792704.6351	-285900.0000	0.0000	0.0000	10942152.1221	
Total	36.8313	846569866.1842	-17339000.0000	0.0000	0.0000	0.0000	10892615.7697	0.0000	0.0000	87368.1369	0.0000	0.0000	0.0000	544.1907	46.2119	2605297.6250	-2755290.0000	0.0000	1633.2961
Heat Duty (Molar)	0.0000																		

Transalkylator, R-301

R-301																			
Stream	In								Out										
Vapor fraction	S-37								S-38										
Pressure (bar)	0.0000								0.0000										
Temperature (°C)	216.0149								229.5292										
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	36.8313	30324962.4364	0.0000	0.0000	0.0000	0.0000	306059.6837	0.0000	0.0000	1128180724.6648	27.6281	32951335.7295	0.0000	0.0000	48660000.0000	0.0000	306059.6837	0.0000	0.0000
Ethylene	0.0092	115353740.1507	-135400000.0000	0.0000	0.0000	0.0000	921411.5436	0.0002	0.0000	127400797.4229	-135400000.0000	0.0000	0.0000	95562.5692	0.0000	0.0000	1049007.3230		
Ethylbenzene	0.0655	39333079.0852	0.0000	0.0000	0.0000	0.0000	421725.8039	0.0000	0.0000	2604791.7700	18.4720	42596938.0973	0.0000	0.0000	12460000.0000	0.0000	421725.8039	0.0000	0.0000
Diethylbenzene	9.2078	52029173.9341	0.0000	0.0000	0.0000	0.0000	501589138.9038	0.0006	0.0000	501589138.9038	52.7835	5829432.9134	0.0000	0.0000	72840000.0000	0.0000	52735.4930	0.0000	0.0000
Methane	0.0000	445530641.1714	-940000.0000	0.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	497717161.0285	-940000.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	210865.9067		
Ethane	0.0000	77829704.6531	-285900.0000	0.0000	0.0000	0.0000	18963.3223	0.0000	0.0000	87609290.9927	-285900.0000	0.0000	0.0000	18963.3223	0.0000	0.0000	0.0000		
Total	46.1139	76049480.1610	-17339000.0000	0.0000	0.0000	0.0000	16332965.8821	0.0000	0.0000	16332965.8821	46.1139	846569866.1842	-17339000.0000	0.0000	-11836000.0000	0.0000	1650287.0311	0.0000	17147954.4484
Total Enthalpy Flow Rate (MJ/hr)	1633.2961																		
Heat Duty (MJ/hr)	533.38																		

Heat Exchanger, E-204

E-204 (Heating Fluid)																			
Stream	In						Out												
Vapor fraction	5.38						5.39												
Pressure (bar)	0.0000						0.0000												
Temperature (°C)	35.000						35.000												
	229.5292						180.6455												
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	
Benzene	27.6281	32951335.7295	0.0000	0.0000	306059.6837	0.0000	0.0000	918838237.8152	27.6281	23877127.0788	0.0000	0.0000	306059.6837	0.0000	0.0000	306059.6837	0.0000	668135205.2250	
Ethylene	0.0092	12740079.4229	-13540000.0000	0.0000	0.0000	95562.5692	0.0000	0.0000	1049007.3230	0.0092	82328983.9839	-13540000.0000	0.0000	0.0000	95562.5692	0.0000	634105.8435		
Ethylbenzene	18.4720	4259639.0973	0.0000	0.0000	421725.0309	0.0000	0.0000	794639446.4035	18.4720	12742380.9896	0.0000	0.0000	421725.0309	0.0000	0.0000	421725.0309	0.0000	243166978.8448	
Diethylbenzene	0.0046	58294324.9134	0.0000	0.0000	0.0000	537535.4930	0.0000	0.0000	270856.9067	0.0046	42975926.1571	0.0000	0.0000	537535.4930	0.0000	0.0000	537535.4930	0.0000	200323.2339
Methane	0.0000	49771716.0285	-940000.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	0.0000	0.0000	328023876.3360	-940000.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	99720.1588	0.0000
Ethane	0.0000	87609290.9927	-2859000.0000	0.0000	0.0000	189683.3223	0.0000	0.0000	0.0000	0.0000	155212214.5670	-2859000.0000	0.0000	0.0000	189683.3223	0.0000	0.0000	189683.3223	0.0000
Total	46.1139	846569866.1842	-17339000.0000	0.0000	0.0000	1650287.0311	0.0000	0.0000	1714797548.4484	46.1139	645160509.1123	-17339000.0000	0.0000	0.0000	1650287.0311	0.0000	0.0000	1650287.0311	0.0000
Total Enthalpy Flow Rate (MJ/hr)		1714.7975						-802.66						912.1366					
Heat Duty (MJ/hr)																			

Heater, E-301

E-301 Cooler																		
Stream	In					Out												
Vapor fraction	S-39					S-40												
Pressure (bar)	0.0000					0.0000												
Temperature (°C)	35.0000					35.0000												
Components	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)
	Benzene	27.6281	23871727.0788	0.0000	0.0000	306059.6837	0.0000	0.0000	668135205.2250	27.6281	13998650.2682	0.0000	0.0000	0.0000	107629.2640	0.0000	0.0000	416506670.9375
Ethylene	0.0092	8232883.9839	-1340000.0000	0.0000	0.0000	95562.5692	0.0000	0.0000	634105.8435	0.0092	-129470.6074	-1354000.0000	0.0000	0.0000	336223.8693	0.0000	0.0000	-133433.7107
Ethylbenzene	18.4720	1724380.9896	0.0000	0.0000	0.0000	421725.8039	0.0000	0.0000	24316978.4448	18.4720	1842873.6811	0.0000	0.0000	0.0000	1483784.7360	0.0000	0.0000	367826018.4308
Diethylbenzene	0.0046	4297926.1571	0.0000	0.0000	0.0000	537353.4930	0.0000	0.0000	200332.2339	0.0046	25558364.9851	0.0000	0.0000	0.0000	1891245.3358	0.0000	0.0000	126375.6444
Methane	0.0000	328023876.3360	-940000.0000	0.0000	0.0000	99720.1588	0.0000	0.0000	36516891.8026	-940000.0000	0.0000	0.0000	0.0000	350851.7814	0.0000	0.0000	0.0000	
Ethane	0.0000	15521224.5670	-2859000.0000	0.0000	0.0000	189683.3223	0.0000	0.0000	2356848.5099	-2859000.0000	0.0000	0.0000	0.0000	667374.9051	0.0000	0.0000	0.0000	
Total	46.1139	645160509.1123	-17339000.0000	0.0000	0.0000	1650287.0311	0.0000	0.0000	912136622.1471	46.1139	22534375.0344	-17339000.0000	0.0000	0.0000	5806309.8916	0.0000	0.0000	78432561.3019
Total Enthalpy Flow Rate (MJ/hr)	912.1366										784.3256							
Heat Duty (MJ/hr)	-177.81																	

Liquid Expander, C-301

Mixing Input Stream before Distillation Column, T-201

Mixing Input Stream, S-11																				
Stream		In							In											
Vapor fraction		5-41							5-12											
Pressure (bar)		0.0000							0.0000											
Temperature (°C)		2.8000							2.8000											
Components		Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)	M
Benzene	27.6281	13998650.2682	0.0000	0.0000	16203.1597	0.0000	0.0000	387203599.8909	239.5763	13998650.2682	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	3357627000.9696			
Ethylene	0.0092	-1291470.6074	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	-136482.1950	0.0576	-1291470.6074	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	-853671.0814		
Ethylbenzene	18.4720	18428873.6811	0.0000	0.0000	22326.6602	0.0000	0.0000	34083009.4661	96.7398	18428873.6811	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	1784956862.5359			
Diethylbenzene	0.0046	25558364.9851	0.0000	0.0000	28457.7614	0.0000	0.0000	117799.5306	9.2078	25558364.9851	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	235599120.1913			
Methane	0.0000	-36516891.8026	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	-116444.5262			
Ethane	0.0000	2356848.5099	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	-30034.6155			
Total	46.1139	22534375.0344	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	728014926.6926	345.6737	22534375.0344	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	5376143833.4737		
Total Enthalpy Flow Rate (MJ/hr)			728.0149														5376.1438			
Heat Duty (MJ/hr)																	0.00			

Out																		
		S-13							2.8000									
		0.0000							2.8000									
		120.6244							120.6244									
ΔH	Molar Flow Rate (kmol/hr)	Sensible Heat, H(T) (J/kmol)	Specific Latent Heat of Vaporization, Hv (J/kmol)	Specific Heat of Formation, Hf (J/kmol)	Specific Heat of Mixing/Solution, Hm (J/kmol)	Specific Heat of Pressure Change (J/kmol)	Kinetic Energy, Ek (J/kmol)	Potential Energy, Ep (J/kmol)	Enthalpy Change, ΔH (J/hr)									
96	267.2044	13998650.2682	0.0000	0.0000	0.0000	16203.1597	0.0000	0.0000	3744830600.8605									
1	0.0668	-1291470.6074	-13540000.0000	0.0000	0.0000	5059.1948	0.0000	0.0000	-990153.2764									
59	115.2118	18428873.6811	0.0000	0.0000	0.0000	22326.6602	0.0000	0.0000	2125795872.0020									
3	9.2124	25558364.9851	0.0000	0.0000	0.0000	28457.7614	0.0000	0.0000	235716919.7219									
2	0.0311	-36516891.8026	-940000.0000	0.0000	0.0000	5279.3025	0.0000	0.0000	-1164444.5262									
?	0.0610	2356848.5099	-2859000.0000	0.0000	0.0000	10042.0582	0.0000	0.0000	-30034.6155									
27	391.7875	22534375.0344	-17339000.0000	0.0000	0.0000	87368.1369	0.0000	0.0000	6104158760.1663									
			6104.1588															

Process Simulation Using Aspen Plus

APPENDIX E: UTILITIES

E.1 Superheated steam

ReboilerE-202

High Pressure Steam to Heat S-14						
Stream	In			Out		
Vapor fraction	1.0000			1.0000		
Pressure (bar)	40.0000			40.0000		
Temperature (°C)	450.0000			250.3000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Steam	4446.2705	732096.2075	3255097786.5349	4446.2705	0.0000	0.0000
Total	4446.2705	732096.2075	3255097786.5349	4446.2705	0.0000	0.0000
Total Enthalpy Flow Rate (MJ/hr)	3255.0978			0.0000		
Heat Duty (MJ/hr)	-3255.10					

Reboiler E-402

High Pressure Steam to Heat S-33						
Stream	In			Out		
Vapor fraction	1.0000			1.0000		
Pressure (bar)	40.0000			40.0000		
Temperature (°C)	450.0000			250.3000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Steam	307.6230	732096.2075	225209623.6444	307.6230	0.0000	0.0000
Total	307.6230	732096.2075	225209623.6444	307.6230	0.0000	0.0000
Total Enthalpy Flow Rate (MJ/hr)	225.2096			0.0000		
Heat Duty (MJ/hr)	-225.21					

Heater E-103

Heat Required For Heating S-7						
Stream	In			Out		
Vapor fraction	1			1		
Pressure (bar)	0			40		
Temperature (°C)	450			250.3		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Steam	3642.403567	732096.2075	2666589838	3642.403567	0	0
Total	3642.403567	732096.2075	2666589838	3642.403567	0	0
Total Enthalpy Flow Rate (MJ/hr)	2666.589838			0		
Heat Duty (MJ/hr)	-2666.59					

Jacketed fixed bed reactor R-301

High Pressure Steam for R-301						
Stream	In			Out		
Vapor fraction	1.0000			1.0000		
Pressure (bar)	40.0000			40.0000		
Temperature (°C)	450.0000			250.3000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Water	728.5652	732096.2075	533379791.0160	728.5652	0.0000	0.0000
Total	728.5652	732096.2075	533379791.0160	728.5652	0.0000	0.0000
Total Enthalpy Flow Rate (MJ/hr)	533.3798			0.0000		
Heat Duty (MJ/hr)	-533.38					

E.2 Cooling Water

CoolerE-101

Cooling Fluid for S-4						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Water	27763.4803	16730.0000	464483024.7582	27763.4803	66920.0000	1857932099.0329
Total	27763.4803	16730.0000	464483024.7582	27763.4803	66920.0000	1857932099.0329
Total Enthalpy Flow Rate (MJ/hr)	464.4830			1857.9321		
Heat Duty (MJ/hr)	2322.42					

Jacketed fixed reactor R-101

Cooling Jacket for R-101						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Water	84016.9003	16730.0000	1405602741.2923	84016.9003	66920.0000	5622410965.1692
Total	84016.9003	16730.0000	1405602741.2923	84016.9003	66920.0000	5622410965.1692
Total Enthalpy Flow Rate (MJ/hr)	1405.6027			5622.4110		
Heat Duty (MJ/hr)	7028.01					

Condenser E201

Cooling Fluid for S-17						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, ΔH (J/hr)
Water	147442.4391	16730.0000	2466712005.7926	147442.4391	66920.0000	9866848023.1705
Total	147442.4391	16730.0000	2466712005.7926	147442.4391	66920.0000	9866848023.1705
Total Enthalpy Flow Rate (MJ/hr)	2466.7120			9866.8480		
Heat Duty (MJ/hr)	12333.56					

Cooler E-203

Cooling Fluid for S-21						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, ΔH (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, ΔH (J/hr)
Water	19374.0370	16730.0000	324127638.5547	19374.0370	66920.0000	1296510554.2187
Total	19374.0370	16730.0000	324127638.5547	19374.0370	66920.0000	1296510554.2187
Total Enthalpy Flow Rate (MJ/hr)	324.1276			1296.5106		
Heat Duty (MJ/hr)	1620.64					

Condenser E-401

Cooling Fluid for S-28						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Water	84035.9111	16730.0000	1405920792.0076	84035.9111	66920.0000	5623683168.0304
Total	84035.9111	16730.0000	1405920792.0076	84035.9111	66920.0000	5623683168.0304
Total Enthalpy Flow Rate (MJ/hr)	1405.9208			5623.6832		
Heat Duty (MJ/hr)	7029.60					

Jacketed fixed bed reactor R-101

Cooling Jacket for R-101						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Water	84016.9003	16730.0000	1405602741.2923	84016.9003	66920.0000	5622410965.1692
Total	84016.9003	16730.0000	1405602741.2923	84016.9003	66920.0000	5622410965.1692
Total Enthalpy Flow Rate (MJ/hr)	1405.6027			5622.4110		
Heat Duty (MJ/hr)	7028.01					

Cooler E-301

Cooling water E-301						
Stream	In			Out		
Vapor fraction	0.0000			0.0000		
Pressure (bar)	1.0000			1.0000		
Temperature (°C)	30.0000			45.0000		
Components	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)	Molar Flow Rate (kmol/hr)	Sensible Heat (J/kmol)	Enthalpy Change, $\Delta\dot{H}$ (J/hr)
Steam	1527.925772	16730	25562198.17	1527.925772	66920	102248792.7
Total	1527.925772	16730	25562198.17	1527.925772	66920	102248792.7
Total Enthalpy Flow Rate (MJ/hr)	25.56219817			102.2487927		
Heat Duty (MJ/hr)	127.81					

APPENDIX F MASS TRANSFER EQUIPMENT DESIGN

DISTILLATION COLUMN T201

Component Distribution

Step 1: Identification of Light Key (LK) and Heavy Key (HK)

Light Key : Benzene Light Non-Key: Ethylene, Ethane, Methane

Heavy Key : Ethylbenzene Heavy Non-Key: Diethylbenzene

Step 2: Determination of Dew Point and Bubble Point

Step 2: Determination of partial vapor pressure and relative volatilities

From Raoult's Law and Dalton's Law, $K = P_{\text{sat}}/P$. Partial pressure of each component is calculated using Antoine's equation.

Antoine Equation
T in K, P in Pa
Vapor pressure = $\exp [C1 + (C2/T) + C3 \times \ln(T) + C4 \times T^{C5}]$
T in K, P in kPa
$T \log P = AC - B + AT - C \log P$

Components	C1	C2	C3	C4	C5
Methane	39.2050	-1324.4000	-3.4366	0.0000	2.0000
Ethane	51.8570	-2598.7000	-5.1283	0.0000	2.0000
Ethylene	53.9630	-2443.0000	-5.5643	0.0000	2.0000
Benzene	83.1070	-6486.2000	-9.2194	0.0000	2.0000
Ethylbenzene	89.0630	-7733.7000	-9.9170	0.0000	2.0000

Components	A	B	C
Diethylbenzene	4.1254	1589.2730	-71.1310

Dew point

$$\sum \frac{y}{K} = 1$$

Bubble point

$$\sum K_x = 1$$

Relative volatilities, α

$$\alpha_{LK,HK}(T) = \frac{K_{LK}(T)}{K_{HK}(T)}$$

Average relative volatility, α_{avg}

$$\alpha_{\frac{LK}{HK}, avg} = \sqrt{(\alpha_{\frac{LK}{HK}})_D \cdot (\alpha_{\frac{LK}{HK}})_B}$$

$$= 4.264431377$$

Feed Temperature	393.7743639	K	Pressure	2.8	bar	
Components	Feed molar fraction	P* (bar)	$K_i = \frac{P_i}{P}$	$\frac{Z_i(K_i - 1)}{1 + (V/F)(K_i - 1)}$	Zi	$y_i = K_i Z_i$
Methane	0.682013537	5427.174532	1938.276619	8283.49	7.9E-05	0.15382
Ethane	0.000170457	223.4963631	79.82012967	341.122	0.00016	0.01243
Ethylene	0.294067015	385.0404661	137.5144522	587.687	0.00017	0.02344
Benzene	0.023513852	3.038679848	1.085242803	4.63793	0.68201	0.74015
Ethylbenzene	7.93593E-05	0.655180031	0.233992868	1	0.29407	0.06881
Diethylbenzene	0.000155779	0.158362158	0.056557914	0.24171	0.02351	0.00133
Total	1	6039.563583	2156.986994	9218.17	1	0.99998

Dew point	390.3962047	K	Pressure	2.8	bar
Components	Distillate Molar Fraction, yi	P* (bar)	$K_i = \frac{P_i}{P}$	$\alpha_i = \frac{K_i}{K_{HK}}$	
Methane	0.000116324	5001.830539	1786.36805	8440.32	6.5E-08
Ethane	0.00022834	212.0883936	75.74585487	357.888	3E-06
Ethylene	0.000249855	363.9673188	129.9883282	614.175	1.9E-06
Benzene	0.99918996	2.800597642	1.000213443	4.72586	0.99898
Ethylbenzene	0.00021552	0.592611517	0.21164697	1	0.00102
Diethylbenzene	0	0.140453131	0.050161833	0.23701	0
Total	1	5581.419914	1993.364255	9418.35	1

Bubble point	454.0629642	K	Pressure	2.8	bar
Components	Bottom Molar Fraction, x_i	P* (bar)	$K_i = \frac{P_i}{P}$	$\alpha_i = \frac{K_i}{K_{HK}}$	$y_i = K_i x_i$
Methane	0	25355.1582	9055.413643	8625.26	0
Ethane	0	553.7374931	197.7633904	188.369	0
Ethylene	0	1053.255981	376.1628502	358.294	0
Benzene	0.001073108	10.40094273	3.714622405	3.53817	0.00399
Ethylbenzene	0.92493157	2.939640617	1.049871649	1	0.97106
Diethylbenzene	0.073995322	0.944419379	0.337292635	0.32127	0.02496
Total	1	26976.43668	9634.441671	9176.78	1

Step 3: Minimum number of stages, N_{\min}

$$N_{\min} = \frac{\ln \left[\left(\frac{x_{Lk}}{x_{Hk}} \right)_D \times \left(\frac{x_{Hk}}{x_{Lk}} \right)_B \right]}{\ln \left[\frac{\alpha_{LK}}{\alpha_{Hk}} \right]} = \frac{\ln \left[\frac{0.9992}{0.0011} \times \frac{0.9249}{0.0002} \right]}{\ln [4.264431377]} = 10.4810811 \text{ stages}$$

Step 4: Determination of reflux ratio, R

Feed enter the distillation column as saturated liquid. $q = 1$

Underwood equation is used to find minimum reflux ratio, R_{\min}

$$\sum_{i=1}^n \frac{\alpha_i x_{F,i}}{\alpha_i - \theta} = 1 - \bar{q}$$

Components	Distillate, $x_{i,D}$ (mol frac)	$K_i = P_{i,sat}/P$	$\alpha_i = K_i/K_{HK}$	Bottom, $x_i = x_{i,B}$ (mol frac)	$\alpha_i x_{i,F}$	$\alpha_i x_{i,F}/(\alpha_i - \theta)$	$\alpha_i x_{i,D}$	$\alpha_i x_{i,D}/(\alpha_i - \theta)$
Methane	0.0001	1938.2766	8283.4859	0.0000	0.6574	0.0001	0.9636	0.0001
Ethane	0.0002	79.8201	341.1221	0.0000	0.0531	0.0002	0.0779	0.0002
Ethylene	0.0002	137.5145	587.6865	0.0000	0.1002	0.0002	0.1468	0.0003
Benzene	0.9992	1.0852	4.6379	0.0011	3.1631	0.9507	4.6342	1.3929
Ethylbenzene	0.0002	0.2340	1.0000	0.9249	0.2941	-0.9458	0.0002	-0.0007
Diethylbenzene	0.0000	0.0566	0.2417	0.0740	0.0057	-0.0053	0.0000	0.0000
Total	1.0000	2156.9870	9218.1741	1.0000	4.2736	0.0000	5.8227	1.3928

q	1.0000	Rmin	0.3928
1-q	0.0000	R/Rmin	1.5000
θ	1.3109	Ract	0.5892

Value of θ is obtained by satisfying $\frac{\sum \alpha_i x_{if}}{\alpha_i - \theta} = 0$. The value of R is set as $1.5R_{min}$.

Finally, R_{act} is **0.5892**.

Step 5: Determination of number of theoretical stages, N

Number of theoretical stages, N is calculated using Gilliland correlation

$$\frac{N - N_{min}}{N + 1} = 0.75 \left(1 - \left(\frac{R - R_{min}}{R + 1} \right)^{0.566} \right)$$

$$\text{Let } X = 0.75 \left(1 - \left(\frac{R - R_{min}}{R + 1} \right)^{0.566} \right)$$

$$X = 0.123582649$$

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

$$N = \frac{0.123582649 + 10.4810811}{1 - 0.123582649}$$

N = 22.4400192 stages (including theoretical stage for reboiler)

$$= 21.4400192 \text{ stages}$$

Step 6: Overall tray efficiency, E_o

Overall tray efficiency is calculated by using O'Connell's correlation of overall column efficiency,

$$E_o = 0.503(\mu_{F,avg} \alpha_{avg})^{-0.226}$$

Liquid viscosity of the components is calculated using properties from Yaws Chemical Properties Handbook and pure component data bank from Aspen Plus.

Properties from yaws Chemical Properties Handbook

Components	A	B	C	D
Benzene	-7.4005	1181.5	0.014888	-0.000013713
Ethylbenzene	-5.2585	830.65	0.010784	-0.000010618
Diethylbenzene	-5.8058	1014	0.010909	-9.7803E-06

Properties from AspenPlus pure component analysis

Component	Temperature (C)		
	117.2462	180.9130	120.6244
Ethylene	2.53E-05	2.02E-05	2.49E-05
Methane	6.33E-07	3.98E-07	6.16E-07
Ethane	8.36E-06	4.24E-06	8.02E-06

Average viscosity for each component

Component	Feed Mole Fraction	Molar average μ in (cP)
Benzene	0.6820	0.147890818
Ethylene	0.0002	0
Ethylbenzene	0.2941	0.08307251
Diethylbenzene	0.0235	0.008313251
Methane	0.0001	0
Ethane	0.0002	0
Total	1	0.239276579

$$E_o = \mathbf{0.494635539}$$

Step 7: Determination of actual number of theoretical stages

N = 21.4400192 stages

Actual number of theoretical stages, N_{act}

$$N_{act} = \frac{N_{eq}}{E_o} = \frac{21.4400192}{0.494635539}$$

N_{act} = 45.36677498 stages = 46 stages

Step 8: Feed point location

By using Kirkbride equation, the location of feed point calculated from

$$\log \frac{N_D}{N_B} = 0.206 \log \left[\frac{B}{D} \left(\frac{x_{HK,F}}{x_{LK,F}} \right) \left(\frac{(x_{LK})_B}{(x_{HK})_D} \right)^2 \right]$$

$$\log \frac{N_D}{N_B} = 0.206 \log \left[\frac{124.5}{267.287} \left(\frac{0.2941}{0.6820} \right) \left(\frac{0.0011}{0.0002} \right)^2 \right]$$

$$\frac{N_D}{N_B} = 1.3919$$

Since $N_D + N_B = N_{act}$,

N_B , Number of stages in stripping section = 19.23142182

$N_B \approx 20$ stages below feed including reboiler

N_D , Number of stages/trays in rectifying section = 26.76857818

$N_D \approx 27$ stages above feed stages

So, the feed located at 27th stage from bottom.

COLUMN SIZING

The distillation column is sized based on the top condition and the bottom condition. Next, the size of distillation column is decided based on the larger diameter calculated from the top or bottom condition. For column sizing, the important information is the flow rate of each stream related to distillation column and their respective density, which is presented in table below:

Properties	Distillate	Bottom	Feed
L (kmol/hr)	157.4825609	549.2701025	
V (kmol/hr)	424.7699	424.7699	
MW _{average} (kg/kmol)	78.09534197	108.2154681	87.66676023
L _w (kg/hr)	12298.65445	59439.52126	
V _w (kg/hr)	33172.54897	45966.67131	
ρ _v (kg/m ³)	6.737015634	8.026408766	7.497828973
ρ _L (kg/m ³)	772.6116412	712.79136	771.6998811
σ (J/m ²)	0.013425218	0.012285994	0.014672601

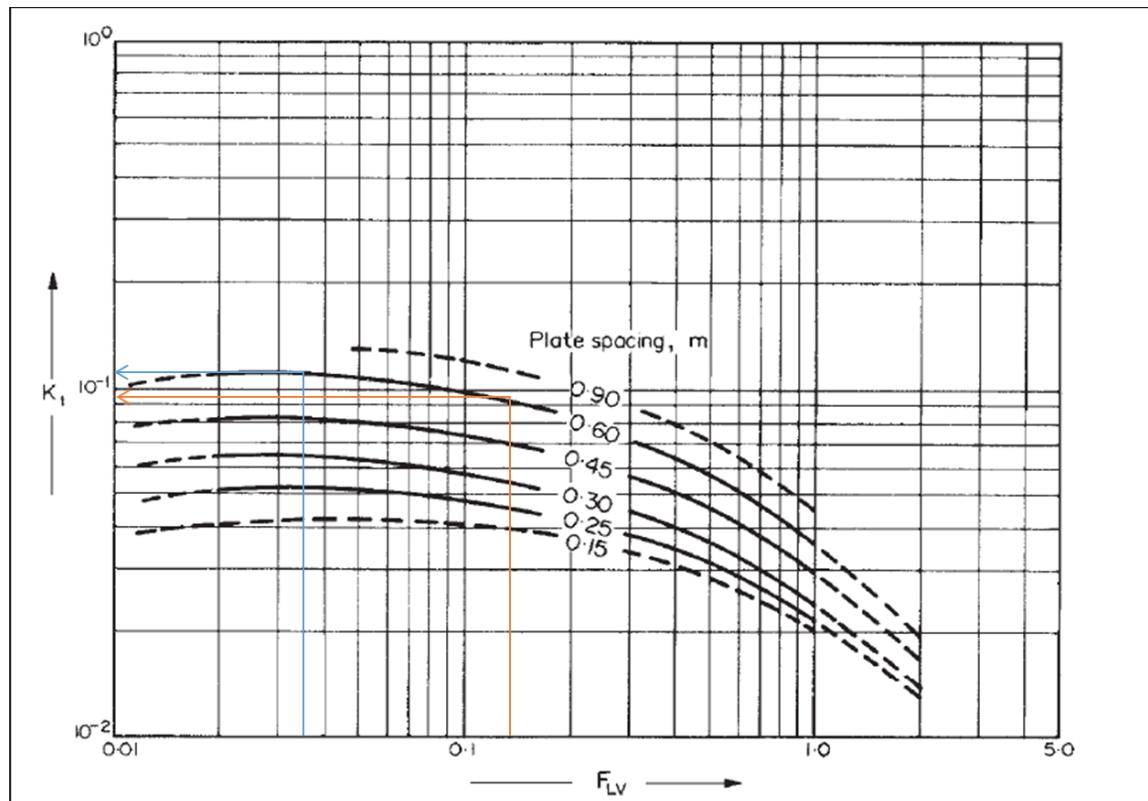
Step 1: Determination of vapor flooding velocity, u_f

Assuming column diameter is larger than 1 m, tray spacing of 0.61 m (2.0013 ft) is typically chosen.

$$u_f = K_1 \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5}$$

Where T_s is tray spacing in ft.

Value of K_1 taken from Figure 11.27 Coulson and Richardson book page 568.



Top Condition	Bottom Condition
$F_{LV} = \frac{L_w}{V_w} \left(\frac{\rho_V}{\rho_L} \right)^{\frac{1}{2}} = \frac{12298.65445}{33172.54897} \left(\frac{6.737015634}{772.6116412} \right)^{0.5} = 0.0346$ $K_1 = 0.097$ $u_f = 0.9550 \text{ m/s}$	$F_{LV} = \frac{L_w}{V_w} \left(\frac{\rho_V}{\rho_L} \right)^{\frac{1}{2}} = \frac{59439.521}{45966.671} \left(\frac{8.026408766}{712.79136} \right)^{0.5} = 0.137$ $K_1 = 0.115625$ $u_f = 0.9829 \text{ m/s}$

Step 2: Determination of actual vapour velocity, u_v

$u_v = 0.8u_f$ (Take 80% flooding velocity for column operation)

Top Condition	Bottom Condition
$u_v = 0.80(0.9550)$	$u_v = 0.80(0.9829)$

= 0.7640 m/s	= 0.7863 m/s
--------------	--------------

Step 3: Determination of net column area, A_n

$$A_n = \frac{\dot{V}}{u_v}$$

Top Condition	Bottom Condition
$A_n = \frac{1.3678}{0.7640}$ = 1.7903 m ²	$A_n = \frac{1.5908}{2.2188}$ = 2.0232 m ²

Step 4: Determination of cross sectional area, A_c

$$A_c = \frac{A_n}{0.88} \text{ (assume downcomer occupies 18% of column cross sectional area)}$$

Top Condition	Bottom Condition
$A_c = \frac{A_n}{0.82} = \frac{1.7903}{0.82}$ = 2.1833 m ²	$A_c = \frac{A_n}{0.82} = \frac{2.0232}{0.82}$ = 2.4673 m ²

Step 5: Determination of column diameter, D_c

$$D_c = \sqrt{\frac{4A_c}{\pi}}$$

Top Condition	Bottom Condition
$D_c = \sqrt{\frac{4A_c}{\pi}} = \sqrt{\frac{4(2.1833)}{\pi}}$ = 1.6673 m	$D_c = \sqrt{\frac{4A_c}{\pi}} = \sqrt{\frac{4(2.4673)}{\pi}}$ = 1.7724 m

Since limiting diameter occurs at distillate,
 $D_c = 1.7724 \text{ m}$

Rule of thumb:

Tray spacing is selected to minimize entrainment

Standard trays spacing for large diameter column = 0.46 or 0.61 m

Therefore, tray spacing of 0.6 m is chosen for column C-3 since the column diameter is 1.7724 m.

Step 9: Height of Column

Tray spacing estimated, $H_s = 0.6 \text{ m}$

Plate thickness, $t_p = 0.003 \text{ m}$

Column height, H_c

$H_c = (\text{No. of stages} - 1) \times (\text{Tray spacing+thickness})$

$$H_c = (N - 1) \times (H_s + t_p) = 31.924 \text{ m}$$

Ratio of column height to column diameter:

$$\text{Ratio} = \frac{H_c}{D_c}$$

Ratio = 18.011 < 30 (acceptable)

PLATE HYDRAULIC DESIGN

Step 1: Liquid flow arrangement

Maximum liquid flow rate, $V_{L\max} = 0.0131 \text{ m}^3/\text{s}$ and $D_c = 3.0 \text{ m}$

From Coulson and Richardson Chemical Engineering Design, Figure 11.28,

The liquid flow arrangement is selected to be **cross flow**.

Step 2: Provisional plate design

Column diameter, $D_c = 1.7724 \text{ m}$

Column area, $A_c = 2.4673 \text{ m}^2$

Downcomer area, $A_d = 0.18(A_c) = \mathbf{0.4441 \text{ m}^2}$

Net area, $A_n = A_c - A_d = 2.0232 \text{ m}^2$

Active area, $A_a = A_c - 2A_d = 2.4673 - 2 \times 0.4441 = \mathbf{1.5791 \text{ m}^2}$

Assume all holes take 10% of active area,

Hole area, $A_h = 0.10(A_a) = 0.10 \times 1.5791 = \mathbf{0.1579 \text{ m}^2}$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.31,

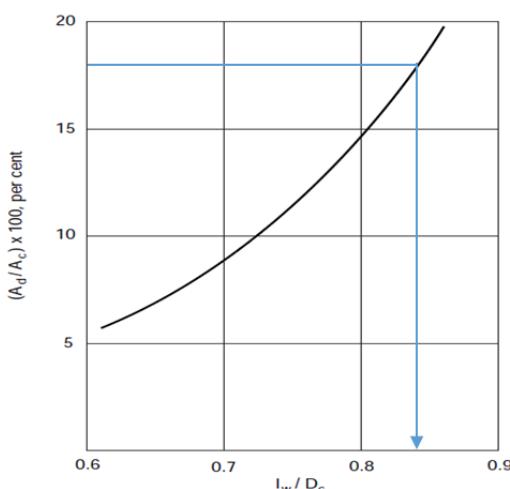


Figure 11.31. Relation between downcomer area and weir length

When $\frac{A_d}{A_c} = 0.1800$; $\frac{l_w}{D_c} = 0.84$

Weir length, $l_w = 0.84 \times D_c = 0.84 \times 1.7724 = \mathbf{1.4888 \text{ m}}$

Take weir height, $h_w = \mathbf{50 \text{ mm}} = 0.05 \text{ m}$ (40-50 mm is recommended for 1 atm.)

Take hole diameter, $d_h = \mathbf{5 \text{ mm}} = 0.005 \text{ m}$ (Preferred size in design)

Take plate thickness = **3 mm** = 0.003 m (Typical for stainless steel plate)

Step 3: Check Weeping Point

Maximum liquid flow rate = 16.511 kg/s

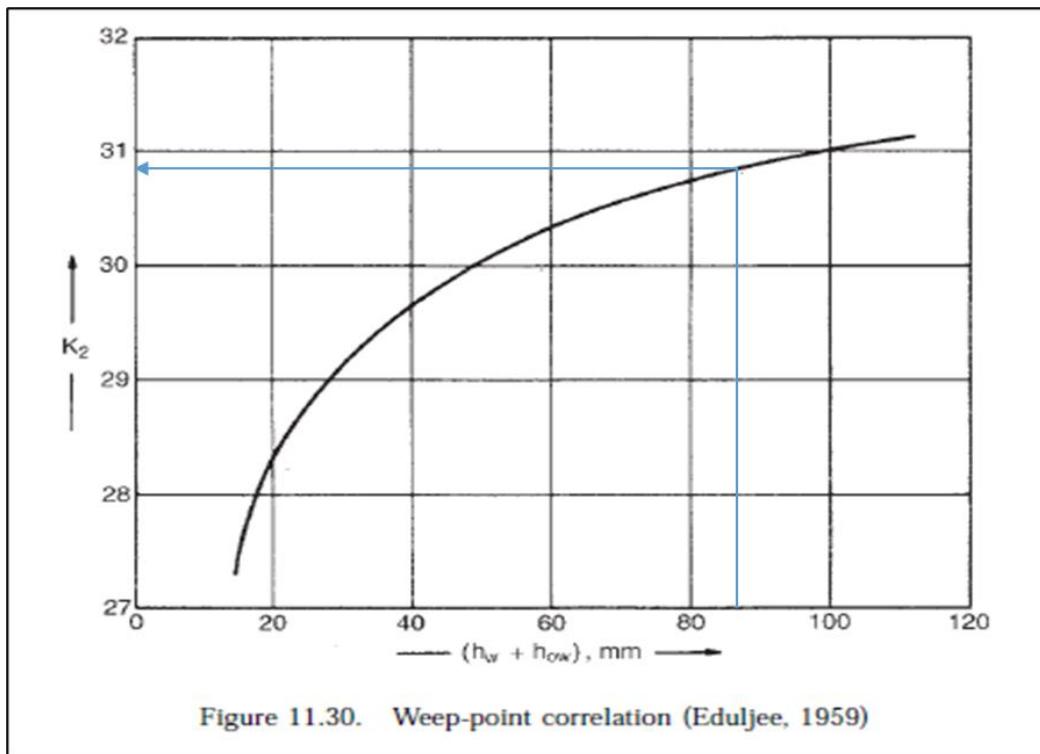
Minimum liquid flow rate at 70% turndown = 0.70 (16.511) = 11.558 kg/s

$$\text{Max } h_{ow} = 750 \left(\frac{L_{w\max}}{\rho_L \times l_w} \right)^2 = 750 \left(\frac{16.511}{712.791 \times 1.4888} \right)^2 = 46.742 \text{ mm liquid}$$

$$\text{Min } h_{ow} = 750 \left(\frac{L_{w\min}}{\rho_L \times l_w} \right)^2 = 750 \left(\frac{11.558}{712.791 \times 1.4888} \right)^2 = 36.850 \text{ mm liquid}$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.30

At minimum liquid flow rate, $h_{ow} + h_w = 36.850 \text{ mm} + 50 \text{ mm} = 86.850 \text{ mm liquid}$



$K_2 = 30.84$

$$\text{Weeping velocity, } u_h = \frac{[K_2 - 0.90(25.4 - d_h)]}{\sqrt{\rho_v}} = \frac{[30.84 - 0.90(25.4 - 5)]}{\sqrt{0.6911}} = 4.405 \text{ m/s}$$

Maximum vapour flow rate = 1.591 m³/s

Minimum vapour velocity at 70% turndown

$$\text{Actual minimum vapour velocity} = u_h = \frac{0.7 * 1.591}{1.4387} = 7.052 \text{ m/s}$$

Note: Since actual minimum vapour velocity > weeping velocity, the minimum operating liquid flow rate is well below weep point, the design is satisfactory.

Step 4: Determination of plate pressure drop

Maximum vapour velocity through holes,

$$u_h = \frac{\text{Maximum Vapour flow rate}}{A_h} = \frac{1.591}{1.4387} = 10.074 \text{ m/s}$$

Percentage of perforated area, $\frac{A_h}{A_p} \times 100\% \approx \frac{A_h}{A_a} \times 100\% \approx 10$ and

$$\frac{\text{plate thickness}}{\text{hole diameter}} = \frac{0.003}{0.005} = 0.6$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.34

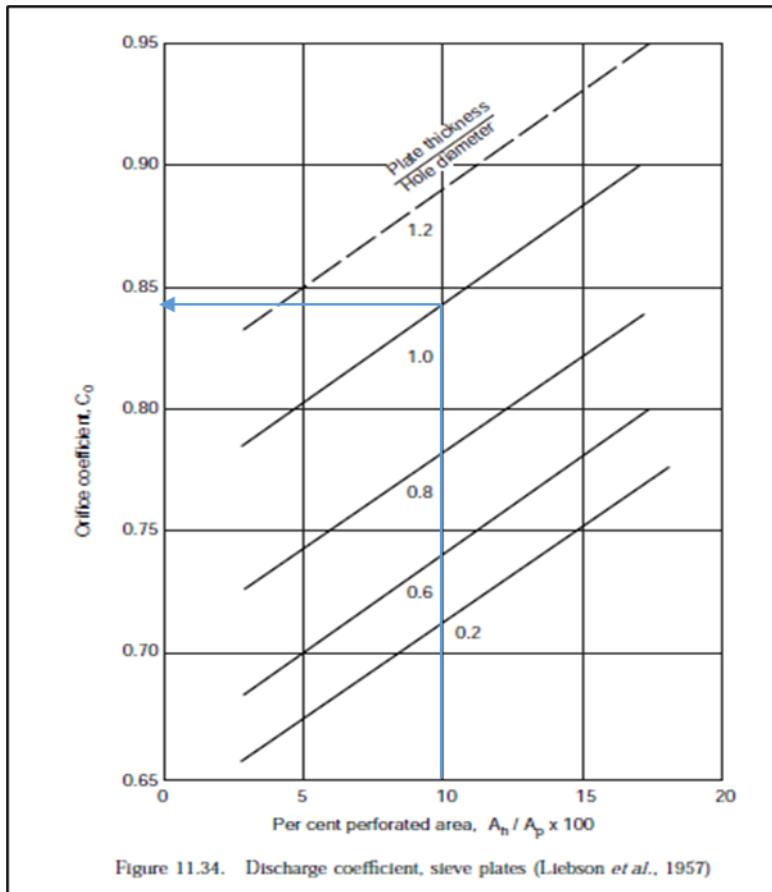


Figure 11.34. Discharge coefficient, sieve plates (Liebson *et al.*, 1957)

Orifice coefficient, $C_0 = 0.844$

$$\text{Dry plate pressure drop, } h_d = 51 \left[\frac{u_h}{C_0} \right]^2 \frac{\rho_v}{\rho_L} = 51 \left[\frac{4.405}{0.844} \right]^2 \frac{8.026}{712.791} = 15.6534 \text{ mm liquid}$$

$$\text{Residual head pressure drop, } h_r = \frac{12500}{\rho_L} = \frac{12500}{712.791} = 17.537 \text{ mm liquid}$$

$$\begin{aligned} \text{Total plate pressure drop, } h_t &= h_d + (h_w + h_{ow,max}) + h_r \\ &= 15.6534 + 17.537 + 86.850 = 120.040 \text{ mm liquid} \end{aligned}$$

Step 5: Downcomer liquid backup

Taking average value range given by Coulson and Richardson's Chemical Engineering Design (5 to 10mm), height of bottom edge of the apron above the plate.

Take $h_{ap} = h_w - 10 = 50 - 10 = 40 \text{ mm} = 0.04 \text{ m}$

Clearance area under downcomer, $A_{ap} = h_{ap}l_w = 0.04 \times 1.4888 = 0.0596 \text{ m}^2$

Since A_{ap} (0.0596 m^2) is less than A_d (0.444 m^2), $A_m = 0.0596 \text{ m}^2$

$$h_{dc} = 166 \left[\frac{L_{wd}}{\rho_L A_m} \right]^2 = 166 \left[\frac{16.511}{(712.791)(0.0596)} \right]^2 = 25.114 \text{ mm}$$

Downcomer backup, $h_b = (h_w + h_{ow}) + h_t + h_{dc} = 86.850 + 120.040 + 25.114 = 232.004 \text{ mm}$

liquid = 0.232 m liquid

$$\frac{1}{2}(l_t + h_w) = \frac{1}{2}(0.6 + 0.05) = 0.325 \text{ m}$$

Since $h_b < \frac{1}{2}(l_t + h_w)$, flooding will not occur, the design is satisfactory.

Step 6: Downcomer residence time

$$\text{Downcomer residence time, } t_r = \left(\frac{A_d h_b \rho_L}{L_{wd}} \right) = \left(\frac{0.4441(232.004)(712.791)}{16.511} \right) = 4.448 \text{ s}$$

Since downcomer residence time $> 3 \text{ s}$, flooding is avoided. The design is satisfactory.

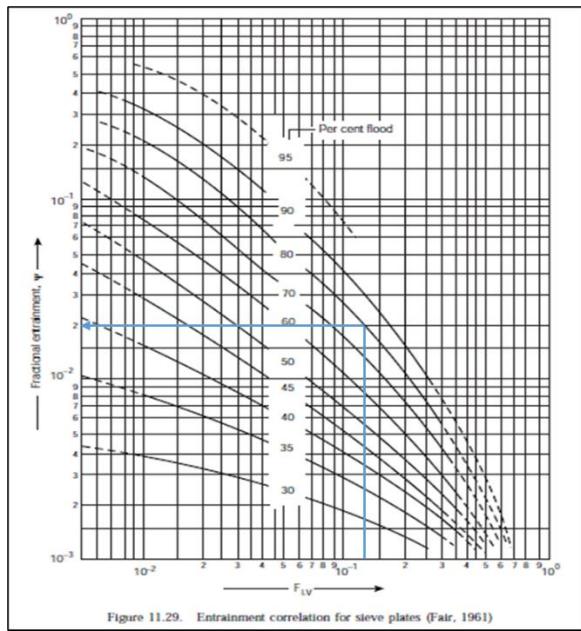
Step 7: Check Entrainment

Actual vapour velocity (based on net area),

$$u_v = \frac{\text{Maximum vapour flow rate}}{A_n} = \frac{1.591}{2.023} = 0.786 \text{ m/s}$$

$$\text{Percentage Flooding} = \frac{u_v}{u_f} = \frac{0.786}{0.983} \times 100\% = 80\%$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.29



When $F_{LV} = 0.137$

Fractional Entrainment, $\varphi = 0.02$

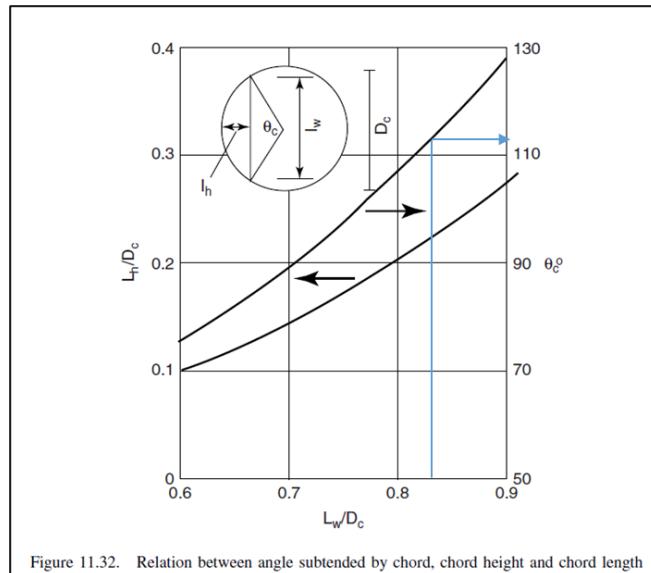
Since $\varphi < 0.1$, the efficiency of plate is not much affected, the design is satisfactory.

Step 8: Determination of perforated area

Allow calming zone width = 50 mm (Coulson and Richardson)

Take unperforated strip round plate edge = 50 mm

From Coulson and Richardson's Chemical Engineering Design, Figure 11.32



When $\frac{l_w}{D_c} = 0.84, \theta_c = 115^\circ$

Angle subtended at plate edge by unperforated strip = $180^\circ - 115^\circ = 65^\circ$

$$\text{Mean length, unperforated edge strips} = (1.772 - 0.05)\pi \times \frac{65}{180} = \mathbf{1.954 \text{ m}}$$

$$\text{Area of unperforated edge strips} = 0.05 \times \mathbf{1.954} = \mathbf{0.0977 \text{ m}^2}$$

Mean length of calming zone = weir length + width of unperforated strip

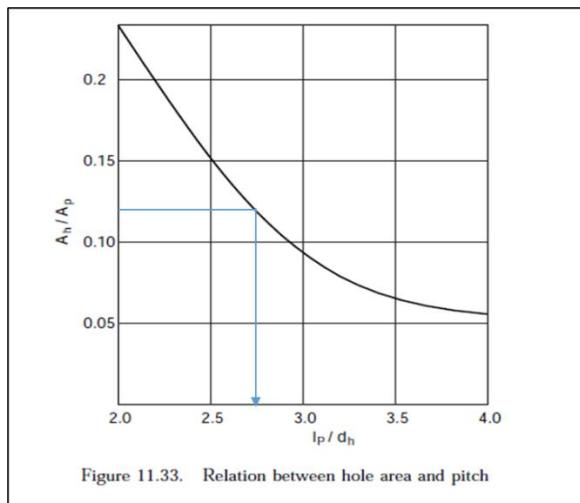
$$\text{Mean length of calming zone} = 1.4888 + 0.05 = 1.539 \text{ m}$$

$$\text{Area of calming zone} = 2 \times 1.539 \times 0.05 = \mathbf{0.1539 \text{ m}^2}$$

$$\text{Total area for perforations, } A_p = 1.579 - 0.0977 - 0.1539 = \mathbf{1.3275 \text{ m}^2}$$

$$\frac{A_h}{A_p} = \frac{0.1579}{1.3275} = 0.1119$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.33



$$\frac{l_p}{d_h} = \mathbf{2.74}$$

This ratio is between 2.5 and 4.0, hence the design is satisfactory.

Step 9: Determination of number of holes

$$\text{Area of one hole} = \frac{\pi d_h^2}{4} = \frac{\pi(0.005)^2}{4} = 1.9635 \times 10^{-5} \text{ m}^2$$

$$\text{Number of holes} = \frac{0.1579}{1.9635 \times 10^{-5}} = 8043.224 \approx 8043 \text{ holes}$$

MECHANICAL DESIGN

Step 1: Design Pressure

Considering pressure drop in distillation column, the operating pressure at bottom = 1.01 bar

Safety margin of 10% is applied to the operating pressure of the column, which is 1.01 bar.

$$\text{Design pressure} = 1.1 \times 2.8 \text{ bar} \times \frac{1 \times 10^5 \text{ N}}{\text{bar.m}^2} \times \frac{1 \text{ m}^2}{10^6 \text{ mm}^2} = 0.308 \frac{\text{N}}{\text{mm}^2}$$

Step 2: Design temperature

Safety margin of 10 °C is applied to the highest temperature of the column, which is 180.913 °C.

$$\text{Design temperature} = 180.913 + 10 = 190.913^\circ\text{C}$$

Step 3: Material of construction

Stainless steel 304 is chosen as the material of construction for this distillation because there is need for corrosion resistance for the column. From Table 13.2 in Coulson and Richardson's Chemical Engineering Design, stainless steel at 191 °C has design stress of about 117.7 N/mm², which is much higher than the column design pressure. Hence, it is a suitable material of construction for this distillation column.

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Step 4: Welded joint efficiency

A double welded butt type of welding is used for this distillation column to balance the tradeoff between higher cost and higher strength of weld joint. The welded joint efficiency, J of this weld joint is 0.85.

Table 13.3. Maximum allowable joint efficiency			
Type of joint	Degree of radiography		
	100 per cent	spot	none
Double-welded butt or equivalent	1.0	0.85	0.7
Single-weld butt joint with bonding strips	0.9	0.80	0.65

Step 5: Minimum Column Thickness

Internal diameter of column, $D_i = 1.773 \text{ m} = 1773 \text{ mm}$

Wall thickness is calculated based on Coulson & Richardson's Chemical Engineering Design.

$$\begin{aligned} \text{Minimum wall thickness, } t &= \frac{P_i D_i}{2J_f - P_i} \\ &= \frac{0.308(1773)}{2(0.85)(117.7) - 0.308} \\ &= \mathbf{2.733 \text{ mm}} \end{aligned}$$

Take corrosion allowance of 1 mm.

Fabrication thickness of column wall = $2.733 + 1 = \mathbf{3.733 \text{ mm}}$

Vessel diameter (m)	Minimum thickness (mm)
1	5
1 to 2	7
2 to 2.5	9
2.5 to 3.0	10
3.0 to 3.5	12

Since the column diameter is 1.733 m, thus the suggested minimum thickness should be used is 7 mm as the calculated wall thickness is smaller. This is due to the condition to make sure the column base able to withstand the wind and dead weight loads. Therefore, the column is divided into 8 section with 2mm increment of thickness as the number of section ascending.

Section 1	2.733399405	mm
Section 2	4.733399405	mm
Section 3	6.733399405	mm

Section 4	8.733399405	mm
Section 5	10.73339941	mm
Section 6	12.73339941	mm
Section 7	14.73339941	mm
Section 8	16.73339941	mm
Average	9.733399405	mm
Average wall thickness + corrosion allowance (1 mm)	10.73339941	mm

Step 6: Column Head Design

Due to low design pressure of the system, the type of head chosen is torispherical head. For torispherical head, the head thickness is designed as below:

Crown radius, $R_c = D_i = 1.773 \text{ m}$

$$R_k / R_c = 0.06$$

$$R_k = 0.1064 \text{ m}$$

$$C_s = \frac{1}{4} \left(3 + \sqrt{\frac{R_c}{R_k}} \right) = \frac{1}{4} \left(3 + \sqrt{0.06} \right) = 1.771$$

$$t = \frac{P_i R_c C_s}{2f_j + P_i (C_s - 0.2)} = \frac{0.308 \times 106.4 \times 1.771}{2 \times 117.7 \times 0.85 + 0.308(1.771 - 0.2)} = 4.116 \text{ mm}$$

The minimum head thickness is comparable with the minimum wall thickness of the cylindrical section. Thus, the head thickness is taken same as the wall thickness, 10.733 mm.

Step 7: Insulation design

Fibreglass with 100 kg/m³ density and 75 mm thickness is chosen for this distillation column.

Step 8: Weight of Vessel

The total weight of the vessel consists of the column weight, tray weight and weight of insulation. Each weight is calculated separately and totalled up to get the total weight of vessel which is required for stress analysis of the column. The weight of column is calculated based on formula in Coulson and Richardson's Chemical Engineering Design:

Weight of Column

Take $C_v = 1.15$ as a factor to account for the weight of nozzle, manway, internal support

$$\text{Mean diameter, } D_m = D_i + t = 1.773 + 2(0.010733) = 1.7837 \text{ m}$$

$$\begin{aligned}
 \text{Weight of column, } W_t &= C_v \pi D_m (H_v + 0.8D_m)t \\
 &= (1.15\pi)(1.7837)[31.92 + 0.8(1.7837)](10.733) \\
 &= 176229.6 \text{ N} = 176.23 \text{ kN}
 \end{aligned}$$

Weight of Plate

$$\begin{aligned}
 \text{Weight of single tray} &= \text{Area of plate} \times \text{Plate thickness} \times \text{construction material density} \times g \\
 &= 2.469 \times 0.003 \times 8000 \times 9.81 \\
 &= 581.283 \text{ N}
 \end{aligned}$$

$$\begin{aligned}
 \text{Weight of Trays} &= \text{Weight of single tray} \times \text{No. of trays} \\
 &= 581.283 \times 46 = 26739.017 \text{ N} = 26.739 \text{ kN}
 \end{aligned}$$

Weight of Insulation

$$\text{Volume of Insulation} = \pi D_i t_I H = \pi(1.773)(0.075)(31.924) = 13.336 \text{ m}^3$$

$$\begin{aligned}
 \text{Weight of Insulation} &= \text{Volume of Insulation} \times \text{Insulation Material Density} \times g \\
 &= 13.336 \times 200 \times 9.81 \\
 &= 26165.544 \text{ N} = 26.166 \text{ kN}
 \end{aligned}$$

$$\text{Total weight of distillation column, } W = 176.23 + 26.739 + 26.166 = \mathbf{229.134 \text{ kN}}$$

Step 9: Stress Analysis

Stress analysis must be made to ensure that the reactor structure is strong and safe. Stress analysis is solely based on Coulson and Richardson's Chemical Engineering Design.

Wind Loading

Typically, wind pressure = **1280 N/m²** for preliminary design.

Effective Column Diameter = Vessel diameter = **1.944 m**

Wind loading per unit length of column, $F_w = 1280(1.944) = 2488.918 \text{ N/m}$

$$\begin{aligned}
 \text{Bending moment at bottom tangent line, } M_x &= \frac{F_w H^2}{2} \\
 &= \frac{2488.918 (31.92)^2}{2} \\
 &= \mathbf{1268242 \text{ Nm}}
 \end{aligned}$$

$$\text{Longitudinal stress, } \sigma_L = \frac{PD_i}{4t} = \frac{0.308 \times 1773}{4 \times 16.733} = \mathbf{8.159 \text{ N/mm}^2}$$

$$\text{Circumferential stress, } \sigma_h = \frac{PD_i}{2t} = \frac{0.308 \times 1773}{2 \times 16.733} = \mathbf{16.317 \text{ N/mm}^2}$$

$$\text{Dead weight stress, } \sigma_w = \frac{W}{\pi(D_i+t)t} = \frac{229.134 \times 1000}{\pi(1773 + 16.733)(16.73)} = \mathbf{2.435 \text{ N/mm}^2}$$

$$\text{Second moment area of the vessel about the plane of bending, } I_v = \frac{\pi}{64}(D_o^4 - D_i^4)$$

$$I_v = \frac{\pi}{64} \times (1806^4 - 1773^4) = 3.77 \times 10^{10} \text{ mm}^4$$

$$\begin{aligned}\text{Bending stress, } \sigma_b &= \pm \frac{M_x}{I_v} \left(\frac{D_i}{2} + t \right) = \pm \frac{1268242 \times 1000}{3.77 \times 10^{10}} \times \left(\frac{1773}{2} + 16.733 \right) \\ &= \pm \mathbf{30.406 \text{ N/mm}^2}\end{aligned}$$

$$\text{Total longitudinal stress, } \sigma_z = \sigma_L + \sigma_w \pm \sigma_b$$

Since σ_w is compressive, hence it is negative.

$$\sigma_z(\text{upwind}) = 8.159 - 2.435 + 30.406 = \mathbf{36.128 \text{ N/mm}^2}$$

$$\sigma_z(\text{downwind}) = 8.159 - 2.435 - 30.406 = \mathbf{-24.683 \text{ N/mm}^2}$$

Principal stress will be σ_z and σ_h due to no torsional shear stress.

Radial stress is negligible.

$$\text{Stress difference} = \sigma_h - \sigma_z(\text{downwind})$$

From calculation, the greatest principle stress difference is 41.00 N/mm^2

This does not exceed the design stress for the material construction of this column (117.7 N/mm^2) hence the design is acceptable.

Step 10: Elastic stability

$$\text{Critical buckling stress, } \sigma_c = 2 \times 10^4 \left(\frac{t}{D_o} \right) = 2 \times 10^4 \left(\frac{16.733}{1806} \right) = \mathbf{185.261 \text{ N/mm}^2}$$

Maximum compressive where the vessel is not under pressure

$$= \sigma_w + \sigma_b = 2.435 + 30.406 = \mathbf{32.841 \text{ N/mm}^2}$$

Since critical buckling stress is smaller than maximum allowable design stress, maximum compressive stress (32.841 N/mm^2) should be less than critical buckling stress (185.261 N/mm^2). Hence, this condition is fulfilled and the design is satisfactory.

Step 11: Vessel support

Type of support chosen: Conical Skirt

Take skirt bottom diameter, $D_s = \mathbf{1.9 \text{ m}}$

Take skirt height, $H_s = \mathbf{3 \text{ m}}$

$$\text{Skirt base angle, } \theta_s = \tan^{-1} \frac{H_s}{\frac{1}{2}(D_s - D_i)} = \tan^{-1} \frac{(3)}{\frac{1}{2}(1.9 - 1.773)} = \mathbf{88.79^\circ}$$

This angle is between 80° and 90° hence the skirt base angle is satisfactory.

The maximum dead weight load on the skirt will occur when the vessel is full of water.

$$\begin{aligned}
\text{Approximate Water Weight, } W_w &= \left(\frac{\pi}{4} \times D_i^2 \times H \right) \times 1000 \times 9.81 \\
&= \left(\frac{\pi}{4} \times 1.773^2 \times 31.92 \right) \times 1000 \times 9.81 \\
&= 1961790 \text{ N} = 773.192 \text{ kN}
\end{aligned}$$

Take skirt thickness, t_s be 16.733 mm,

$$\begin{aligned}
\text{Bending moment at bottom of skirt, } M_s &= \frac{F_w(H+H_s)^2}{2} \\
&= \frac{2.490 (31.92 + 3)^2}{2} \\
&= \mathbf{1517.807 \text{ kNm}}
\end{aligned}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \frac{4M_s}{\pi(D_s + t_s)D_s t_s} = \frac{4(1517.807 \times 1000)10^3}{\pi(3000 + 16.733)(3000)(16.733)}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \mathbf{31.712 \frac{N}{mm^2}}$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(\text{test})} = \frac{W_w}{\pi(D_s + t_s)t_s} = \frac{(773.192 \times 1000)}{\pi(3000 + 16.733)(16.733)}$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(\text{test})} = \mathbf{7.673 \text{ N/mm}^2}$$

$$\sigma_{ws(\text{operating})} = \frac{W}{\pi(D_s + t_s)t_s} = \frac{(229.134 \times 10^3)}{\pi(3000 + 16.733)(16.733)} = \mathbf{2.274 \text{ N/mm}^2}$$

$$\sigma_{s(\text{compressive})} = 31.712 + 7.673 = \mathbf{39.386 \text{ N/mm}^2}$$

$$\sigma_{s(\text{tensile})} = 31.712 - 2.274 = \mathbf{29.438 \text{ N/mm}^2}$$

The skirt thickness should be such that under the worst combination of wind and dead-weight loading, 2 design criteria must be satisfied. Choosing the skirt material to be stainless steel 304, maximum allowable design stress is 117.7 N/mm².

$$\sigma_{s(\text{tensile})} < f_s J \sin \theta$$

$$29.438 < (0.85)(117.7) \sin(88.79^\circ)$$

$$29.438 < 100.02$$

$$\sigma_{s(\text{compressive})} < 0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta$$

$$39.385 < 0.125(197500) \left(\frac{16.733}{3000} \right) \sin(88.79^\circ)$$

$$39.385 < 220.127$$

Since both design criteria are satisfied, the skirt thickness is acceptable

Take corrosion allowance of 2mm, skirt thickness = $16.733 + 2 = \mathbf{18.733 \text{ mm}}$

Step 12: Base ring and anchor bolt design

Take pitch circle diameter, $D_b = 3.2 \text{ m}$

Circumference of bolt circle = $3.2 \times 10^3(\pi) = 10053.096 \text{ mm}$

Minimum bolt spacing is recommended at 630 mm

No. of bolts required = $\frac{10053.096}{630} = 15.957 \approx 16 \text{ bolts (Must be multiple of 4)}$

Bolt stress, $f_b = 125 \frac{\text{N}}{\text{mm}^2}$ (from Coulson & Richardson's Chemical Engineering Design)

$$\begin{aligned} \text{Area of bolt, } A_b &= \frac{1}{N_b f_b} \left[\frac{4M_s}{D_b} - W \right] = \frac{1}{16(125)} \left[\frac{4(15178007)}{3.2} - 229.134 \times 10^3 \right] \\ &= 834.063 \text{ mm}^2 \end{aligned}$$

$$\text{Diameter of bolt} = \sqrt{\frac{A_b \times 4}{\pi}} = \sqrt{\frac{834.063 \times 4}{\pi}} = \mathbf{32.587 \text{ mm}}$$

From Coulson & Richardson's Chemical Engineering Design Figure 13.30, the bolt type selected is **M36** as it is the closest standard size bolt larger than 32.587 mm. Its root area is 817 mm^2 .

Total compressive load on base ring, F_b

$$= \frac{4M_s}{\pi D_s^2} + \frac{W}{\pi D_s} = \frac{4(15178007)}{\pi(3)^2} + \frac{229134}{\pi(3)} = \mathbf{573714.848 \text{ N/m}}$$

From Coulson and Richardson's Chemical Engineering Design, maximum allowable bearing pressure on concrete foundation pad, $f_c = 6 \text{ N/mm}^2$

$$\text{Minimum base ring width, } L_b = \frac{F_b}{f_c} \times \frac{1}{1000} = \frac{573714.848}{6} \times \frac{1}{1000} = \mathbf{95.619 \text{ mm}}$$

From Figure 13.26 in Coulson and Richardson's Chemical Engineering Design, distance from skirt edge to ring edge, $L_r = \mathbf{102 \text{ mm}}$

Actual base ring width = $L_r + t_s + 50 = 102 + 18.7333 + 50 = \mathbf{170.7333 \text{ mm}}$

$$\text{Actual bearing pressure on concrete foundation pad, } f'_c = \frac{573714.848}{170.733 \times 1000} = 3.36 \text{ N/mm}^2$$

Allowable design stress in ring material, $f_r = 140 \text{ N/mm}^2$ (From Coulson and Richardson's Chemical Engineering Design)

$$\text{Minimum base ring thickness, } t_b = L_r \sqrt{\frac{3f'_c}{f_r}} = 102 \sqrt{\frac{3 \times 3.36}{140}} = \mathbf{27.371 \text{ mm}}$$

Step 13: Nozzles design

Stream	W (kg/hr)	ρ (kg/m³)	D_{opt} (mm)	D_{opt} (in)	NPS (in)
Feed	34346.74	771.70	117.72	4.63	5
Top outlet	20873.89	6.74	409.07	16.10	18
Reflux	12298.65	772.61	74.12	2.92	3
Bottom outlet	23445.87	712.79	101.60	4.00	4
Boilup	9973.02	8.03	277.89	10.94	12

DISTILLATION COLUMN T-401

Component Distribution

Step 1: Identification of Light Key (LK) and Heavy Key (HK)

Light Key : EthylBenzene

Light Non-Key: Benzene

Heavy Key : Diethylbenzene

Step 2: Determination of Dew Point and Bubble Point

Step 2: Determination of partial vapor pressure and relative volatilities

From Raoult's Law and Dalton's Law, $K = P_{\text{sat}}/P$. Partial pressure of each component is calculated using Antoine's equation.

Antoine Equation					
T in K, P in Pa					
Vapor pressure = $\exp [C1 + (C2/T) + C3 \times \ln(T) + C4 \times T^{C5}]$					
T in K, P in kPa					
$T \log P = AC - B + AT - C \log P$					

Components	C1	C2	C3	C4	C5
Benzene	83.1070	-6486.2000	-9.2194	0.0000	2.0000
Ethylbenzene	89.0630	-7733.7000	-9.9170	0.0000	2.0000

Components	A	B	C
Diethylbenzene	4.1254	1589.2730	-71.1310

Dew point
$$\sum \frac{y}{K} = 1$$

Bubble point
$$\sum Kx = 1$$

Relative volatilities, α
$$\alpha_{LK,HK}(T) = \frac{K_{LK}(T)}{K_{HK}(T)}$$

Average relative volatility, α_{avg}

$$\alpha_M = \sqrt[3]{\alpha_{(LK,HK)F} \times \alpha_{(LK,HK)D} \times \alpha_{(LK,HK)B}}$$

$$\alpha_M = 2.9604$$

Feed temperature	454.0630	K	Pressure	2.8000	bar	
Components	Molar Flow Rate (kmol/hr)	P* (bar)	$K_i = \frac{P_i}{P}$	$\alpha_i = \frac{K_i}{K_{HK}}$	Zi	$y_i = K_i z_i$
Methane	0.0000	25355.1582	9055.4136	26847.3506	0.0000	0.0000
Ethane	0.0000	553.7375	197.7634	586.3258	0.0000	0.0000
Ethylene	0.0000	1053.2560	376.1629	1115.2418	0.0000	0.0000
Benzene	0.1336	10.4009	3.7146	11.0131	0.0011	0.0040
Ethylbenzene	115.1542	2.9396	1.0499	3.1126	0.9249	0.9711
Diethylbenzene	9.2124	0.9444	0.3373	1.0000	0.0740	0.0250
Total	124.5002	26976.4367	9634.4417	28564.0440	1.0000	1.0000

Dew point	451.7356	K	Pressure	2.8000	bar	
Components	Distillate Mole Fraction	P* (bar)	$K_i = \frac{P_i}{P}$	$\alpha_i = \frac{K_i}{K_{HK}}$	$x_i = \frac{y_i}{K_i}$	
Methane	0.0000	23813.7423	8504.9079	26732.6145	0.0000	
Ethane	0.0000	534.9358	191.0485	600.5033	0.0000	
Ethylene	0.0000	1012.6185	361.6495	1136.7361	0.0000	
Benzene	0.0012	9.9838	3.5656	11.2075	0.0003	
Ethylbenzene	0.9988	2.7979	0.9993	3.1408	0.9995	
Diethylbenzene	0.0000	0.8908	0.3181	1.0000	0.0001	
Total	1.0000	25374.9691	9062.4890	28485.2024	1.0000	

Bubble point	502.6792	K	Pressure	2.8000	bar
Components	Bottom Mole Fraction,	P* (bar)	$K_i = \frac{P_i}{P}$	$\alpha_i = \frac{K_i}{K_{HK}}$	$y_i = K_i x_i$
Methane	0.0000	100226.0548	35795.0196	36163.0025	0.0000
Ethane	0.0000	1143.2412	408.3004	412.4979	0.0000
Ethylene	0.0000	2444.1197	872.8999	881.8735	0.0000
Benzene	0.0000	22.4287	8.0102	8.0926	0.0000
Ethylbenzene	0.0062	7.3554	2.6269	2.6539	0.0163
Diethylbenzene	0.9938	2.7715	0.9898	1.0000	0.9837
Total	1.0000	103845.9713	37087.8469	37469.1204	1.0000

Step 3: Minimum number of stages, N_{min}

$$N_{min} = \frac{\ln\left(\frac{x_{D,LK} \times x_{B,HK}}{x_{B,LK} \times x_{D,DH}}\right)}{\ln(\alpha_M)} = \frac{\ln\left(\frac{0.9988}{0.0062} \times \frac{0.9938}{4 \times 10^{-5}}\right)}{\ln(4.264)} = 14.006 \text{ stages}$$

Step 4: Determination of reflux ratio, R

Feed enters the distillation column as saturated liquid. q = 1

Underwood equation is used to find minimum reflux ratio, R_{min}

$$\sum_{i=1}^n \frac{\alpha_i x_{F,i}}{\alpha_i - \theta} = 1 - \bar{q}$$

Components	Distillate, x _{i,D} (mol frac)	K _i = P _{i,sat} /P	$\alpha_i = K_i/K_{HK}$	Bottom, x _{i=B} (mol frac)	$\alpha_i x_{i,F}$	$\alpha_i x_{i,F}/(\alpha_i - \theta)$	$\alpha_i x_{i,D}$	$\alpha_i x_{i,D}/(\alpha_i - \theta)$
Methane	0.0000	9055.4136	26847.3506	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	197.7634	586.3258	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	0.0000	376.1629	1115.2418	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0012	3.7146	11.0131	0.0000	0.0118	0.0012	0.0128	0.0013
Ethylbenzene	0.9988	1.0499	3.1126	0.0062	2.8790	1.3977	3.1089	1.5094
Diethylbenzene	0.0000	0.3373	1.0000	0.9938	0.0740	-1.3989	0.0000	-0.0008
Total	1.0000	9634.4417	28564.0440	1.0000	2.9648	0.0000	3.1217	1.5099

q	1.0000	Rmin	0.5099
1-q	0.0000	R/Rmin	1.5000
θ	1.0529	R _{act}	0.7648

Value of θ is obtained by satisfying $\frac{\sum \alpha_i x_{if}}{\alpha_i - \theta} = 0$. The value of R is set as $1.5R_{min}$.

Finally, R_{act} is **0.7648**.

Step 5: Determination of number of theoretical stages, N

Number of theoretical stages, N is calculated using Gilliland correlation

$$Y = \frac{N - N_{min}}{N + 1} = 1 - \exp\left[\frac{1 + 54.4X}{11 + 117.2X} \times \frac{X - 1}{X^{0.5}}\right]$$

$$X = \left(\frac{R_{act} - R_{min}}{R_{act} + 1}\right)$$

$$X = 0.1444$$

$$Y = 1 - \exp\left[\frac{1 + 54.4(0.1444)}{11 + 117.2(0.1444)} \times \frac{(0.1444) - 1}{(0.1444)^{0.5}}\right]$$

$$Y = 0.5102 = \frac{N - N_{min}}{N + 1}$$

N = 29.641 stages (including theoretical stage for reboiler)

= 28.641 stages

Step 6: Overall tray efficiency, E_o

Overall tray efficiency is calculated by using O'Connell's correlation of overall column efficiency,

$$E_o = 0.503(\mu_{F,avg} \alpha_{avg})^{-0.226}$$

Liquid viscosity of the components is calculated using properties from Yaws Chemical Properties Handbook and pure component data bank from Aspen Plus.

Properties from yaws Chemical Properties Handbook

Components	A	B	C	D
Benzene	-7.4005	1181.5	0.014888	-0.000013713
Ethylbenzene	-5.2585	830.65	0.010784	-0.000010618
Diethylbenzene	-5.8058	1014	0.010909	-9.7803E-06

Average viscosity for each component

Component	Feed Mole Fraction	Molar average μ in (cP)
-----------	--------------------	-----------------------------

Benzene	0.0011	0.000146232
Ethylene	0.0000	0
Ethylbenzene	0.9249	0.175569742
Diethylbenzene	0.0740	0.017120329
Methane	0.0000	0
Ethane	0.0000	0
Total	1	0.192836303

$$E_o = \mathbf{0.568}$$

Step 7: Determination of actual number of theoretical stages

N = 28.641 stages

Actual number of theoretical stages, N_{act}

$$N_{act} = \frac{N_{eq}}{E_o} = \frac{28.641}{0.568}$$

N_{act} = 50.433 stages = 51 stages

Step 8: Feed point location

By using Kirkbride equation, the location of feed point calculated from

$$\log \frac{N_D}{N_B} = 0.206 \log \left[\frac{B}{D} \left(\frac{x_{HK,F}}{x_{LK,F}} \right) \left(\frac{(x_{LK})_B}{(x_{HK})_D} \right)^2 \right]$$

$$\log \frac{N_D}{N_B} = 0.206 \log \left[\frac{9.2654}{115.235} \left(\frac{0.025}{0.9711} \right) \left(\frac{0.0163}{0.0001} \right)^2 \right]$$

$$\frac{N_D}{N_B} = 2.0787$$

Since N_D + N_B = N_{act},

N_B, Number of stages in stripping section = 16.566

N_B ≈ 17 stages below feed including reboiler

N_D, Number of stages/trays in rectifying section = 34.434

N_D ≈ 35 stages above feed stages

So, the feed located at 35th stage from bottom.

COLUMN SIZING

The distillation column is sized based on the top condition and the bottom condition. Next, the size of distillation column is decided based on the larger diameter calculated from the top or bottom condition. For column sizing, the important information is the flow rate of each stream related to distillation column and their respective density, which is presented in table below:

Properties	Distillate	Bottom	Feed
L (kmol/hr)	88.13562662	212.63585	
V (kmol/hr)	203.3704	203.3704	

MW _{average} (kg/kmol)	106.1386003	134.0456916	108.2154681
L _w (kg/hr)	9354.592047	28502.91958	
V _w (kg/hr)	21585.45437	27260.93195	
ρ _v (kg/m ³)	7.912925174	8.980694434	8.026408766
ρ _L (kg/m ³)	714.5536299	670.6869939	712.79136
σ (J/m ²)	0.012424659	0.009245586	0.007896538

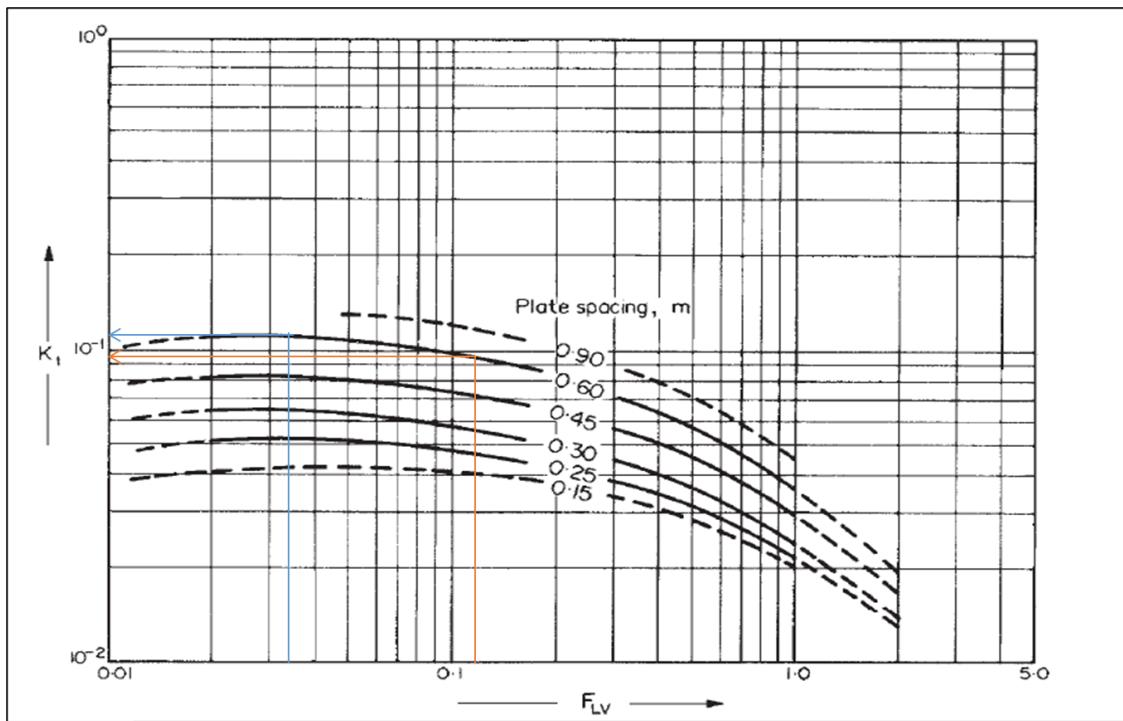
Step 1: Determination of vapor flooding velocity, u_f

Assuming column diameter is larger than 1 m, tray spacing of 0.61 m (2.0013 ft) is typically chosen.

$$u_f = K_1 \left(\frac{\rho_L - \rho_v}{\rho_v} \right)^{0.5}$$

Where Ts is tray spacing in ft.

Value of K₁ taken from Figure 11.27 Coulson and Richardson book page 568.



Top Condition	Bottom Condition
$F_{LV} = \frac{L_w}{V_w} \left(\frac{\rho_v}{\rho_L} \right)^{\frac{1}{2}} = \frac{9354.592}{21585.454} \left(\frac{7.912925174}{714.5536299} \right)^{0.5} = 0.0456$ $K_1 = 0.095$ $u_f = 0.816 \text{ m/s}$	$F_{LV} = \frac{L_w}{V_w} \left(\frac{\rho_v}{\rho_L} \right)^{\frac{1}{2}} = \frac{28502.920}{27260.932} \left(\frac{8.980694434}{670.6869939} \right)^{0.5} = 0.1210$ $K_1 = 0.118$ $u_f = 0.868 \text{ m/s}$

Step 2: Determination of actual vapour velocity, u_v

$u_v = 0.8u_f$ (Take 80% flooding velocity for column operation)

Top Condition	Bottom Condition
$u_v = 0.80(0.816)$ $= \mathbf{0.653 \text{ m/s}}$	$u_v = 0.80(0.868)$ $= \mathbf{0.694 \text{ m/s}}$

Step 3: Determination of net column area, A_n

$$A_n = \frac{\dot{V}}{u_v}$$

Top Condition	Bottom Condition
$A_n = \frac{0.7577}{0.653}$ $= 1.1604 \text{ m}^2$	$A_n = \frac{0.8432}{0.694}$ $= 1.2142 \text{ m}^2$

Step 4: Determination of cross sectional area, A_c

$$A_c = \frac{A_n}{0.88} \text{ (assume downcomer occupies 18% of column cross sectional area)}$$

Top Condition	Bottom Condition
$A_c = \frac{A_n}{0.82} = \frac{1.1604}{0.82}$ $= 1.4152 \text{ m}^2$	$A_c = \frac{A_n}{0.82} = \frac{1.2142}{0.82}$ $= 1.4808 \text{ m}^2$

Step 5: Determination of column diameter, D_c

$$D_c = \sqrt{\frac{4A_c}{\pi}}$$

Top Condition	Bottom Condition
$D_c = \sqrt{\frac{4A_c}{\pi}} = \sqrt{\frac{4(1.4152)}{\pi}}$ $= 1.3423 \text{ m}$	$D_c = \sqrt{\frac{4A_c}{\pi}} = \sqrt{\frac{4(1.4808)}{\pi}}$ $= 1.3731 \text{ m}$

Since limiting diameter occurs at distillate,

$$D_c = 1.3731 \text{ m}$$

Rule of thumb:

Tray spacing is selected to minimize entrainment

Standard trays spacing for large diameter column = 0.46 or 0.61 m

Therefore, tray spacing of 0.6 m is chosen for column C-3 since the column diameter is 1.3731 m.

Step 9: Height of Column

Tray spacing estimated, $H_s = 0.6 \text{ m}$

Plate thickness, $t_p = 0.003 \text{ m}$

Column height, H_c

$H_c = (\text{No. of stages} - 1) \times (\text{Tray spacing} + \text{thickness})$

$$H_c = (N - 1) \times (H_s + t_p) = 35.471 \text{ m}$$

Ratio of column height to column diameter:

$$\text{Ratio} = \frac{H_c}{D_c}$$

Ratio = $25.833 < 30$ (acceptable)

PLATE HYDRAULIC DESIGN

Step 1: Liquid flow arrangement

Maximum liquid flow rate, $V_{L\max} = 0.0118 \text{ m}^3/\text{s}$ and $D_c = 1.3731 \text{ m}$

From Coulson and Richardson Chemical Engineering Design, Figure 11.28,

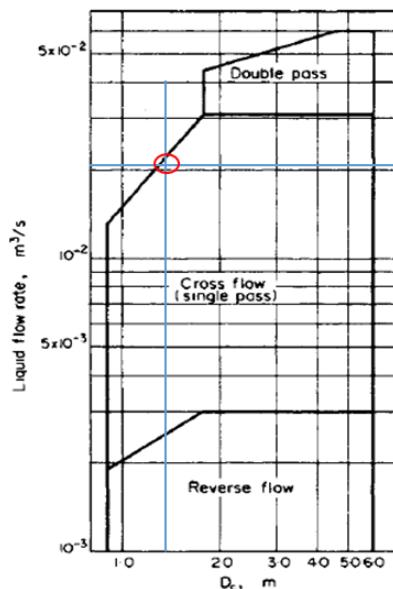


Figure 11.28. Selection of liquid-flow arrangement

The liquid flow arrangement is selected to be **cross flow**.

Step 2: Provisional plate design

Column diameter, $D_c = 1.3731 \text{ m}$

Column area, $A_c = 1.4808 \text{ m}^2$

Downcomer area, $A_d = 0.18(A_c) = 0.2665 \text{ m}^2$

Net area, $A_n = A_c - A_d = 1.214 \text{ m}^2$

Active area, $A_a = A_c - 2A_d = 2.4673 - 2 \times 0.2665 = 0.948 \text{ m}^2$

Assume all holes take 10% of active area,

$$\text{Hole area, } A_h = 0.10(A_a) = 0.10 \times 0.948 = \mathbf{0.0948 \text{ m}^2}$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.31,

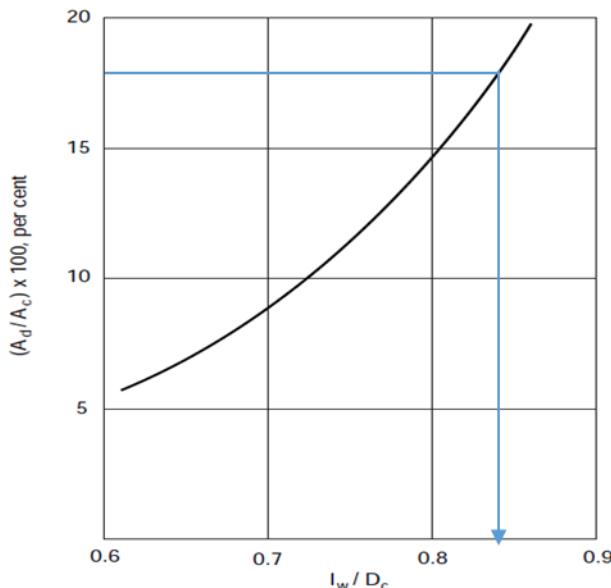


Figure 11.31. Relation between downcomer area and weir length

$$\text{When } \frac{A_d}{A_c} = 0.1800; \frac{l_w}{D_c} = 0.84$$

$$\text{Weir length, } l_w = 0.84 \times D_c = 0.84 \times 1.3731 = \mathbf{1.1534 \text{ m}}$$

Take weir height, $h_w = \mathbf{50 \text{ mm}} = 0.05 \text{ m}$ (40-50 mm is recommended for 1 atm.)

Take hole diameter, $d_h = \mathbf{5 \text{ mm}} = 0.005 \text{ m}$ (Preferred size in design)

Take plate thickness = **3 mm** = 0.003 m (Typical for stainless steel plate)

Step 3: Check Weeping Point

Maximum liquid flow rate = 7.9174 kg/s

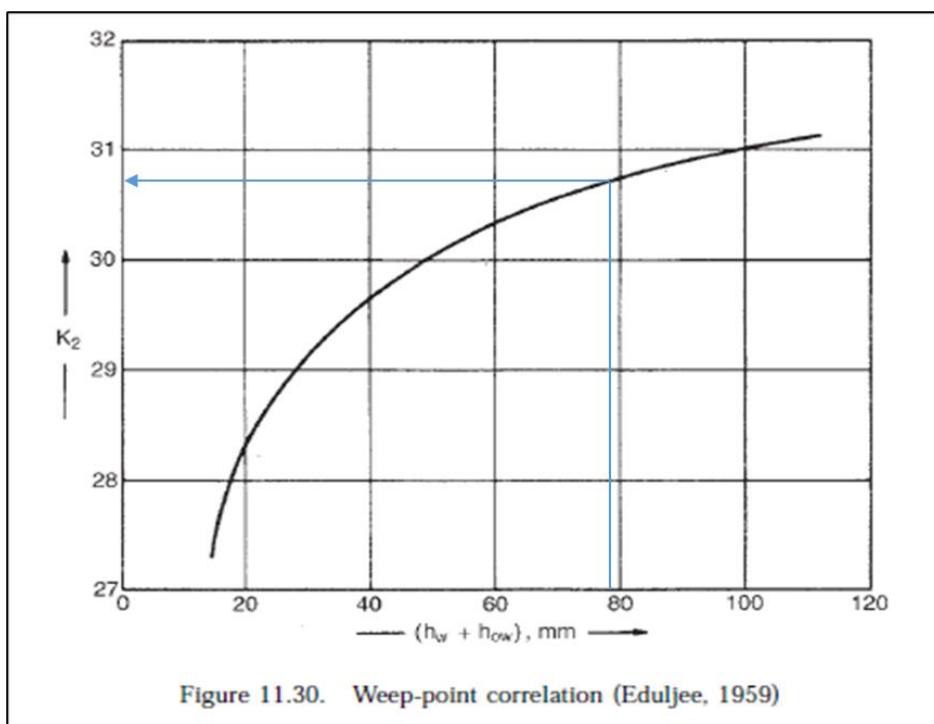
Minimum liquid flow rate at 70% turndown = 0.70 (7.9174) = 5.542 kg/s

$$\text{Max } h_{ow} = 750 \left(\frac{L_{w\max}}{\rho_L \times l_w} \right)^{\frac{2}{3}} = 750 \left(\frac{7.9174}{670.687 \times 1.4888} \right)^{\frac{2}{3}} = 35.355 \text{ mm liquid}$$

$$\text{Min } h_{ow} = 750 \left(\frac{L_{w\min}}{\rho_L \times l_w} \right)^{\frac{2}{3}} = 750 \left(\frac{5.542}{670.687 \times 1.4888} \right)^{\frac{2}{3}} = 27.873 \text{ mm liquid}$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.30

At minimum liquid flow rate, $h_{ow} + h_w = 27.873 \text{ mm} + 50 \text{ mm} = 77.873 \text{ mm liquid}$



$$K_2 = 30.71$$

$$\text{Weeping velocity, } u_h = \frac{[K_2 - 0.90(25.4 - d_h)]}{\sqrt{\rho_v}} = \frac{[30.71 - 0.90(25.4 - 5)]}{\sqrt{8.980}} = 4.121 \text{ m/s}$$

Maximum vapour flow rate = 0.8432 m³/s

Minimum vapour velocity at 70% turndown

$$\text{Actual minimum vapour velocity} = u_h = \frac{0.7 * 0.8432}{0.0948} = 6.228 \text{ m/s}$$

Note: Since actual minimum vapour velocity > weeping velocity, the minimum operating liquid flow rate is well below weep point, the design is satisfactory.

Step 4: Determination of plate pressure drop

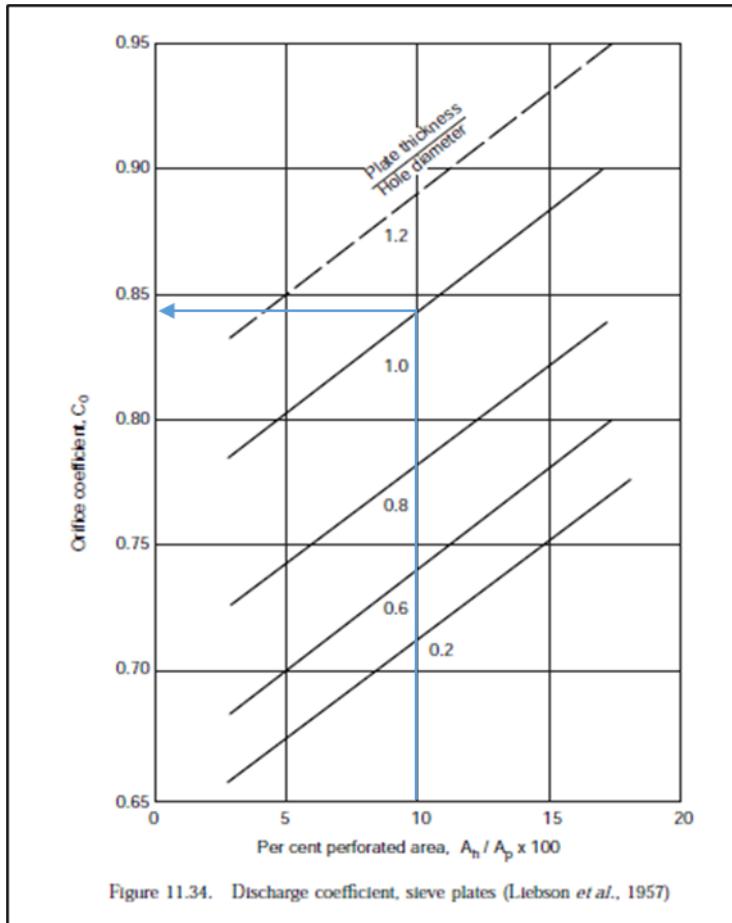
Maximum vapour velocity through holes,

$$u_h = \frac{\text{Maximum Vapour flow rate}}{A_h} = \frac{0.8432}{0.0948} = 8.8974 \text{ m/s}$$

Percentage of perforated area, $\frac{A_h}{A_p} \times 100\% \approx \frac{A_h}{A_a} \times 100\% \approx 10$ and

$$\frac{\text{plate thickness}}{\text{hole diameter}} = \frac{0.003}{0.005} = 0.6$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.34



Orifice coefficient, $C_o = 0.84375$

$$\text{Dry plate pressure drop, } h_d = 51 \left[\frac{u_h}{C_o} \right]^2 \frac{\rho_v}{\rho_L} = 51 \left[\frac{4.121}{0.84375} \right]^2 \frac{8.981}{670.687} = 16.291 \text{ mm liquid}$$

$$\text{Residual head pressure drop, } h_r = \frac{12500}{\rho_L} = \frac{12500}{670.687} = 18.638 \text{ mm liquid}$$

$$\begin{aligned} \text{Total plate pressure drop, } h_t &= h_d + (h_w + h_{ow,max}) + h_r \\ &= 16.291 + 18.638 + 77.873 = 112.802 \text{ mm liquid} \end{aligned}$$

Step 5: Downcomer liquid backup

Taking average value range given by Coulson and Richardson's Chemical Engineering Design (5 to 10mm), height of bottom edge of the apron above the plate.

Take $h_{ap} = h_w - 10 = 50 - 10 = 40 \text{ mm} = 0.04 \text{ m}$

Clearance area under downcomer, $A_{ap} = h_{ap}l_w = 0.04 \times 1.1534 = 0.0461 \text{ m}^2$

Since A_{ap} (0.0461 m^2) is less than A_d (0.2665 m^2), $A_m = 0.0461 \text{ m}^2$

$$h_{dc} = 166 \left[\frac{L_{wd}}{\rho_L A_m} \right]^2 = 166 \left[\frac{7.917}{(670.687)(0.0461)} \right]^2 = \mathbf{10.868 \text{ mm}}$$

$$\begin{aligned} \text{Downcomer backup, } h_b &= (h_w + h_{ow}) + h_t + h_{dc} = 77.873 + 112.802 + 10.868 \\ &= \mathbf{201.544 \text{ mm liquid}} = 0.232 \text{ m liquid} \end{aligned}$$

$$\frac{1}{2}(l_t + h_w) = \frac{1}{2}(0.6 + 0.05) = 0.325 \text{ m}$$

Since $h_b < \frac{1}{2}(l_t + h_w)$, flooding will not occur, the design is satisfactory.

Step 6: Downcomer residence time

$$\text{Downcomer residence time, } t_r = \left(\frac{A_d h_b \rho_L}{L_{wd}} \right) = \left(\frac{0.2665(201.544)(670.687)}{7.917} \right) = \mathbf{4.550 \text{ s}}$$

Since downcomer residence time $> 3 \text{ s}$, flooding is avoided. The design is satisfactory.

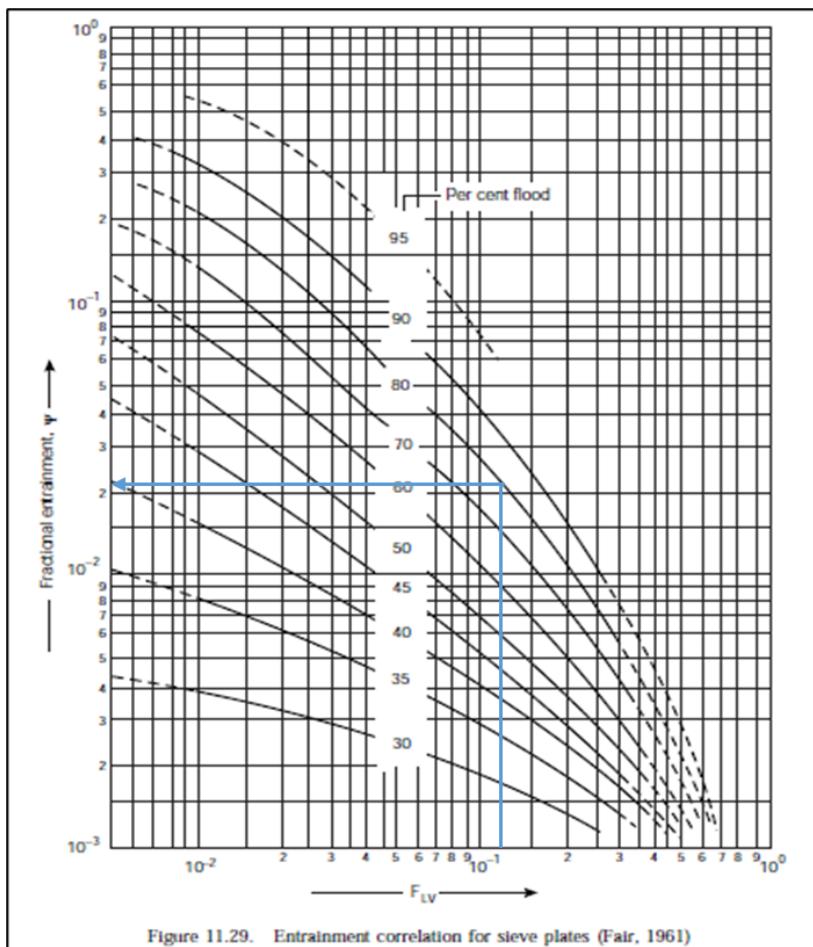
Step 7: Check Entrainment

Actual vapor velocity (based on net area),

$$u_v = \frac{\text{Maximum vapour flow rate}}{A_n} = \frac{0.8432}{1.2142} = 0.6744 \text{ m/s}$$

$$\text{Percentage Flooding} = \frac{u_v}{u_f} = \frac{0.6744}{0.868} \times 100\% = 80\%$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.29



When $F_{LV} = 0.1210$

Fractional Entrainment, $\varphi = 0.0214$

Since $\varphi < 0.1$, the efficiency of plate is not much affected, the design is satisfactory.

Step 8: Determination of perforated area

Allow calming zone width = 50 mm (Coulson and Richardson)

Take unperforated strip round plate edge = 50 mm

From Coulson and Richardson's Chemical Engineering Design, Figure 11.32

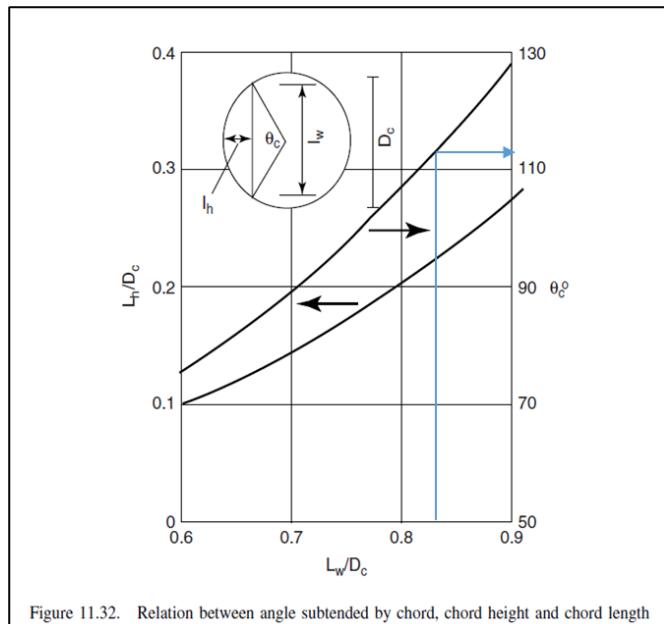


Figure 11.32. Relation between angle subtended by chord, chord height and chord length

$$\text{When } \frac{l_w}{D_c} = 0.84, \theta_c = 115^\circ$$

Angle subtended at plate edge by unperforated strip = $180^\circ - 115^\circ = 65^\circ$

$$\text{Mean length, unperforated edge strips} = (1.3731 - 0.05)\pi \times \frac{65}{180} = \mathbf{1.501 \text{ m}}$$

$$\text{Area of unperforated edge strips} = 0.05 \times \mathbf{1.501} = \mathbf{0.075 \text{ m}^2}$$

Mean length of calming zone = weir length + width of unperforated strip

$$\text{Mean length of calming zone} = 1.1534 + 0.05 = 1.2034 \text{ m}$$

$$\text{Area of calming zone} = 2 \times 1.2034 \times 0.05 = \mathbf{0.1204 \text{ m}^2}$$

$$\text{Total area for perforations, } A_p = 0.948 - 0.1204 - 0.075 = \mathbf{0.7523 \text{ m}^2}$$

$$\frac{A_h}{A_p} = \frac{0.0948}{0.7523} = 0.1260$$

From Coulson and Richardson's Chemical Engineering Design, Figure 11.33

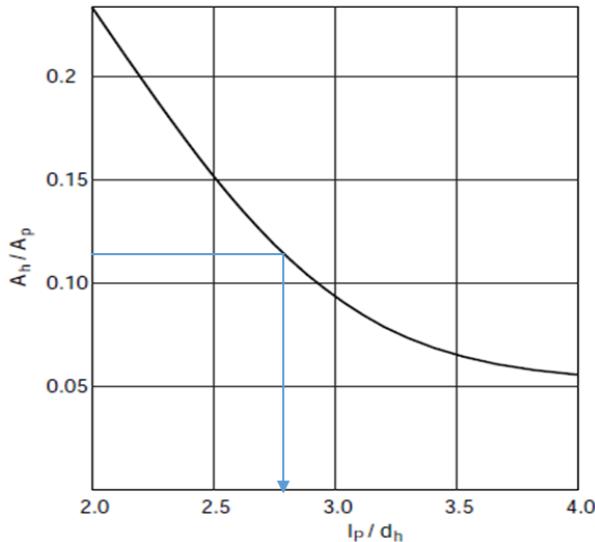


Figure 11.33. Relation between hole area and pitch

$$\frac{l_p}{d_h} = 2.79$$

This ratio is between 2.5 and 4.0, hence the design is satisfactory.

Step 9: Determination of number of holes

$$\text{Area of one hole} = \frac{\pi d_h^2}{4} = \frac{\pi(0.005)^2}{4} = 1.9635 \times 10^{-5} \text{ m}^2$$

$$\text{Number of holes} = \frac{0.0948}{1.9635 \times 10^{-5}} = 4826.5 \approx 4827 \text{ holes}$$

MECHANICAL DESIGN

Step 1: Design Pressure

Considering pressure drop in distillation column, the operating pressure at bottom = 1.01 bar

Safety margin of 10% is applied to the operating pressure of the column, which is 1.01 bar.

$$\text{Design pressure} = 1.1 \times 2.8 \text{ bar} \times \frac{1 \times 10^5 \text{ N}}{\text{bar.m}^2} \times \frac{1 \text{ m}^2}{10^6 \text{ mm}^2} = 0.308 \frac{\text{N}}{\text{mm}^2}$$

Step 2: Design temperature

Safety margin of 10 °C is applied to the highest temperature of the column, which is 229.529 °C.

$$\text{Design temperature} = 229.529 + 10 = 239.529 \text{ }^\circ\text{C}$$

Step 3: Material of construction

Stainless steel 304 is chosen as the material of construction for this distillation because there is need for corrosion resistance for the column. From Table 13.2 in Coulson and Richardson's Chemical Engineering Design, stainless steel at 240 °C has design stress of about 111 N/mm², which is much higher than the column design pressure. Hence, it is a suitable material of construction for this distillation column.

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Step 4: Welded joint efficiency

A double welded butt type of welding is used for this distillation column to balance the tradeoff between higher cost and higher strength of weld joint. The welded joint efficiency, J of this weld joint is 0.85.

Table 13.3. Maximum allowable joint efficiency			
Type of joint	Degree of radiography		
	100 per cent	spot	none
Double-welded butt or equivalent	1.0	0.85	0.7
Single-weld butt joint with bonding strips	0.9	0.80	0.65

Step 5: Minimum Column Thickness

Internal diameter of column, $D_i = 1.3731 \text{ m} = 1.3731 \text{ mm}$

Wall thickness is calculated based on Coulson & Richardson's Chemical Engineering Design.

$$\begin{aligned}\text{Minimum wall thickness, } t &= \frac{P_i D_i}{2J_f - P_i} \\ &= \frac{0.308(1373.1)}{2(0.85)(111) - 0.308} \\ &= \mathbf{2.246 \text{ mm}}\end{aligned}$$

Take corrosion allowance of 1 mm.

Fabrication thickness of column wall = $2.246 + 1 = \mathbf{3.246 \text{ mm}}$

Vessel diameter (m)	Minimum thickness (mm)
1	5
1 to 2	7
2 to 2.5	9
2.5 to 3.0	10
3.0 to 3.5	12

Since the column diameter is 1.3731 m, thus the suggested minimum thickness should be used is 7 mm as the calculated wall thickness is smaller. This is due to the condition to make sure the column base able to withstand the wind and dead weight loads. Therefore, the column is divided into 8 section with 2mm increment of thickness as the number of section ascending.

Section 1	2.246337424	mm
Section 2	4.246337424	mm
Section 3	6.246337424	mm
Section 4	8.246337424	mm

Section 5	10.24633742	mm
Section 6	12.24633742	mm
Section 7	14.24633742	mm
Section 8	16.24633742	mm
Average	9.246337424	mm
Average wall thickness + corrosion allowance	10.24633742	mm

Step 6: Column Head Design

Due to low design pressure of the system, the type of head chosen is torispherical head. For torispherical head, the head thickness is designed as below:

Crown radius, $R_c = D_i = 1.3731 \text{ m}$

$$R_k / R_c = 0.06$$

$$R_k = 0.0823 \text{ m}$$

$$C_s = \frac{1}{4} \left(3 + \sqrt{\frac{R_c}{R_k}} \right) = \frac{1}{4} \left(3 + \sqrt{0.06} \right) = 1.771$$

$$t = \frac{P_i R_c C_s}{2fj + P_i (C_s - 0.2)} = \frac{0.308 \times 82.3 \times 1.771}{2 \times 111 \times 0.85 + 0.308(1.771 - 0.2)} = 3.383 \text{ mm}$$

The minimum head thickness is comparable with the minimum wall thickness of the cylindrical section. Thus, the head thickness is taken same as the wall thickness, 10.246 mm.

Step 7: Insulation design

Fibreglass with 100 kg/m³ density and 75 mm thickness is chosen for this distillation column.

Step 8: Weight of Vessel

The total weight of the vessel consists of the column weight, tray weight and weight of insulation. Each weight is calculated separately and totalled up to get the total weight of vessel which is required for stress analysis of the column. The weight of column is calculated based on formula in Coulson and Richardson's Chemical Engineering Design:

Weight of Column

Take $C_v = 1.15$ as a factor to account for the weight of nozzle, manway, internal support

$$\text{Mean diameter, } D_m = D_i + t = 1.3731 + 2(0.010733) = 1.3842 \text{ m}$$

$$\begin{aligned}
 \text{Weight of column, } W_t &= C_v \pi D_m (H_v + 0.8D_m)t \\
 &= (1.15\pi)(1.3842)[35.471 + 0.8(1.3842)](10.246) \\
 &= 134189.4 \text{ N} = 143.189 \text{ kN}
 \end{aligned}$$

Weight of Plate

$$\begin{aligned}
 \text{Weight of single tray} &= \text{Area of plate} \times \text{Plate thickness} \times \text{construction material density} \times g \\
 &= 1.4827 \times 0.003 \times 8000 \times 9.81 \\
 &= 349.095 \text{ N}
 \end{aligned}$$

$$\begin{aligned}
 \text{Weight of Trays} &= \text{Weight of single tray} \times \text{No. of trays} \\
 &= 349.095 \times 51 = 17803.844 \text{ N} = 17.804 \text{ kN}
 \end{aligned}$$

Weight of Insulation

$$\text{Volume of Insulation} = \pi D_i t_I H = \pi(1.3731)(0.075)(35.471) = 11.483 \text{ m}^3$$

$$\begin{aligned}
 \text{Weight of Insulation} &= \text{Volume of Insulation} \times \text{Insulation Material Density} \times g \\
 &= 11.483 \times 200 \times 9.81 \\
 &= 22530.21 \text{ N} = 22.530 \text{ kN}
 \end{aligned}$$

$$\text{Total weight of distillation column, } W = 143.189 + 17.804 + 22.530 = \mathbf{183.523 \text{ kN}}$$

Step 9: Stress Analysis

Stress analysis must be made to ensure that the reactor structure is strong and safe. Stress analysis is solely based on Coulson and Richardson's Chemical Engineering Design.

Wind Loading

Typically, wind pressure = **1280 N/m²** for preliminary design.

Effective Column Diameter = Vessel diameter = **1.5445 m**

Wind loading per unit length of column, $F_w = 1280(1.5445) = 1976.95 \text{ N/m}$

$$\begin{aligned}
 \text{Bending moment at bottom tangent line, } M_x &= \frac{F_w H^2}{2} \\
 &= \frac{1976.95 (35.471)^2}{2} \\
 &= \mathbf{1243662.698 \text{ Nm}}
 \end{aligned}$$

$$\text{Longitudinal stress, } \sigma_L = \frac{PD_i}{4t} = \frac{0.308 \times 1373.1}{4 \times 16.246} = \mathbf{6.512 \text{ N/mm}^2}$$

$$\text{Circumferential stress, } \sigma_h = \frac{\text{PD}_i}{2t} = \frac{0.308 \times 1373.1}{2 \times 16.246} = 13.024 \text{ N/mm}^2$$

$$\text{Dead weight stress, } \sigma_w = \frac{W}{\pi(D_i+t)t} = \frac{183.523 \times 1000}{\pi(1373 + 16.2246)(16.246)} = 2.586 \text{ N/mm}^2$$

$$\text{Second moment area of the vessel about the plane of bending, } I_v = \frac{\pi}{64}(D_o^4 - D_i^4)$$

$$I_v = \frac{\pi}{64} \times (1406^4 - 1373^4) = 1.71 \times 10^{10} \text{ mm}^4$$

$$\text{Bending stress, } \sigma_b = \pm \frac{M_x}{I_v} \left(\frac{D_i}{2} + t \right) = \pm \frac{1243622.698 \times 1000}{1.71 \times 10^{10}} \times \left(\frac{1373}{2} + 16.246 \right)$$

$$= \pm 51.011 \text{ N/mm}^2$$

$$\text{Total longitudinal stress, } \sigma_z = \sigma_L + \sigma_w \pm \sigma_b$$

Since σ_w is compressive, hence it is negative.

$$\sigma_z(\text{upwind}) = 6.512 - 2.586 + 51.011 = 54.936 \text{ N/mm}^2$$

$$\sigma_z(\text{downwind}) = 6.512 - 2.586 + 51.011 = -47.085 \text{ N/mm}^2$$

Principal stress will be σ_z and σ_h due to no torsional shear stress.

Radial stress is negligible.

$$\text{Stress difference} = \sigma_h - \sigma_z(\text{downwind})$$

From calculation, the greatest principle stress difference is 60.110 N/mm²

This does not exceed the design stress for the material construction of this column (111 N/mm²) hence the design is acceptable.

Step 10: Elastic stability

$$\text{Critical buckling stress, } \sigma_c = 2 \times 10^4 \left(\frac{t}{D_o} \right) = 2 \times 10^4 \left(\frac{16.246}{1406} \right) = 231.019 \text{ N/mm}^2$$

Maximum compressive where the vessel is not under pressure

$$\sigma_w + \sigma_b = 2.586 + 51.011 = 53.597 \text{ N/mm}^2$$

Since critical buckling stress is smaller than maximum allowable design stress, maximum compressive stress (53.597 N/mm²) should be less than critical buckling stress (231.019 N/mm²). Hence, this condition is fulfilled and the design is satisfactory.

Step 11: Vessel support

Type of support chosen: Conical Skirt

Take skirt bottom diameter, $D_s = 1.5 \text{ m}$

Take skirt height, $H_s = 3 \text{ m}$

$$\text{Skirt base angle, } \theta_s = \tan^{-1} \frac{H_s}{\frac{1}{2}(D_s - D_i)} = \tan^{-1} \frac{(3)}{\frac{1}{2}(1.5 - 1.373)} = 88.65^\circ$$

This angle is between 80° and 90° hence the skirt base angle is satisfactory.

The maximum dead weight load on the skirt will occur when the vessel is full of water.

$$\begin{aligned}
\text{Approximate Water Weight, } W_w &= \left(\frac{\pi}{4} \times D_i^2 \times H \right) \times 1000 \times 9.81 \\
&= \left(\frac{\pi}{4} \times 1.373^2 \times 35.47 \right) \times 1000 \times 9.81 \\
&= 515941 \text{ N} = 545.941 \text{ kN}
\end{aligned}$$

Take skirt thickness, t_s be 16.246 mm,

$$\begin{aligned}
\text{Bending moment at bottom of skirt, } M_s &= \frac{F_w(H+H_s)^2}{2} \\
&= \frac{1.977 (35.47 + 3)^2}{2} \\
&= \mathbf{1425.150 \text{ kNm}}
\end{aligned}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \frac{4M_s}{\pi(D_s + t_s)D_s t_s} = \frac{4(1425.150 \times 1000)10^3}{\pi(3000 + 16.246)(3000)(16.246)}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \mathbf{49.108 \frac{N}{mm^2}}$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(\text{test})} = \frac{W_w}{\pi(D_s + t_s)t_s} = \frac{(515.942 \times 1000)}{\pi(3000 + 16.246)(16.246)}$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(\text{test})} = \mathbf{6.667 \text{ N/mm}^2}$$

$$\sigma_{ws(\text{operating})} = \frac{W}{\pi(D_s + t_s)t_s} = \frac{(183.523 \times 10^3)}{\pi(3000 + 16.246)(16.246)} = \mathbf{2.371 \text{ N/mm}^2}$$

$$\sigma_{s(\text{compressive})} = 49.108 + 6.667 = \mathbf{55.775 \text{ N/mm}^2}$$

$$\sigma_{s(\text{tensile})} = 49.108 - 2.371 = \mathbf{46.767 \text{ N/mm}^2}$$

The skirt thickness should be such that under the worst combination of wind and dead-weight loading, 2 design criteria must be satisfied. Choosing the skirt material to be stainless steel 304, maximum allowable design stress is 111 N/mm².

$$\sigma_{s(\text{tensile})} < f_s J \sin \theta$$

$$29.438 < (0.85)(111)\sin(88.65^\circ)$$

$$29.438 < 94.32$$

$$\sigma_{s(\text{compressive})} < 0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta$$

$$39.385 < 0.125(197500) \left(\frac{16.246}{3000} \right) \sin(88.65^\circ)$$

$$39.385 < 270.687$$

Since both design criteria are satisfied, the skirt thickness is acceptable

Take corrosion allowance of 2mm, skirt thickness = $16.246 + 2 = \mathbf{18.246 \text{ mm}}$

Step 12: Base ring and anchor bolt design

Take pitch circle diameter, $D_b = 3.2 \text{ m}$

Circumference of bolt circle = $3.2 \times 10^3(\pi) = 10053.096 \text{ mm}$

Minimum bolt spacing is recommended at 630 mm

No. of bolts required = $\frac{10053.096}{630} = 15.957 \approx 16 \text{ bolts (Must be multiple of 4)}$

Bolt stress, $f_b = 125 \frac{\text{N}}{\text{mm}^2}$ (from Coulson & Richardson's Chemical Engineering Design)

$$\begin{aligned} \text{Area of bolt, } A_b &= \frac{1}{N_b f_b} \left[\frac{4M_s}{D_b} - W \right] = \frac{1}{16(125)} \left[\frac{4(1425149.672)}{3.2} - 229.134 \times 10^3 \right] \\ &= 798.957 \text{ mm}^2 \end{aligned}$$

$$\text{Diameter of bolt} = \sqrt{\frac{A_b \times 4}{\pi}} = \sqrt{\frac{798.957 \times 4}{\pi}} = \mathbf{31.895 \text{ mm}}$$

From Coulson & Richardson's Chemical Engineering Design Figure 13.30, the bolt type selected is **M36** as it is the closest standard size bolt larger than 31.895 mm. Its root area is 817 mm^2 .

Total compressive load on base ring, F_b

$$= \frac{4M_s}{\pi D_s^2} + \frac{W}{\pi D_s} = \frac{4(1425149)}{\pi(3)^2} + \frac{183523}{\pi(3)} = \mathbf{845414.631 \text{ N/m}}$$

From Coulson and Richardson's Chemical Engineering Design, maximum allowable bearing pressure on concrete foundation pad, $f_c = 6 \text{ N/mm}^2$

$$\text{Minimum base ring width, } L_b = \frac{F_b}{f_c} \times \frac{1}{1000} = \frac{845414.631}{6} \times \frac{1}{1000} = \mathbf{140.902 \text{ mm}}$$

From Figure 13.26 in Coulson and Richardson's Chemical Engineering Design, distance from skirt edge to ring edge, $L_r = \mathbf{102 \text{ mm}}$

Dimensions mm								
Bolt size	Root area	A	B	C	D	E	F	G
M24	353	45	76	64	13	19	30	36
M30	561	50	76	64	13	25	36	42
M36	817	57	102	76	16	32	42	48
M42	1120	60	102	76	16	32	48	54
M48	1470	67	127	89	19	38	54	60
M56	2030	75	150	102	25	45	60	66
M64	2680	83	152	102	25	50	70	76
70	—	89	178	127	32	64	76	83
76	—	95	178	127	32	64	83	89

Bolt size = Nominal dia. (BS 4190: 1967)

Figure 13.30. Anchor bolt chair design

$$\text{Actual base ring width} = L_r + t_s + 50 = 102 + 18.246 + 50 = \mathbf{170.246 \text{ mm}}$$

$$\text{Actual bearing pressure on concrete foundation pad, } f'_c = \frac{845414.631}{170.246 \times 1000} = 4.966 \text{ N/mm}^2$$

Allowable design stress in ring material, $f_r = 140 \text{ N/mm}^2$ (From Coulson and Richardson's Chemical Engineering Design)

$$\text{Minimum base ring thickness, } t_b = L_r \sqrt{\frac{3f'_c}{f_r}} = 102 \sqrt{\frac{3 \times 4.966}{140}} = \mathbf{33.273 \text{ mm}}$$

Step 13: Nozzles design

Stream	W (kg/hr)	ρ (kg/m ³)	D _{opt} (mm)	D _{opt} (in)	NPS (in)
Feed	21585.45	712.79	97.89	3.85	4
Top outlet	21585.45	7.91	395.08	15.55	16
Reflux	9354.59	714.55	67.14	2.64	3
Bottom outlet	1418.23	670.69	29.30	1.15	1.5
Boilup	176.24	8.98	43.65	1.72	2

HEAT TRANSFER EQUIPMENT DESIGN

Design Parameters for all heat exchanger equipment:

Cooler design	Tube design
Overall heat transfer coefficient Total heat transfer area	Shell inner diameter Baffle cut Baffle spacing Shell side heat transfer coefficient Shell side pressure drop
Mechanical design	Shell design
Design pressure and temperature Material of construction Shell wall thickness Exchanger head design Insulation Exchanger support Nozzle size	Tube size Number of tube Number of tube passes Tube configuration Tube side heat transfer coefficient Tube side pressure drop

APPENDIX G: HEAT TRANSFER EQUIPMENT

E102 HEAT EXCHANGER SHELL AND TUBE

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE	SHELL
Heat duty, Q	J/s	140827.7778	
Inlet temperature	K	333.27	473.15
Outlet temperature	K	428.75	393.77
Pressure	bar	40	40
Mass flow rate	ton/hr	26.99474	30.22639
	kg/s	7.498538889	8.396219444

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (COLD)	SHELL (HOT)
Mean temperature	K	381.01	433.46
Density	kg/m ³	782.6291524	745.0564244
Specific heat capacity, Cp	kJ/kg.K	2.187402181	0.818627916
Viscosity, μ	kg/m.s	0.000243515	0.000100005
Thermal conductivity, Kf	W/m.K	0.117948386	0.089369733

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² °C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 100 W/m².C.

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{\left(T_{in_h} - T_{out_c}\right) - \left(T_{out_h} - T_{in_c}\right)}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

$$\Delta T_{lm} = \frac{(473.15 - 428.75) - (393.77 - 333.27)}{\ln\frac{473.15 - 428.75}{393.77 - 333.27}} = 52.0355$$

□ Mean temperature difference, ΔT_m

$$\Delta T_m = F_t \Delta T_{lm}$$

□ F_t depends on R & S

$$R = \frac{T_{hi} - T_{ho}}{T_{co} - T_{ci}}$$

$$S = \frac{T_{co} - T_{ci}}{T_{hi} - T_{ci}}$$

$$R = \frac{(473.15 - 393.77)}{(428.75 - 333.27)} = 0.08311783$$

$$S = \frac{(428.75 - 393.77)}{(473.15 - 393.77)} = 0.06825$$

Temperature correction factor, F_t can be obtained from figure 12.19 C&R 3rd edition. If correction factor less than 0.75, proceed to second shell and find the F_t value from figure 12.20 C&R 3rd edition.

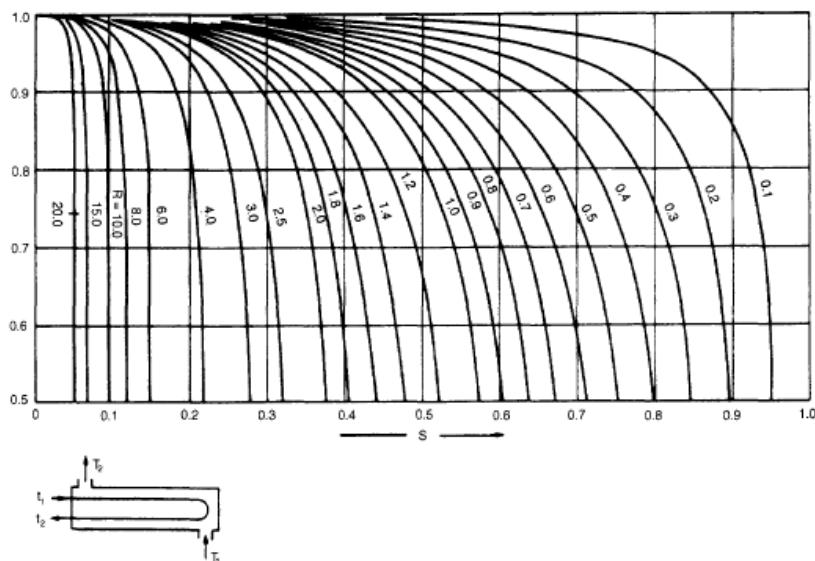


Figure 12.19. Temperature correction factor: one shell pass; two or more even tube 'passes'

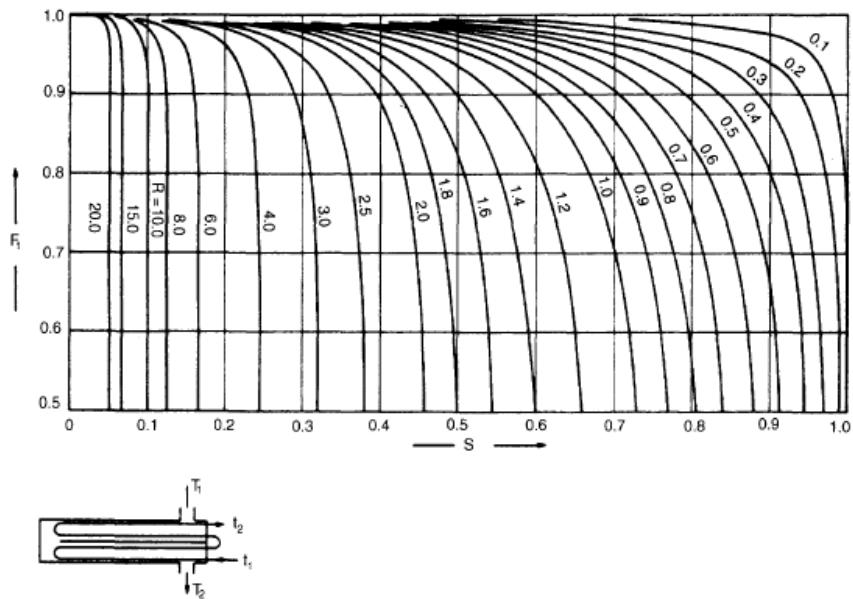


Figure 12.20. Temperature correction factor: two shell passes; four or multiples of four tube passes
Ft value is 0.85.

So,

$$\Delta T_m = 0.85 \times 52.0355 = 44.2302123$$

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{U \times \text{LMTD}}$$

$$A = 31.8397 \text{ m}^2$$

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Parameter	Unit	Value
Tube inner diameter, d_i	m	0.026
Tube outer diameter, d_o	m	0.03
Wall thickness	m	0.002
Nominal length, L	m	4.88
Pitch arrangement, p_t	m	0.0375

STEP 7: NUMBER OF TUBES

$$\text{Area of one tube, } = \pi \times d_o \times L = \pi \times 0.03 \times 4.88 = 0.45999 \text{ m}^2$$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}} = \frac{31.8397}{0.045999} = 69$$

Number of passes, $N_p = 4$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p} = \frac{69}{4} = 17$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi x (d_i^2)}{4} = 0.000530929 \text{ m}^2$$

$$\text{Area per pass} = \frac{A_i}{\text{Number of tubes per pass}} = \frac{0.000530929}{17} = 0.009025796 \text{ m}^2$$

$$\text{Volumetric flow} = \frac{m}{\rho} = 0.009581216 \text{ m}^3/\text{s}$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}} = 1.06165 \text{ m/s}$$

Parameter	Unit	Value
Area of one tube	m ²	0.459929164
Number of tubes, N _t		69
Number of passes, N _p		4
N _t / N _p		17
tube cross-sectional area	m ²	0.000530929
Area per pass	m ²	0.009025796
Volumetric flow	m ³ /s	0.009581216
Tube-side velocity, u _t	m/s	1.061536981

STEP 8: BUNDLE AND SHELL DIAMETER

K₁ and n₁ from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, p _t = 1.25d _o					
No. passes	1	2	4	6	8
K ₁	0.319	0.249	0.175	0.0743	0.0365
n ₁	2.142	2.207	2.285	2.499	2.675
Square pitch, p _t = 1.25d _o					
No. passes	1	2	4	6	8
K ₁	0.215	0.156	0.158	0.0402	0.0331
n ₁	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition

HEAT-TRANSFER EQUIPMENT

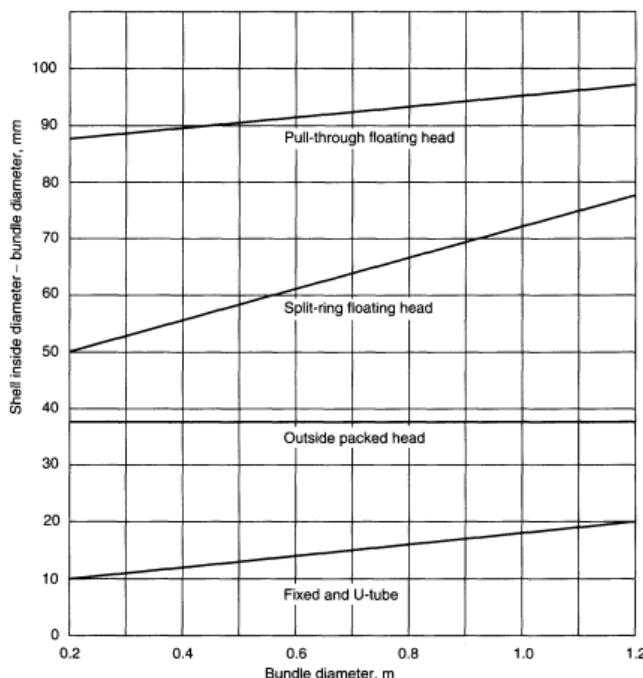


Figure 12.10. Shell-bundle clearance

*Using fixed and utube – shell bundle clearance

Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$+\frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

$$D_{si} = \text{bundle diameter} + \text{shell bundle clearance}$$

Parameter	Unit	Value
K_1		0.249
n_1		2.285
Bundle diameter, D_b	m	0.351653203
Tube in centre row		9.377418757
Shell-bundle clearance	m	0.012
Shell diameter, D_{si}	m	0.363653203
Baffle diameter	m	0.362053203
Tolerance	m	0.0008

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$Re = \frac{\rho u t d_i}{\mu}$$

$Pr = C_p \mu / k$
Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition
 $Nu = j_h x Re x Pr^{0.33}$

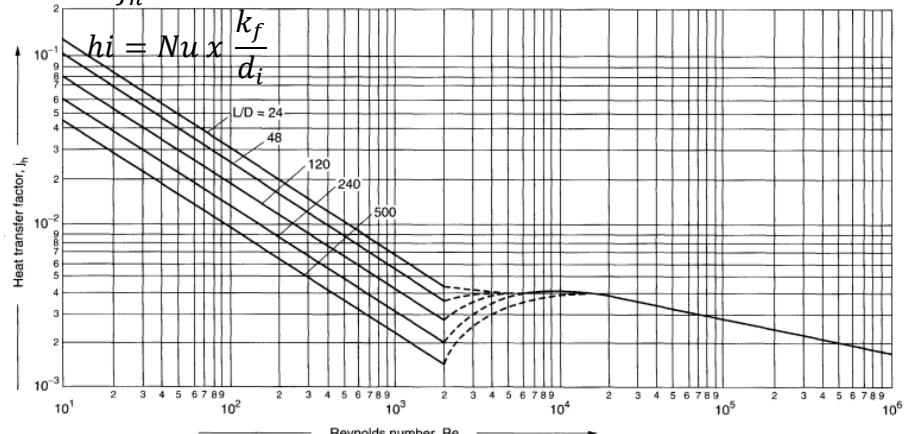


Figure 12.23. Tube-side heat-transfer factor

Reynolds number, Re		8.87E+04
Prandtl number, Pr		0.00451609
L/di		187.6923077
Tube-side heat transfer factor, j_h		0.0029
Nu		43.29205525
Tube side heat transfer coefficient, h_i	W/m²·°C	196.3933856

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{4 \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, l_B	m	0.181826602
Tube pitch, p_t	m	0.0375
Cross-flow area, A_s	m ²	0.013224365
Shell-side mass velocity, G_s	kg/s.m ²	634.9052901
Shell-side linear velocity, u_s	m/s	0.852157326
Equilateral diameter, d_e	m	0.004279688
Reynolds number, Re		2.72E+04
Prandtl number, Pr		0.000916047
Shell-side heat-transfer factors, j_h		0.004
Shell-side heat transfer coefficient, h_s	W/m ² .°C	220.4162289

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m²°C,

h_o = outside fluid film coefficient, W/m²°C,

h_i = inside fluid film coefficient, W/m²°C,

h_{od} = outside dirt coefficient (fouling factor), W/m²°C,

h_{id} = inside dirt coefficient, W/m²°C,

k_w = thermal conductivity of the tube wall material, W/m°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (A356), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel (C max ≈ 1.5%):														
Carbon steel C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² ·°C	220.4162289	
outside dirt/fouling coefficient, h_{od}	W/m ² ·°C	5000	(organic liquid)
inside fluid film coefficient, h_i	W/m ² ·°C	196.3933856	
inside dirt/fouling coefficient, h_{id}	W/m ² ·°C	5000	(organic liquid)
thermal conductivity tube wall material, k_w	W/m ² ·°C	54	Carbon steel 0.5%
overall coefficient based on the outside area of	W/m ² ·°C	91.89006951	
Error	%	-8.109930491	below 30%, design

STEP 12: PRESSURE DROP

Friction factor, f_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

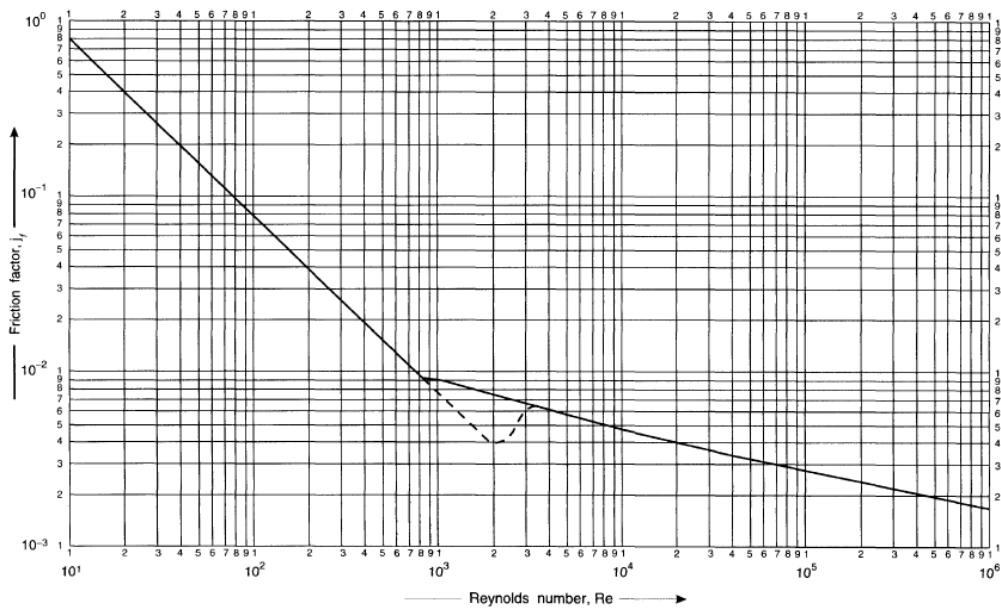


Figure 12.24. Tube-side friction factors

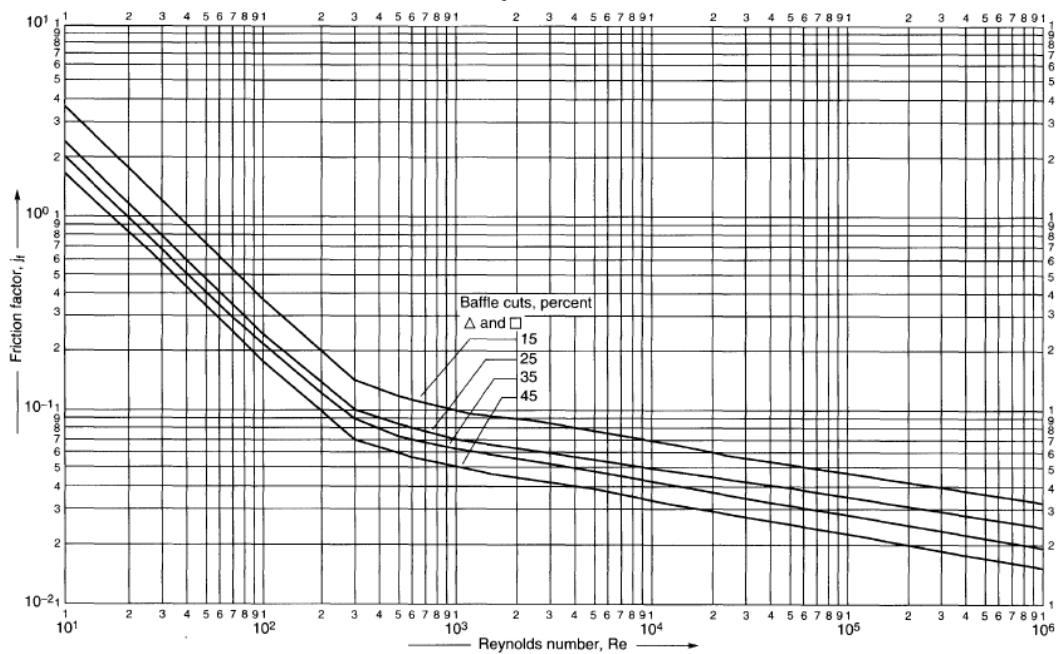


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and sell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8 j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8 j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side

Reynolds number, Re		8.87E+04
Friction factor, j_f		0.003
Tube side pressure drop, ΔP_t	kg/m ²	6014.796254
	bar	0.58985014

Shell side		
Reynolds number, Re		2.72E+04
Friction factor, j_f		0.042
Tube side pressure drop, ΔP_s	kg/m ² bar	207288.7671 20.32808813

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube			
Operating pressure, P_o	40 bar	4000000 Pa	
Design pressure, P_d	44 bar	4400000 Pa	
Shell (steam)			
Operating pressure, P_o	40 bar	4000000 Pa	
Design pressure, P_d	44 bar	4400000 Pa	

The maximum normal operating temperature should have additional 25°C

Tube		
Inlet temperature, T_i	333.27 K	
Outlet temperature, T_o	428.75 K	
Design temperature, T_d	453.75 K	
Shell		
Inlet temperature	473.15 K	
Outlet temperature	393.77 K	
Design temperature, T_d	498.15 K	

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate

(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

minimum allowable stress	360 N/mm ²	360000000 N/m ²
max allowable for tube, f	109.298 N/mm ²	109298000 N/m ²
max allowable for shell, f	101.75 N/mm ²	101750000 N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_i}{4Jf - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

For tube MAWP = $\frac{2 \times \text{tensile strength} \times E \times t_t}{D_i + t_t}$

Design pressure, Pd	$D_i + t_t$	4400000.0000 Pa
Design temperature, Td		453.7500 K
Tube inner diameter, dti		0.0260 m
Tube outer diameter, do		0.0300 m
Wall thickness		0.0020 m
Minimum wall thickness, e		0.0003 m
Corrosion allowance		0.0020 m
Fabrication wall thickness, tt		0.0023 m
design tube outer diameter, do		0.0306 m
MAWP	49982467.42	N/m ²
	499.8246742	bar

The design can be accepted as the MAWP is greater than the operating pressure

For shell,

Design pressure, Pd	4400000	Pa
Design temperature, Td	498.15	K
Shell inner diameter, dti	0.363653203	m
Minimum wall thickness, e	0.004696845	m
Corrosion allowance	0.002	m
Fabrication wall thickness, ts	0.006696845	m
design shell outer diameter, do	0.377046893	m
MAWP	11066473.45	N/m ²
	110.6647345	bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

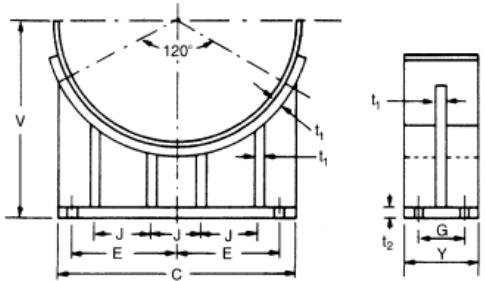
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radius, Rc	0.363653203	m
knuckle radius, Rk	0.021819192	m
Joint efficiency, E	1	
Design pressure, Pd	4400000	Pa
Minimum wall thickness	0.409949883	m
Corrosion allowance	0.002	m
Head wall thickness, th	0.411949883	m
External diameter	1.187552969	
MAWP	382417142.2	N/m ²
	3824.171422	bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm		
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24
All contacting edges fillet welded										

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter	
Vol.flow rate, Q	0.008957228 m ³ /s
Min cross section area	0.00843798 m ²
Min diamter	0.103651194 m
Operate nozzle diameter	0.207302389 m
Tube outlet nozzle diameter	
Vol.flow rate, Q	0.010360629 m ³ /s
Min cross section area	0.009760026 m ²
Min diamter	0.111475787 m
Operate nozzle diameter	0.222951573 m
Shell inlet nozzle diameter	
Vol.flow rate, Q	0.011704684 m ³ /s
Min cross section area	0.013735355 m ²
Min diamter	0.132243705 m
Operate nozzle diameter	0.26448741 m
Shell outlet nozzle diameter	
Vol.flow rate, Q	0.010919344 m ³ /s
Min cross section area	0.012813765 m ²
Min diamter	0.127730153 m
Operate nozzle diameter	0.255460306 m

E204 HEAT EXCHANGER SHELL AND TUBE

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE	SHELL
Heat duty, Q	J/s	22296.11111	
Inlet temperature	K	350.2881	502.6792
Outlet temperature	K	483.15	454.15
Pressure	bar	40	35
Mass flow rate	ton/hr	2.87836	4.12035
	kg/s	0.799544444	1.144541667

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (COLD)	SHELL (HOT)
Mean temperature	K	416.71905	478.4146
Density	kg/m ³	739.1970213	664.5604567
Specific heat capacity, Cp	kJ/kg.K	2.411264643	0.687449172
Viscosity, μ	kg/m.s	0.000177358	9.47018E-05
Thermal conductivity, Kf	W/m.K	0.107022464	0.087275178

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² .°C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 100 W/m³.

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{(T_{in_h} - T_{out_c}) - (T_{out_h} - T_{in_c})}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

Mean temperature difference, ΔT_m

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t depends on R & S

$$R = \frac{T_{hi} - T_{ho}}{T_{co} - T_{ci}}$$

$$S = \frac{T_{co} - T_{ci}}{T_{hi} - T_{ci}}$$

Temperature correction factor, F_t can be obtained from figure 12.19 C&R 3rd edition. If correction factor less than 0.75, proceed to second shell and find the F_t value from figure 12.20 C&R 3rd edition.

HEAT-TRANSFER EQUIPMENT

65

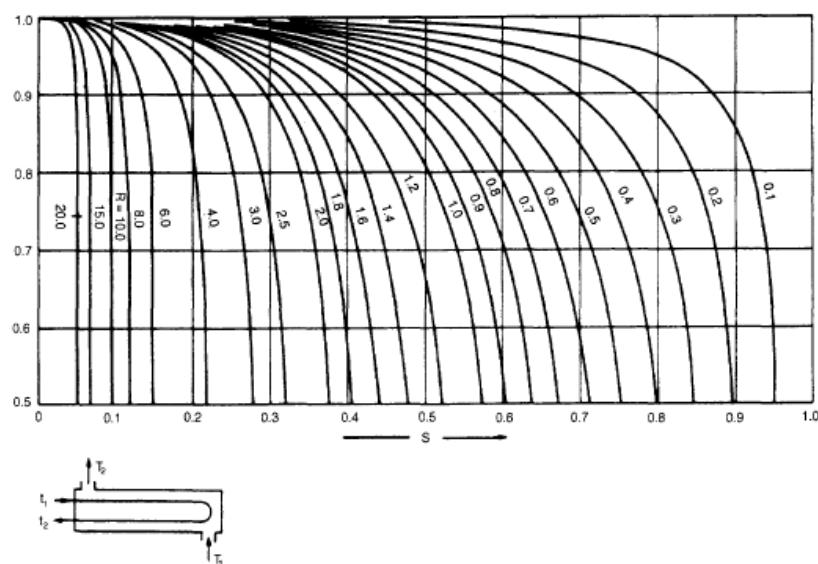


Figure 12.19. Temperature correction factor: one shell pass; two or more even tube 'passes'

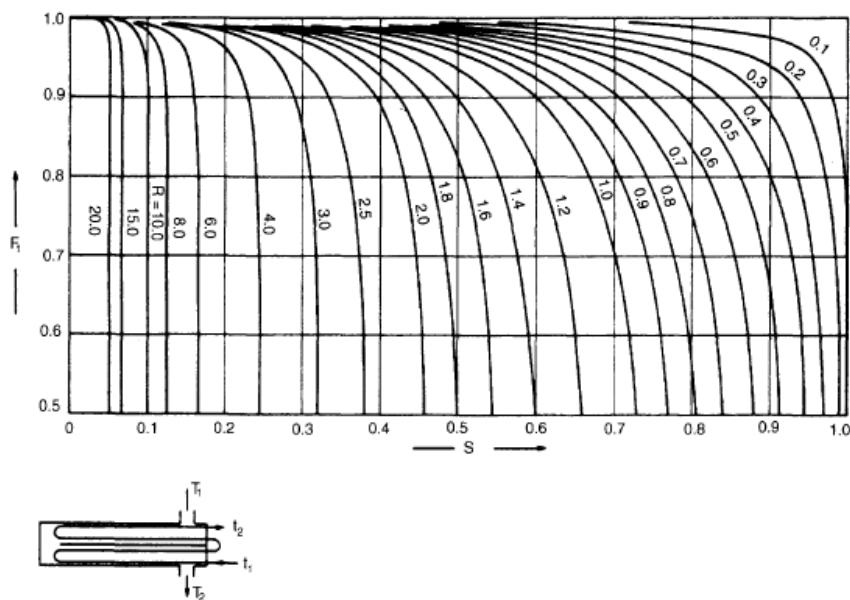


Figure 12.20. Temperature correction factor: two shell passes; four or multiples of four tube passes

So,

Log mean temperature difference, ΔT_m	50.4638314
R	0.36526047
S	0.87184816
Temperature correction factor, F_t (1 shell)	-
Temperature correction factor, F_t (2 shell)	0.91
True temperature difference, ΔT_m	45.9220866

equation :(invalid)

Figure 12.20

F_t (1 shell) cannot be calculated by using formula and out of range from Figure 12.19

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{U_x LMTD}$$

A (m ²)	4.85520428
---------------------	------------

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Parameter	Unit	Value
Tube inner diameter, d_i	m	0.0136
Tube outer diameter, d_o	m	0.016
Wall thickness	m	0.0012
Nominal length, L	m	4.88 *optimum 5 to 10m
Pitch arrangement, p_t	m	0.02 1.25 d_o

STEP 7: NUMBER OF TUBES

Area of one tube, $= \pi \times d_o \times L = \pi \times 0.03 \times 4.88 = 0.45999 m^2$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}}$$

Number of passes, $N_p = 4$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p}$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi \times (d_i^2)}{4}$$

$$\text{Area per pass} = \frac{A_i}{\text{Number of tubes per pass}}$$

$$\text{Volumetric flow} = \frac{m}{\rho}$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}}$$

Parameter	Unit	Value
Area of one tube	m ²	0.245295554
Number of tubes, N _t		20
Number of passes, N _p		4
N _t / N _p		5
tube cross-sectional area	m ²	0.000145267
Area per pass	m ²	0.000726336
Volumetric flow	m ³ /s	0.001081639
Tube-side velocity, u _t	m/s	1.489171443

STEP 8: BUNDLE AND SHELL DIAMETER

K₁ and n₁ from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, p _t = 1.25d _o					
No. passes	1	2	4	6	8
K ₁	0.319	0.249	0.175	0.0743	0.0365
n ₁	2.142	2.207	2.285	2.499	2.675
Square pitch, p _t = 1.25d _o					
No. passes	1	2	4	6	8
K ₁	0.215	0.156	0.158	0.0402	0.0331
n ₁	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition
HEAT-TRANSFER EQUIPMENT

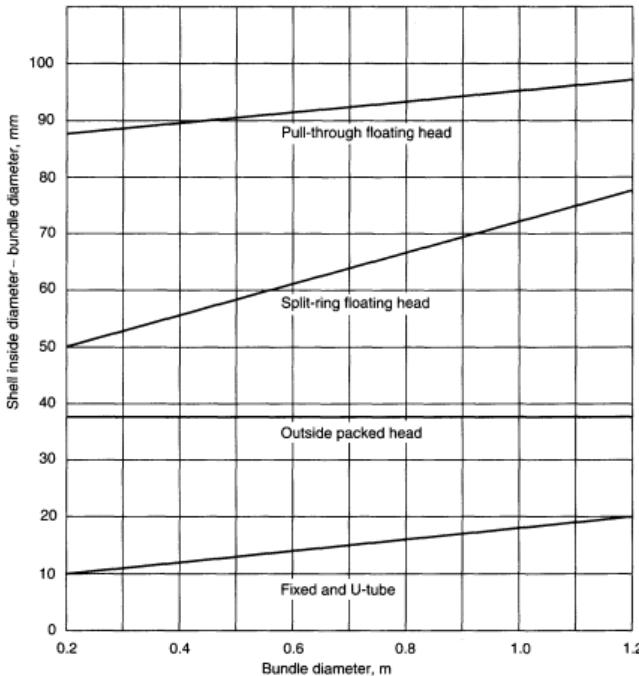


Figure 12.10. Shell-bundle clearance

*Using split floating head—shell bundle clearance
Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D _s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	D _s - $\frac{1}{16}$ in. (1.6 mm)	+ $\frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	D _s - $\frac{1}{8}$ in. (3.2 mm)	+0, - $\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	D _s - $\frac{3}{16}$ in. (4.8 mm)	+0, - $\frac{1}{16}$ in. (1.6 mm)

$$D_{si} = \text{bundle diameter} + \text{shell bundle clearance}$$

Parameter	Unit	Value	
K ₁		0.249	table 12.4
n ₁		2.207	table 12.4
Bundle diameter, D _b	m	0.116736297	
Tube in centre row		5.836814853	
Shell bundle clearance	m	0.03	figure 12.10
Shell diameter, D _{si}	m	0.23	Assume
Baffle diameter	m	0.2284	table 12.5
Tolerance	m	0.0008	table 12.5

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$Re = \frac{\rho \cdot u_t \cdot d_i}{\mu}$$

$Pr = C_p \mu / k_f$
Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition
 $Nu = j_h x Re x Pr^{0.33}$

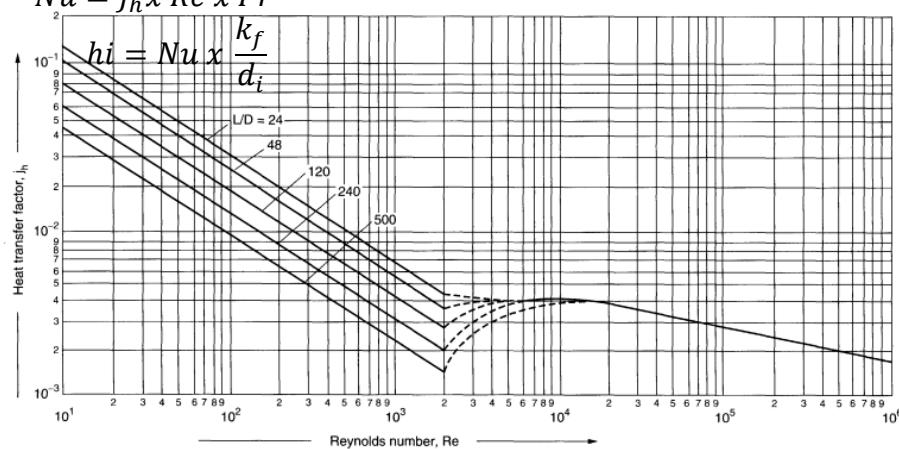


Figure 12.23. Tube-side heat-transfer factor

Assumed 25% baffle cut

Reynolds number, Re		8.44E+04	Re>2000, turbulent
Prandtl number, Pr		0.00399596	
L/di		358.8235294	
Tube-side heat transfer factor, j _h		0.0029	Figure 12.23
Nu		39.56631602	
Tube side heat transfer coefficient, h _i	W/m ² .°C	311.3591648	

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{4 \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, l_B	m	0.046	
Tube pitch, p_t	m	0.02	
Cross-flow area, A_s	m ²	0.002116	
Shell-side mass velocity, G_s	kg/s.m ²	540.8987083	
Shell-side linear velocity, u_s	m/s	0.81391949	
Equivalent diameter, d_e	m	0.0022825	
Reynolds number, Re		1.30E+04	
Prandtl number, Pr		0.000745947	
Shell-side heat-transfer factors, j_h		0.0052	Baffle cut 25% Figure 12.29
Shell-side heat transfer coefficient, h_s	W/m ² .°C	235.0829117	without viscosity correction term

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m².°C,

h_o = outside fluid film coefficient, W/m².°C,

h_i = inside fluid film coefficient, W/m².°C,

h_{od} = outside dirt coefficient (fouling factor), W/m².°C,

h_{id} = inside dirt coefficient, W/m².°C,

k_w = thermal conductivity of the tube wall material, W/m.°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Alusil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel (C max ≈ 1.5%):														
Carbon steel C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² ·°C	235.0829117		
outside dirt/fouling coefficient, h_{od}	W/m ² ·°C	5000	(organic liquid)	
inside fluid film coefficient, h_i	W/m ² ·°C	311.3591648		
inside dirt/fouling coefficient, h_{id}	W/m ² ·°C	5000	(organic liquid)	table 12.2
thermal conductivity tube wall material, k_w	W/m ² ·°C	54	Carbon steel 0.5%	table A-2
overall coefficient based on the outside area of	W/m ² ·°C	117.7621987		
Error	%	17.76219869	below 30%, design can be accepted	

STEP 12: PRESSURE DROP

Friction factor, j_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

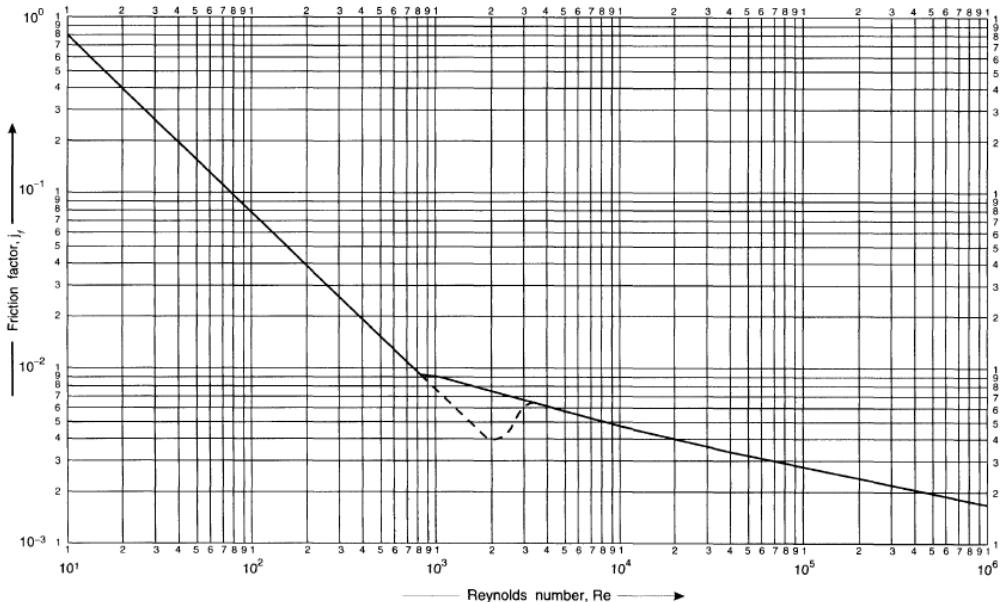


Figure 12.24. Tube-side friction factors

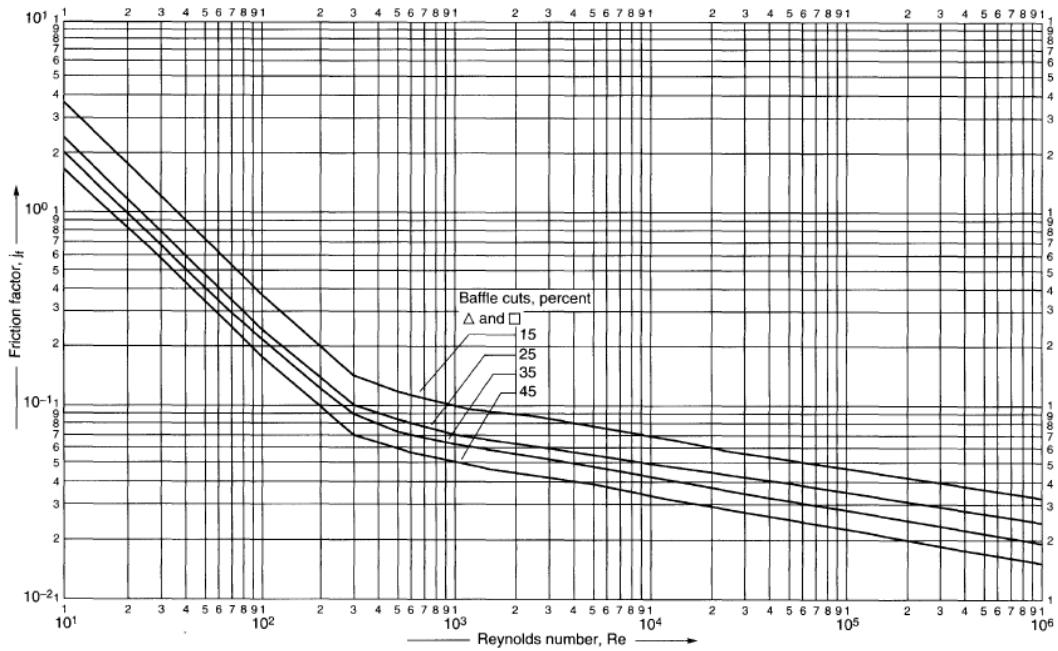


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and sell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side

Reynolds number, Re		8.44E+04
Friction factor, j_f		0.0028
Tube side pressure drop, ΔP_t	kg/m ²	19476.29739

Figure 12.24

Shell side

Reynolds number, Re		1.30E+04
Friction factor, j_f		0.043
Tube side pressure drop, ΔP_s	kg/m ²	809477.6826

Figure 12.30

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube			
Operating pressure, P_o	40	bar	4000000 Pa
Design pressure, P_d	44	bar	4400000 Pa

Shell (steam)			
Operating pressure, P_o	35	bar	3500000 Pa
Design pressure, P_d	38.5	bar	3850000 Pa

The maximum normal operating temperature should have additional 25°C

Tube		
Inlet temperature, T_i	350.2881	K
Outlet temperature, T_o	483.15	K
Design temperature, T_d	508.15	K

Shell			
Inlet temperature		502.6792 K	
Outlet temperature		454.15 K	
Design temperature, Td		527.6792 K	

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Minimum allowable stress	360 N/mm ²	360000000 N/m ²
max allowable for tube, f	100.05 N/mm ²	100050000 N/m ²
max allowable for shell, f	96.730036 N/mm ²	96730036 N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_i}{4Jf - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

$$\text{For tube } \text{MAWP} = \frac{2 \times \text{tensile strength} \times E \times t_t}{D_i + t_t}$$

Design pressure, P _d	D _i + t _t	4400000.0000 Pa
Design temperature, T _d		508.1500 K
Tube inner diameter, d _{ti}		0.0136 m
Tube outer diameter, d _o		0.0160 m
Wall thickness		0.0012 m
Minimum wall thickness, e		0.0002 m
Corrosion allowance		0.0020 m
Fabrication wall thickness, t _f		0.0022 m
design tube outer diameter, d _o		0.0180 m
MAWP		84503588.49 N/m ²
		845.0358849 bar

The design can be accepted as the MAWP is greater than the operating pressure
For shell,

Design pressure, Pd	3850000 Pa
Design temperature, Td	527.6792 K
Shell inner diameter, dti	0.23 m
Minimum wall thickness, e	0.002730815 m
Corrosion allowance	0.002 m
Fabrication wall thickness, ts	0.004730815 m
design shell outer diameter, do	0.239461631 m
MAWP	12334379.81 N/m ²
	123.3437981 bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

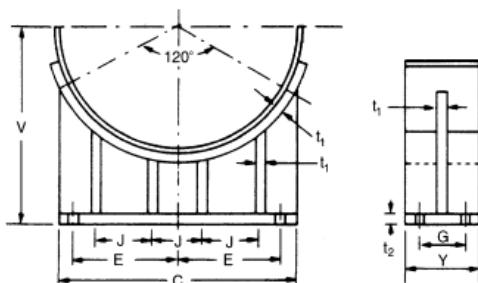
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radiusm, Rc	0.23 m
knuckle radius, Rk	0.0138 m
Joint efficiency, E	1
Design pressure, Pd	3850000 Pa
Minimum wall thickness	0.259280733 m
Corrosion allowance	0.002 m
Head wall thickness, th	0.261280733 m
External diameter	0.752561465
MAWP	382417142.2 N/m ²
	3824.171422 bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)					mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam. Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20 25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20 25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20 25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20 25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24 30

All contacting edges fillet welded

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter		
Vol.flow rate, Q	0.000977226	m ³ /s
Min cross section area	0.000656221	m ²
Min diamter	0.028905477	m
Operate nozzle diameter	0.057810953	m
Tube outlet nozzle diameter		
Vol.flow rate, Q	0.001248285	m ³ /s
Min cross section area	0.000838241	m ²
Min diamter	0.032669285	m
Operate nozzle diameter	0.06533857	m
Shell inlet nozzle diameter		
Vol.flow rate, Q	0.001828706	m ³ /s
Min cross section area	0.002246789	m ²
Min diamter	0.053485523	m
Operate nozzle diameter	0.106971047	m
Shell outlet nozzle diameter		
Vol.flow rate, Q	0.001638266	m ³ /s
Min cross section area	0.002012811	m ²
Min diamter	0.050624008	m
Operate nozzle diameter	0.101248016	m

E201 CONDENSER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE (cooling water)	SHELL
Heat duty, Q	J/s	342598.8889	
Inlet temperature	K	303.15	390.3962
Outlet temperature	K	318.15	390.3962
Pressure	bar	1	2.8
Mass flow rate	ton/hr	1726.03733	0.09254793
	kg/s	479.4548139	0.025707758

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (COLD)	SHELL (HOT)
Mean temperature	K	310.65	390.3962
Density	kg/m³	989.7802221	389.3143734
Specific heat capacity, Cp	kJ/kg.K	1.828200103	1.828200103
Viscosity, μ	kg/m.s	0.000715554	0.000116365
Thermal conductivity, Kf	W/m.K	0.6225055	0.066855472

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m²°C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 200 W/m².C but a bit lower than the range of coefficient value for condenser.

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{(T_{in_h} - T_{out_c}) - (T_{out_h} - T_{in_c})}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

Log mean temperature difference, ΔT_{lm}	79.5105219
--	------------

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{U_x \text{ LMTD}}$$

A (m ²)	21.5442485
---------------------	------------

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Parameter	Unit	Value	
Tube inner diameter, d_i	m	0.046	
Tube outer diameter, d_o	m	0.05	Table 12.3
Wall thickness	m	0.002	Table 12.3
Nominal length, L	m	1.83	*the shell and tube
Pitch arrangement, p_t	m	0.0625	1.25 d_o

STEP 7: NUMBER OF TUBES

Area of one tube, $= \pi x d_o x L$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}}$$

Number of passes, $N_p = 1$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p}$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi x (d_i^2)}{4}$$

$$\text{Area per pass} = \frac{A_i}{\text{Number of tubes per pass}}$$

$$\text{Volumetric flow} = \frac{m}{\rho}$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}}$$

Parameter	Unit	Value
Area of one tube	m ²	0.287455728
Number of tubes, N_t		75
Number of passes, N_p		1
N_t / N_p		75
tube cross-sectional area	m ²	0.001661903
Area per pass	m ²	0.124642689
Volumetric flow	m ³ /s	0.484405329
Tube-side velocity, u_t	m/s	3.886351734

STEP 8: BUNDLE AND SHELL DIAMETER

K₁ and n₁ from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition
HEAT-TRANSFER EQUIPMENT

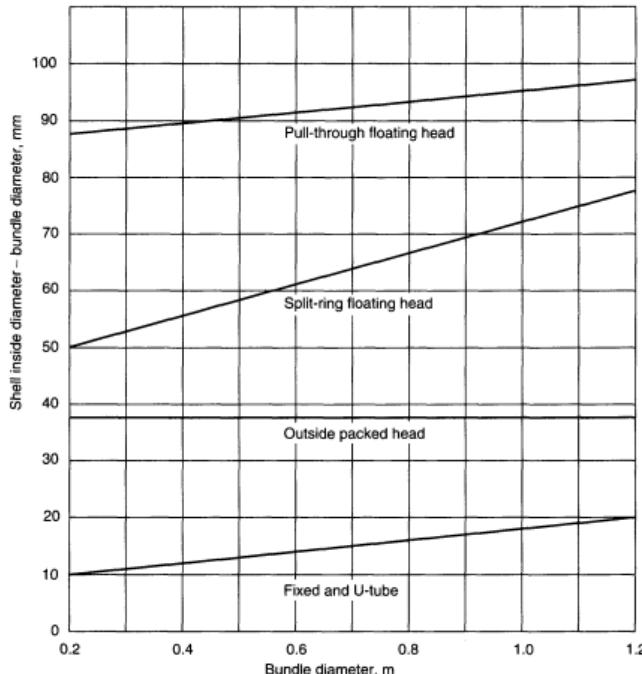


Figure 12.10. Shell-bundle clearance

*Using split floating head—shell bundle clearance

Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$\pm \frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm) 27 to 42 in. (686 to 1067 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm) $D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm) $+0, -\frac{1}{16}$ in. (1.6 mm)

$D_{si} = \text{bundle diameter} + \text{shell bundle clearance}$

K ₁		0.319	table 12.4
n ₁		2.142	table 12.4
Bundle diameter, D _b	m	0.64	
Tube in centre row		10.23589303	
Shell-bundle clearance	m	0.063	Figure 12.10
Shell diameter, D _{si}	m	0.702743315	Bundle diameter +
Baffle diameter	m	0.701143315	table 12.5
Tolerance	m	0.0008	table 12.5

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$Re = \frac{\rho \cdot u_t \cdot d_i}{\mu}$$

330

$$Pr = C_p \mu / k_f$$

$$Nu = j_h x Re x Pr^{0.33}$$

$$hi = Nu x \frac{k_f}{d}$$

Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition

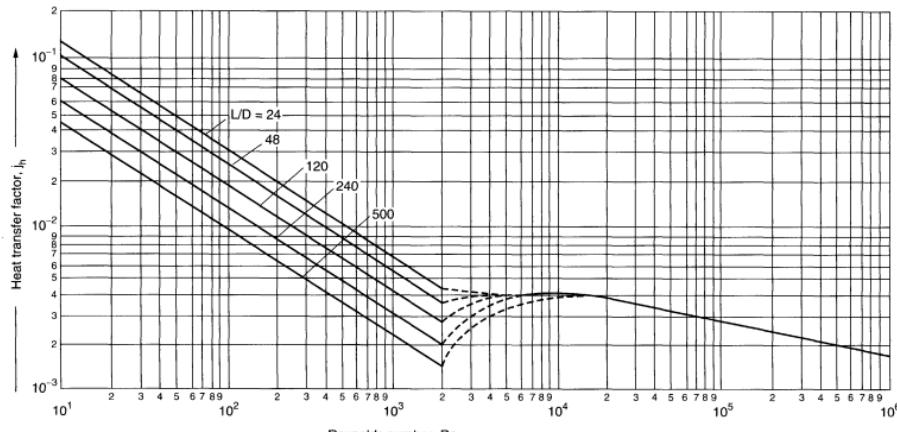


Figure 12.23. Tube-side heat-transfer factor

Assumed 25% baffle cut

Reynolds number, Re		2.47E+05	Re>2000, turbulent
Prandtl number, Pr		0.002101467	
L/d _i		39.7826087	
Tube-side heat transfer factor, j_h		0.0026	Figure 12.23
Nu		84.06252251	
Tube side heat transfer coefficient, h_i	W/m ² .°C	1137.595274	

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{\frac{4}{2} \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, l_B	m	0.070274331	choose 0.5
Tube pitch, p_t	m	0.0625	
Cross-flow area, A_s	m ²	0.009876963	
Shell-side mass velocity, G_s	kg/s.m ²	2.602799817	
Shell-side linear velocity, u_s	m/s	0.006685599	
Equilateral diameter, d_e	m	0.007132813	
Reynolds number, Re		1.60E+02	
Prandtl number, Pr		0.00318206	
Shell-side heat-transfer factors, j_h		0.5	Baffle cut 25%
Shell-side heat transfer coefficient, h_s	W/m ² .°C	1.10E+02	without viscosity correction

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m².°C,

h_o = outside fluid film coefficient, W/m².°C,

h_i = inside fluid film coefficient, W/m².°C,

h_{od} = outside dirt coefficient (fouling factor), W/m².°C,

h_{id} = inside dirt coefficient, W/m².°C,

k_w = thermal conductivity of the tube wall material, W/m°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Alusil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel (C max ≈ 1.5%):														
Carbon steel C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² · °C	109.9754168		
outside dirt/fouling coefficient, h_{od}	W/m ² · °C	5000	(organic liquid)	
inside fluid film coefficient, h_i	W/m ² · °C	1137.595274		
inside dirt/fouling coefficient, h_{id}	W/m ² · °C	12000	river water	table 12.2
thermal conductivity tube wall material, k_w	W/m · °C	54	Carbon steel 0.5%	table A-2
overall coefficient based on the outside area of tube	W/m ² · °C	96.361304		
Error	%	-51.819348	below 30%, design can be acc	

STEP 12: PRESSURE DROP

Friction factor, j_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

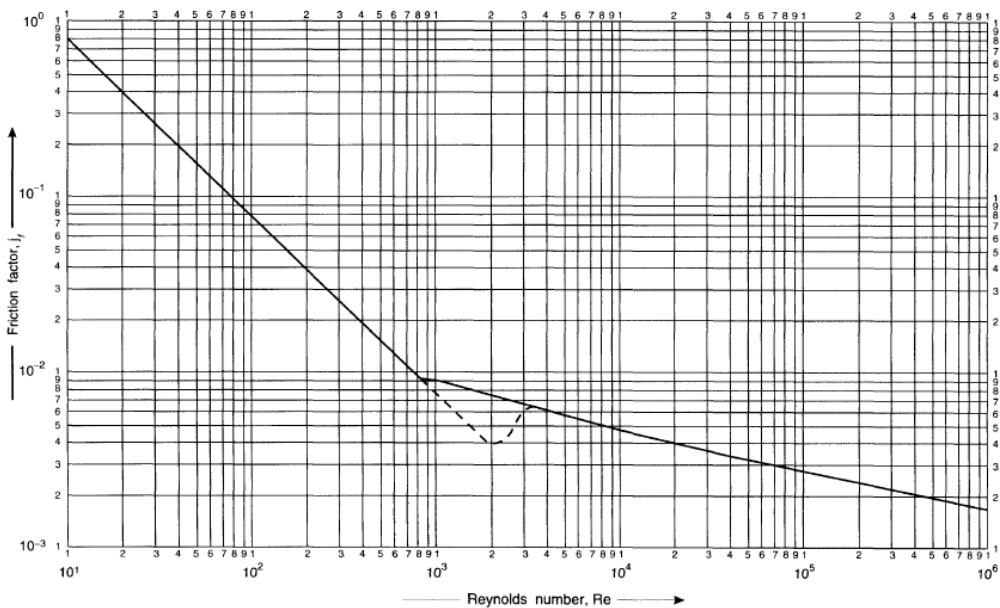


Figure 12.24. Tube-side friction factors

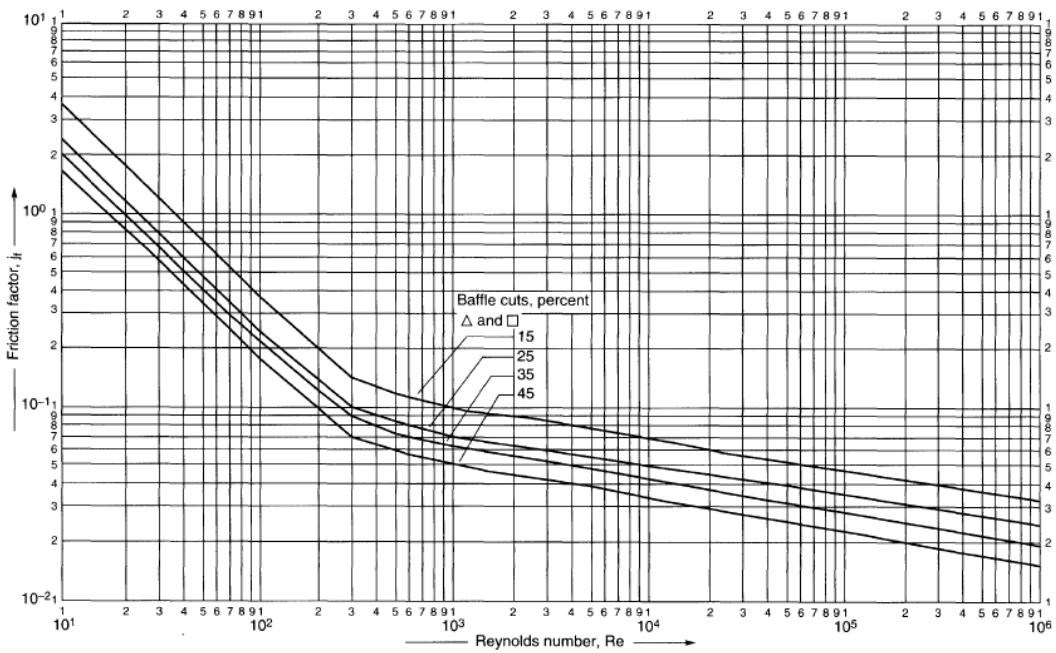


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and shell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side		
Reynolds number, Re		2.47E+05
Friction factor, j_f		0.0023
Tube side pressure drop, ΔP_t	kg/m ²	7582.22944
	bar	0.743562859
Shell side		
Reynolds number, Re		1.60E+02
Friction factor, j_f		0.032
Tube side pressure drop, ΔP_s	kg/m ²	5.714540943
	bar	0.000560405

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube			
Operating pressure, P_o	1 bar	100000	Pa
Design pressure, P_d	1.1 bar	110000	Pa
Shell (steam)			
Operating pressure, P_o	2.8 bar	280000	Pa
Design pressure, P_d	3.08 bar	308000	Pa

The maximum normal operating temperature should have additional 25°C

Tube			
Inlet temperature, T_i		303.15	K
Outlet temperature, T_o		318.15	K
Design temperature, T_d		343.15	K
<hr/>			
Shell			
Inlet temperature		390.3962	K
Outlet temperature		390.3962	K
Design temperature, T_d		415.3962	K

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)								
		0 to 50	100	150	200	250	300	350	400	450
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70	
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100	
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110	
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	95

minimum allowable stress	360	N/mm ²	360000000	N/m ²
maximum allowable for tube, f	128.1	N/mm ²	128100000	N/m ²
maximum allowable for shell, f	115.818146	N/mm ²	115818146	N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_i}{4Jf - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

$$MAWP = \frac{2 \times \text{tensile strength} \times E \times t_t}{D_i + t_t}$$

For tube,

Design pressure, Pd	110000.0000	Pa
Design temperature, Td	343.1500	K
Tube inner diameter, dti	0.0460	m
Tube outer diameter, do	0.0500	m
Wall thickness	0.0020	m
Minimum wall thickness, e	0.0000	m
Corrosion allowance	0.0020	m
Fabrication wall thickness, tt	0.0020	m
design tube outer diameter, do	0.0500	m

MAWP	25641963.19	N/m ²
	256.4196319	bar

The design can be accepted as the MAWP is greater than the operating pressure
For shell,

Design pressure, Pd	308000	Pa
Design temperature, Td	415.3962	K
Shell inner diameter, dti	0.702743315	m
Minimum wall thickness, e	0.000550174	m
Corrosion allowance	0.002	m
Fabrication wall thickness, ts	0.002550174	m
design shell outer diameter, do	0.707843662	m
MAWP	2212846.505	N/m ²
	22.12846505	bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

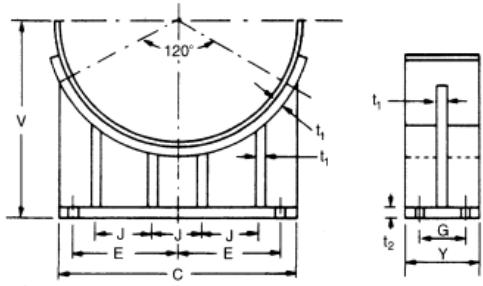
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radiusm, Rc	0.702743315	m
knuckle radius, Rk	0.042164599	m
Joint efficiency, E	1	
Design pressure, Pd	308000	Pa
Minimum wall thickness	0.791907063	m
Corrosion allowance	0.002	m
Head wall thickness, th	0.793907063	m
External diameter	2.290557441	
MAWP	381928267.3	N/m ²
	3819.282673	bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter		
Vol.flow rate, Q	0.004829046	m ³ /s
Min cross section area	0.001242565	m ²
Min diamter	0.03977541	m
Operate nozzle diameter	0.079550819	m
Tube outlet nozzle diameter		
Vol.flow rate, Q	0.004859155	m ³ /s
Min cross section area	0.001250313	m ²
Min diamter	0.039899216	m
Operate nozzle diameter	0.079798432	m
Shell inlet nozzle diameter		
Vol.flow rate, Q	3.81603E-05	m ³ /s
Min cross section area	0.00570784	m ²
Min diamter	0.085249326	m
Operate nozzle diameter	0.170498652	m
Shell outlet nozzle diameter		
Vol.flow rate, Q	3.33049E-07	m ³ /s
Min cross section area	4.98158E-05	m ²
Min diamter	0.007964137	m
Operate nozzle diameter	0.015928275	m

E401 CONDENSER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE (cooling water)	SHELL
Heat duty, Q	J/s	195275	
Inlet temperature	K	303.15	451.7356
Outlet temperature	K	318.15	451.7356
Pressure	bar	1	2.8
Mass flow rate	ton/hr	983.76777	21.58545
	kg/s	273.268825	5.995958333

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (COLD)	SHELL (HOT)
Mean temperature	K	310.65	451.7356
Density	kg/m³	989.7802221	393.900382
Specific heat capacity, Cp	kJ/kg.K	1.971554561	1.971554561
Viscosity, μ	kg/m.s	0.000715554	0.000140324
Thermal conductivity, Kf	W/m.K	0.6225055	0.065807464

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m²°C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 110 W/m³.C but a bit lower than the range of coefficient value for condenser.

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{(T_{in_h} - T_{out_c}) - (T_{out_h} - T_{in_c})}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

Log mean temperature difference, ΔT_{lm}	140.952602
--	------------

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{Ux LMTD}$$

A (m ²)	12.0469112
---------------------	------------

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)			
16	1.2	1.6	2.0	—
20	—	1.6	2.0	2.6
25	—	1.6	2.0	2.6
30	—	1.6	2.0	2.6
38	—	—	2.0	2.6
50	—	—	2.0	2.6

Parameter	Unit	Value	
Tube inner diameter, d_i	m	0.046	
Tube outer diameter, d_o	m	0.05	Table 12.3
Wall thickness	m	0.002	Table 12.3
Nominal length, L	m	1.83	*the shell and tube
Pitch arrangement, p_t	m	0.0625	1.25 d_o

STEP 7: NUMBER OF TUBES

Area of one tube, $= \pi x d_o x L$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}}$$

Number of passes, $N_p = 1$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p}$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi x (d_i^2)}{4}$$

$$\text{Area per pass} = \frac{A_i}{\text{Number of tubes per pass}}$$

$$\text{Volumetric flow} = \frac{m}{\rho} =$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}}$$

Parameter	Unit	Value
Area of one tube	m ²	0.287455728
Number of tubes, N_t		42
Number of passes, N_p		1
N_t / N_p		42
tube cross-sectional area	m ²	0.001661903
Area per pass	m ²	0.069799906
Volumetric flow	m ³ /s	0.276090408
Tube-side velocity, u_t	m/s	3.955455317

STEP 8: BUNDLE AND SHELL DIAMETER

K1 and n1 from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition
HEAT-TRANSFER EQUIPMENT

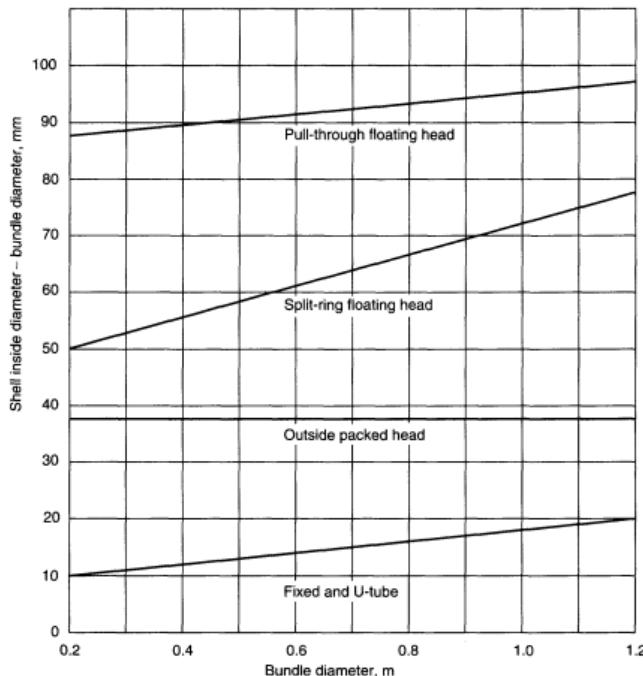


Figure 12.10. Shell-bundle clearance

*Using split floating head— shell bundle clearance

Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$\pm \frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

$$D_{si} = \text{bundle diameter} + \text{shell bundle clearance}$$

Parameter	Unit	Value	
K ₁		0.319	table 12.4
n ₁		2.142	table 12.4
Bundle diameter, D _b	m	0.5	
Tube in centre row		7.808479258	
Shell-bundle clearance	m	0.058	Figure 12.10
Shell diameter, D _{si}	m	0.546029954	Bundle diameter +
Baffle diameter	m	0.544429954	table 12.5
Tolerance	m	0.0008	table 12.5

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$Re = \frac{\rho \cdot u_t \cdot d_i}{\mu}$$

340

$$Pr = C_p \mu / k_f$$

$$Nu = j_h x Re x Pr^{0.33}$$

$$hi = Nu x \frac{k_f}{?}$$

Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition

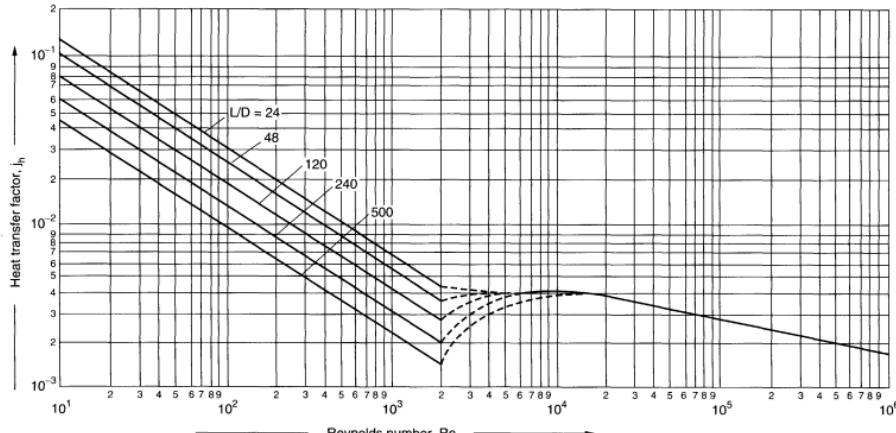


Figure 12.23. Tube-side heat-transfer factor

Assumed 25% baffle cut

Reynolds number, Re		2.52E+05	Re>2000, turbulent
Prandtl number, Pr		0.002266249	
L/di		39.7826087	
Tube-side heat transfer factor, j_h		0.0032	Figure 12.23
Nu		107.9574209	
Tube side heat transfer coefficient, h_t	W/m ² .°C	1460.958441	

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{\frac{4}{2} \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, l_B	m	0.109205991	choose 0.1		
Tube pitch, p_t	m	0.0625			
Cross-flow area, A_s	m ²	0.011925948			
Shell-side mass velocity, G_s	kg/s.m ²	502.7657447			
Shell-side linear velocity, u_s	m/s	1.276377906			
Equilateral diameter, d_e	m	0.007132813			
Reynolds number, Re		2.56E+04			
Prandtl number, Pr		0.004204021			
Shell-side heat-transfer factors, j_h		0.004	Baffle cut 25% Figure 12.29		
Shell-side heat transfer coefficient, h_s	W/m ² .°C	1.52E+02	without viscosity correction term		

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m²°C,

h_o = outside fluid film coefficient, W/m²°C,

h_i = inside fluid film coefficient, W/m²°C,

h_{od} = outside dirt coefficient (fouling factor), W/m²°C,

h_{id} = inside dirt coefficient, W/m²°C,

k_w = thermal conductivity of the tube wall material, W/m°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Alusil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel														
(C max ≈ 1.5%):														
Carbon steel														
C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² · °C	152.2151471		
outside dirt/fouling coefficient, h_{od}	W/m ² · °C	5000	(organic liquid)	
inside fluid film coefficient, h_i	W/m ² · °C	1460.958441		
inside dirt/fouling coefficient, h_{id}	W/m ² · °C	6000	cooling water	table 12.2
thermal conductivity tube wall material, k_w	W/m ² · °C	54	Carbon steel 0.5%	table A-2
overall coefficient based on the outside area of	W/m ² · °C	129.3090162		
Error	%	12.44262282	below 30%, design can be accepted	

STEP 12: PRESSURE DROP

Friction factor, j_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

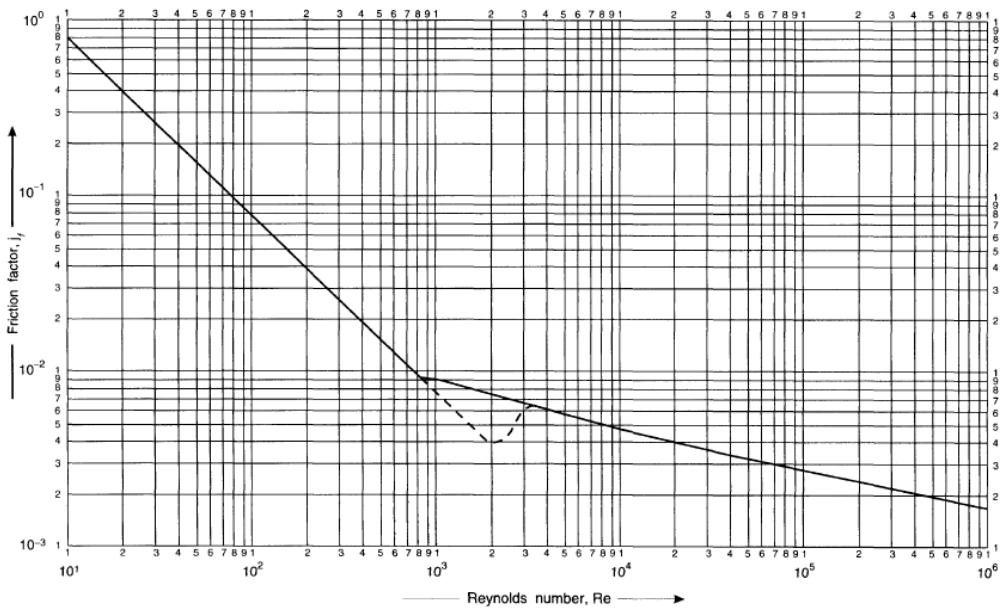


Figure 12.24. Tube-side friction factors

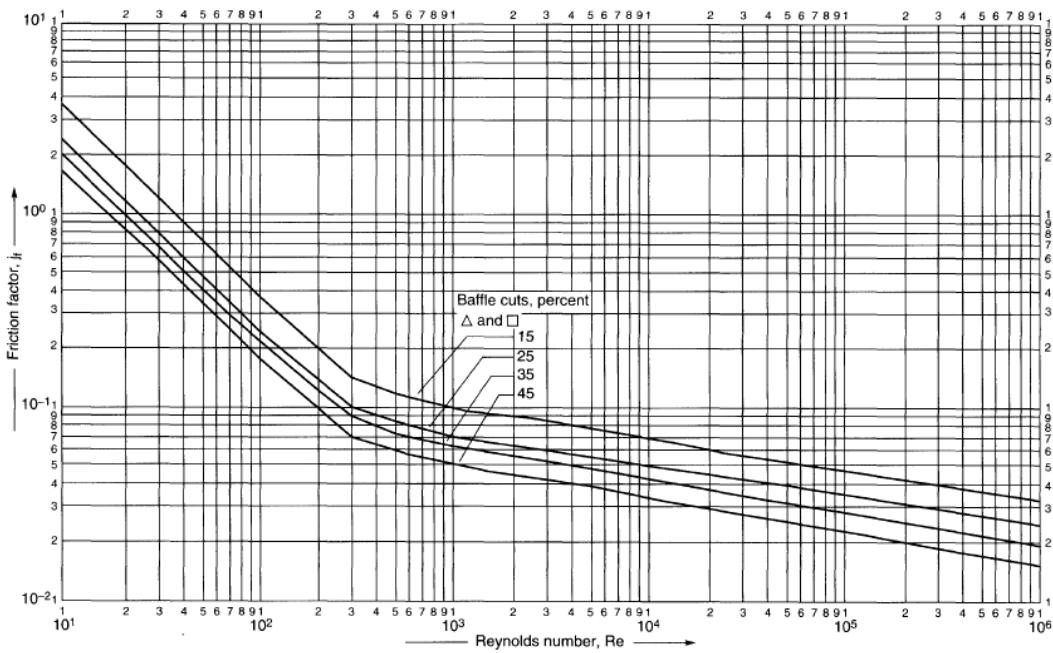


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and shell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side		
Reynolds number, Re		2.52E+05
Friction factor, j_f		0.0025
Tube side pressure drop, ΔP_t	kg/m ²	8008.952125
	bar	0.785410068
Shell side		
Reynolds number, Re		2.56E+04
Friction factor, j_f		0.049
Tube side pressure drop, ΔP_s	kg/m ²	161347.1562
	bar	15.8227542

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube				
Operating pressure, P_o	1	bar	100000	Pa
Design pressure, P_d	1.1	bar	110000	Pa
Shell (steam)				
Operating pressure, P_o	2.8	bar	280000	Pa
Design pressure, P_d	3.08	bar	308000	Pa

The maximum normal operating temperature should have additional 25°C

Tube	
Inlet temperature, Ti	303.15 K
Outlet temperature, To	318.15 K
Design temperature, Td	343.15 K
Shell	
Inlet temperature	451.7356 K
Outlet temperature	451.7356 K
Design temperature, Td	476.7356 K

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Min allowable stress	360 N/mm ²	360000000 N/m ²
Max allowable for tube, f	128.1 N/mm ²	128100000 N/m ²
Max allowable for shell, f	105.390448 N/mm ²	105390448 N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_i}{4Jf - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

$$\text{For tube MAWP} = \frac{2 \times \text{tensile strength} \times E \times t_t}{D_i + t_t}$$

Design pressure, P _d	D _i + t _t	110000.0000 Pa
Design temperature, T _d		343.1500 K
Tube inner diameter, d _{ti}		0.0460 m
Tube outer diameter, d _o		0.0500 m
Wall thickness		0.0020 m
Minimum wall thickness, e		0.0000 m
Corrosion allowance		0.0020 m
Fabrication wall thickness, t _t		0.0020 m
design tube outer diameter, d _o		0.0500 m
MAWP		25641963.19 N/m ²
		256.4196319 bar

The design can be accepted as the MAWP is greater than the operating pressure

For shell,

Design pressure, Pd	308000	Pa
Design temperature, Td	476.7356	K
Shell inner diameter, dti	0.546029954	m
Minimum wall thickness, e	0.000469824	m
Corrosion allowance	0.002	m
Fabrication wall thickness, ts	0.002469824	m
design shell outer diameter, do	0.550969602	m
MAWP	2755757.347	N/m ²
	27.55757347	bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

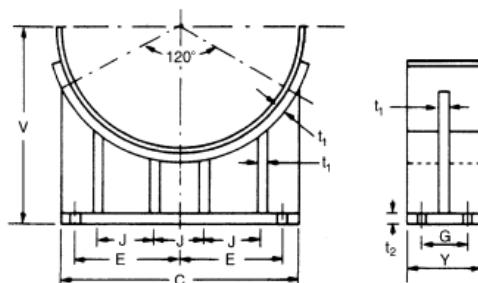
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radiusm, Rc	0.546029954	m
knuckle radius, Rk	0.032761797	m
Joint efficiency, E	1	
Design pressure, Pd	308000	Pa
Minimum wall thickness	0.615332523	m
Corrosion allowance	0.002	m
Head wall thickness, th	0.617332523	m
External diameter	1.780694999	
MAWP	382064425.7	N/m ²
	3820.644257	bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter		
Vol.flow rate, Q	0.00275235	m ³ /s
Min cross section area	0.000695837	m ²
Min diamter	0.029765191	m
Operate nozzle diameter	0.059530382	m
Tube outlet nozzle diameter		
Vol.flow rate, Q	0.002769511	m ³ /s
Min cross section area	0.000700175	m ²
Min diamter	0.029857839	m
Operate nozzle diameter	0.059715679	m
Shell inlet nozzle diameter		
Vol.flow rate, Q	0.007581172	m ³ /s
Min cross section area	0.005939598	m ²
Min diamter	0.086962814	m
Operate nozzle diameter	0.173925629	m
Shell outlet nozzle diameter		
Vol.flow rate, Q	7.68819E-05	m ³ /s
Min cross section area	6.02345E-05	m ²
Min diamter	0.008757448	m
Operate nozzle diameter	0.017514896	m

E203 COOLER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	Tube	Shell
Heat Duty, Q	MJ/hr	-1620.6382	
	J/s	-450177.2758	
Inlet temperature	K	390.40 (S21)	303.15
Outlet temperature	K	350.29 (S22)	313.15
Pressure	bar	2.8	2.8
Mass flow rate, \dot{m}	ton/hr	20.8739	348.9264
	kg/s	5.7983	96.9240

Design method:

Coulson and Richardson's Chemical Engineering Design is used as a reference on designing the heat exchanger. While for properties of the components in stream, it being manually calculated based on formulas gained from related references.

Heat duty = -1620.6382 MJ/hr

$$\dot{m}(\text{tube}) = 20.8739 \frac{\text{ton}}{\text{hr}} \times \frac{1000\text{kg}}{1\text{ton}} \times \frac{1\text{hr}}{3600\text{s}} = 5.7983 \text{ kg.s}^{-1}$$

$$\dot{m}(\text{shell}) = 348.9264 \frac{\text{ton}}{\text{hr}} \times \frac{1000\text{kg}}{1\text{ton}} \times \frac{1\text{hr}}{3600\text{s}} = 96.9240 \text{ kg.s}^{-1}$$

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE	SHELL
Mean temperature	K	370.34	308.15
Density, ρ	kg/m ³	772.8696	999.8
Specific heat capacity, C_p	kJ/kg.K	1.9569	4.2186
Viscosity, μ	kg/m.s	0.0002	0.5824
Thermal conductivity, k_f	W/m.K	0.1151	0.5694

The physical properties of the components determined from data gained from running an ASPEN for specific temperature.

STEP 3: INITIAL ESTIMATION OF OVERALL HEAT TRANSFER COEFFICIENT

HEAT-TRANSFER EQUIPMENT

Table 12.1. Typical overall coefficients

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² °C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on the figure, value of overall heat transfer coefficient can be assumed based on the range given by the type of hot and cold fluid. For this cooler, E-203, since the hot fluid is organic solvents and cold fluid is water; thus, U is in the range of 250 - 750 W/m²°C.

$$U_o = 750 \text{ W/m}^2\text{°C}$$

STEP 4: MEAN TEMPERATURE DIFFERENCE FOR COUNTER-CURRENT FLOW

	Unit	TUBE (HOT)	SHELL (COLD)
Inlet temperature	K	390.40	303.15
Outlet temperature	K	350.29	313.15

$$\text{Log mean temperature difference, } \Delta T_{lm} = \frac{(T_{hot,in} - T_{cold,out}) - (T_{hot,out} - T_{cold,in})}{\ln \left(\frac{T_{hot,in} - T_{cold,out}}{T_{hot,out} - T_{cold,in}} \right)}$$

$$= 60.9579K$$

$$R = \frac{(T_{shell,in} - T_{shell,out})}{(T_{tube,out} - T_{tube,in})}$$

$$= 0.2493$$

$$S = \frac{(T_{tube,out} - T_{tube,in})}{(T_{shell,in} - T_{tube,in})}$$

$$= 0.4597$$

$$F_t = \frac{\sqrt{(R^2 + 1)} \ln \left[\frac{(1-S)}{(1-RS)} \right]}{(R-1) \ln \left[\frac{2 - S[R+1 - \sqrt{(R^2 + 1)}]}{2 - S[R+1 + \sqrt{(R^2 + 1)}]} \right]}$$

Temperature correction factor, $F_t = 0.9815$

If the value for temperature correction factor less than 0.75, Figure 12.20 can be used in order to find the F_t .

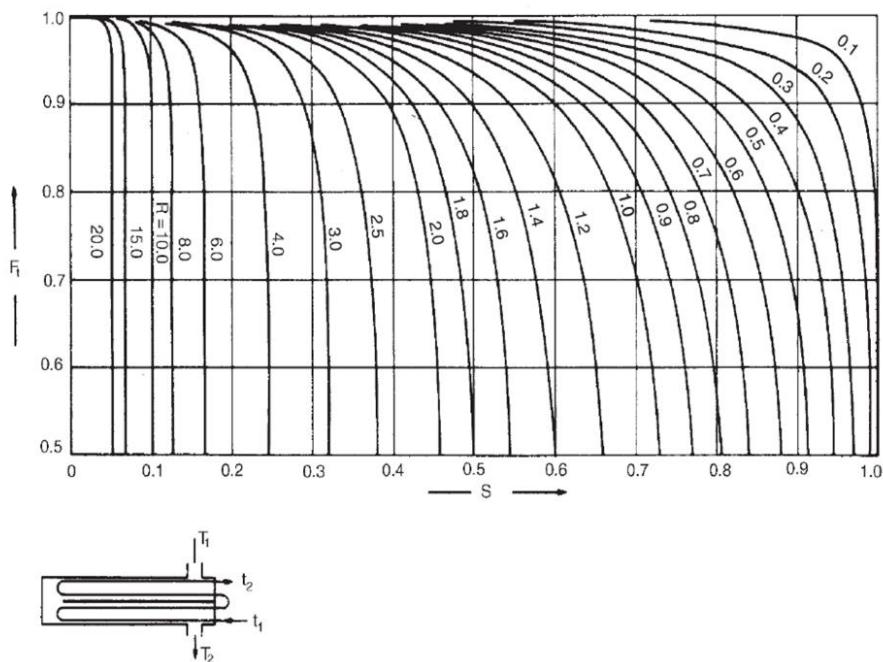


Figure 12.20. Temperature correction factor: two shell passes; four or multiples of four tube passes

$$\Delta T_m = F_t \times \Delta T_{lm} = 0.9815 \times 60.9579 = 59.83 \text{ K}$$

STEP 5: HEAT TRANSFER AREA

$$A = \frac{Q}{U\Delta T_{lm}} = 10.0321 m^2$$

STEP 6: LAYOUT AND TUBE SIZE

3.66 m is chosen to be the nominal length of tube which taken from the recommended value by Coulson and Richardson Engineering Material Design.

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

While for tube outer diameter, d_o , 0.03 m is chosen from Table 12.3 with wall thickness of 0.002 m.

$$\text{Tube inner diameter, } d_i = d_o - (2 \times t) = 0.0260 \text{m}$$

$$\text{Pitch arrangement, } P_t = 1.25 \times d_o = 1.25 \times 0.03 = 0.0375 \text{m}$$

STEP 7: TUBE SHEET LAYOUT

$$\text{Area of one tube} = \pi \times d_o \times L = 0.1725 \text{m}^2$$

$$\text{Number of tubes, } N_t = \frac{A}{\text{Area of one tube}} \sim 58$$

Number of passes, N_p chosen is 8

$$\text{Total number of tubes per pass} = \frac{N_t}{N_p} \sim 7$$

$$\text{Inner cross-sectional area of tube, } A_i = \frac{\pi \times (d_i^2)}{4} = \frac{\pi \times (0.0148^2)}{4} = 0.0005 \text{m}^2$$

$$\text{Area per pass} = \text{total number of tubes per pass} \times A_i = 0.0037 \text{m}^2$$

$$\text{Volumetric flow rate} = \frac{\dot{m}}{\rho} = \frac{8.3962}{720.5329453} = 0.0075 \frac{\text{m}^3}{\text{s}}$$

$$\text{Tube-side velocity, } u_t = \frac{\text{volumetric flow rate}}{\text{area per pass}} = 2.0186 \frac{\text{m}}{\text{s}}$$

Based on the reference book, velocity for tube must be in a range between 1 m/s to 4 m/s.

Area of one tube	m^2	0.1725
Number of tubes, N_t		58
Number of passes, N_p		8
Total number of tubes per pass		7
Inner cross-sectional area of tube, A_i	m^2	0.0005

Area per pass	m^2	0.0037
Volumetric flow rate	m^3/s	0.0075
Tube-side velocity, u_t	m/s	2.0186

STEP 8: BUNDLE AND SHELL DIAMETER (TRIANGULAR PITCH ARRANGEMENT)

Type of floating head chosen: split-ring floating head.

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

From Table 12.4 above, for the number of passes = 8 for this heat exchanger with triangular pitch arrangement, K_1 and n_1 values are 0.0365 and 2.675 respectively.

$$\text{Bundle diameter, } D_b = d_o \times \left(\frac{N_t}{K_1} \right)^{\frac{1}{n_1}} = 0.4719\text{m}$$

From Figure 12.10 in Coulson and Richardson's Chemical Engineering Design,
For split-ring floating head,

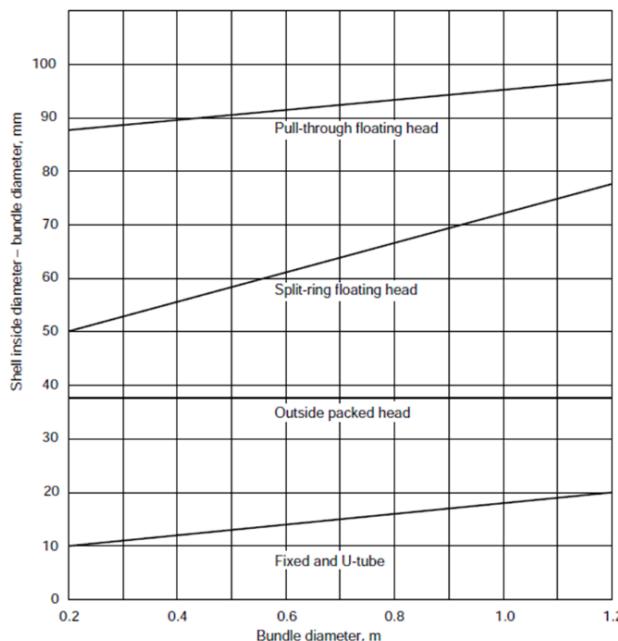


Figure 12.10. Shell-bundle clearance

$$\text{Shell bundle clearance} = 57.5 \text{ mm} = 0.0575 \text{ m}$$

$$\begin{aligned}\text{Shell inside diameter} &= \text{Shell bundle clearance} + \text{bundle diameter} \\ &= 0.0575 \text{ m} + 0.4719 \text{ m} \\ &= 0.5294 \text{ m}\end{aligned}$$

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$\pm \frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

Based on Table 12.5, the formulas of baffle diameter and tolerance for pipe shells are used.

$$\text{Baffle diameter} = D_s - (1.6 \times 10^{-3}) = 0.5278$$

$$\text{tolerance} = 0.8 \times 10^{-3} = 0.0008 \text{ m}$$

STEP 9: TUBE SIDE HEAT TRANSFER COEFFICIENT

$$\text{Reynold number, } \text{Re} = \frac{\rho u d_i}{\mu} = 193800.8900$$

$$\text{Prandtl, } \text{Pr} = \frac{C_p \mu}{k_f} = 3.5598$$

$$L/d_i = 2.44/0.0228 = 70.3846$$

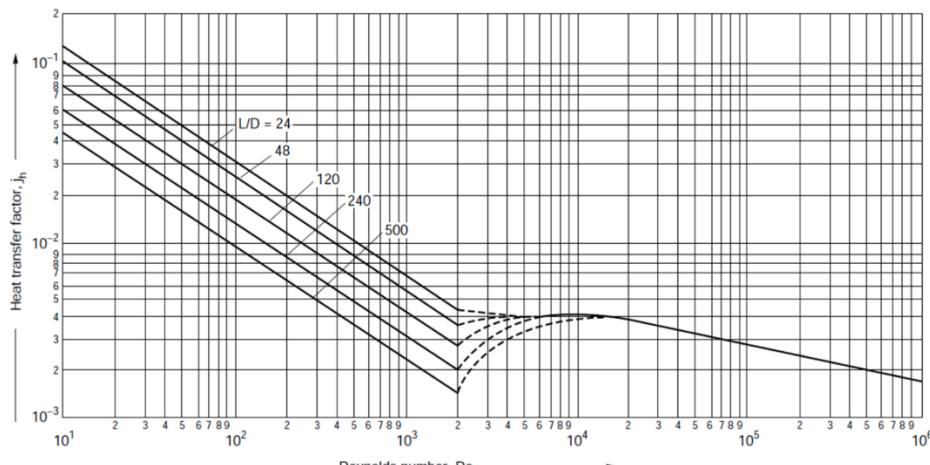


Figure 12.23. Tube-side heat-transfer factor

Based on Figure 12.23 above, tube-side heat transfer factor, $j_h = 0.004$

$$\text{Nusselt number } (j_h \times \text{Re} \times \text{Pr}^{0.33}) = 1178.6575$$

$$\text{Tube side heat transfer coefficient, } h_i = \frac{Nu \times k_f}{d_i} = 5216.0123 \frac{W}{m^2 \cdot ^\circ C}$$

STEP 10: SHELL-SIDE HEAT TRANSFER COEFFICIENT

$$Prandtl, \text{Pr} = \frac{C_p \mu}{k_f} = 4314.8986$$

Baffle spacing can choose from 0.3 to 0.5 of shell diameter to be multiplied with D_s for this heat exchanger, 0.5 is used.

$$l_B = 0.5 \times D_s = 0.2647m$$

$$\text{number of baffles}, N_b = \left(\frac{L}{l_B} \right) - 1 \sim 6$$

$$\text{cross flow area}, A_s = \frac{(P_t - d_o)D_s l_B}{P_t} = 0.0280m^2$$

$$\text{Shell side equivalent diameter, } d_e = \frac{1.1}{d_o} (p_t^2 - 0.917 d_o^2) = 0.0213m$$

$$\text{Shell side mass velocity, } G_s = \frac{W_s}{A_s} = 3458.9125 \frac{kg}{sm^2}$$

$$\text{Shell side linear velocity, } U_s = \frac{G_s}{\rho} = 3.4596 \frac{m}{s}$$

$$\text{Reynolds number, } Re = \frac{G_s d_e}{\mu} = \frac{u_s d_e \rho}{\mu} = 126.5178$$

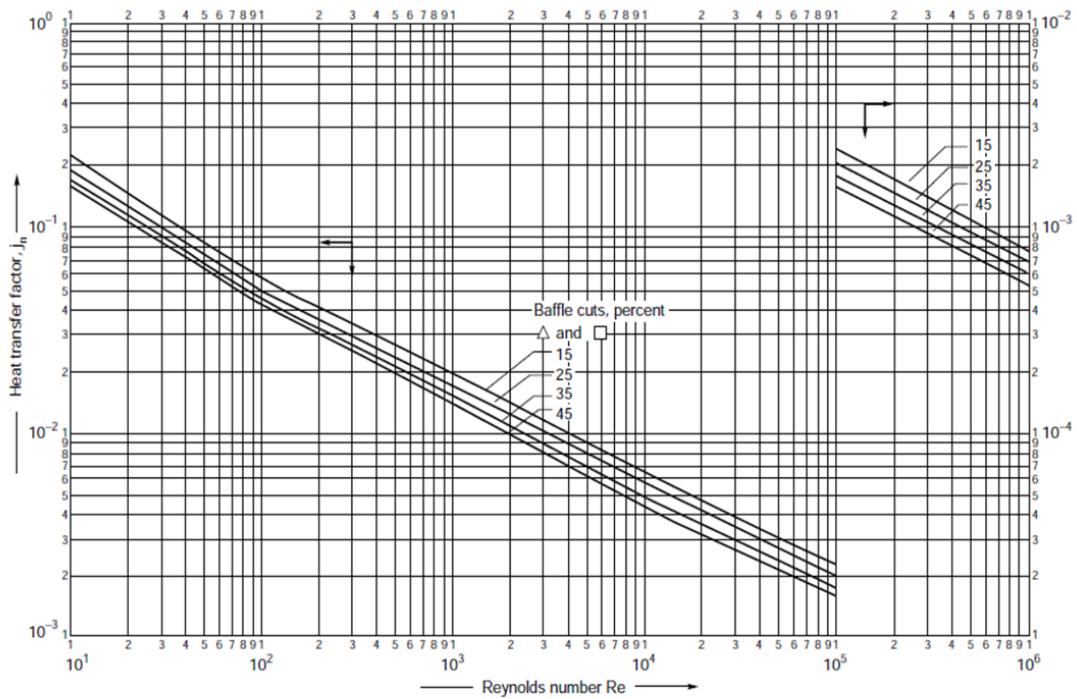


Figure 12.29. Shell-side heat-transfer factors, segmental baffles

Based on Figure 12.29, for the baffle cut for this heat exchanger of 25%, shell side heat transfer factor, $j_h = 0.055$.

$$Nu = j_h Re Pr^{1/3} \left(\frac{\mu}{\mu_w} \right)^{0.14} = 113.2847$$

$$\text{shell side heat transfer coefficient, } h_s = \frac{Nu k_f}{d_e} = 3028.0250$$

STEP 11: OVERALL COEFFICIENT

Fouling factor can be gained from Table 12.2

Table 12.2. Fouling factors (coefficients), typical values

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

outside fouling factor, $h_{od} = 3000 \text{ W/m}^2\text{.}^\circ\text{C}$

inside fouling factor, $h_{id} = 5000 \text{ W/m}^2\text{.}^\circ\text{C}$

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C								
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F
Aluminum:													
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249			
Al-Cu (Duralumin), 94–98% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194					
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161				
Al-Si (Alusil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178				
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204						
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8				
Iron:													
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33
Steel (C max ≈ 1.5%):													
Carbon steel C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28

Thermal conductivity of the tube wall gained from table A-2 where mean temperature of the tube is used to find the thermal conductivity of metal. Thus, $k_w = 52.0842 \text{ W/m.}^\circ\text{C}$

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \frac{d_o}{d_i}}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} = 0.0012$$

Overall coefficient based on outside area of tube, $U_o = \frac{1}{0.001156775} = 864.4720 W/m^2.^{\circ}C$

Overall coefficient error must not exceed 30% for the heat exchanger to function properly.

$$= \frac{(864.4719951 - 750)}{750} \times 100\% = 15.2629\%$$

STEP 12: PRESSURE DROP

Tube side:

Reynolds number, $Re = 193800.8900$

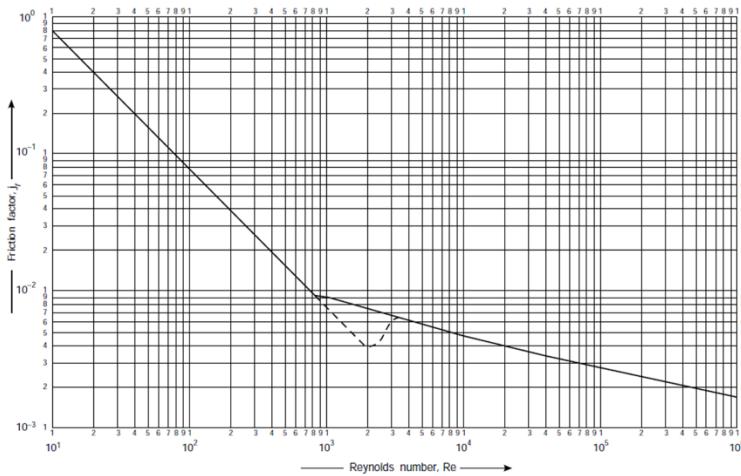


Figure 12.24. Tube-side friction factors

From Figure 12.24, friction factor, $j_f = 0.0048$

Tube side pressure drop, ΔP_t

$$= N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2} = 0.6554 \text{ bar}$$

Shell side:

$Re = 126.5178$

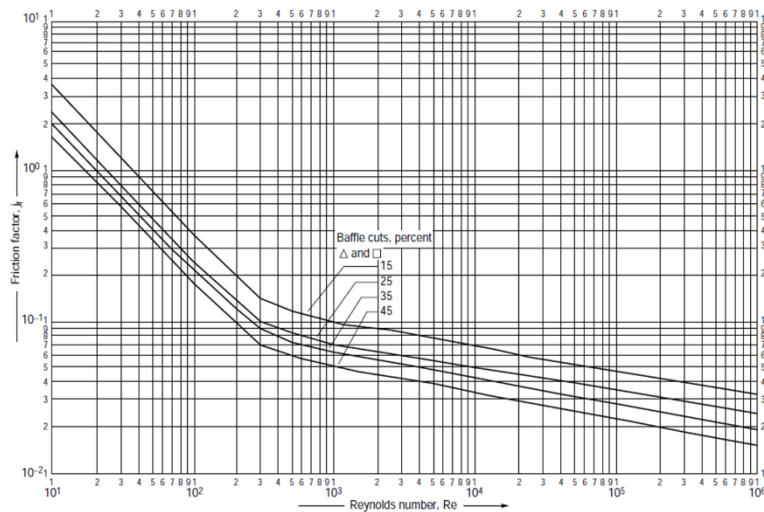


Figure 12.30. Shell-side friction factors, segmental baffles

$$\text{friction factor, } j_f = 0.056$$

$$\begin{aligned} & \text{Shell side pressure drop, } \Delta P_s \\ &= 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14} = 4.6056 \text{ bar} \end{aligned}$$

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE:

Maximum allowable working pressure

The design pressure is set at 10 % above normal working pressure as a safety margin, thus,

$$\text{Tube side design pressure, } P_d = 3.08 \text{ bar}$$

$$\text{Shell side design pressure, } P_d = 3 \text{ bar}$$

Minimum design metal temperature (MDMT)

Additional of 10 °C is applied to the design temperature, thus,

$$\text{Tube side design temperature, } T_d = 127.25 \text{ °C}$$

$$\text{Shell side design temperature, } T_d = 50.00 \text{ °C}$$

STEP 2: MATERIAL OF CONSTRUCTION:

Carbon steel

Table 13.2. Typical design stresses for plate
 (The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Minimum tensile strength 360 N/mm²

Maximum allowable stress at 127.25 °C 113.0256 N/mm²

Maximum allowable stress at 50 °C 135 N/mm²

STEP 3: WALL DESIGN

Tube

The equation specified by ASME BPV Code (Sec. VIII D.1 Part UG-27) is

$$t = \frac{P_d D_d}{2SE_{\text{f}} + 1.2 P_d}$$

With the following useful data, the minimum wall thickness obtained is **0.0000418 m.**

Design pressure, P_d 0.308 N/mm²

Design temperature, T_d 400.3962 K

Tube inner diameter, d_i 0.026 m

Welded joint efficiency, E

Corrosion allowance 2 mm

allowance, which is **0.0020 m**. Besides, the outer diameter of tube is obtained as **0.03 m**.

The maximum allowable working pressure for the tube can be calculated by using the equation below:

$$MAWP = \frac{Z \times Tensile\ strength \times E \times t_t}{d_i + t_t} = 44.5605 N/mm^2$$

The MAWP is acceptable because it is greater than the operating pressure, 0.308 N/mm^2 .

Shell

The equation specified by ASME BPV Code (Sec. VIII D.1 Part UG-27) is

$$t = \frac{P_d D_d}{2SE - 0.12P_d}$$

With the following useful data, the minimum wall thickness obtained is **0.000711564 m.**

Design pressure, P _d	0.308	N/mm ²
Design temperature, T _d	323.15	K
Shell inner diameter, d _{s<i>i</i>}	0.5294	m
Welded joint efficiency, E	0.85	-
Corrosion allowance	2	mm

The fabrication wall thickness, t_s is addition of minimum wall thickness with corrosion allowance, which is **0.0027 m**. Besides, the outer diameter of shell is obtained as **0.5348 m**. The maximum allowable working pressure for the shell can be calculated by using the equation below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times E \times t_s}{ds_i + t_s} = 3.1189 \text{ N/mm}^2$$

The MAWP is acceptable because it is greater than the operating pressure, 0.308 N/mm².

STEP 4: HEAD DESIGN

Torispherical head is used to design the closure of the vessel because is the most commonly used head type and can withstand up to 15 bar. The ASME BPV Code gives the design equation (Sec. VIII D.1 Part UG-32):

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

With the following useful data, the minimum wall thickness obtained is **0.0011 m.**

Design pressure, P _d	0.308	N/mm ²
Crown radius, R _c = d _i	0.5294	m
Welded joint efficiency, E	1	-
Corrosion allowance	2	mm

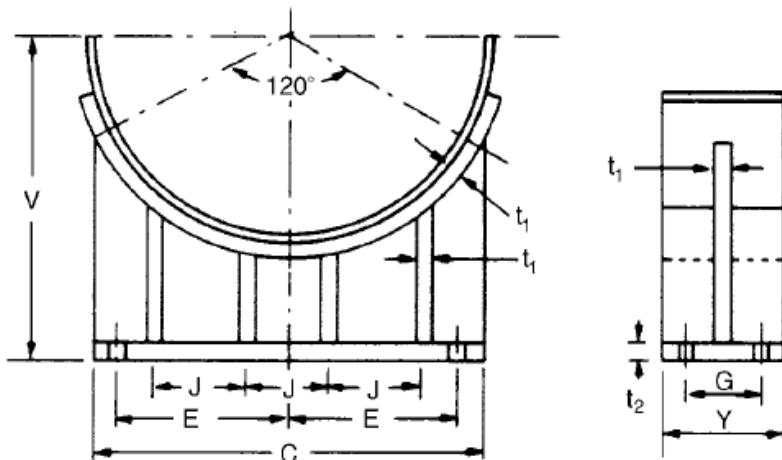
The fabrication wall thickness, t_h is addition of minimum wall thickness with corrosion allowance, which is **0.0031 m**. Besides, the outer diameter of head is obtained as **0.5355 m**. The maximum allowable working pressure for the head can be calculated by using the equation below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times E \times t_h}{d_i + t_h} = 4.1503 \text{ N/mm}^2$$

The MAWP is acceptable because it is greater than the operating pressure, 0.308 N/mm².

STEP 5: VESSEL SUPPORT

The type of vessel support used is saddle support which is suitable for horizontal vessel.



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

From the table above, the dimensions of the saddle chosen will be according to the vessel with vessel 0.8 m with maximum 50 kN as both the vessel diameter (0.6348m) and total weight (6.655 kN) do not exceed these values.

STEP 6: NOZZLE DIMENSION

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}}$$

Tube Inlet		
Mass flow rate, W	20873.89	kg/hr
Density, ρ	771.90	kg/m ³
Optimum pipe diameter, D _{opt}	94.07	mm

Tube Outlet		
Mass flow rate, W	20873.89	kg/hr
Density, ρ	773.83	kg/m ³
Optimum pipe diameter, D _{opt}	94.00	mm

Shell Inlet		
Mass flow rate, W	348926.41	kg/hr
Density, ρ	999.80	kg/m ³
Optimum pipe diameter, D _{opt}	308.36	mm

Shell Outlet		
Mass flow rate, W	348926.41	kg/hr
Density, ρ	999.80	kg/m ³
Optimum pipe diameter, D _{opt}	308.36	mm

E-301 COOLER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	Tube	Shell
Heat Duty, Q	MJ/hr	-127.8110	
	J/s	-35503.0530	
Inlet temperature	K	453.80 (S39)	303.15
Outlet temperature	K	393.77 (S40)	318.15
Pressure	bar	35	1
Mass flow rate, \dot{m}	ton/hr	4.1204	27.5179
	kg/s	1.1445	7.6439

Design method:

Coulson and Richardson's Chemical Engineering Design is used as a reference on designing the heat exchanger. While for properties of the components in stream, it being manually calculated based on formulas gained from related references.

Heat duty = -127.8110 MJ/hr

$$\dot{m}(\text{tube}) = 4.1204 \frac{\text{ton}}{\text{hr}} \times \frac{1000\text{kg}}{1\text{ton}} \times \frac{1\text{hr}}{3600\text{s}} = 1.1445 \text{ kg.s}^{-1}$$

$$\dot{m}(\text{shell}) = 27.5179 \frac{\text{ton}}{\text{hr}} \times \frac{1000\text{kg}}{1\text{ton}} \times \frac{1\text{hr}}{3600\text{s}} = 7.6439 \text{ kg.s}^{-1}$$

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE	SHELL
Mean temperature	K	423.78	310.65
Density, ρ	kg/m ³	701.8555	999.8000
Specific heat capacity, C_p	kJ/kg.K	2.2833	4.2133
Viscosity, μ	kg/m.s	0.0005	1.0662
Thermal conductivity, k_f	W/m.K	0.0925	0.5722

The physical properties of the components determined from data gained from running an ASPEN for specific temperature.

STEP 3: INITIAL ESTIMATION OF OVERALL HEAT TRANSFER COEFFICIENT

HEAT-TRANSFER EQUIPMENT

Table 12.1. Typical overall coefficients

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² °C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on the figure, value of overall heat transfer coefficient can be assumed based on the range given by the type of hot and cold fluid. For this cooler, E-301, since the hot fluid is organic solvents and cold fluid is water; thus, U is in the range of 250 - 750 W/m²°C.

$$U_o = 500 \text{ W/m}^2\text{°C}$$

STEP 4: MEAN TEMPERATURE DIFFERENCE FOR COUNTER-CURRENT FLOW

	Unit	TUBE (HOT)	SHELL (COLD)
Inlet temperature	K	453.80	303.15
Outlet temperature	K	393.77	318.15

$$\text{Log mean temperature difference, } \Delta T_{lm} = \frac{(T_{hot,in} - T_{cold,out}) - (T_{hot,out} - T_{cold,in})}{\ln \left(\frac{T_{hot,in} - T_{cold,out}}{T_{hot,out} - T_{cold,in}} \right)}$$

$$= 111.6259K$$

$$R = \frac{(T_{shell,in} - T_{shell,out})}{(T_{tube,out} - T_{tube,in})}$$

$$= 0.2499$$

$$S = \frac{(T_{tube,out} - T_{tube,in})}{(T_{shell,in} - T_{tube,in})}$$

$$= 0.3984$$

$$F_t = \frac{\sqrt{(R^2 + 1)} \ln \left[\frac{(1-S)}{(1-RS)} \right]}{(R-1) \ln \left[\frac{2-S[R+1-\sqrt{(R^2+1)}]}{2-S[R+1+\sqrt{(R^2+1)}]} \right]}$$

Temperature correction factor, $F_t = 0.9877$

If the value for temperature correction factor less than 0.75, Figure 12.20 can be used in order to find the F_t .

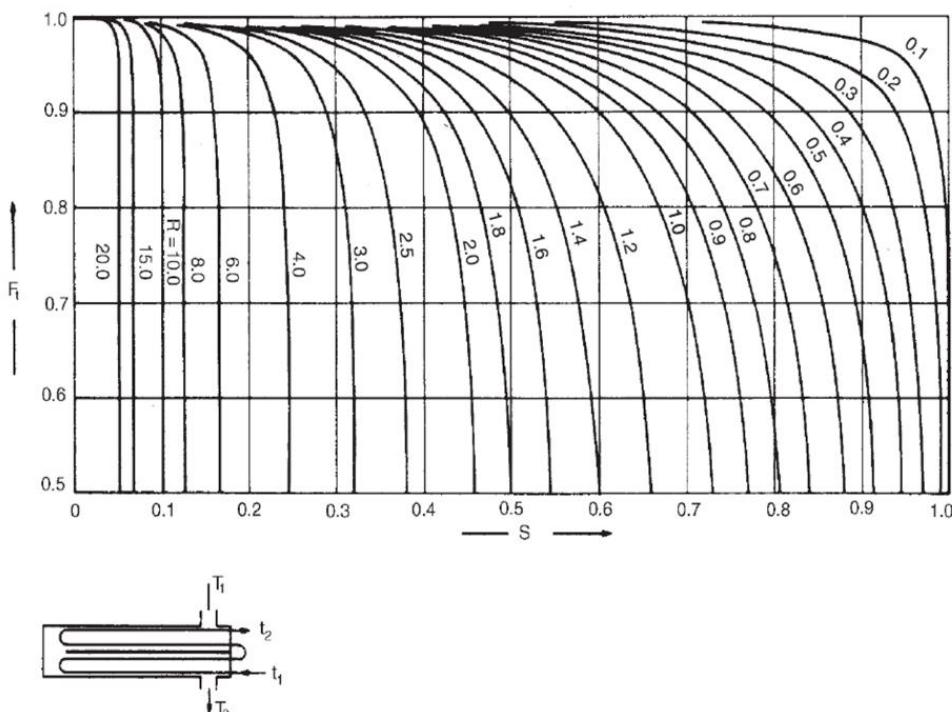


Figure 12.20. Temperature correction factor: two shell passes; four or multiples of four tube passes

$$\Delta T_m = F_t \times \Delta T_{lm} = 0.987738147 \times 111.6258696 = 110.26 \text{ K}$$

STEP 5: HEAT TRANSFER AREA

$$A = \frac{Q}{U\Delta T_{lm}} = 0.64400 \text{ m}^2$$

STEP 6: LAYOUT AND TUBE SIZE

3.66 m is chosen to be the nominal length of tube which taken from the recommended value by Coulson and Richardson Engineering Material Design.

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)			
16	1.2	1.6	2.0	—
20	—	1.6	2.0	2.6
25	—	1.6	2.0	2.6
30	—	1.6	2.0	2.6
38	—	—	2.0	2.6
50	—	—	2.0	2.6

While for tube outer diameter, d_o , 0.03 m is chosen from Table 12.3 with wall thickness of 0.002 m.

$$\text{Tube inner diameter, } d_i = d_o - (2 \times t) = 0.0260 \text{ m}$$

$$\text{Pitch arrangement, } P_t = 1.25 \times d_o = 1.25 \times 0.03 = 0.0375 \text{ m}$$

STEP 7: TUBE SHEET LAYOUT

$$\text{Area of one tube} = \pi \times d_o \times L = 0.1725 \text{ m}^2$$

$$\text{Number of tubes, } N_t = \frac{A}{\text{Area of one tube}} \sim 4$$

Number of passes, N_p chosen is 4

$$\text{Total number of tubes per pass} = \frac{N_t}{N_p} \sim 1$$

$$\text{Inner cross-sectional area of tube, } A_i = \frac{\pi \times (d_i^2)}{4} = \frac{\pi \times (0.0148^2)}{4} = 0.0005 \text{ m}^2$$

$$\text{Area per pass} = \text{total number of tubes per pass} \times A_i = 0.0005 \text{ m}^2$$

$$\text{Volumetric flow rate} = \frac{\dot{m}}{\rho} = \frac{8.3962}{720.5329453} = 0.0016 \frac{\text{m}^3}{\text{s}}$$

$$\text{Tube-side velocity, } u_t = \frac{\text{volumetric flow rate}}{\text{area per pass}} = 3.0715 \frac{\text{m}}{\text{s}}$$

Based on the reference book, velocity for tube must be in a range between 1 m/s to 4 m/s.

Area of one tube	m^2	0.1725
Number of tubes, N_t		4
Number of passes, N_p		4

Total number of tubes per pass		1
Inner cross-sectional area of tube, A_i	m^2	0.0005
Area per pass	m^2	0.0005
Volumetric flow rate	m^3/s	0.0016
Tube-side velocity, u_t	m/s	3.0715

STEP 8: BUNDLE AND SHELL DIAMETER (TRIANGULAR PITCH ARRANGEMENT)

Type of floating head chosen: split-ring floating head.

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

From Table 12.4 above, for the number of passes = 4 for this heat exchanger with triangular pitch arrangement, K_1 and n_1 values are 0.0175 and 2.285 respectively.

$$\text{Bundle diameter, } D_b = d_o \times \left(\frac{N_t}{K_1} \right)^{\frac{1}{n_1}} = 0.3232m$$

From Figure 12.10 in Coulson and Richardson's Chemical Engineering Design,

For split-ring floating head,

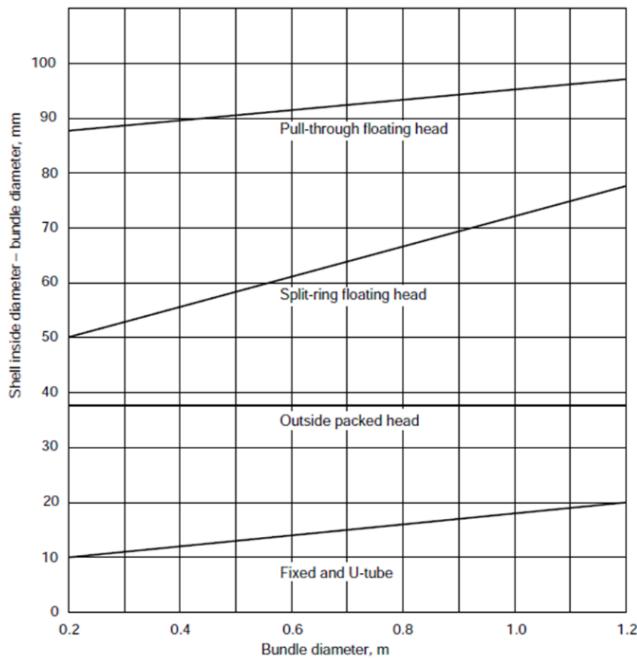


Figure 12.10. Shell-bundle clearance

$$\text{Shell bundle clearance} = 53 \text{ mm} = 0.0530 \text{ m}$$

$$\begin{aligned}\text{Shell inside diameter} &= \text{Shell bundle clearance} + \text{bundle diameter} \\ &= 0.0530 \text{ m} + 0.3232m \\ &= 0.3762 \text{ m}\end{aligned}$$

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells		
6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$+\frac{1}{32}$ in. (0.8 mm)
Plate shells		
6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

Based on Table 12.5, the formulas of baffle diameter and tolerance for pipe shells are used.

$$\text{Baffle diameter} = D_s - (1.6 \times 10^{-3}) = 0.3746m$$

$$\text{tolerance} = 0.8 \times 10^{-3} = 0.0008 m$$

STEP 9: TUBE SIDE HEAT TRANSFER COEFFICIENT

$$\text{Reynold number, } \text{Re} = \frac{\rho u d_i}{\mu} = 392293.3404$$

$$\text{Prandtl, } \text{Pr} = \frac{C_p \mu}{k_f} = 3.5275$$

$$L/d_i = 1.28/0.026 = 70.3846$$

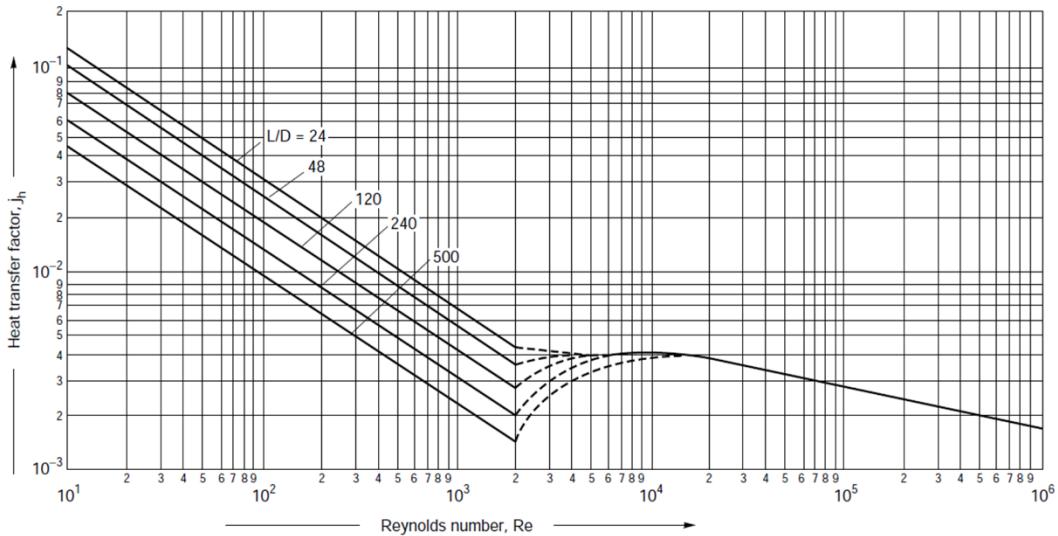


Figure 12.23. Tube-side heat-transfer factor

Based on Figure 12.23 above, tube-side heat transfer factor, $j_h = 0.0021$

$$\text{Nusselt number } (j_h \times Re \times P_r^{0.33}) = 1248.7991$$

$$\text{Tube side heat transfer coefficient, } h_i = \frac{Nu \times k_f}{d_i} = 4441.9293 \frac{W}{m^2 \cdot ^\circ C}$$

STEP 10: SHELL-SIDE HEAT TRANSFER COEFFICIENT

$$Prandtl, Pr = \frac{C_p \mu}{k_f} = 7850.8670$$

Baffle spacing can choose from 0.3 to 0.5 of shell diameter to be multiplied with D_s for this heat exchanger, 0.5 is used.

$$l_B = 0.5 \times D_s = 0.1881m$$

$$\text{number of baffles, } N_b = \left(\frac{L}{l_B} \right) - 1 \sim 9$$

$$\text{cross flow area, } A_s = \frac{(P_t - d_o)D_s l_B}{P_t} = 0.0142m^2$$

$$\text{Shell side equivalent diameter, } d_e = \frac{1.1}{d_o} (P_t^2 - 0.917 d_o^2) = 0.0213m$$

$$\text{Shell side mass velocity, } G_s = \frac{W_s}{A_s} = 540.0068 \frac{kg}{sm^2}$$

$$\text{Shell side linear velocity, } U_s = \frac{G_s}{\rho} = 0.5401 \frac{m}{s}$$

$$\text{Reynolds number, } Re = \frac{G_s d_e}{\mu} = \frac{u_s d_e \rho}{\mu} = 10.7889$$

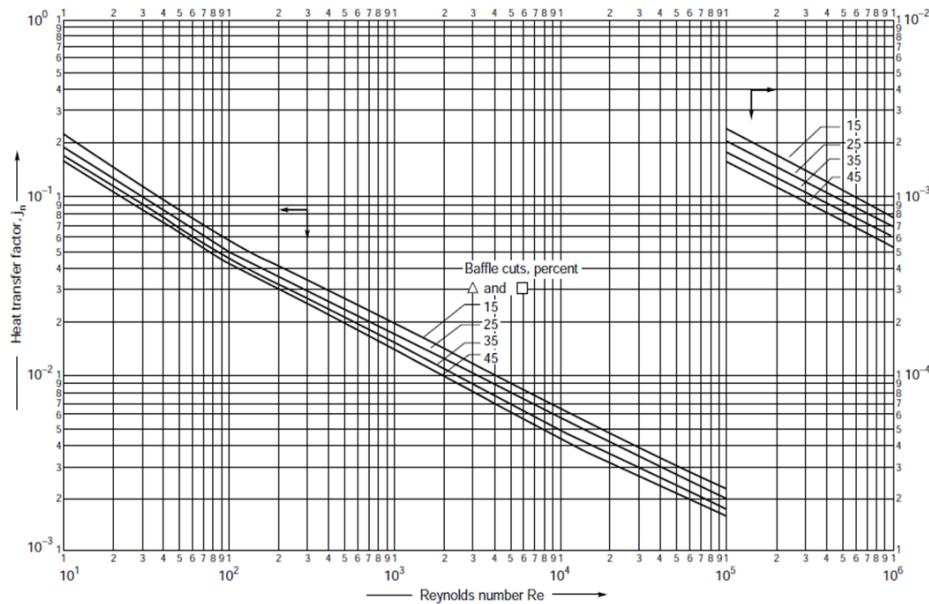


Figure 12.29. Shell-side heat-transfer factors, segmental baffles

Based on Figure 12.29, for the baffle cut for this heat exchanger of 25%, *shell side heat transfer factor*, $j_h = 0.15$.

$$Nu = j_h Re Pr^{1/3} \left(\frac{\mu}{\mu_w} \right)^{0.14} = 32.1643$$

$$\text{shell side heat transfer coefficient, } h_s = \frac{Nu k_f}{d_e} = 863.9774$$

STEP 11: OVERALL COEFFICIENT

Fouling factor can be gained from Table 12.2

Table 12.2. Fouling factors (coefficients), typical values

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

$$\text{outside fouling factor, } h_{od} = 6000 \text{ W/m}^2 \cdot ^\circ\text{C}$$

$$\text{inside fouling factor, } h_{id} = 5000 \text{ W/m}^2 \cdot ^\circ\text{C}$$

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Alasil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead:	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel (C max ≈ 1.5%: Carbon steel)														
C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

Thermal conductivity of the tube wall gained from table A-2 where mean temperature of the tube is used to find the thermal conductivity of metal. Thus, $k_w = 49.9746$ W/m · °C

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \frac{d_o}{d_i}}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} = 0.0019$$

Overall coefficient based on outside area of tube, $U_o = \frac{1}{0.0019} = 538.3325 W/m^2 \cdot ^\circ C$

Overall coefficient error must not exceed 30% for the heat exchanger to function properly.

$$= \frac{(538.3325 - 500)}{500} \times 100\% = 7.6665\%$$

STEP 12: PRESSURE DROP

Tube side:

Reynolds number, $Re = 392293.3403619$

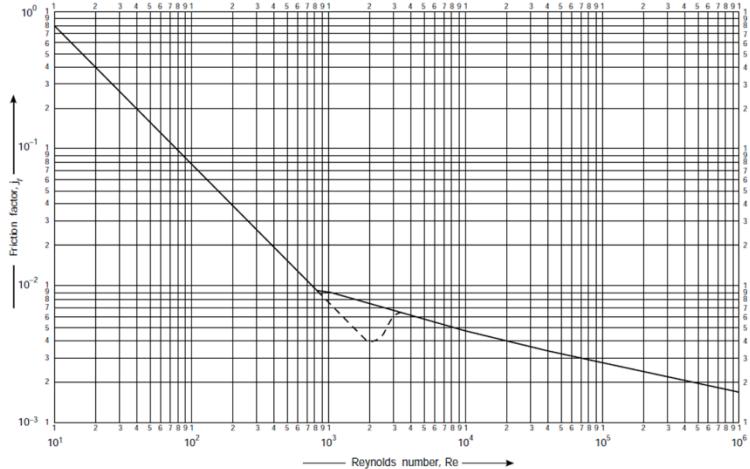


Figure 12.24. Tube-side friction factors

From Figure 12.24, friction factor, $j_f = 0.0048$

$$\text{Tube side pressure drop, } \Delta P_t \\ = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2} = 0.6890 \text{ bar}$$

Shell side:

$$Re = 10.7890$$

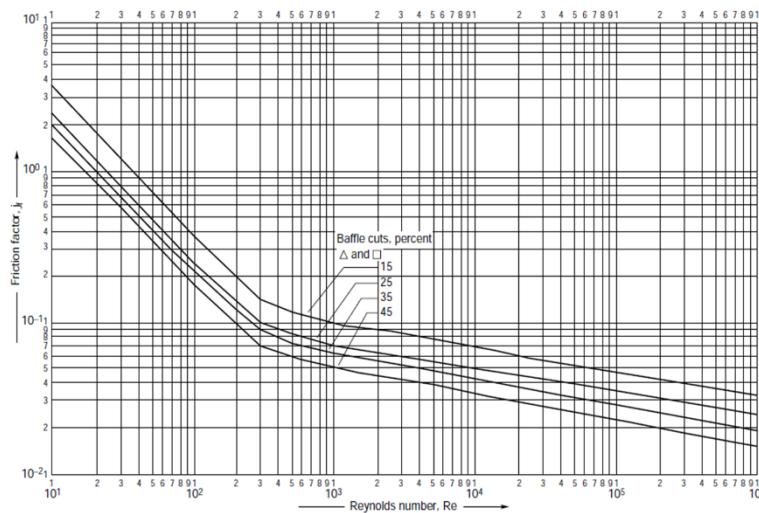


Figure 12.30. Shell-side friction factors, segmental baffles

friction factor, $j_f = 0.056$

Shell side pressure drop, ΔP_s

$$= 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14} = 0.1123 \text{ bar}$$

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE:

Maximum allowable working pressure

The design pressure is set at 10 % above normal working pressure as a safety margin, thus,

Tube side design pressure, P_d = 38.5 bar
 Shell side design pressure, P_d = 1 bar

Minimum design metal temperature (MDMT)

Additional of 10 °C is applied to the design temperature, thus,

Tube side design temperature, T_d = 190.65 °C
 Shell side design temperature, T_d = 55.00 °C

STEP 2: MATERIAL OF CONSTRUCTION:

Carbon steel

Table 13.2. Typical design stresses for plate
 (The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Minimum tensile strength 360 N/mm²
 Maximum allowable stress at 127.25 °C 71.5496 N/mm²
 Maximum allowable stress at 50 °C 150.5160 N/mm²

STEP 3: WALL DESIGN

Tube

The equation specified by ASME BPV Code (Sec. VIII D.1 Part UG-27) is

$$t = \frac{P_d D_d}{2S_F + 1.2R_g}$$

With the following useful data, the minimum wall thickness obtained is **0.00004 m**.

Design pressure, P _d	3.85	N/mm ²
Design temperature, T _d	463.7955	K
Tube inner diameter, d _i	0.0260	m
Welded joint efficiency, E	0.85	-

Corrosion allowance	2	mm
---------------------	---	----

The fabrication wall thickness, t_t is addition of minimum wall thickness with corrosion allowance, which is **0.0020 m**. Besides, the outer diameter of tube is obtained as **0.03 m**.

The maximum allowable working pressure for the tube can be calculated by using the equation below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times E \times t_t}{d_i + t_t} = 60.5617 \text{ N/mm}^2$$

The MAWP is acceptable because it is greater than the operating pressure, 3.85 N/mm^2 .

Shell

The equation specified by ASME BPV Code (Sec. VIII D.1 Part UG-27) is

$$t = \frac{P_d D_d}{2SE - 1.2P_o}$$

With the following useful data, the minimum wall thickness obtained is **0.0002 m**.

Design pressure, P_d	0.11	N/mm ²
Design temperature, T_d	328.15	K
Shell inner diameter, d_{si}	0.3762	m
Welded joint efficiency, E	0.85	-
Corrosion allowance	2	mm

The fabrication wall thickness, t_s is addition of minimum wall thickness with corrosion allowance, which is **0.0022 m**. Besides, the outer diameter of shell is obtained as **0.3806 m**.

The maximum allowable working pressure for the shell can be calculated by using the equation below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times E \times t_s}{ds_i + t_s} = 3.4964 \text{ N/mm}^2$$

The MAWP is acceptable because it is greater than the operating pressure, 3.85 N/mm^2 .

STEP 4: HEAD DESIGN

Ellipsoidal head is used to design the closure of the vessel because it can withstand the highest pressure compared to other types of head. The ASME BPV Code gives the design equation (Sec. VIII D.1 Part UG-32):

$$t = \frac{P_i D}{2SE - 0.2P_o}$$

With the following useful data, the minimum wall thickness obtained is **0.0003 m**.

Design pressure, P_d	3.85	N/mm ²
------------------------	------	-------------------

Crown radius, $R_c = d_i$	0.3762	m
Welded joint efficiency, E	1	-
Corrosion allowance	2	mm

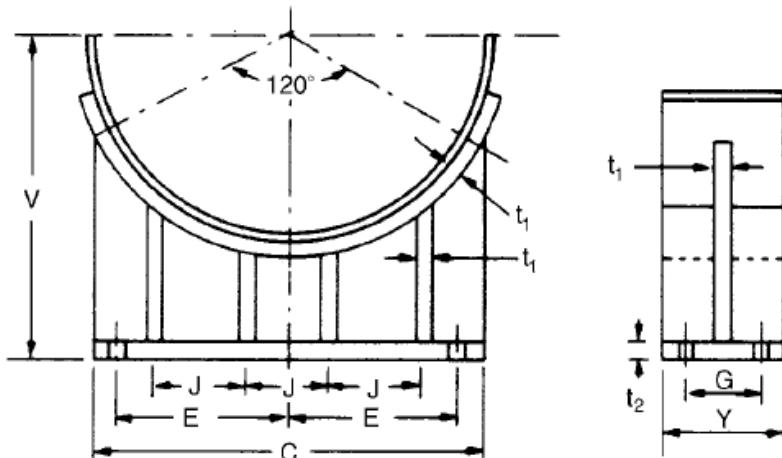
The fabrication wall thickness, t_h is addition of minimum wall thickness with corrosion allowance, which is **0.0023 m**. Besides, the outer diameter of head is obtained as **0.3808 m**. The maximum allowable working pressure for the head can be calculated by using the equation below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times E \times t_h}{d_i + t_h} = 4.3275 \text{ N/mm}^2$$

The MAWP is acceptable because it is greater than the operating pressure, 3.85 N/mm².

STEP 5: VESSEL SUPPORT

The type of vessel support used is saddle support which is suitable for horizontal vessel.



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

From the table above, the dimensions of the saddle chosen will be according to the vessel with vessel 0.6 m with maximum 35 kN as both the vessel diameter (0.4806 m) and total weight (2.7781 kN) do not exceed these values.

STEP 6: NOZZLE DIMENSION

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}}$$

Tube Inlet		
Mass flow rate, W	4120.35	kg/hr
Density, ρ	699.40	kg/m ³
Optimum pipe diameter, D _{opt}	46.74	mm

Tube Outlet		
Mass flow rate, W	4120.35	kg/hr
Density, ρ	704.31	kg/m ³
Optimum pipe diameter, D _{opt}	46.63	mm

Shell Inlet		
Mass flow rate, W	27517.94	kg/hr
Density, ρ	999.80	kg/m ³
Optimum pipe diameter, D _{opt}	98.32	mm

Shell Outlet		
Mass flow rate, W	27517.94	kg/hr
Density, ρ	999.80	kg/m ³
Optimum pipe diameter, D _{opt}	98.32	mm

E103 HEATER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE (steam)	SHELL (PROCESS FLUID)
Heat duty, Q	J/s	74071.94444	
Inlet temperature	K	723.15	428.7498
Outlet temperature	K	523.45	473.15
Pressure	bar	40	40
Mass flow rate	ton/hr	65.5633	26.99472
	kg/s	18.21202778	7.498533333

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (steam)	SHELL (PROCESS FLUID)
Mean temperature	K	623.3	450.9499
Density	kg/m ³	14.27181292	450.699561
Specific heat capacity, Cp	kJ/kg.K	2.698683049	2.698683049
Viscosity, μ	kg/m.s	2.2314E-05	0.000137519
Thermal conductivity, Kf	W/m.K	0.05736345	0.066855638

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² °C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 60 W/m².C

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{(T_{in_h} - T_{out_c}) - (T_{out_h} - T_{in_c})}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

Mean temperature difference, ΔT_m

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t depends on R & S

$$R = \frac{T_{hi} - T_{ho}}{T_{co} - T_{ci}}$$

$$S = \frac{T_{co} - T_{ci}}{T_{hi} - T_{ci}}$$

Temperature correction factor, F_t can be obtained from figure 12.19 C&R 3rd edition. If correction factor less than 0.75, proceed to second shell and find the F_t value from figure 12.20 C&R 3rd edition.

HEAT-TRANSFER EQUIPMENT

65

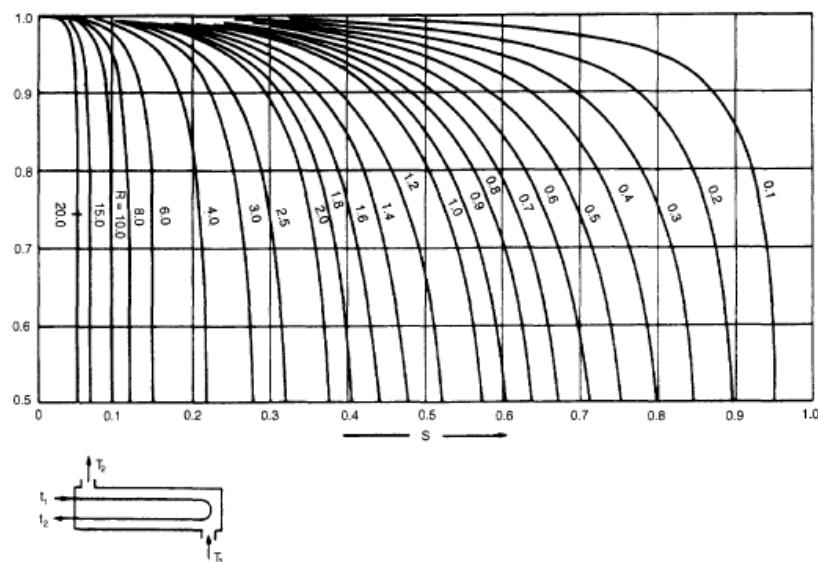


Figure 12.19. Temperature correction factor: one shell pass; two or more even tube 'passes'

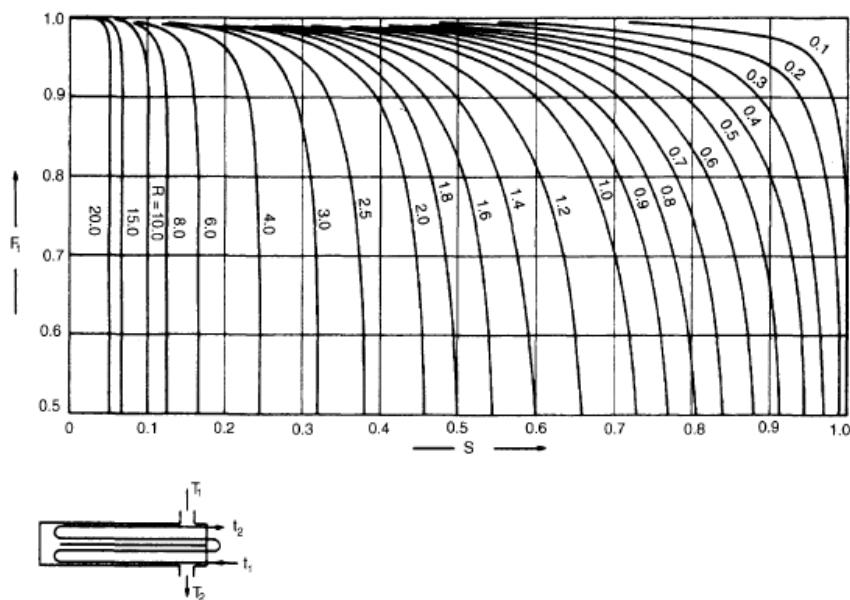


Figure 12.20. Temperature correction factor: two shell passes; four or multiples of four tube passes

So,

Log mean temperature difference, ΔT_{lm}	159.980047
R	0.2223345
S	0.67832834
Temperature correction factor, F_t (1 shell)	0.9
True temperature difference, ΔT_m	143.982043

figure 12.19

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{Ux LMTD}$$

A (m ²)	8.57421096
---------------------	------------

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Parameter	Unit	Value	
Tube inner diameter, d_i	m	0.046	
Tube outer diameter, d_o	m	0.05	Table 12.3
Wall thickness	m	0.002	Table 12.3
Nominal length, L	m	1.83	*the shell and tube pressure
Pitch arrangement, p_t	m	0.0625	1.25 d_o

STEP 7: NUMBER OF TUBES

Area of one tube, $= \pi \times d_o \times L = \pi \times 0.03 \times 4.88 = 0.45999 m^2$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}} = \frac{31.8397}{0.045999} = 69$$

Number of passes, $N_p = 1$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p}$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi \times (d_i^2)}{4}$$

$$\text{Area per pass} = \frac{m}{\text{Number of tubes per pass}}$$

$$\text{Volumetric flow} = \frac{m}{\rho}$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}}$$

Parameter	Unit	Value	
Area of one tube	m ²	0.287455728	
Number of tubes, N_t		30	
Number of passes, N_p		1	
N_t / N_p		30	
tube cross-sectional area	m ²	0.001661903	
Area per pass	m ²	0.049857075	
Volumetric flow	m ³ /s	1.276083696	
Tube-side velocity, u_t	m/s	25.59483656	*in the range for vapor

STEP 8: BUNDLE AND SHELL DIAMETER

K₁ and n₁ from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition
HEAT-TRANSFER EQUIPMENT

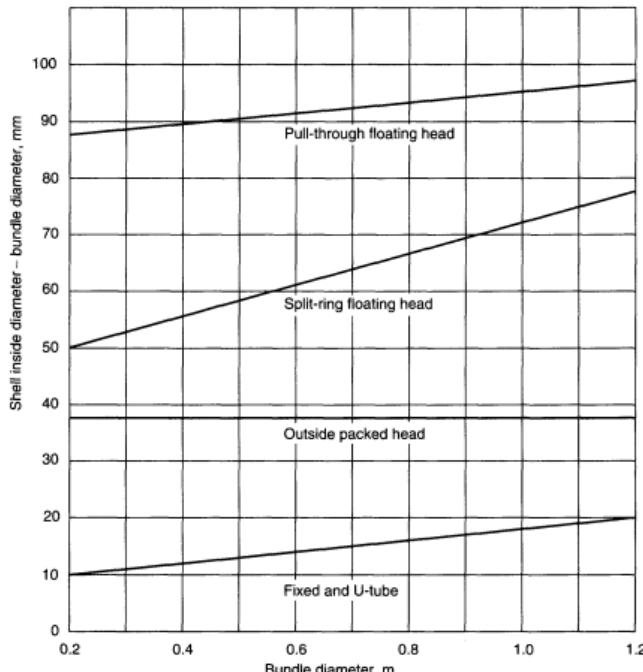


Figure 12.10. Shell-bundle clearance

*Using split floating head – shell bundle clearance

Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$\pm \frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

$$D_{si} = \text{bundle diameter} + \text{shell bundle clearance}$$

Parameter	Unit	Value	
K ₁		0.319	table 12.4
n ₁		2.142	table 12.4
Bundle diameter, D _b	m	0.42	
Tube in centre row		6.673383597	
Shell-bundle clearance	m	0.057	Figure 12.10 (split floating)
Shell diameter, D _{si}	m	0.474086475	Bundle diameter + shell clearance
Baffle diameter	m	0.472486475	table 12.5
Tolerance	m	0.0008	table 12.5

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$\text{Re} = \frac{\rho u_t d_i}{\mu}$$

$$Pr = C_p \mu / k_f$$

$$Nu = j_h x \text{Re} x Pr^{0.33}$$

$$hi = Nu x \frac{k_f}{d_i}$$

Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition

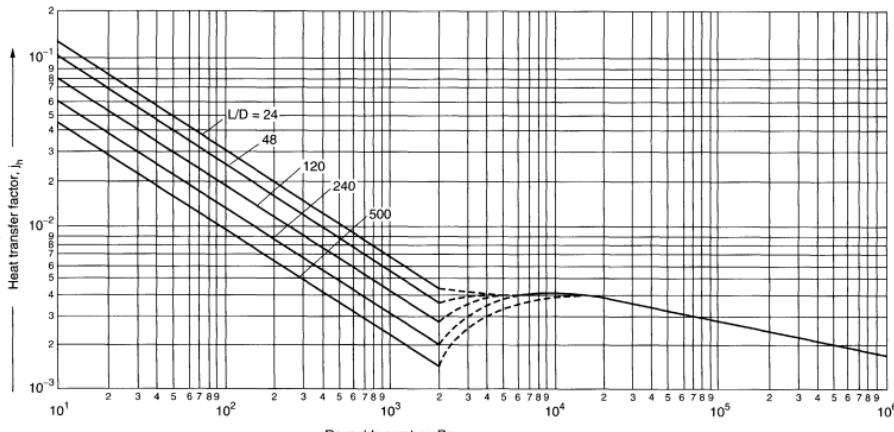


Figure 12.23. Tube-side heat-transfer factor

Assumed 25% baffle cut

Reynolds number, Re		7.53E+05	Re>2000, turbulent
Prandtl number, Pr		0.001049767	
L/di		39.7826087	
Tube-side heat transfer factor, j_h		0.0018	Figure 12.23
Nu		140.9438401	
Tube side heat transfer coefficient, h_t	W/m ² .°C	175.7614115	

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{4 \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, lb	m	0.237043237	choose 0.5	
Tube pitch, pt	m	0.0625		
Cross-flow area, As	m ²	0.022475799		
Shell-side mass velocity, G _s	kg/s.m ²	333.6270039		
Shell-side linear velocity, u _s	m/s	0.740242576		
Equilateral diameter, d _e	m	0.007132813		
Reynolds number, Re		1.73E+04		
Prandtl number, Pr		0.00555107		
Shell-side heat-transfer factors, j _h		0.0048	Baffle cut 25%	Figure 12.29
Shell-side heat transfer coefficient, h _s	W/m ² .°C	1.38E+02	without viscosity correction term	

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m²°C,

h_o = outside fluid film coefficient, W/m²°C,

h_i = inside fluid film coefficient, W/m²°C,

h_{od} = outside dirt coefficient (fouling factor), W/m²°C,

h_{id} = inside dirt coefficient, W/m²°C,

k_w = thermal conductivity of the tube wall material, W/m°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k, W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dunlumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Solumn, copper-bearing), 86.5% Al, 1% Cu	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Ahasil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	36	33	33	
Steel (C max ≈ 1.5%):														
Carbon steel														
C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² .°C	137.8488672	
outside dirt/fouling coefficient, h_{od}	W/m ² .°C	5000	(organic liquid)
inside fluid film coefficient, h_i	W/m ² .°C	175.7614115	
inside dirt/fouling coefficient, h_{id}	W/m ² .°C	5000	steam condensate
thermal conductivity tube wall material, k_w	W/m ² .°C	54	Carbon steel 0.5%
overall coefficient based on the outside area of tube, h_o	W/m ² .°C	71.97046677	table 12.2
Error	%	19.95077795	table A-2
			below 30%, design can be accepted

STEP 12: PRESSURE DROP

Friction factor, j_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

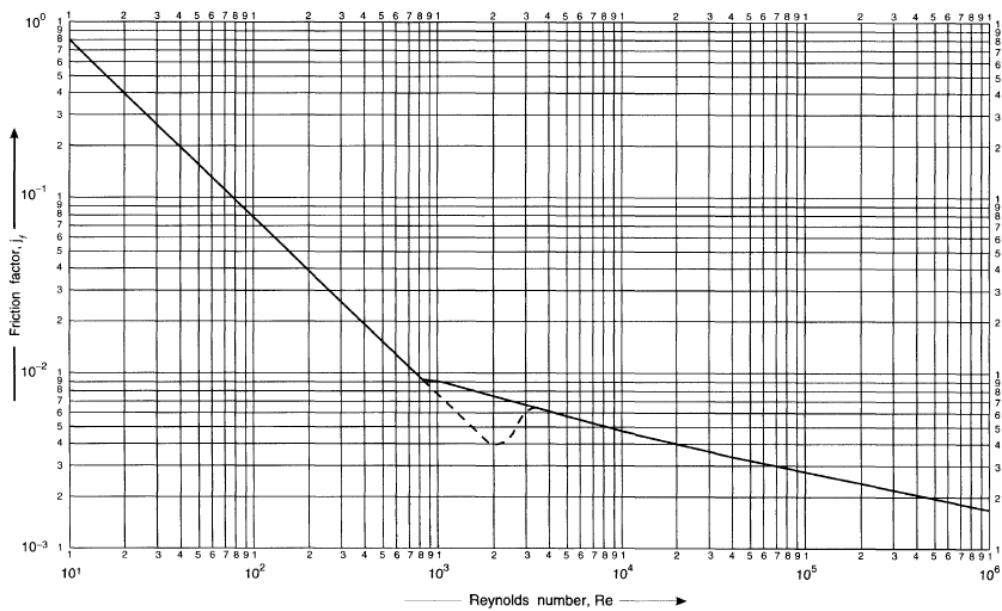


Figure 12.24. Tube-side friction factors

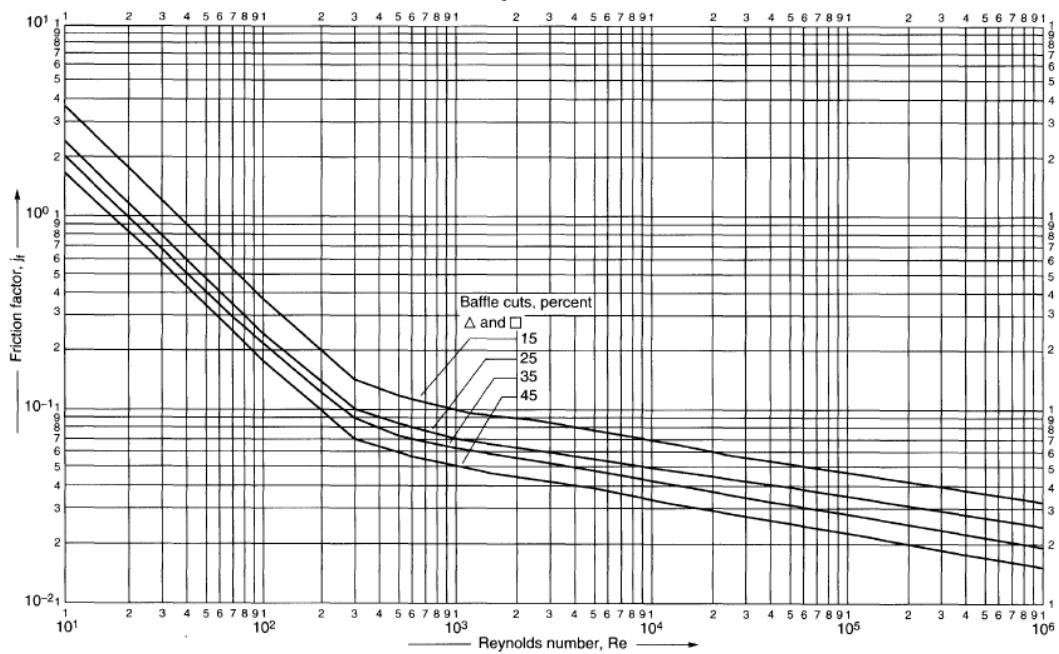


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and shell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side

Reynolds number, Re		7.53E+05	
Friction factor, j_f		0.0018	
Tube side pressure drop, ΔP_t	kg/m ²	627358.7771	Figure 12.24
	bar	61.52289237	
<u>Shell side</u>			
Reynolds number, Re		1.73E+04	
Friction factor, j_f		0.048	Figure 12.30
Tube side pressure drop, ΔP_s	kg/m ²	24330.82089	
	bar	2.386038946	

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube				
Operating pressure, P_o		40 bar	4000000 Pa	
Design pressure, P_d		44 bar	4400000 Pa	
<u>Shell (steam)</u>				
Operating pressure, P_o		40 bar	4000000 Pa	
Design pressure, P_d		44 bar	4400000 Pa	

The maximum normal operating temperature should have additional 25°C

Tube			
Inlet temperature, T_i		723.15 K	
Outlet temperature, T_o		523.45 K	
Design temperature, T_d		548.45 K	
<u>Shell</u>			
Inlet temperature		428.7498 K	
Outlet temperature		473.15 K	
Design temperature, T_d		453.7498 K	

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Minimum allowable stress	360 N/mm ²	360000000 N/m ²
Maximum allowable for tube, f	93.199 N/mm ²	93199000 N/m ²
Maximum allowable for shell, f	109.298034 N/mm ²	109298034 N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_l}{4Jf - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

For tube MAWP = $\frac{2 \times \text{tensile strength} \times E \times t_t}{D_i + t_t}$

Design pressure, Pd	D _i + t _t	4400000.0000 Pa
Design temperature, Td		548.4500 K
Tube inner diameter, d _{ti}		0.0460 m
Tube outer diameter, d _o		0.0500 m
Wall thickness		0.0020 m
Minimum wall thickness, e		0.0006 m
Corrosion allowance		0.0020 m
Fabrication wall thickness, t _f		0.0026 m
design tube outer diameter, d _o		0.0513 m
MAWP	33330814.16 N/m ²	
	333.3081416 bar	

The design can be accepted as the MAWP is greater than the operating pressure
For shell,

Design pressure, Pd	4400000 Pa
Design temperature, Td	453.7498 K
Shell inner diameter, d _{ti}	0.474086475 m
Minimum wall thickness, e	0.005694215 m
Corrosion allowance	0.002 m
Fabrication wall thickness, t _s	0.007694215 m
design shell outer diameter, d _o	0.489474904 m
MAWP	9773864.743 N/m ²
	97.73864743 bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

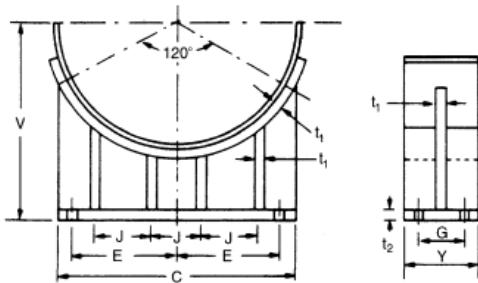
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radius, R _c	0.474086475 m
knuckle radius, R _k	0.028445188 m
Joint efficiency, E	1
Design pressure, Pd	4400000 Pa
Minimum wall thickness	0.534441419 m
Corrosion allowance	0.002 m
Head wall thickness, t _h	0.536441419 m
External diameter	1.546969313
MAWP	382213914.2 N/m ²
	3822.139142 bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t ₂	t ₁	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter	
Vol.flow rate, Q	1.519502967 m ³ /s
Min cross section area	0.059367559 m ²
Min diamter	0.274934763 m
Operate nozzle diameter	0.549869525 m
Tube outlet nozzle diameter	
Vol.flow rate, Q	1.099885702 m ³ /s
Min cross section area	0.042972953 m ²
Min diamter	0.233912083 m
Operate nozzle diameter	0.467824167 m
Shell inlet nozzle diameter	
Vol.flow rate, Q	0.030718144 m ³ /s
Min cross section area	0.041497402 m ²
Min diamter	0.229861117 m
Operate nozzle diameter	0.459722233 m
Shell outlet nozzle diameter	
Vol.flow rate, Q	0.011408231 m ³ /s
Min cross section area	0.015411477 m ²
Min diamter	0.14008034 m
Operate nozzle diameter	0.280160681 m

E202 REBOILER

STEP 1: SPECIFICATION

Type heat exchanger: Horizontal (higher heat transfer compared to vertical)

Material construction: Carbon Steel

Type: Shell and tube

Design method: All values are taken from mass and energy balance part

	Unit	TUBE (steam)	SHELL (PROCESS FLUID)
Heat duty, Q	J/s	90419.44444	
Inlet temperature	K	723.15	502.6792
Outlet temperature	K	523.45	502.6792
Pressure	bar	40	2.8
Mass flow rate	ton/hr	5.5372	1.41823
	kg/s	1.538111111	0.393952778

STEP 2: PHYSICAL PROPERTIES

	Unit	TUBE (steam)	SHELL (PROCESS FLUID)
Mean temperature	K	623.3	502.6792
Density	kg/m ³	14.27181292	693.2019754
Specific heat capacity, Cp	kJ/kg.K	2.878804977	3.863530147
Viscosity, μ	kg/m.s	2.2314E-05	0.000174236
Thermal conductivity, Kf	W/m.K	0.05736345	0.1050421

The physical properties are taken from APSEN 10 Simulation of standard method at specific temperature and pressure

STEP 3: INITIAL QUSS OVERALL COEFFICIENT VALUE

Shell and tube exchangers		
Hot fluid	Cold fluid	U (W/m ² .C)
<i>Heat exchangers</i>		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
<i>Coolers</i>		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
<i>Heaters</i>		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue gases	Hydrocarbon vapours	30–100
<i>Condensers</i>		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
<i>Vaporisers</i>		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Based on table 12.1 Coulson and Richardson 3rd edition, the initial guess of heat transfer coefficient is taken at 50 W/m².C for heater.

STEP 4: HEAT EXCHANGER TYPE AND DIMENSION

Log mean temperature difference from equation 12.4, R value calculated by using equation 12.6 and S value from equation 12.7 C&R 3rd edition.

$$\Delta T_{LM} = \frac{(T_{in_h} - T_{out_c}) - (T_{out_h} - T_{in_c})}{\ln\left(\frac{T_{in_h} - T_{out_c}}{T_{out_h} - T_{in_c}}\right)}$$

So,

Log mean temperature difference, ΔT_{lm}	84.5392236
--	------------

STEP 5: HEAT TRANSFER AREA

From equation 12.1 C&R 3rd edition

$$A = \frac{Q}{U_x LMTD}$$

A (m ²)	21.3911225
---------------------	------------

STEP 6: LAYOUT AND TUBE SIZE

From table 12.3 C&R 3rd edition

Table 12.3. Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Parameter	Unit	Value	
Tube inner diameter, d_i	m	0.026	
Tube outer diameter, d_o	m	0.03	Table 12.3
Wall thickness	m	0.002	Table 12.3
Nominal length, L	m	7.32	*the shell and tube pressure drop
Pitch arrangement, p_t	m	0.0375	1.25 d_o

STEP 7: NUMBER OF TUBES

Area of one tube, $= \pi x d_o x L$

$$\text{Number of tubes, } N_t = \frac{A}{\text{area of one tube}}$$

Number of passes, $N_p = 2$

$$\text{Number of tubes per pass} = \frac{N_t}{N_p}$$

$$\text{Cross sectional area of tube, } A_i = \frac{\pi x (d_i^2)}{4}$$

$$\text{Area per pass} = \frac{A_i}{\text{Number of tubes per pass}}$$

$$\text{Volumetric flow} = \frac{m}{\rho}$$

$$\text{Tube side velocity, } U_t = \frac{\text{Volumetric flow}}{\text{Area per pass}}$$

Parameter	Unit	Value	
Area of one tube	m ²	0.689893747	
Number of tubes, N_t		31	
Number of passes, N_p		2	
N_t / N_p		16	
tube cross-sectional area	m ²	0.000530929	
Area per pass	m ²	0.008494867	
Volumetric flow	m ³ /s	0.107772651	
Tube-side velocity, U_t	m/s	12.68679743	*in the range for vapor

STEP 8: BUNDLE AND SHELL DIAMETER

K1 and n1 from Table 12.4 C&R 3rd edition

Table 12.4. Constants for use in equation 12.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Shell bundle clearance from figure 12.10 C&R 3rd edition
HEAT-TRANSFER EQUIPMENT

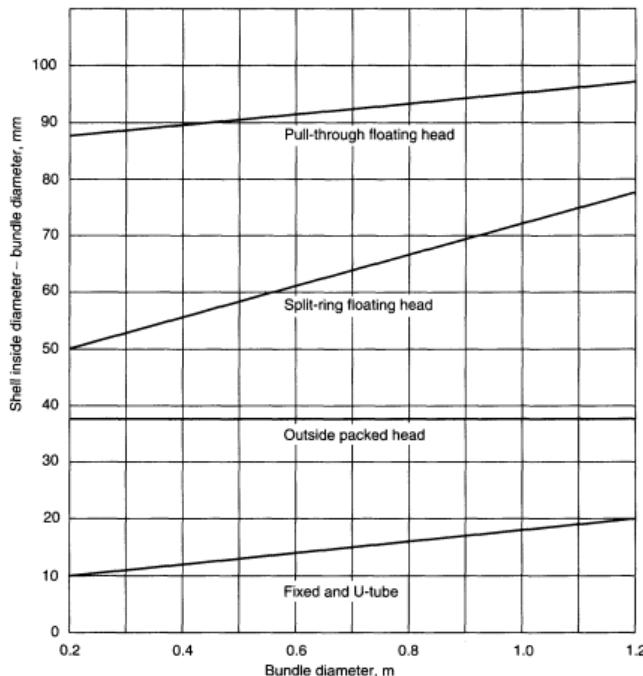


Figure 12.10. Shell-bundle clearance

*Using fixed and tube head– shell bundle clearance

Baffle diameter and tolerance from figure 12.10 C&R 3rd edition

Table 12.5. Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$\pm \frac{1}{32}$ in. (0.8 mm)
Plate shells 6 to 25 in. (152 to 635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27 to 42 in. (686 to 1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

$$D_{SI} = \text{bundle diameter} + \text{shell bundle clearance}$$

Parameter	Unit	Value	
K_1		0.249	table 12.4
n_1		2.207	table 12.4
Bundle diameter, D_b	m	0.27	
Tube in centre row		7.118949722	
Shell-bundle clearance	m	0.0105	Figure 12.10
Shell diameter, D_{SI}	m	0.277460615	Bundle diameter + shell clear.
Baffle diameter	m	0.275860615	table 12.5
Tolerance	m	0.0008	table 12.5

STEP 9: TUBE AND SIDE HEAT TRANSFER COEFFICIENT

$$Re = \frac{\rho \cdot u_t \cdot d_i}{\mu}$$

$$Pr = C_p \mu / k_f$$

$$Nu = j_h x Re x Pr^{0.33}$$

$$hi = Nu x \frac{k_f}{d_i}$$

Tube side heat transfer factor, j_h can be obtained from figure 12.23 C&R 3rd edition

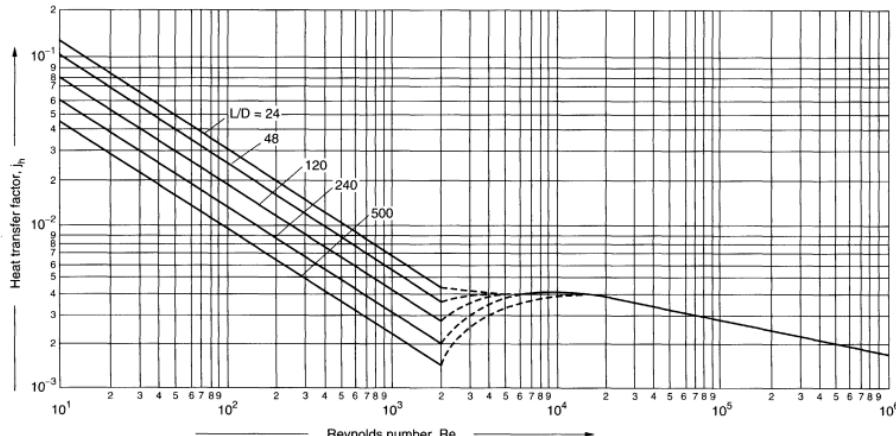


Figure 12.23. Tube-side heat-transfer factor

Assumed 25% baffle cut

Reynolds number, Re		2.11E+05	Re>2000, turbulent
Prandtl number, Pr		0.001119833	
L/di		281.5384615	
Tube-side heat transfer factor, j_h		0.0025	Figure 12.23
Nu		56.02587976	
Tube side heat transfer coefficient, h_i	W/m ² .°C	123.6091443	

STEP 10: SHELL SIDE HEAT TRANSFER COEFFICIENT

Baffle diameter can be chosen from 0.3 to 0.5 of shell diameter

Area flow area from equation 12.2 C&R 3rd edition

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t}$$

p_t = tube pitch,

d_o = tube outside diameter,

D_s = shell inside diameter, m,

l_B = baffle spacing, m.

Shell-side mass velocity, G_s and shell side linear velocity are calculated as shown below

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

W_s = fluid flow-rate on the shell-side, kg/s,

ρ = shell-side fluid density, kg/m³.

Equilateral diameter from equation 12.23 C&R 3rd edition

For an equilateral triangular pitch arrangement:

$$d_e = \frac{4 \left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi \frac{d_o^2}{4} \right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2)$$

Reynolds number are calculated as:

$$Re = \frac{G_s d_e}{\mu}$$

Then, shell side heat transfer area factor, j_h can be obtained from figure 12.29 C&R 3rd edition

Baffle spacing, l_B	m	0.055492123	choose 0.3
Tube pitch, p_t	m	0.0375	
Cross-flow area, A_s	m ²	0.003079376	
Shell-side mass velocity, G_s	kg/s.m ²	127.9326771	
Shell-side linear velocity, u_s	m/s	0.184553249	
Equilateral diameter, d_e	m	0.004279688	
Reynolds number, Re		3.14E+03	
Prandtl number, Pr		0.006408535	
Shell-side heat-transfer factors, j_h		0.01	Baffle cut 25%
Shell-side heat transfer coefficient, h_s	W/m ² .°C	1.43E+02	without viscosity correction to

STEP 11: OVERALL COEFFICIENT

The equation for overall heat coefficient (equation 12.2 C&R 3rd edition);

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln \left(\frac{d_o}{d_i} \right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (12.2)$$

where U_o = the overall coefficient based on the outside area of the tube, W/m².°C,

h_o = outside fluid film coefficient, W/m².°C,

h_i = inside fluid film coefficient, W/m².°C,

h_{od} = outside dirt coefficient (fouling factor), W/m².°C,

h_{id} = inside dirt coefficient, W/m².°C,

k_w = thermal conductivity of the tube wall material, W/m.°C,

d_i = tube inside diameter, m,

d_o = tube outside diameter, m.

Outside dirt/fouling coefficient, h_{od} and inside dirt/fouling coefficient, h_{id} can be obtained from Table 12.2 C&R 3rd edition while thermal conductivity tube wall material is referred to Table 12 A-2

Table 12.2. Fouling factors (coefficients), typical values

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

Table A-2 | Property values for metals.[†]

Metal	Properties at 20°C				Thermal conductivity k , W/m · °C									
	ρ kg/m ³	c_p kJ/kg · °C	k W/m · °C	$\alpha \times 10^5$ m ² /s	-100°C -148°F	0°C 32°F	100°C 212°F	200°C 392°F	300°C 572°F	400°C 752°F	600°C 1112°F	800°C 1472°F	1000°C 1832°F	
Aluminum:														
Pure	2,707	0.896	204	8.418	215	202	206	215	228	249				
Al-Cu (Dumilumin), 94–96% Al, 3–5% Cu, trace Mg	2,787	0.883	164	6.676	126	159	182	194						
Al-Si (Silumin, copper-bearing), 86.5% Al, 1% Cu, 1% Si	2,659	0.867	137	5.933	119	137	144	152	161					
Al-Si (Alusil), 78–80% Al, 20–22% Si	2,627	0.854	161	7.172	144	157	168	175	178					
Al-Mg-Si, 97% Al, 1% Mg, 1% Si, 1% Mn	2,707	0.892	177	7.311	175	189	204							
Lead	11,373	0.130	35	2.343	36.9	35.1	33.4	31.5	29.8					
Iron:														
Pure	7,897	0.452	73	2.034	87	73	67	62	55	48	40	36	35	
Wrought iron, 0.5% C	7,849	0.46	59	1.626		59	57	52	48	45	40	33	33	
Steel (C max ≈ 1.5%):														
Carbon steel														
C ≈ 0.5%	7,833	0.465	54	1.474		55	52	48	45	42	35	31	29	
1.0%	7,801	0.473	43	1.172		43	43	42	40	36	33	29	28	
1.5%	7,753	0.486	36	0.970		36	36	36	35	33	31	28	28	

outside fluid film coefficient, h_o	W/m ² .°C	143.2605549		
outside dirt/fouling coefficient, h_{od}	W/m ² .°C	5000	(organic liquid)	
inside fluid film coefficient, h_i	W/m ² .°C	123.6091443		
inside dirt/fouling coefficient, h_{id}	W/m ² .°C	5000	steam condensate	table 12.2
thermal conductivity tube wall material, k_w	W/m ² .°C	54	Carbon steel 0.5%	table A-2
overall coefficient based on the outside area of tube, h_{oi}	W/m ² .°C	59.57543376		
Error	%	19.15086752	below 30%, design can be accepted	

STEP 12: PRESSURE DROP

Friction factor, j_f tube side is obtained from Figure 12.24 C&R 3rd edition while for shell side is referred to Figure 12.30 C&R 3rd edition. It is assumed that baffle cut is 25%.

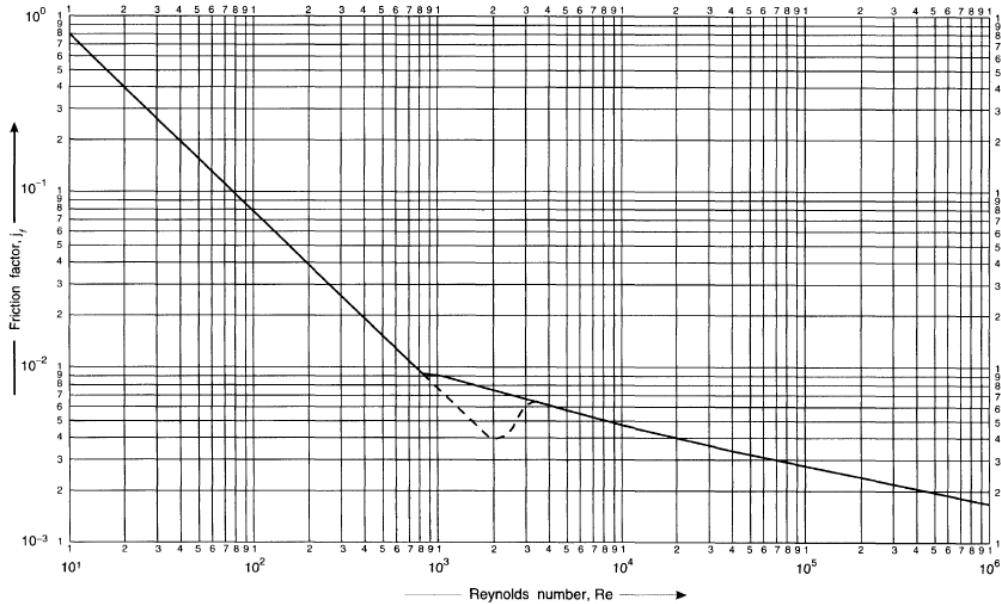


Figure 12.24. Tube-side friction factors

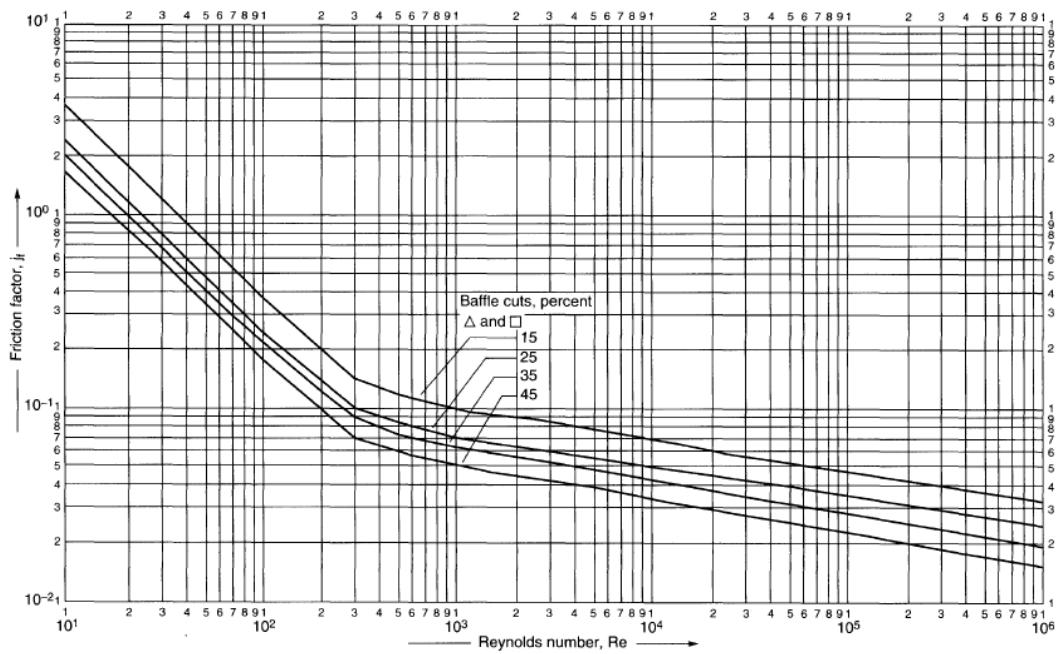


Figure 12.30. Shell-side friction factors, segmental baffles

The equations for tube side pressure drop, ΔP_t and shell side pressure drop, ΔP_s are;

$$\Delta P_t = N_p \left[8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2}$$

$$\Delta P_s = 8 j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14}$$

Tube side		
Reynolds number, Re		2.11E+05
Friction factor, j_f		0.0025
Tube side pressure drop, ΔP_t	kg/m ² bar	815704.3397 79.99328633
Shell side		
Reynolds number, Re		3.14E+03
Friction factor, j_f		0.06
Tube side pressure drop, ΔP_s	kg/m ² bar	48460.00483 4.752304056

Figure 12.24

Figure 12.30

MECHANICAL DESIGN

STEP 1: DESIGN PRESSURE AND TEMPERATURE

The design pressure should be 5 - 10% above operating pressure

Tube		
Operating pressure, P_o	40 bar	4000000 Pa
Design pressure, P_d	44 bar	4400000 Pa
Shell (steam)		
Operating pressure, P_o	2.8 bar	280000 Pa
Design pressure, P_d	3.08 bar	308000 Pa

The maximum normal operating temperature should have additional 25°C

Tube		
Inlet temperature, T_i	723.15 K	
Outlet temperature, T_o	523.45 K	
Design temperature, T_d	548.45 K	
Shell		
Inlet temperature	502.6792 K	
Outlet temperature	502.6792 K	
Design temperature, T_d	527.6792 K	

STEP 2: MATERIAL OF CONSTRUCTION

For carbon steel, the minimum and maximum allowable stress can be obtained by plotting data Table 13.2 C&R 3rd edition design stress

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

minimum allowable stress	360 N/mm ²	360000000 N/m ²
max allowable for tube, f	93.199 N/mm ²	93199000 N/m ²
max allowable for shell, f	96.730036 N/mm ²	96730036 N/m ²

STEP 3: SHELL WALL DESIGN

The minimum corrosion allowance is 0.002m while the minimum wall thickness for both shell and tube can be calculated by using equation 13.40b C&R 3rd edition.

$$e = \frac{P_i D_i}{4J_f - 1.2P_i} \quad (13.40b)$$

Then, the maximum allowable working pressure can be calculated by using equation below

For tube $MAWP = \frac{2 \times \text{tensile strength} \times E \times t}{D_i + t}$

Design pressure, Pd	$D_i + t$	4400000.0000 Pa
Design temperature, Td		548.4500 K
Tube inner diameter, d _i		0.0260 m
Tube outer diameter, d _o		0.0300 m
Wall thickness		0.0020 m
Minimum wall thickness, e		0.0004 m
Corrosion allowance		0.0020 m
Fabrication wall thickness, tt		0.0024 m
design tube outer diameter, d _o		0.0307 m
MAWP		51069316.25 N/m ²
		510.6931625 bar

The design can be accepted as the MAWP is greater than the operating pressure

For shell,

Design pressure, Pd	308000	Pa
Design temperature, Td	527.6792	K
Shell inner diameter, d _i	0.277460615	m
Minimum wall thickness, e	0.000260136	m
Corrosion allowance	0.002	m
Fabrication wall thickness, t _s	0.002260136	m
design shell outer diameter, d _o	0.281980886	m
MAWP	4944942.806	N/m ²
	49.44942806	bar

The design can be accepted as the MAWP is greater than the operating pressure

STEP 4: HEAD AND CLOSURE

Torispherical head is used as it can withstand high pressure up to 15 bar and commonly used in industry. The equation for minimum wall thickness torispherical head is;

$$e = \frac{P_i R_c C_s}{2fJ + P_i(C_s - 0.2)} \quad (13.44)$$

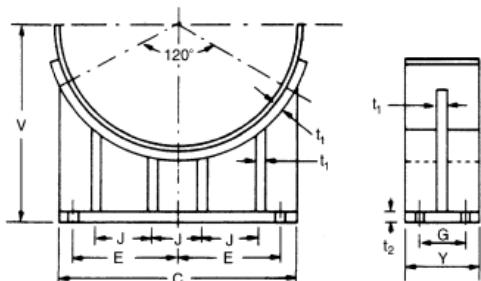
where C_s = stress concentration factor for torispherical heads = $\frac{1}{4}(3 + \sqrt{R_c/R_k})$,

R_c = crown radius,

R_k = knuckle radius.

Crown radiusm, R_c	0.277460615	m
knuckle radius, R_k	0.016647637	m
Joint efficiency, E	1	
Design pressure, P_d	308000	Pa
Minimum wall thickness	0.312685656	m
Corrosion allowance	0.002	m
Head wall thickness, t_h	0.314685656	m
External diameter	0.906831927	
MAWP	382631257.8	N/m ²
	3826.312578	bar

STEP 5: VESSEL SUPPORT



Vessel diam. (m)	Maximum weight (kN)	Dimensions (m)						mm			
		V	Y	C	E	J	G	t_2	t_1	Bolt diam.	Bolt holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

All contacting edges fillet welded

(a)

Figure 13.26. Standard steel saddles (adapted from Bhattacharyya, 1976). (a) for vessels up to 1.2 m

Saddle support had been chosen as the best type or support for horizontal vessel. The dimension of saddle support is related to the dead weight of vessel. Saddle support at 0.6m diameter is used for this heat exchanger.

STEP 6: NOZZLE DIAMETER

The volumetric flow rate is calculated by dividing mass flow rate with density of fluid.

Tube inlet nozzle diameter		
Vol.flow rate, Q	0.128330817	m3/s
Min cross section area	0.010115304	m2
Min diamter	0.113486587	m
Operate nozzle diameter	0.226973174	m
Tube outlet nozzle diameter		
Vol.flow rate, Q	0.092891711	m3/s
Min cross section area	0.00732192	m2
Min diamter	0.096553392	m
Operate nozzle diameter	0.193106785	m
Shell inlet nozzle diameter		
Vol.flow rate, Q	0.000572014	m3/s
Min cross section area	0.003099453	m2
Min diamter	0.062819951	m
Operate nozzle diameter	0.125639902	m
Shell outlet 1 nozzle diameter		
Vol.flow rate, Q	0.04386647	m3/s
Min cross section area	0.237690045	m2
Min diamter	0.550123954	m
Operate nozzle diameter	1.100247907	m
Shell outlet 2 nozzle diameter		
Vol.flow rate, Q	1.006519947	m3/s
Min cross section area	0.0070258	m2
Min diamter	0.09458079	m
Operate nozzle diameter	0.18916158	m

APPENDIX H
REACTOR DESIGN

R-101, Packed-Bed Reactor

Design Criteria

Type of reactor: Packed bed reactor with cooling jacket

Orientation: Vertical

Material of construction: Stainless steel 304

Operating temperature: 182.4655°C

Operating pressure: 40 bar

Benzene/Ethylene feed ratio: 3

Ethylene conversion: 0.9995

Selectivity towards ethylbenzene production: 0.92

Selectivity towards diethylbenzene production: 0.08

WHSV: 5-135 h⁻¹

Catalyst type: MWW MCM-22 zeolite

Bulk density: 892.89kg/m³

Effective particle size of the catalyst, D_p: 0.005m

Void fraction, ε: 0.48

Reaction Kinetics and design equation

Reaction kinetics applied in determining the weight of catalyst are show as follows:

Let benzene, ethylene, ethylbenzene and diethylbenzene be a,b,c, and d respectively



$$r_1 = k_1 C_b C_e$$

$$k_1 = 1.528E + 06 \exp \frac{-7.113E + 04}{RT}$$

$$r_2 = k_2 C_{eb} C_e$$

$$k_2 = 2.778E + 07 \exp \frac{-8.368E + 04}{RT}$$

Design Equation:

$$\frac{dW}{dX_e} = -\frac{F_{eo}}{r_e}$$

Nomenclature

F = molar flow rate, kmol/hr

F_o = initial molar flow rate, kmol/hr
 C = molar concentration, kmol/m³
 C_0 = initial molar concentration, kmol/m³
 W = mass of catalyst, kg
 X = conversion
 R = universal gas constant, J/mol.K
 r_i = rate of the i th reaction, kmol/m³.hr
 T = temperature, K

Subscripts

a = Benzene
 b = Ethylene
 c = Ethylbenzene

Step 1: Weight of Catalyst

Design assumptions:

- The system is to be operated under isobaric and isothermal condition.
- The initial concentration of ethylene and ethylbenzene which need to be specified in Polymath is calculated beforehand in which the initial concentration of each component is obtained by dividing its molar flow rate by total volumetric flow rate.
- Molar and mass flow rate data extracted at the inlet stream of the reactor (Stream 9).

Table: Information of inlet stream of reactor R-101.

Reactor Inlet					
Stream	S-9				
Pressure (bar)	40				
Temperature (K)	455.6155				
Components	Molar flow rate (kmol/hr)	Mass flow rate (kg/hr)	Density (kg/m ³)	Volumetric flow rate (m ³ /hr)	Initial Concentration, C_0 (kmol/m ³)
Benzene	345.4664	26987.8326	685.0238813	39.3969223	6.326100042
Ethylene	115.1555	3230.1105	212.617	15.1921555	2.108700014
Ethylbenzene	0.0576	6.1160	710.1108001	0.00861277	0.001054866
Diethylbenzene	0.0000	0.0000	718.3159557	0	0
Methane	0.0311	0.4987	161.745	0.00308334	0.000569349
Ethane	0.0610	1.8352	205.817	0.00891687	0.001117611
Total	460.7716	30226.3931		54.6096908	8.437541882

Table: Information of outlet stream of reactor R-101.

Reactor Outlet				
Stream	S-10			
Pressure (bar)	40			
Temperature (K)	473.15			
Molar Flow rate (kmol/hr)	Mass Flow Rate (kg/hr)	Density (kg/m ³)	Volumetric flow rate (m ³ /hr)	Final concentration, C (kmol/m ³)
239.5763	18715.7021	657.4016667	28.46920387	5.306209479
0.0576	1.6151	212.617	0.007596078	0.001275249
96.7398	10270.8671	689.4763333	14.89662016	2.142623149
9.2078	1235.8750	700.3073333	1.764760864	0.203937836
0.0311	0.4987	161.745	0.003083343	0.000688635
0.0610	1.8352	205.817	0.008916873	0.001351764
345.6737	30226.3931		45.15018119	7.656086111

Polymath coding:

#a=benzene

#b=ethylene

#c=ethylbenzene

Mole Balance for the PBR

d(W) / d(Xb) = 1/(-r/Fbo)

W(0)=0

Xb(0)=0

Xb(f)=0.9995

r=-r1+(-r2)

Rate of reaction and Rate constant

r1=k1*Ca*Cb

k1=1.528E+06*exp((-7.113E+04)/(R*T))

r2=k2*Cc*Cb

k2=2.778E+07*exp((-8.368E+04)/(R*T))

Initial Molar Flows and Concentration

Fbo=115.1555

Fco=0.0576

Fao=345.4664

Cbo=2.046651444

Cco=0.001023826

Cao=6.139954331

Operating Temperature and Gas Constant Value

T=473.15

R=8.314

Concentration

Cb=Cbo*(1-Xb)

$$Cc = Cco + 0.92 * Cbo * Xb - 0.08 * Cbo * Xb$$

$$Ca = 5.306209479$$

Table 1: Calculated weight of catalyst from polymath.

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	5.306209	5.306209	5.306209	5.306209
2	Cao	6.139954	6.139954	6.139954	6.139954
3	Cb	2.046651	0.0010233	2.046651	0.0010233
4	Cbo	2.046651	2.046651	2.046651	2.046651
5	Cc	0.0010238	0.0010238	1.70135	1.70135
6	Cco	0.0010238	0.0010238	0.0010238	0.0010238
7	Fao	345.4664	345.4664	345.4664	345.4664
8	Fbo	115.1555	115.1555	115.1555	115.1555
9	Fco	0.0576	0.0576	0.0576	0.0576
10	k1	0.0214415	0.0214415	0.0214415	0.0214415
11	k2	0.0160444	0.0160444	0.0160444	0.0160444
12	R	8.314	8.314	8.314	8.314
13	r	-0.232888	-0.232888	-0.0001444	-0.0001444
14	r1	0.2328544	0.0001164	0.2328544	0.0001164
15	r2	3.362E-05	2.793E-05	0.0139815	2.793E-05
16	T	473.15	473.15	473.15	473.15
17	W	0	0	3116.987	3116.987
18	Xb	0	0	0.9995	0.9995

From Polymath, the weight of catalyst required is calculated to be 3116.987 kg with the specified conversion and selectivity.

Step 2: Reactor bed sizing

The size of reactor depends on the weight of catalyst.

$$\text{Volume of catalyst bed, } V = \frac{\text{Mass of catalyst}}{\rho_c(1 - \varepsilon)} = \frac{3116.987}{892.89(1 - 0.48)} = 7.22 \text{ m}^3$$

Separating catalyst bed into 2 stages,

$$\text{Volume of each catalyst bed, } V_{bed} = \frac{7.22}{2} = 3.61 \text{ m}^3$$

Let reactor cross sectional area, $A_c = 1.50 \text{ m}^2$

$$\text{Internal diameter, } D_i = \sqrt{\frac{4 A_c}{\pi}} = \sqrt{\frac{4(1.5)}{\pi}} = 1.38 \text{ m}$$

$$\text{Length of each catalyst bed, } L_{bed} = \frac{3.61}{1.50} = 2.41 \text{ m}$$

For catalytic fixed bed reactor, 0.3 m of quench zone and 0.15 m of support grid to prevent catalyst migration downstream while minimizing possible pressure drop of the reacting fluid passing through the reactor vessel are included.

$$\begin{aligned} \text{Functional height of the reactor, } L &= L_{bed} + L_{quench} + L_{support} \\ &= (2.41 \times 2) + (0.3 \times 3) + (0.15 \times 4) \\ &= 6.02 \text{ m} \end{aligned}$$

Step 3: Cooling requirement Design

Cooling system is required for the reactor as the reaction that takes place in the reactor is exothermic reaction. Cooling water operating from 30°C to 40°C is used as the utility in

reactor shell side.

Properties of cooling water at average temperature (calculated using www.engineeringtoolbox.com):

Average temperature = 35°C = 308.15 K

Density, $\rho = 994.06 \text{ kg/m}^3$

Viscosity, $\mu = 0.7198 \text{ cP} = 0.0007198 \text{ kg/m.s}$

Thermal Conductivity, $k = 0.62153 \text{ W/m.K}$

Specific heat capacity, $C_p = 4180 \text{ J/kg.K}$

From energy balance calculation, the cooling duty required is 7028.01371 MJ/hr

Temperature of reactor wall, $T_w = 200^\circ\text{C} = 473.15 \text{ K}$

Temperature of surrounding, $T_\infty = 35^\circ\text{C} = 308.15 \text{ K}$

For a vessel type reactor, cooling jacket length is typically 80% of reactor bed length.

$$L_{jacket} = 0.80 \times 6.02 = 4.81 \text{ m}$$

$$\text{Heat transfer area, } A = \frac{\pi D_o^2 L_{jacket}}{4} = \frac{\pi (1.44698)^2 (4.81)}{4} = 7.91 \text{ m}^2$$

$$Q = hA(T_w - T_\infty)$$

$$h = \frac{7028.01371 \times 10^6}{3600 \times 7.91 \times (473.15 - 308.15)} = 1495.16 \text{ W/m}^2 \cdot \text{K}$$

The heat transfer system represents a cross flow system across a tube in which the correlation of heat transfer is given as such: $Nu = C(Re)^n Pr^{1/3}$

$$Nu = \frac{hD_o}{k} = \frac{(1151.35)(1.44698)}{0.62} = 3480.87$$

$$Pr = \frac{\mu C_p}{k} = \frac{(0.0007198)(4180)}{0.62} = 4.84$$

For large Nu value, the Re is expected to be large. From Heat Transfer by J. P. Holman, for high Re, $C = 0.0266$, $n = 0.805$

$$Re = \sqrt[0.805]{\frac{3480.87}{4.84^{1/3} \times 0.0266}} = 1182136.38$$

$$Re = \frac{\rho u D_o}{\mu}$$

$$u = \frac{Re \mu}{\rho D_o} = \frac{(1190071.76)(0.0007198)}{(994.06)(1.44698)} = 0.59 \text{ m/s}$$

$$\text{Amount of cooling water required, } m = \frac{Q}{C_p(T_{out} - T_{in})}$$

$$= \frac{7028.01371 \times 10^6}{3600 \times 4180 \times (313.15 - 303.15)} = 46.70 \text{ kg/s}$$

$$\text{Volumetric flow rate of cooling water, } V_{H2O} = \frac{m}{\rho} = \frac{46.70}{994.06} = 0.0470 \text{ m}^3/\text{s}$$

$$\text{Cross sectional area for cooling water flow, } A_w = \frac{V_{H2O}}{u} = \frac{0.0470}{0.59} \times 10 = 0.7942 \text{ m}^2$$

*Extra 10 times for the cross-sectional area for water flow

$$A_w = \frac{\pi(D_t^2 - D_o^2)}{4}$$

$$D_t = \sqrt{\frac{0.7942 \times 4}{\pi}} + 1.44698^2 = 1.48 \text{ m}$$

$$\text{Jacket thickness, } t_j = \frac{D_t - D_o}{2} = \frac{1.44698 - 1.48}{2} = 0.01727 \text{ m} = 17.27 \text{ mm}$$

Mechanical Design

Step 1: Design Pressure

According to Coulson Richardson's Chemical Engineering Design 4th edition (Chapter 13), safety factor of 10.0% is applied to the operating pressure of the reactor.

Tube (Reactor Vessel)

Operating pressure = 40 bar = 4.00 N/mm²

Design pressure, Pd = 1.10 x 4.00 = 4.40 N/mm²

Shell (Cooling Jacket)

Operating pressure = 1.01325 bar = 0.101325 N/mm²

Design pressure, Pd = 1.10 x 0.101325 = 0.11 N/mm²

Step 2: Design Temperature

Safety factor of 10°C above the operating temperature will be applied to the reactor design.

Tube (Reactor Vessel)

Design temperature, Td = Operating temperature + 10 °C

= 200 + 10

= 210 °C

Shell (Cooling Jacket)

Design temperature, Td = Operating temperature + 10 °C

= 45 + 10

= 55 °C

Step 3: Material of construction

The material of construction for the packed bed reactor is stainless steel type 304. Based on table 13.2 in Coulson and Richardson's Chemical Engineering Design 4th edition, design stress, f of stainless steel type 304 is 115 N/mm² at temperature of 200°C which is higher than the reactor design pressure (4.40 N/mm²). Stainless steel type 304 also has good tensile strength of 510 N/mm². This makes it suitable to be used as the material of construction for high operating temperature and pressure reactor.

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Step 4: Welded joint efficiency

A double-welded butt type of welding is used for the reactor in order to balance the trade-off between the higher cost and higher strength of weld joint. As shown in table 13.3 in Coulson and Richardson's Chemical Engineering Design 4th edition, the welded joint efficiency, J of the double welded butt type of welding is 0.85.

Table 13.3. Maximum allowable joint efficiency

Type of joint	Degree of radiography		
	100 per cent	spot	none
Double-welded butt or equivalent	1.0	0.85	0.7
Single-weld butt joint with bonding strips	0.9	0.80	0.65

Step 5: Wall Thickness

The minimum wall thickness is calculated based on Coulson and Richardson's Chemical Engineering Design 4th edition.

Reactor tube

$$\begin{aligned}
 e &= \frac{P_d D_i}{2Jf - P_d} \\
 &= \frac{4.40(1.38)(1000)}{2(0.85)(115) - 4.40}
 \end{aligned}$$

With the following useful data, the minimum wall thickness obtained is **31.82 mm**.

Design pressure, P _d	N/mm ²	4.40
---------------------------------	-------------------	------

Design temperature, T_d	$^{\circ}\text{C}$	190
Vessel inner diameter, D_i	m	1.4273
Maximum allowable stress, f	N/mm^2	121
Welded joint efficiency, J	-	0.85
Corrosion allowance	mm	2
Tensile strength of Stainless Steel Type 304	N/mm^2	510

The fabrication wall thickness, t is the addition of minimum wall thickness, e and corrosion allowance (2 mm) which is **33.82 mm**. Besides, the outer diameter of vessel obtained is **1.4496 m**.

The maximum allowable working pressure, MAWP for the vessel is calculated as below:

$$\begin{aligned} \text{MAWP} &= \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.03182}{1.38 + 0.03182} \\ &= 20.71 \text{ N/mm}^2 \end{aligned}$$

Since the MAWP is greater than the operating pressure of 4.0 N/mm^2 , thus the thickness of the reactor wall is acceptable.

Cooling Jacket

$$\begin{aligned} t &= \frac{P_a D_i}{2Jf - P_a} \\ &= \frac{0.11(1.45)(1000)}{2(0.85)(165.00) - 0.11} \\ &= 0.58 \text{ mm} \end{aligned}$$

With the following useful data, the minimum wall thickness obtained is **0.58 mm**.

Design pressure, P_d	N/mm^2	0.11
Design temperature, T_d	$^{\circ}\text{C}$	90
Vessel inner diameter, D_i	m	1.45
Maximum allowable stress, f	N/mm^2	1.54
Welded joint efficiency, J	-	0.85
Corrosion allowance	mm	2
Tensile strength of Stainless Steel Type 304	N/mm^2	510

The fabrication wall thickness, t is the addition of minimum wall thickness, e and corrosion allowance (2 mm) which is **2.58 mm**. Besides, the outer diameter of vessel obtained is **1.4496 m**.

The maximum allowable working pressure, MAWP for the vessel is calculated as below:

$$\text{MAWP} = \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.00258}{1.45 + 0.00258} = 1.54 \text{ N/mm}^2$$

Since the MAWP is greater than the operating pressure of 0.11 N/mm^2 , the thickness of the cooling jacket wall is acceptable.

Step 6: Reactor Vessel Head Design

Hemispherical head is chosen as the type of head for the reactor due to the high pressure of the reactor. According to Coulson and Richardson's Chemical Engineering Design 4th edition, the head thickness for hemispherical head is 0.6 times of the reactor wall thickness.

$$\text{Head thickness} = 0.6t = 0.6(33.82) = 20.29 \text{ mm}$$

$$\text{Corrosion allowance} = 2.00 \text{ mm}$$

$$\text{Fabrication thickness of vessel head} = 20.29 + 2 = 22.29 \text{ mm}$$

$$MAWP = \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.01953}{1.4273 + 0.01953}$$

$$= 13.76 \text{ N/mm}^2$$

Since the MAWP is greater than the reactor operating pressure (4.0 N/mm²), thus the thickness of the reactor head is acceptable.

Step 7: L/D ratio of reactor

$$\text{Functional height of reactor, } L = 6.02 \text{ m}$$

$$\text{Length of head, } L_H = D_i/2 = 1.38/2 = 0.6910 \text{ m}$$

$$\text{Total length of reactor, } L_T = 6.02 + (0.6910 \times 2) = 6.7063 \text{ m}$$

$$\text{Reactor shell outer diameter, } D_o = D_i + 2 \times t = 1.38 + 2 \times 0.0338 = 1.4496 \text{ m}$$

$$L_T / D = 6.7063 / 1.4496 = 4.63$$

Since L_T / D ratio is in between 2 to 5, thus the reactor size is acceptable.

Step 8: Total weight of reactor

The weight of vessel is calculated based on Coulson and Richardson's Chemical Engineering Design.

Let factor account for the weight of nozzle, $C_v = 1.15$,

Reactor tube

$$\text{Mean diameter of vessel, } D_m = D_i + t = 1.38 + (33.82/1000) = 1.42 \text{ m}$$

$$\text{Weight of vessel, } W_v = 240 C_v D_m (H_v + 0.8D_m) t$$

$$= 240 (1.15)(1.42)[6.0153 + 0.8(1.42)](0.03382)$$

$$= 94.46 \text{ kN}$$

Cooling jacket

$$\text{Mean diameter of vessel, } D_m = D_i + t_t = (1485 + 2.65)/1000 = 1.488 \text{ m}$$

$$\text{Weight of shell, } W_s = 240 C_v D_m (H_v + 0.8D_m) t_t$$

$$= 240 (1.15)(1.45)[4.81 + 0.8(1.45)](0.00258)$$

$$= 6.17 \text{ kN}$$

$$\text{Weight of catalyst, } W = (3116.987 \times 9.81)/1000 = 30.58 \text{ kN}$$

$$\text{Total weight of reactor, } W_R = W_v + W_s + W = 94.46 + 6.17 + 30.58 = 131.208 \text{ kN}$$

Step 9: Stress Analysis

Stress analysis is conducted based on Coulson and Richardson's Chemical Engineering Design to ensure the reactor structure is strong and safe against stresses.

For wind loading,

Let wind speed, $u_w = 160 \text{ km/hr}$

Wind pressure, $P_w = 0.05 u_w^2 = 0.05(160)^2 = 1280 \text{ N/m}^2$

Wind loading per unit length of column, $F_w = P_w D_o = 1280 (1.4496) = 1855.51 \text{ N/m}$

Bending moment at bottom tangent line, $M_x = \frac{F_w L_T^2}{2} = \frac{(1855.51)(6.7063)^2}{2} = 41724.60 \text{ Nm}$

Longitudinal stress, $\sigma_L = \frac{P_d D_i}{4t} = \frac{4.40 \times 1380}{4 \times 33.82} = 44.95 \text{ N/mm}^2$

Circumferential stress, $\sigma_h = \frac{P_d D_i}{2t} = \frac{4.40 \times 1380}{2 \times 33.82} = 89.90 \text{ N/mm}^2$

Dead weight stress, $\sigma_w = \frac{W_R}{\pi(D_i + t)t} = \frac{131.208 \times 1000}{\pi(1380 + 33.82)(33.82)} = 0.87 \text{ N/mm}^2$

Second moment area of the vessel about the plane of bending, I_v

$$I_v = \frac{\pi}{64} (D_o^4 - D_i^4) = \frac{\pi}{64} (1449.62^4 - 1380^4) = 3.77 \times 10^{10} \text{ mm}^4$$

$$\text{Bending stress, } \sigma_b = \pm \frac{M_x}{I_v} \left(\frac{D_i}{2} + t \right) = \pm \frac{41724.60 \times 1000}{3.77 \times 10^{10}} \left(\frac{1380}{2} + 33.82 \right) = \pm 0.80 \text{ N/mm}^2$$

Total longitudinal stress, $\sigma_z = \sigma_L + \sigma_w \pm \sigma_b$

Since σ_w is compressive, therefore σ_w is negative value.

$$\sigma_z(\text{upwind}) = 44.95 - 0.87 + 0.80 = 44.88 \text{ N/mm}^2$$

$$\sigma_z(\text{downwind}) = 44.95 - 0.87 - 0.80 = 43.28 \text{ N/mm}^2$$

No torsional shear stress is considered in preliminary design.

The 3 principal stresses and their differences are calculated under this condition.

Principal Stress (N/mm ²)	Upwind	Downwind
$\sigma_1 = \sigma_h$	89.90	89.90
$\sigma_2 = \sigma_z$	44.88	43.28
$\sigma_3 = 0.5P$	2.2	2.2
$\sigma_1 - \sigma_2$	45.02	46.62
$\sigma_1 - \sigma_3$	87.70	87.70
$\sigma_2 - \sigma_3$	42.68	41.08

From the calculation the greatest principal stress difference is 87.70 N/mm^2 . This does not exceed the design stress for the material construction of the reactor which is 115 N/mm^2 . Thus, the design is acceptable.

$$\text{Critical buckling stress, } \sigma_c = 2 \times 10^4 \left(\frac{t}{D_o} \right) = 2 \times 10^4 \left(\frac{33.82}{1449.62} \right) = 466.60 \text{ N/mm}^2$$

Maximum compressive where the vessel is not under pressure = $\sigma_w + \sigma_b = 0.87 + 0.80 = 1.67 \text{ N/mm}^2$.

As the maximum allowable design stress is smaller than critical buckling stress, the design is satisfactory.

Step 10: Vessel Support

Type of support chosen: Conical skirt

Let skirt bottom diameter, $D_s = 1.8 \text{ m}$

Let skirt height, $H_s = 2.0 \text{ m}$

$$\text{Skirt base angle, } \theta_s = \tan^{-1} \frac{D_s}{0.5 \times (D_s - D_i)} = \tan^{-1} \frac{1.8}{0.5 \times (1.8 - 1.38)} = 83.38^\circ$$

The skirt base angle is satisfactory as the angle is in between 80° and 90° .

The maximum dead weight load on the skirt will occur when the vessel is full of water.

$$\begin{aligned} \text{Approximate water weight, } W_w &= \left(\frac{\pi}{4} \times D_i^2 \times L_T \right) \times 1000 \times 9.81 \\ &= \left(\frac{\pi}{4} \times 1.38^2 \times 6.7063 \right) \times 9.81 = 98.68 \text{ kN} \end{aligned}$$

Taking skirt thickness, t_s same as thickness of vessel (33.82 mm),

$$\text{Bending moment at bottom of skirt, } M_s = \frac{F_w(L_T + H_s)^2}{2} = \frac{1855.51(6.7063+2)^2}{2} = 70322.62 \text{ Nm}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \frac{4M_s}{\pi(D_s + t_s)D_s t_s} = \frac{4 \times 70322.62 \times 1000}{\pi(1800 + 33.82)(1800 \times 33.82)} = 0.80 \text{ N/mm}^2$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(test)} = \frac{W_w}{\pi(D_s + t_s)t_s} = \frac{98.68 \times 1000}{\pi(1800 + 33.82)(33.82)} = 0.51 \text{ N/mm}^2$$

$$\sigma_{ws(operating)} = \frac{W}{\pi(D_s + t_s)t_s} = \frac{131.208 \times 1000}{\pi(1800 + 33.82)(33.82)} = 0.67 \text{ N/mm}^2$$

$$\sigma_s(\text{compressive}) = \sigma_{bs} + \sigma_{ws(operating)} = 0.80 + 0.51 = 1.31 \text{ N/mm}^2$$

$$\sigma_s(\text{tensile}) = \sigma_{bs} - \sigma_{ws(test)} = 0.80 - 0.67 = 0.13 \text{ N/mm}^2$$

The skirt thickness should be such that under the worst combination of wind and dead weight loading. 2 design criteria must be satisfied:

$$\sigma_s(\text{tensile}) < f_s J \sin \theta_s$$

$$\sigma_s(\text{compressive}) < 0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta_s$$

The skirt material is chosen to be stainless steel 304 with maximum allowable design stress at ambient temperature is $f_s = 165 \text{ N/mm}^2$. The Young modulus, E of stainless steel type 304 is 193000 MPa.

$$\begin{aligned} f_s J \sin \theta_s &= 165 \times 0.85 \times \sin(83.38) = 139.17 \text{ N/mm}^2 \\ 0.13 \text{ N/mm}^2 &< 139.50 \text{ N/mm}^2 \text{ [Satisfy]} \end{aligned}$$

$$0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta_s = 0.125 \times 193000 \left(\frac{33.82}{1800} \right) \sin(83.38) = 449.77 \text{ N/mm}^2$$

$$1.31 \text{ N/mm}^2 < 449.77 \text{ N/mm}^2 \text{ [Satisfy]}$$

Since both design criteria are satisfied, the skirt thickness is acceptable.

Step 11: Base ring and anchor bolt design

Take pitch circle diameter, $D_b = 0.62 \text{ m}$

Circumference of bolt circle = $620 \times \pi = 1947.79$ mm

Bolt spacing is taken at 250 mm for conical skirt

$$\text{Number of bolts required, } N_b = \frac{1947.79}{250} = 7.79 \approx 8 \text{ bolts}$$

$$\text{Maximum allowable bolt stress, } f_b = 125 \text{ N/mm}^2$$

$$\begin{aligned} \text{Area of bolt, } A_b &= \frac{1}{N_b f_b} \left[\frac{4M_s}{D_b} - W \right] = \frac{1}{8(125)} \left[\frac{4(70322.62)}{0.62} - 131.21 \times 1000 \right] \\ &= 322.49 \text{ mm}^2 \end{aligned}$$

$$\text{Diameter of bolt} = \sqrt{\frac{A_b \times 4}{\pi}} = \sqrt{\frac{322.49 \times 4}{\pi}} = 20.26 \text{ mm}$$

From Coulson & Richardson's Chemical Engineering Design Figure 13.30, the bolt type selected is M30 as it is the closest standard size bolt larger than 21.99 mm. Its root area is 561 mm².

$$\begin{aligned} \text{Total compressive load on base ring, } F_b &= \frac{4M_s}{\pi D_s^2} + \frac{W}{\pi D_s} \\ &= \frac{4(70322.62)}{\pi(1.8)^2} + \frac{131.21 \times 1000}{\pi(1.8)} = 50837.65 \text{ N/m} \end{aligned}$$

Maximum allowable bearing pressure on concrete foundation pad, $f_c = 7 \text{ N/mm}^2$

$$\text{Minimum width base ring, } L_b = \frac{F_b}{f_c} \times \frac{1}{10^3} = \frac{50837.65}{7} \times \frac{1}{1000} = 7.26 \text{ mm}$$

Using bolt M30 distance from skirt edge to ring edge, $L_r = 76$ mm

Actual base ring width = $L_r + t_s + 50 = 76 + 33.82 + 50 = 159.82$ mm

$$\text{Actual bearing pressure on concrete foundation pad, } f'_c = \frac{F_b}{\text{Actual base width}}$$

$$= \frac{50837.65}{159.82 \times 1000} = 0.32 \text{ N/mm}^2$$

Allowable design stress in the ring material, $f_r = 140 \text{ N/mm}^2$

$$\text{Minimum base ring thickness, } t_b = L_r \sqrt{\frac{3f'_c}{f_r}} = 76 \sqrt{\frac{3(0.32)}{140}} = 6.27 \text{ mm}$$

Dimensions mm								
Bolt size	Root area	A	B	C	D	E	F	G
M24	353	45	76	64	13	19	30	36
M30	561	50	76	64	13	25	36	42
M36	817	57	102	76	16	32	42	48
M42	1120	60	102	76	16	32	48	54
M48	1470	67	127	89	19	38	54	60
M56	2030	75	150	102	25	45	60	66
M64	2680	83	152	102	25	50	70	76
70	—	89	178	127	32	64	76	83
76	—	95	178	127	32	64	83	89

Bolt size = Nominal dia. (BS 4190: 1967)

Figure 13.30. Anchor bolt chair design

Step 12: Nozzles design

Benzene Feed Inlet

Calculated according to the Harker equation (1978), modified for SI unit, for the optimum pipe (and nozzle) diameter.

W = Mass flow rate = 26987.8326 kg/hr

At Temperature = 182.4655°C, Pressure = 40 bar

$\rho = 657.40 \text{ kg/m}^3$

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{26987.8326^{0.45}}{657.40^{0.31}} = 110.99 \text{ mm} = 4.37 \text{ in}$$

By referring to ASME B36.19, the 5 in. stainless steel Sch. 80 is used. (OD = 141.3mm, wall thickness = 9.53 mm)

Ethylene Feed Inlet

W = Mass flow rate = 3230.11 kg/hr

At Temperature = 182.4655°C, Pressure = 40 bar

$\rho = 212.62 \text{ kg/m}^3$

$$\text{Volumetric flow rate, } Q = \frac{W}{\rho} = \frac{3230.11}{212.62 \times 3600} = 0.0042 \text{ m}^3/\text{s}$$

$$\text{Minimum nozzle cross sectional area, } A = \frac{Q}{c} = \frac{0.0042}{440.48} = 9.58 \times 10^{-6} \text{ m}^2$$

$$\text{Minimum nozzle diameter} = \sqrt{\frac{4 \times A}{\pi}} = \sqrt{\frac{4 \times 9.58 \times 10^{-6}}{\pi}} \times 1000 = 3.49 \text{ mm} = 0.14 \text{ in}$$

By referring to ASME B36.19, the 0.25 in. stainless steel Sch. 80 is used. (OD = 13.7 mm, wall thickness = 3.03 mm)

Product Outlet

At Temperature = 200°C, Pressure = 40 bar

W = Mass flow rate = 30217.94 kg/hr

$\rho = 657.40 \text{ kg/m}^3$

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{30217.94^{0.45}}{657.40^{0.31}} = 116.79 \text{ mm} = 4.60 \text{ in}$$

By referring to B36.19, the 5 in. stainless steel Sch. 80 is used. (OD = 141.3mm, wall thickness = 9.53 mm)

Cooling Water Inlet

At Temperature = 30°C, Pressure = 1.01325 bar

W = Mass flow rate = 168134.30 kg/hr

$\rho = 995.67 \text{ kg/m}^3$

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{168134.30^{0.45}}{995.67^{0.31}} = 222.29 \text{ mm} = 8.75 \text{ in}$$

By referring to B36.19, the 10 in. stainless steel Sch. 80 is used. (OD = 273.1 mm, wall thickness = 12.70 mm)

Cooling Water Outlet

At Temperature = 80°C, Pressure = 1.01325 bar

W = Mass flow rate = 1688134.30 kg/hr

$\rho = 992.25 \text{ kg/m}^3$

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{1688134.30^{0.45}}{992.25^{0.31}} = 222.53 \text{ mm} = 8.76 \text{ in}$$

By referring to B36.19, the 10 in. stainless steel Sch. 80 is used. (OD = 273.1 mm, wall thickness = 12.70 mm)

H.1 R-301, Packed-Bed Reactor

Design Criteria

Type of reactor: Packed bed reactor with heating jacket

Orientation: Vertical

Material of construction: Stainless steel 304

Operating temperature: 229.5292°C

Operating pressure: 35 bar

Benzene/Ethylene feed ratio: 3

Diethylbenzene conversion: 0.9995

Selectivity towards ethylbenzene production: 1

Catalyst type: MWW MCM-22 zeolite

Bulk density: 720.00 kg/m³ [Ali, A. (2012). Liquid Phase Alkylation of Benzene with Ethylene. Retrieved from <https://ar.scribd.com/doc/106876722/Liquid-Phase-Alkylation-of-Benzene-with-Ethylene.>]

Effective particle size of the catalyst, D_p: 0.005m [Ng, Q. H., Sharma, S. and Rangaiah, G. P. (2017) ‘Design and analysis of an ethyl benzene production process using conventional distillation columns and dividing-wall column for multiple objectives’, *Chemical Engineering Research and Design*. Institution of Chemical Engineers, 118, pp. 142–157. doi: 10.1016/j.cherd.2016.10.046.]

Void fraction, ε: 0.48 [Ng, Q. H., Sharma, S. and Rangaiah, G. P. (2017) ‘Design and analysis of an ethyl benzene production process using conventional distillation columns and dividing-wall column for multiple objectives’, *Chemical Engineering Research and Design*. Institution of Chemical Engineers, 118, pp. 142–157. doi: 10.1016/j.cherd.2016.10.046.]

Reaction Kinetics and design equation

Reaction kinetics applied in determining the weight of catalyst are show as follows:

Let benzene, ethylene, ethylbenzene and diethylbenzene be a,b,c, and d respectively



$$r_3 = 1000 \exp \frac{-6.276E + 04}{RT} [d][a]$$

$$R = 8.314 \text{ J/mol.K} ; T (\text{K})$$

Design Equation:

$$\frac{dW}{dX_d} = -\frac{F_{do}}{r_d}$$

Nomenclature

F = molar flow rate, kmol/s

F_o = initial molar flow rate, kmol/s

C = molar concentration, kmol/m³

C_o = initial molar concentration, kmol/m³

W = mass of catalyst, kg

X = conversion

R = universal gas constant, J/mol.K

r_i = rate of the ith reaction, kmol/m³.s

T = temperature, K

Subscripts

a = Benzene

c = Ethylbenzene

d = Diethylbenzene

Step 1: Weight of Catalyst

Design assumptions:

- The system is to be operated under isobaric and isothermal condition.
- The initial concentration of ethylene and ethylbenzene which need to be specified in Polymath is calculated beforehand in which the initial concentration of each component is obtained by dividing its molar flow rate by total volumetric flow rate.
- Molar and mass flow rate data extracted at the inlet stream of the reactor (Stream 37).

Table: Information of inlet stream of reactor R-101.

Stream	Reactor Inlet				
	S-37				
Pressure (bar)		35			
Temperature (K)		489.1649			
Components	Molar Flow rate (kmol/hr)	Mass flow rate (kg/hr)	Density (kg/m ³)	Volumetric flow rate (m ³ /hr)	Initial Concentration, C _o (kmol/m ³)
Benzene	36.8313	2877.2621	629.9067	4.5678	5.7655
Ethylene	0.0092	0.2582	212.6170	0.0012	0.0014
Ethylbenzene	0.0655	6.9564	669.6685	0.0104	0.0103
Diethylbenzene	9.2078	1235.8747	683.2515	1.8088	1.4414
Methane	0.0000	0.0000	161.7450	0.0000	0.0000
Ethane	0.0000	0.0000	205.8170	0.0000	0.0000
Total	46.1139	4120.3514		6.3882	7.2186

Table: Information of outlet stream of reactor R-101.

<u>Reactor Outlet</u>	
Stream	S-38
Pressure (bar)	35
Temperature (K)	502.6792

Molar Flow rate (kmol/hr)	Mass Flow Rate (kg/hr)	Density (kg/m ³)	Volumetric flow rate (m ³ /hr)	Final concentration, C (kmol/m ³)
27.6281	2158.3062	603.9288	3.5738	4.1961
0.0092	0.2582	212.6170	0.0012	0.0014
18.4720	1961.1690	651.9229	3.0083	2.8055
0.0046	0.6179	668.2334	0.0009	0.0007
0.0000	0.0000	161.7450	0.0000	0.0000
0.0000	0.0000	205.8170	0.0000	0.0000
46.1139	4120.3514	2504.2642	6.5842	7.0037

Polymath coding:

#a=benzene

#d=diethylbenzene

#c=ethylbenzene

Mole Balance for the PFR

$$d(W) / d(X_d) = 1 / ((8.8215E-07) / F_{do})$$

$$W(0)=0$$

$$X_d(0)=0$$

$$X_d(f)=0.9995$$

Rate of reaction and Rate constant

$$r=(1000 * \exp(-6.276E+04 / R * T)) * C_d * C_a$$

Initial Molar Flows and Concentration

$$F_{do}=0.0025577$$

$$F_{co}=1.82994E-05$$

$$F_{ao}=0.01023092$$

$$C_{do}=1.441386294$$

$$C_{co}=0.010256674$$

$$C_{ao}=5.765545177$$

Operating Temperature and Gas Constant Value

$$T=502.6792$$

$$R=8.314$$

Concentration

$$C_d=C_{do}*(1-X_d)$$

$$C_c=C_{co}+1*C_{do}*X_d$$

$$C_a=4.19612$$

Table 1: Calculated weight of catalyst from polymath.

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	4.19612	4.19612	4.19612	4.19612
2	Cao	5.765545	5.765545	5.765545	5.765545
3	Cc	0.0102567	0.0102567	1.450922	1.450922
4	Cco	0.0102567	0.0102567	0.0102567	0.0102567
5	Cd	1.441386	0.0007207	1.441386	0.0007207
6	Cdo	1.441386	1.441386	1.441386	1.441386
7	Fao	0.0102309	0.0102309	0.0102309	0.0102309
8	Fco	1.83E-05	1.83E-05	1.83E-05	1.83E-05
9	Fdo	0.0025577	0.0025577	0.0025577	0.0025577
10	R	8.314	8.314	8.314	8.314
11	r	0	0	0	0
12	T	502.6792	502.6792	502.6792	502.6792
13	W	0	0	2897.944	2897.944
14	Xd	0	0	0.9995	0.9995

From Polymath, the weight of catalyst required is calculated to be 2897.944 kg with the specified conversion and selectivity.

Step 2: Reactor bed sizing

The size of reactor depends on the weight of catalyst.

$$\text{Volume of catalyst bed, } V = \frac{\text{Mass of catalyst}}{\rho_c(1 - \varepsilon)} = \frac{2897.944}{720(1 - 0.48)} = 7.74 \text{ m}^3$$

Separating catalyst bed into 2 stages,

$$\text{Volume of each catalyst bed, } V_{\text{bed}} = \frac{9.10}{2} = 3.87 \text{ m}^3$$

Let reactor cross sectional area, $A_c = 1.50 \text{ m}^2$

$$\text{Internal diameter, } D_i = \sqrt{\frac{4 A_c}{\pi}} = \sqrt{\frac{4(1.5)}{\pi}} = 1.38 \text{ m}$$

$$\text{Length of each catalyst bed, } L_{\text{bed}} = \frac{3.87}{1.50} = 2.58 \text{ m}$$

For catalytic fixed bed reactor, 0.3 m of quench zone and 0.15 m of support grid to prevent catalyst migration downstream while minimizing possible pressure drop of the reacting fluid passing through the reactor vessel are included

$$\begin{aligned} \text{Functional height of the reactor, } L &= L_{\text{bed}} + L_{\text{quench}} + L_{\text{support}} \\ &= (2.58 \times 2) + (0.3 \times 3) + (0.15 \times 4) \\ &= 6.36 \text{ m} \end{aligned}$$

Step 3: Heating Jacket Design

Steam circulates in the annular space between a steam jacket and the vessel walls and heat is transferred through the wall of the vessel. The diameter of the steam jacket is calculated using equations from Engineering Principles and Heat Transfer [Engineering Principles and Heat Transfer, Available at <https://www.spiraxsarco.com/learn-about-steam/steam-engineering-principles-and-heat-transfer/heating-with-coils-and-jackets> [Accessed 5 February 2022].

The minimum steam pressure in the heating jacket should be taken as 58% of upstream absolute pressure as critical pressure drop (CPD) will occur across the control valve during start-up [Engineering Principles and Heat Transfer, Available at <https://www.spiraxsarco.com/learn-about-steam/steam-engineering-principles-and-heat-transfer/heating-with-coils-and-jackets> [Accessed 5 February 2022]]..

Steam pressure = 40 bar g + 1 bar = 41 bar a

Minimum steam pressure = 41 bar a x 58% = 23.78 bar a = 22.78 bar g

Enthalpy of evaporation (h_{fg}) = 1862.64 kJ/kg (from steam table at 22.78 bar g)

Mean heat load = 533.38 MJ x 0.28 = 149.35 kW

Average steam flowrate = $\frac{149.35}{1862.64} = 0.08 \text{ kg/s} = 288.65 \text{ kg/h}$

Mean liquid temperature, $T_m = \frac{216.0149 + 229.5292}{2} = 222.77 \text{ }^\circ\text{C}$

Steam temperature in the jacket, $T_s = \frac{450 + 250}{2} = 350 \text{ }^\circ\text{C}$ (taking average of steam temperature in jacket)

$\Delta T_m = T_s - T_m = 350 - 222.77 = 127.23 \text{ }^\circ\text{C}$

Since $Q = UA \Delta T$, Heat transfer area, $A = \frac{149.35 \times 1000}{850 \times 127.23} = 1.38 \text{ m}^2$

Extra 10% heat transfer area is applied to allow for future fouling of the heat exchange surface [Engineering Principles and Heat Transfer, Available at <https://www.spiraxsarco.com/learn-about-steam/steam-engineering-principles-and-heat-transfer/heating-with-coils-and-jackets> [Accessed 5 February 2022]]...

Recommended heat transfer area, $A = 1.38 \text{ m}^2 + 10\% = 1.52 \text{ m}^2$

Consider maximum heating capacity of jacket, $Q_{jacket} = UA \Delta T$,

Initial liquid temperature, $T_1 = 216.01 \text{ }^\circ\text{C}$

$\Delta T = T_s - T_1 = 6.25 \text{ }^\circ\text{C}$

Table 2.10.4 Overall heat transfer coefficients for steam jackets

Process fluid or product	Wall material	U (W/m ² °C)
Water	Stainless steel	850 - 1 700
	Glass-lined Carbon steel	400 - 570
Aqueous solution	Stainless steel	450 - 1 140
	Glass-lined carbon steel	285 - 480
Organics	Stainless steel	285 - 850
	Glass-lined carbon steel	170 - 400
Light oil	Stainless steel	340 - 910
	Glass-lined carbon steel	230 - 425
Heavy oil	Stainless steel	57 - 285
	Glass-lined carbon steel	57 - 230

Based on table above [Engineering Principles and Heat Transfer, Available at <https://www.spiraxsarco.com/learn-about-steam/steam-engineering-principles-and-heat-transfer/heating-with-coils-and-jackets> [Accessed 5 February 2022]], U is selected between 285 and 850 W/m.°C for organic fluid and stainless steel wall where 850 W/m.°C is selected in this case.

Maximum heating capacity of jacket, $Q_{jacket} = \frac{850 \times 1.38 \times 133.99}{1000} = 157.28 \text{ kW}$

Maximum recommended steam velocity = 25.00 m/s [Engineering Principles and Heat Transfer, Available at <https://www.spiraxsarco.com/learn-about-steam/steam-engineering-principles-and-heat-transfer/heating-with-coils-and-jackets> [Accessed 5 February 2022]].,

$$\text{Maximum steam flowrate, } m_s = \frac{157.28 \times 3600}{1862.64} \text{ kg/h}$$

$$Vg = 82.61 \text{ cm}^3/\text{g} = 0.08 \text{ m}^3/\text{kg} \text{ (from steam table at 22.78 bar g)}$$

$$\text{Diameter of jacket} = \sqrt{\frac{0.08 \times 303.98 \times 4}{3600 \times \pi \times 25}} = 0.06 \text{ m} = 18.85 \text{ mm}$$

Consider heating jacket length as 80% of total height of one reactor,
Heating jacket length, L_jacket = 0.8 (6.36) = 5.09 m

Mechanical Design

Step 1: Design Pressure

According to Coulson Richardson's Chemical Engineering Design 4th edition (Chapter 13), safety factor of 10.0% is applied to the operating pressure of the reactor.

Tube (Reactor Vessel)

$$\text{Operating pressure} = 35 \text{ bar} = 3.50 \text{ N/mm}^2$$

$$\text{Design pressure, } P_d = 1.10 \times 3.50 = 3.85 \text{ N/mm}^2$$

Shell (Heating Jacket)

$$\text{Operating pressure} = 40 \text{ bar} = 4.00 \text{ N/mm}^2$$

$$\text{Design pressure, } P_d = 1.10 \times 4.00 = 4.40 \text{ N/mm}^2$$

Step 2: Design Temperature

Safety factor of 10°C or K above the operating temperature will be applied to the reactor design.

Tube (Reactor Vessel)

$$\text{Design temperature, } T_d = \text{Operating temperature} + 10 \text{ K}$$

$$= 502.69 + 10$$

$$= 512.69 \text{ K}$$

Shell (Heating Jacket)

$$\text{Design temperature, } T_d = \text{Operating temperature} + 10 \text{ K}$$

$$= 523.45 + 10$$

$$= 533.45 \text{ K}$$

Step 3: Material of construction

The material of construction for the packed bed reactor is stainless steel type 304. Based on table 13.2 in Coulson and Richardson's Chemical Engineering Design 4th edition, design stress, f of stainless steel type 304 is 115 N/mm² at temperature of 200°C which is higher than the reactor design pressure (3.85 N/mm²). Stainless steel type 304 also has good tensile strength of 510 N/mm². This makes it suitable to be used as the material of construction for high operating temperature and pressure reactor.

Table 13.2. Typical design stresses for plate
(The appropriate material standards should be consulted for particular grades and plate thicknesses)

Material	Tensile strength (N/mm ²)	Design stress at temperature °C (N/mm ²)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon steel (semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70		
Carbon-manganese steel (semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100		
Carbon-molybdenum steel, 0.5 per cent Mo	450	180	170	145	140	130	120	110	110		
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	235	230	220	190	170	
Stainless steel 18Cr/8Ni unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless steel 18Cr/8Ni Ti stabilised (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless steel 18Cr/8Ni Mo 2½ per cent (316)	520	175	150	135	120	115	110	105	105	100	95

Step 4: Welded joint efficiency

A double-welded butt type of welding is used for the reactor in order to balance the trade-off between the higher cost and higher strength of weld joint. As shown in table 13.3 in Coulson and Richardson's Chemical Engineering Design 4th edition, the welded joint efficiency, J of the double welded butt type of welding is 0.85.

Table 13.3. Maximum allowable joint efficiency

Type of joint	Degree of radiography		
	100 per cent	spot	none
Double-welded butt or equivalent	1.0	0.85	0.7
Single-weld butt joint with bonding strips	0.9	0.80	0.65

Step 5: Wall Thickness

The minimum wall thickness is calculated based on Coulson and Richardson's Chemical Engineering Design 4th edition.

Reactor tube

$$\begin{aligned}
 e &= \frac{P_d D_i}{2Jf - P_d} \\
 &= \frac{3.85(1.38)(1000)}{2(0.85)(110) - 3.85} \\
 &= 29.05 \text{ mm}
 \end{aligned}$$

With the following useful data, the minimum wall thickness obtained is **29.05 mm**.

Design pressure, P _d	N/mm ²	3.85
---------------------------------	-------------------	------

Design temperature, T_d	K	512.69
Vessel inner diameter, D_i	m	1.38
Maximum allowable stress, f	N/mm ²	110
Welded joint efficiency, J	-	0.85
Corrosion allowance	mm	2
Tensile strength of Stainless Steel Type 304	N/mm ²	510

The fabrication wall thickness, t is the addition of minimum wall thickness, e and corrosion allowance (2 mm) which is **31.05 mm**. Besides, the outer diameter of vessel obtained is **1.44408 m**.

The maximum allowable working pressure, MAWP for the vessel is calculated as below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.03105}{1.38 + 0.03105}$$

$$= 19.05 \text{ N/mm}^2$$

Since the MAWP is greater than the operating pressure of 4.0 N/mm², thus the thickness of the reactor wall is acceptable.

Cooling Jacket

$$t = \frac{P_d D_i}{2Jf - P_d}$$

$$= \frac{4.40(1.44)(1000)}{2(0.85)(105) - 4.40}$$

$$= 38.50 \text{ mm}$$

With the following useful data, the minimum wall thickness obtained is **38.50 mm**.

Design pressure, P_d	N/mm ²	4.40
Design temperature, T_d	°C	90
Vessel inner diameter, D_i	m	1.45
Maximum allowable stress, f	N/mm ²	105
Welded joint efficiency, J	-	0.85
Corrosion allowance	mm	2
Tensile strength of Stainless Steel Type 304	N/mm ²	510

The fabrication wall thickness, t is the addition of minimum wall thickness, e and corrosion allowance (2 mm) which is **40.50 mm**. Besides, the outer diameter of vessel obtained is **1.44408 m**.

The maximum allowable working pressure, MAWP for the vessel is calculated as below:

$$MAWP = \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.03850}{1.44 + 0.03850} = 22.51 \text{ N/mm}^2$$

Since the MAWP is greater than the operating pressure of 4.40 N/mm², the thickness of the cooling jacket wall is acceptable.

Step 6: Reactor Vessel Head Design

Hemispherical head is chosen as the type of head for the reactor due to the high pressure of the reactor. According to Coulson and Richardson's Chemical Engineering Design 4th edition, the head thickness for hemispherical head is 0.6 times of the reactor wall thickness.

$$\text{Head thickness} = 0.6t = 0.6(31.05) = 18.63 \text{ mm}$$

$$\text{Corrosion allowance} = 2.00 \text{ mm}$$

$$\text{Fabrication thickness of vessel head} = 18.639 + 2 = 20.63 \text{ mm}$$

$$MAWP = \frac{2 \times \text{Tensile strength} \times J \times t}{D_i + t} = \frac{2 \times 510 \times 0.85 \times 0.02063}{1.38 + 0.02063}$$

$$= 12.75 \text{ N/mm}^2$$

Since the MAWP is greater than the reactor operating pressure (3.85 N/mm^2), thus the thickness of the reactor head is acceptable.

Step 7: L/D ratio of reactor

$$\text{Functional height of reactor, } L = 6.36 \text{ m}$$

$$\text{Length of head, } L_H = D_i/2 = 1.38/2 = 0.6910 \text{ m}$$

$$\text{Total length of reactor, } L_T = 6.36 + (0.6910 \times 2) = 7.0511 \text{ m}$$

$$\text{Reactor shell outer diameter, } D_o = D_i + 2 \times t = 1.38 + 2 \times 0.03105 = 1.44408 \text{ m}$$

$$L_T / D = 7.0511 / 1.44408 = 4.88$$

Since L_T / D ratio is in between 2 to 5, thus the reactor size is acceptable.

Step 8: Total weight of reactor

The weight of vessel is calculated based on Coulson and Richardson's Chemical Engineering Design.

Let factor account for the weight of nozzle, $C_v = 1.15$,

Reactor tube

$$\text{Mean diameter of vessel, } D_m = D_i + t = 1.38 + (31.05/1000) = 1.41 \text{ m}$$

$$\text{Weight of vessel, } W_v = 240 C_v D_m (H_v + 0.8D_m) t$$

$$= 240 (1.15)(1.41)[6.3602 + 0.8(1.41)](0.03105)$$

$$= 90.71 \text{ kN}$$

Cooling jacket

$$\text{Mean diameter of vessel, } D_m = D_i + t_t = (1440 + 38.50)/1000 = 1.48 \text{ m}$$

$$\text{Weight of shell, } W_s = 240 C_v D_m (H_v + 0.8D_m) t_t$$

$$= 240 (1.15)(1.48)[4.81 + 0.8(1.48)](0.00385)$$

$$= 98.83 \text{ kN}$$

$$\text{Weight of catalyst, } W = (2897.944 \times 9.81)/1000 = 28.43 \text{ kN}$$

$$\text{Total weight of reactor, } W_R = W_v + W_s + W = 90.71 + 28.43 + 98.83 = 217.97 \text{ kN}$$

Step 9: Stress Analysis

Stress analysis is conducted based on Coulson and Richardson's Chemical Engineering Design to ensure the reactor structure is strong and safe against stresses.

For wind loading,

Let wind speed, $u_w = 160 \text{ km/hr}$

Wind pressure, $P_w = 0.05 u_w^2 = 0.05(160) = 1280 \text{ N/m}^2$

Wind loading per unit length of column, $F_w = P_w D_o = 1280 (1.44408) = 1848.42 \text{ N/m}$

$$\text{Bending moment at bottom tangent line, } M_x = \frac{F_w L_T^2}{2} = \frac{(1848.42)(7.0511)^2}{2} = 45950.46 \text{ Nm}$$

$$\text{Longitudinal stress, } \sigma_L = \frac{P_d D_i}{4t} = \frac{4.40 \times 1380}{4 \times 33.82} = 42.84 \text{ N/mm}^2$$

$$\text{Circumferential stress, } \sigma_h = \frac{P_d D_i}{2t} = \frac{3.85 \times 1380}{2 \times 31.05} = 85.68 \text{ N/mm}^2$$

$$\text{Dead weight stress, } \sigma_w = \frac{W_R}{\pi(D_i + t)t} = \frac{217.97 \times 1000}{\pi(1380 + 31.05)(31.05)} = 1.58 \text{ N/mm}^2$$

Second moment area of the vessel about the plane of bending, I_v

$$I_v = \frac{\pi}{64} (D_o^4 - D_i^4) = \frac{\pi}{64} (1444.08^4 - 1380^4) = 3.44 \times 10^{10} \text{ mm}^4$$

$$\text{Bending stress, } \sigma_b = \pm \frac{M_x}{I_v} \left(\frac{D_i}{2} + t \right) = \pm \frac{45940.46 \times 1000}{3.44 \times 10^{10}} \left(\frac{1380}{2} + 31.05 \right) = \pm 0.96 \text{ N/mm}^2$$

Total longitudinal stress, $\sigma_z = \sigma_L + \sigma_w \pm \sigma_b$

Since σ_w is compressive, therefore σ_w is negative value.

$$\sigma_z(\text{upwind}) = 42.84 - 1.58 + 0.96 = 42.22 \text{ N/mm}^2$$

$$\sigma_z(\text{downwind}) = 42.84 - 1.58 - 0.96 = 40.29 \text{ N/mm}^2$$

No torsional shear stress is considered in preliminary design.

The 3 principal stresses and their differences are calculated under this condition.

Principal Stress (N/mm ²)	Upwind	Downwind
$\sigma_1 = \sigma_h$	85.68	85.68
$\sigma_2 = \sigma_z$	42.22	40.29
$\sigma_3 = 0.5P$	1.93	1.925
$\sigma_1 - \sigma_2$	43.46	45.38
$\sigma_1 - \sigma_3$	83.75	83.75
$\sigma_2 - \sigma_3$	40.30	38.37

From the calculation the greatest principal stress difference is 83.75 N/mm^2 . This does not exceed the design stress for the material construction of the reactor which is 110 N/mm^2 . Thus, the design is acceptable.

$$\text{Critical buckling stress, } \sigma_c = 2 \times 10^4 \left(\frac{t_o}{D_o} \right) = 2 \times 10^4 \left(\frac{31.05}{1444.08} \right) = 430.04 \text{ N/mm}^2$$

Maximum compressive where the vessel is not under pressure = $\sigma_w + \sigma_b = 1.58 + 0.96 = 2.55 \text{ N/mm}^2$.

As the maximum allowable design stress is smaller than critical buckling stress, the design is satisfactory.

Step 10: Vessel Support

Type of support chosen: Conical skirt

Let skirt bottom diameter, $D_s = 1.8 \text{ m}$

Let skirt height, $H_s = 2.0 \text{ m}$

$$\text{Skirt base angle, } \theta_s = \tan^{-1} \frac{D_s}{0.5 \times (D_s - D_i)} = \tan^{-1} \frac{1.8}{0.5 \times (1.8 - 1.38)} = 83.38^\circ$$

The skirt base angle is satisfactory as the angle is in between 80° and 90° .

The maximum dead weight load on the skirt will occur when the vessel is full of water.

$$\begin{aligned} \text{Approximate water weight, } W_w &= \left(\frac{\pi}{4} \times D_i^2 \times L_T \right) \times 1000 \times 9.81 \\ &= \left(\frac{\pi}{4} \times 1.38^2 \times 7.0511 \right) \times 9.81 = 103.76 \text{ kN} \end{aligned}$$

Taking skirt thickness, t_s same as thickness of vessel (31.05 mm),

$$\text{Bending moment at bottom of skirt, } M_s = \frac{F_w(L_T + H_s)^2}{2} = \frac{1848.42(7.0511+2)^2}{2} = 75714.24 \text{ Nm}$$

$$\text{Bending stress in skirt, } \sigma_{bs} = \frac{4M_s}{\pi(D_s + t_s)D_s t_s} = \frac{4 \times 75714.22 \times 1000}{\pi(1800 + 31.05)(1800 \times 31.05)} = 0.94 \text{ N/mm}^2$$

$$\text{Dead weight stress in the skirt, } \sigma_{ws(test)} = \frac{W_w}{\pi(D_s + t_s)t_s} = \frac{103.76 \times 1000}{\pi(1800 + 31.05)(31.05)} = 0.58 \text{ N/mm}^2$$

$$\sigma_{ws(operating)} = \frac{W}{\pi(D_s + t_s)t_s} = \frac{217.97 \times 1000}{\pi(1800 + 31.05)(31.05)} = 1.22 \text{ N/mm}^2$$

$$\sigma_s(\text{compressive}) = \sigma_{bs} + \sigma_{ws(operating)} = 0.94 + 0.58 = 1.52 \text{ N/mm}^2$$

$$\sigma_s(\text{tensile}) = \sigma_{ws(test)} - \sigma_{bs} = 0.94 - 1.22 = 0.28 \text{ N/mm}^2$$

The skirt thickness should be such that under the worst combination of wind and dead weight loading. 2 design criteria must be satisfied:

$$\sigma_s(\text{tensile}) < f_s J \sin \theta_s$$

$$\sigma_s(\text{compressive}) < 0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta_s$$

The skirt material is chosen to be stainless steel 304 with maximum allowable design stress at ambient temperature is $f_s = 165 \text{ N/mm}^2$. The Young modulus, E of stainless steel type 304 is 193000 MPa.

$$\begin{aligned} f_s J \sin \theta_s &= 165 \times 0.85 \times \sin(83.38) = 139.17 \text{ N/mm}^2 \\ 0.28 \text{ N/mm}^2 &< 139.17 \text{ N/mm}^2 \text{ [Satisfy]} \end{aligned}$$

$$0.125 E \left(\frac{t_s}{D_s} \right) \sin \theta_s = 0.125 \times 193000 \left(\frac{33.82}{1800} \right) \sin(83.38) = 412.95 \text{ N/mm}^2$$

$$1.52 \text{ N/mm}^2 < 412.95 \text{ N/mm}^2 \text{ [Satisfy]}$$

Since both design criteria are satisfied, the skirt thickness is acceptable.

Step 11: Base ring and anchor bolt design

Take pitch circle diameter, $D_b = 0.62 \text{ m}$

Circumference of bolt circle = $620 \times \pi = 1947.79 \text{ mm}$

Bolt spacing is taken at 250 mm for conical skirt

$$\text{Number of bolts required, } N_b = \frac{1947.79}{250} = 7.79 \approx 8 \text{ bolts}$$

$$\text{Maximum allowable bolt stress, } f_b = 125 \text{ N/mm}^2$$

$$\text{Area of bolt, } A_b = \frac{1}{N_b f_b} \left[\frac{4M_s}{D_b} - W \right] = \frac{1}{8(125)} \left[\frac{4(75714.24)}{0.62} - 217.97 \times 1000 \right]$$

$$= 270.51 \text{ mm}^2$$

$$\text{Diameter of bolt} = \sqrt{\frac{A_b \times 4}{\pi}} = \sqrt{\frac{270.51 \times 4}{\pi}} = 18.56 \text{ mm}$$

From Coulson & Richardson's Chemical Engineering Design Figure 13.30, the bolt type selected is M30 as it is the closest standard size bolt larger than 21.99 mm. Its root area is 561 mm².

$$\text{Total compressive load on base ring, } F_b = \frac{4M_s}{\pi D_s^2} + \frac{W}{\pi D_s}$$

$$= \frac{4(75714.24)}{\pi(1.8)^2} + \frac{217.97 \times 1000}{\pi(1.8)} = 68299.12 \text{ N/m}$$

Maximum allowable bearing pressure on concrete foundation pad, $f_c = 7 \text{ N/mm}^2$

$$\text{Minimum width base ring, } L_b = \frac{F_b}{f_c} \times \frac{1}{10^3} = \frac{68299.12}{7} \times \frac{1}{1000} = 9.76 \text{ mm}$$

Using bolt M30 distance from skirt edge to ring edge, $L_r = 76 \text{ mm}$

$$\text{Actual base ring width} = L_r + t_s + 50 = 76 + 31.05 + 50 = 157.05 \text{ mm}$$

$$\text{Actual bearing pressure on concrete foundation pad, } f'_c = \frac{F_b}{\text{Actual base width}}$$

$$= \frac{68299.12}{157.05 \times 1000} = 0.43 \text{ N/mm}^2$$

Allowable design stress in the ring material, $f_r = 140 \text{ N/mm}^2$

$$\text{Minimum base ring thickness, } t_b = L_r \sqrt{\frac{3f'_c}{f_r}} = 76 \sqrt{\frac{3(0.43)}{140}} = 7.34 \text{ mm}$$

Dimensions mm								
Bolt size	Root area	A	B	C	D	E	F	G
M24	353	45	76	64	13	19	30	36
M30	561	50	76	64	13	25	36	42
M36	817	57	102	76	16	32	42	48
M42	1120	60	102	76	16	32	48	54
M48	1470	67	127	89	19	38	54	60
M56	2030	75	150	102	25	45	60	66
M64	2680	83	152	102	25	50	70	76
70	—	89	178	127	32	64	76	83
76	—	95	178	127	32	64	83	89

Bolt size = Nominal dia. (BS 4190: 1967)

Figure 13.30. Anchor bolt chair design

Step 12: Nozzles design

Benzene Feed Inlet

Calculated according to the Harker equation (1978), modified for SI unit, for the optimum pipe (and nozzle) diameter.

W = Mass flow rate = 2877.2621 kg/hr

At Temperature = 489.1649 K, Pressure = 35 bar

ρ = 629.91 kg/m³

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{2877.2621^{0.45}}{629.91^{0.31}} = 41.07 \text{ mm} = 1.62 \text{ in}$$

By referring to ASME B36.19, the 2 in. stainless steel Sch. 80 is used. (OD = 60.3 mm, wall thickness = 5.54 mm)

Ethylene Feed Inlet

W = Mass flow rate = 0.26 kg/hr

At Temperature = 489.1649 K, Pressure = 35 bar

ρ = 212.62 kg/m³

$$\text{Volumetric flow rate, } Q = \frac{W}{\rho} = \frac{0.26}{212.62 \times 3600} = 3.37 \times 10^{-7} \text{ m}^3/\text{s}$$

$$\text{Minimum nozzle cross sectional area, } A = \frac{Q}{c} = \frac{3.37 \times 10^{-7}}{440.48} = 7.76 \times 10^{-10} \text{ m}^2$$

$$\text{Minimum nozzle diameter} = \sqrt{\frac{4 \times A}{\pi}} = \sqrt{\frac{4 \times 7.76 \times 10^{-10}}{\pi}} \times 1000 = 0.0305 \text{ mm} = 0.0012 \text{ in}$$

By referring to ASME B36.19, the 0.125 in. stainless steel Sch. 80 is used. (OD = 10.3 mm, wall thickness = 2.42 mm)

Product Outlet

At Temperature = 502.6792 K, Pressure = 35 bar

W = Mass flow rate = 2877.52 kg/hr

ρ = 604.06 kg/m³

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{2877.52^{0.45}}{604.06^{0.31}} = 41.61 \text{ mm} = 1.64 \text{ in}$$

By referring to ASME B36.19, the 2 in. stainless steel Sch. 80 is used. (OD = 60.3 mm, wall thickness = 5.54 mm)

High Pressure Steam Inlet

At temperature = 723.15 K, pressure = 40 bar

W = Mass flow rate = 303.98 kg/hr

ρ = 0.44 kg/m³

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{303.98^{0.45}}{0.44^{0.31}} = 142.54 \text{ mm} = 5.61 \text{ in}$$

By referring to ASME B36.19, the 6 in. stainless steel Sch. 80 is used. (OD = 168.3 mm, wall thickness = 10.98 mm)

High Pressure Steam Outlet

At temperature = 523.45 K, pressure = 40 bar

W = Mass flow rate = 303.98 kg/hr

ρ = 0.42 kg/m³

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{303.98^{0.45}}{0.42^{0.31}} = 144.06 \text{ mm} = 5.67 \text{ in}$$

By referring to ASME B36.19, the 6 in. stainless steel Sch. 80 is used. (OD = 168.3 mm, wall thickness = 10.98 mm)

APPENDIX I

AUXILIARY EQUIPMENT

H.1 R-101, Packed-Bed Reactor

Design Basis

Stream	7 (Input)	8 (Output)
Molar Flowrate (kmol/hr)	115.2269	115.2269
Mass Flowrate (kg/s)	2.5004	2.5004

Design Parameters

Pump Design
Operating temperature
Operating pressure
Friction loss
Net positive suction head, NPSH
Nozzle size
Motor power

Design Criteria

Operating Temperature (°C)	25.00
Operating Pressure – Inlet (bar)	1.0
Operating Pressure – Outlet (bar)	40.0

Design Method

The design of the pump power is based on the Bernoulli's Equation.

$$\frac{P_1}{\rho g} + z_1 + \frac{v_1^2}{2g} + h_p = \frac{P_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_f$$

Design Procedure

Step 1: Properties of Components at Streams and Operating Conditions

Properties of component at pump P-101

Component	Mass Fraction	Density (kg/m³)	Viscosity (Pa.s)	Vapor Pressure (bar)
Benzene	1.00	873.7	0.000600396	0.1264
Ethylene	0.00	1.138	0.00	69.7529
Ethylbenzene	0.00	866	0.00	0.0128
Diethylbenzene	0.00	870	0.00	0.0013
Methane	0.00	0.648	0.00	618.3406
Ethane	0.00	1.219	0.00	41.8744

Volumetric Flow Rate (m ³ /hr)	10.30276
Operating temperature (K)	298
Pressure inlet	1.0 bar
Pressure outlet	40.0 bar
Density (kg/m ³)	873.7
Viscosity (Pa.s)	0.000600396
Length inlet, L ₁ (m)	5
Length outlet, L ₂ (m)	5
Total length pipe, L (m)	10
Inlet elevation, z ₁ (m)	0.5
Outlet elevation, z ₂ (m)	3

Design Equation

$$\frac{P_1}{\rho g} + z_1 + \frac{v_1^2}{2g} + h_p = \frac{P_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_f$$

Step 2: Nozzles Design

Determination of the optimum diameter for the nozzle is done by using the equation from the Harker Equation (1978), modified SI unit:

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}}$$

Where: W = mass flowrate (kg/hr)
 ρ = density (kg/m³)

Liquid Inlet and Outlet

$$W = 2.5004 \text{ kg/s} = 9001.5234 \text{ kg/hr}$$

$$\rho = 873.7 \text{ kg/m}^3$$

$$D_{opt} = 8.41 \frac{W^{0.45}}{\rho^{0.31}} = 8.41 \frac{9001.5234^{0.45}}{873.7^{0.31}} = 62.0034 \text{ mm}$$

$$D_{opt} = 62.0034 \text{ mm} = 2.4410 \text{ in}$$

Based on Scheduled 40 pipe dimension, the pipe size to be choose is 2.5 in nominal size.

Schedule 40 pipe dimensions

Nominal sizes (Inches)	Internal Diameter (mm)
2.5	62.71

Area of Pipeline

The calculation of area for pipeline is based in the internal diameter of the pipeline.

$$A = \frac{\pi D^2}{4} = \frac{\pi(0.06271)^2}{4} = 0.003088 \text{ m}^2$$

Step 3: Velocity of Liquid

Velocity of liquid:

$$V = \frac{Q}{A} = \frac{10.3027}{0.003088} \div 3600 = 0.9265 \frac{m}{s}$$

Step 4: Friction in Pipe

Friction loss in pipe is determined by considering the total length of the pipelines at the inlet and outlet of the pump. The friction loss is calculated with the equation stated below.

$$\text{Friction loss, } h_f = 8f \left[\frac{L}{D} \right] \left[\frac{v^2}{2g} \right]$$

The Reynolds Number, Re and the relative roughness, ϵ/D need to determine to find the friction factor, f. The equation to determine Reynolds Number is stated as below.

$$\text{Reynolds Number, } Re = \frac{\rho v D}{\mu}$$
$$Re = \frac{873.7 \times 0.9265 \times 0.06271}{0.000600396} = 84556.85088$$

The material construction selected for the pump is commercial steel. Hence, the value of roughness, ϵ for the material is 0.046 mm. From this value, the relative roughness of the pump is determined.

$$\text{Relative Roughness, } \frac{\epsilon}{D} = \frac{0.046}{0.06271 \times 1000} = 0.0007335$$

From these values, the friction factor, f is determined based on the Moody Chart. From the Moody Chart, the value of friction factor is 0.0185.

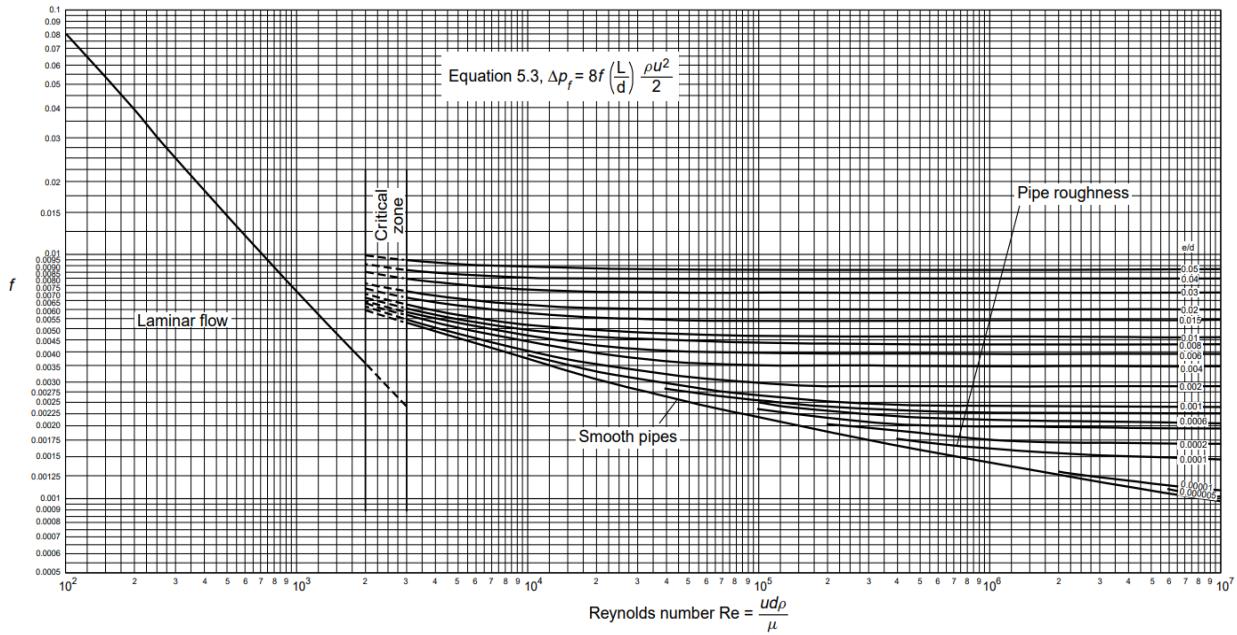


Figure 5.7. Pipe friction versus Reynolds number and relative roughness

Moody chart

Then, the value of friction loss in the pipe is determined based on the equation stated earlier.

$$\text{Friction loss, } h_f = 8 \times 0.0185 \left[\frac{10}{0.06271} \right] \left[\frac{0.9265^2}{2 \times 9.81} \right] = 1.0328 \text{ m}$$

Step 5: Total Head

The total head is calculated by arranging the Bernoulli's equation. As there is no reaction happened at the pump, the velocity of the fluid at inlet and outlet of the pump is the same.

$$h_p = \left(\frac{P_2 - P_1}{\rho g} \right) + (z_2 - z_1) + h_f$$

$$h_p = \left(\frac{4000,000 - 10,000}{873.7 \times 9.81} \right) + (3 - 0.5) + 1.0328 = 458.5557 \text{ m}$$

Step 6: Power Required

$$P = \dot{m}gh_p = 2.5004 \times 9.81 \times 458.5557 = 11247.8782 \text{ W}$$

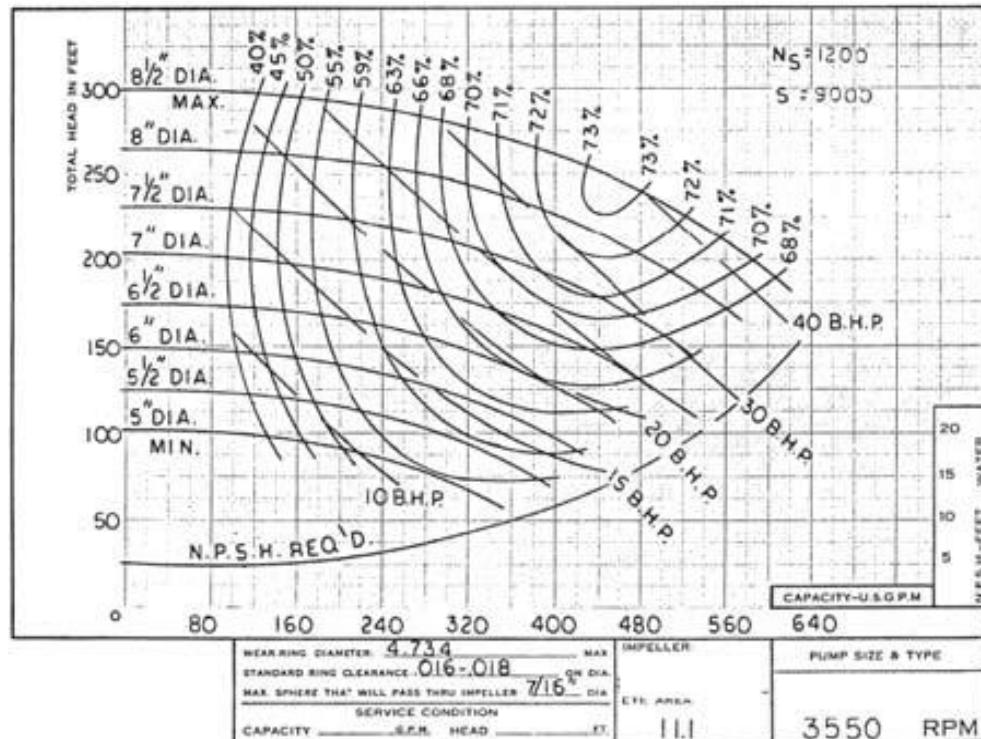
Step 7: Net Positive Suction Head Available, NPSH_A

The calculation of NPSH_A of the piping is involved for the inlet section only. Thus, the parameters used for the calculation of NPSH_A is based on the inlet section of the pump.

$$NPSH_A = \frac{P_1 - P_v}{\rho g} + z_1 - h_{f1}$$

$$\text{Friction loss, } h_f = 8 \times 0.0023 \left[\frac{5.0}{0.0779} \right] \left[\frac{0.473^2}{2 \times 9.81} \right] = 0.135 \text{ m}$$

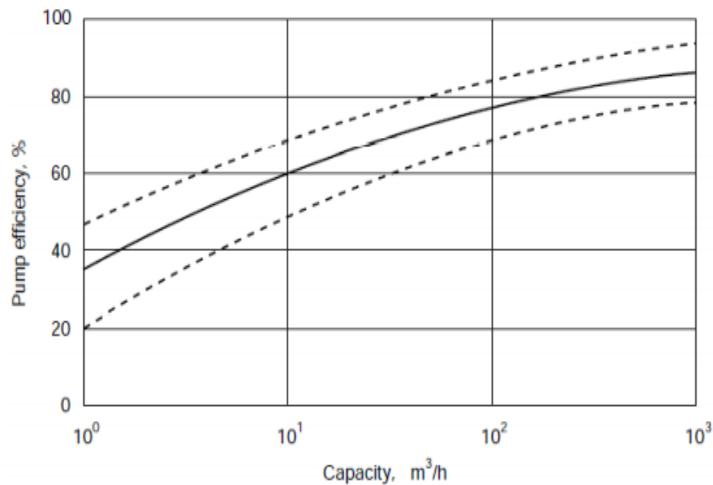
$$NPSH_A = 8.9694$$



Step 8: Actual Motor Power

In calculating the actual motor power of the pump, the pump efficiency should be known. The pump efficiency is obtained from the graph which are shown at below.

Pump Efficiency



Centrifugal pump efficiency in Chemical Engineering Design

From the graph above, the pump efficiency obtained is 60.0 %.

$$\text{Actual Power} = \frac{11247.8782}{0.6} = 18746.4636 \text{ W}$$

$$\text{Actual Power} = 18746.4636 \text{ W} \times 0.00134102 = 25.13938 \text{ hp}$$

**** Same step 1 to 8 is applied to other pumps (P-201 & P-401) to get the result.

C-101, Compressor

Design Basis: Total molar flow rate of ethylene feed = 115.1960 kmol/hr

Step 1: Stages of compressor

The type of compressor used is centrifugal compressor. The typical value of compression ratio, CR for centrifugal type of compressor is between 6 to 8. Let the compression ratio, CR = 6.

$$n = \frac{\log_{10} \frac{P_2}{P_1}}{\log_{10} CR}$$

$$n = \frac{\log_{10} \frac{50}{40}}{\log_{10} 6} = 0.1245 \approx 1 \text{ stage}$$

Step 2: Determination of inter-stage pressure

$$P_i = \sqrt{P_1 \times P_2}$$

$$P_i = \sqrt{40 \times 50} = 44.7214 \text{ bar}$$

Step 3: Determination of inlet volumetric flow rate

Components	Mole fraction	Tc (K)	Pc (bar)
Ethylene	0.9992	282.40	50.60
Ethylbenzene	0.0001	617.10	36.06
Methane	0.0003	190.56	45.99
Ethane	0.0005	303.35	48.80
Average		282.4446	50.60132

Critical temperature and pressure for ethylene, methane and ethane were obtained from The Engineering ToolBox whereas ethylbenzene was obtained from <https://cameochemicals.noaa.gov/chris/ETB.pdf>

Using Kay's Rule,

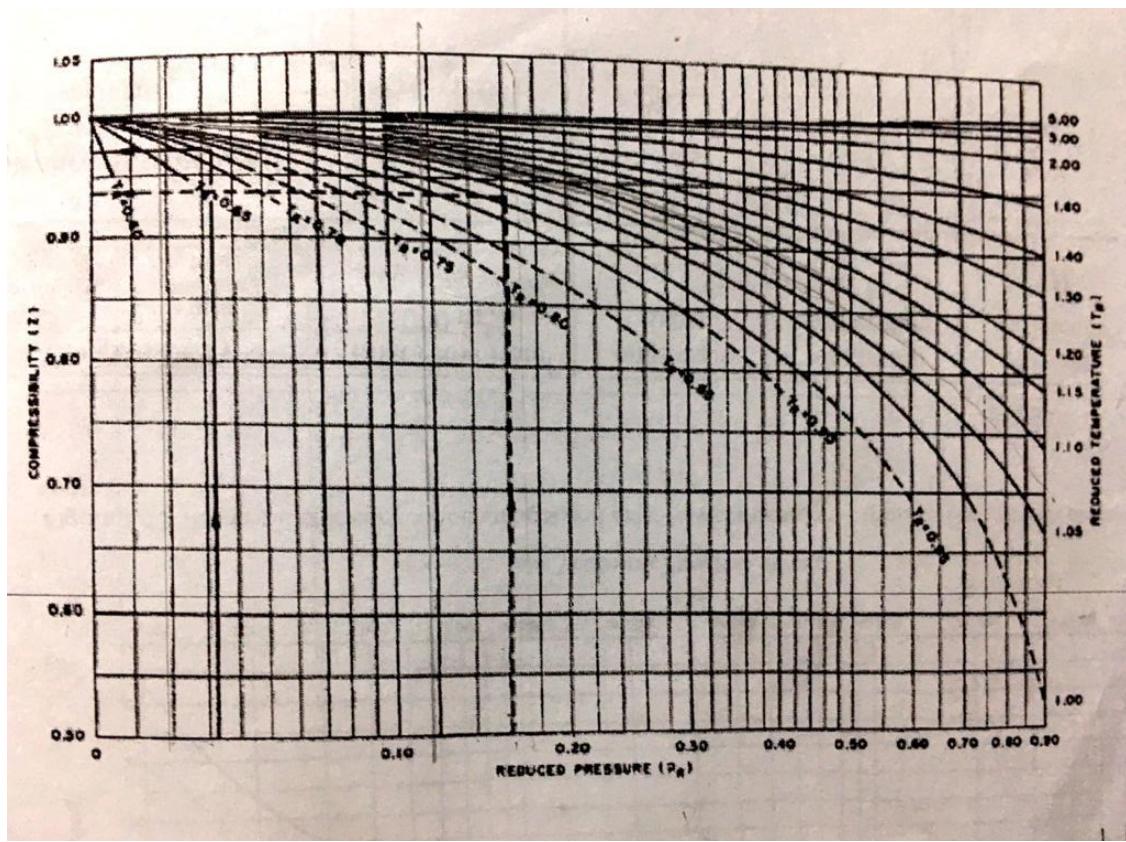
$$\begin{aligned} \text{Average } T_c &= \sum(T_{ci} \times x_i) \\ &= (0.9992 \times 282.4) + (0.0001 \times 617.1) + (0.0003 \times 190.56) + (0.0005 \times \\ &303.35) = 282.4446 \text{ K} \end{aligned}$$

$$T_r = \frac{T_1}{T_c} = \frac{298.15}{282.4446} = 1.0556$$

$$\begin{aligned} \text{Average } P_c &= \sum(P_{ci} \times x_i) \\ &= (0.9992 \times 50.6) + (0.0001 \times 36.06) + (0.0003 \times 45.99) + (0.0005 \times 48.8) = \\ &50.6013 \text{ bar} \end{aligned}$$

$$P_r = \frac{P_1}{P_c} = \frac{40}{50.6013} = 0.7905$$

Based on the values of T_r and P_r , compressibility factor, Z can be obtained from the graph.
 $Z = 0.73$



Using the real gas law equation,

$$PV = nZRT$$

$$\frac{V}{n} = \frac{ZRT}{P}$$

$$= \frac{(0.73) \times (8.314 \text{ Pa.m}^3/\text{mol.K}) \times (298.15 \text{ K})}{40 \times 10^5} \times 1000 = 0.4524 \text{ m}^3/\text{kmol}$$

Inlet volumetric flow rate = Molar flow rate × molar volume

$$= \left(115.1960 \frac{\text{kmol}}{\text{hr}} \times 0.4524 \frac{\text{m}^3}{\text{kmol}} \right) \times \frac{1 \text{ hr}}{3600 \text{ s}} = 0.0145 \text{ m}^3/\text{s}$$

The polytropic efficiency, E_p of centrifugal compressor correlated to volumetric flow rate can be obtained from Figure 3.6 in Coulson and Richardson's Chemical Engineering Design.

From the figure, $E_p = 0.655$

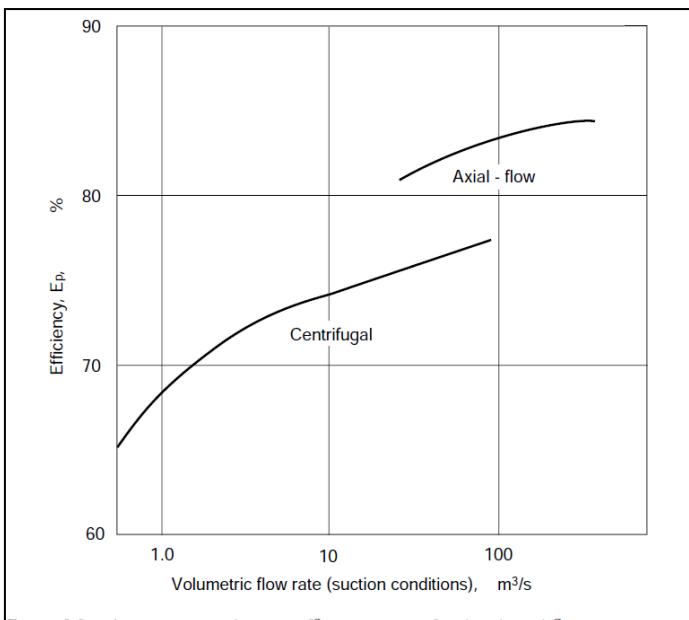


Figure 3.6. Approximate polytropic efficiencies centrifugal and axial-flow compressors

Step 4: Determination of the ratio of specific heats, γ

$$\gamma = \frac{C_p}{C_p - R}$$

Since the compressor works with gas mixture, the average specific heat capacity is determined.

$$\text{Heat capacity, } C_p \left[\frac{\text{kJ}}{\text{mol.}^\circ\text{C}} \right] = a + bT + cT^2 + dT^3$$

Components	Mole fraction	a	b	c	d
Ethylene	0.998821735	4.08E-02	1.15E-04	-6.89E-08	1.77E-11
Methane	0.00092646	3.43E-02	5.47E-05	3.66E-09	-1.10E-11
Ethane	0.000251805	4.94E-02	1.39E-04	-5.82E-08	7.28E-12
Average		4.07E-02	1.15E-04	-6.88E-08	1.76E-11

Besides, the ratio of specific heats, is calculated at the average inlet and outlet temperature of the process stream for a more accurate calculation as the outlet temperature will increase significantly after compression in which the outlet temperature is approximated by isentropic compression relation.

$$\frac{T_{out}}{T_{in}} = \left(\frac{P_{out}}{P_{in}} \right)^{\frac{\gamma-1}{\gamma}}$$

T_{out} and γ are iterated until constant values are obtained. From the table below, $\gamma = 1.24$

C-101					
P _{in} (bar)	40.00000	C1	C2	C3	C4
P _{out} (bar)	50.00000	4.07E-02	1.15E-04	-6.88E-08	1.76E-11
T _{in} (°C)	T _{out} (°C)	T _{in} (K)	T _{out} (K)	C _{pave} (kJ/mol.K)	gamma, γ
25.00	-	298.15	-	0.04	1.25
25.00	26.12	298.15	299.12	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24
25.00	26.09	298.15	299.09	0.04	1.24

Step 5: Determination of power requirement and outlet temperature

Work by compressor, $W = \text{Molar flow rate} \times \frac{ZRT_1}{(n-1)/n} \left\{ \left[\frac{P_2}{P_1} \right]^{\frac{n-1}{n}} - 1 \right\}$

$$\frac{n-1}{n} = \frac{(\gamma-1)/\gamma}{E_p} = \frac{(1.23-1)/1.23}{0.675} = 0.2955$$

$$W = 83.8198 \times \frac{0.98333 \times 8.314 \times 303.15}{0.2749} \left\{ \left[\frac{5.9551}{1.01325} \right]^{0.2749} - 1 \right\} \times \frac{1000}{3600}$$

$$= 13356.2289 \text{ W}$$

The approximate electric motor efficiency for compressor can be obtained from Table 3.1 in Coulson and Richardson's Chemical Engineering Design to estimate the actual power required.

Table 3.1. Approximate efficiencies of electric motors

Size(kW)	Efficiency (%)
5	80
15	85
75	90
200	92
750	95
>4000	97

$$\text{Efficiency, } N_m = 0.85$$

Therefore, the actual power required is determined as

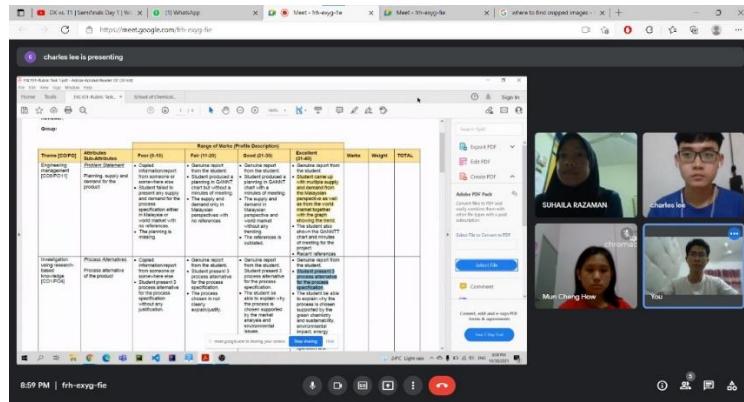
$$\frac{W}{N_m} = \frac{131.1584 \text{ kW}}{0.85} = 15.7132 \text{ kW}$$

$$T_2 = T_1 \left(\frac{P_2}{P_1} \right)^{\frac{n-1}{n}} = 298.15 \left[\frac{50}{40} \right]^{0.2855} = \mathbf{318.4790 \text{ K} = 45.3219 \text{ }^{\circ}\text{C}}$$

APPENDIX J

MINUTE MEETING

MEETING MINUTE 1



Date: 26 Oct 2021

Time: 2015 – 2115H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

- Decide roles: Kah hoe as the team leader
- Discuss on the overview of the process and point out relevant information
- Work distribution of part 1 and 2: (General info + 1 alternative)
(Related News)
(Scope + 1 alternative)
(Gantt chart + 1 alternative)

Prepared by,

Suhaila

(Noor Suhaila binti Razaman)

MEETING MINUTES 2



Date: 2 Nov Oct 2021

Time: 2015 – 2115H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

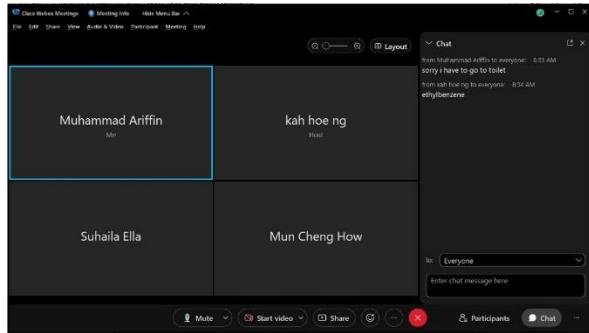
- Explain each section of the task clearly to avoid any mistakes
- Briefly explain the progress of the project
- Proposed 3 alternatives to supervisor (facing problem due to biological product)
- Decided to have another meeting to propose new product

Prepared by,

MunCheng

(How Mun Cheng)

MEETING MINUTES 3



Date: 5 Nov 2021

Time: 0830 – 0900H

Meeting platform: Webex

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

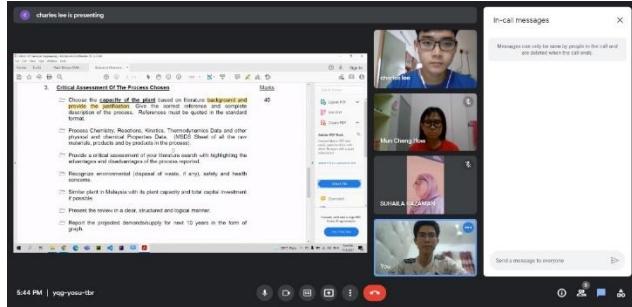
- Discussion on the suitable product to propose to Prof Azmier
- Decided to change the assigned product to ethylbenzene
- Proposed 3 alternatives:
 1. Liquid Phase Alkylation of Benzene with Ethylene with EBZ-500 Zeolite Catalyst
 2. Mixed Xylenes Isomerization and Ethylbenzene Produced by Xylenes Separation
 3. Vapor Phase Alkylation of Benzene with Ethylene with ZSM-5 and Kaolinite Mixed Catalyst

Prepared by,

Ariffin

(Muhammad Ariffin bin Samsu)

MEETING MINUTES 4



Date: 8 Nov 2021

Time: 1730 – 1630H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

- Updates of part 1
- Discuss on the best alternative for ethylbenzene plant, based on the comparison of the literature review of three alternatives
- Work distribution and set new date line on part 2, 3 and 4 due to change of product
- Discuss roughly on the basic equipment and process needed for the plant

Prepared by,

Kah Hoe

Ng Kah Hoe

MEETING MINUTES 5



Date: 12 Nov 2021

Time: 0900 – 1000H

Meeting platform: Webex

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

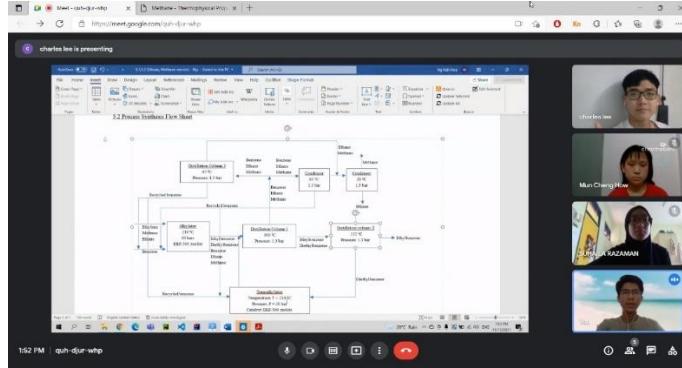
- Update the current progress of the report
- Discuss on the suitable platform to get the current data of supply and demand as well as plant capacity
- Consult with Prof regarding to the chosen site plant and its capacity
- Confirmation of the process block diagram and its operating condition

Prepared by,

Suhaila

Noor Suhaila binti Razaman

MEETING MINUTES 6



Date: 13 Nov 2021

Time: 1300 – 1400H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

- Discussion on several changes in report (data, parameter used, etc)
- Discussion of the process synthesis flow sheet (improvement of stream, operating condition, equipment)

Prepared by,

MunCheng

(How Mun Cheng)

MEETING MINUTES 7



Date: 19 Nov 2021

Time: 1300 – 1400H

Meeting platform: Webex

Attendance:

No.	Name
1	Ng Kah Hoe
2	How Mun Cheng
3	Muhammad Ariffin bin Samsu

Note: Noor Suhaila binti Razaman did not attending meeting due to connection problem (float occurred at hometown area)

Meeting agenda:

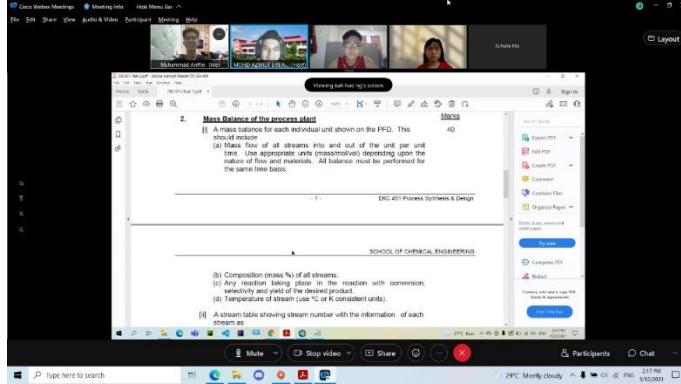
- Meeting to finalise the format of report before submitting on 22nd November 2021
- To be corrected on:
 1. Design of Process flow diagram
 2. Signature part of letter transmittal
 3. Real example of plant capacity

Prepared by,

Ariffin

(Muhammad Ariffin bin Samsu)

Meeting minute 7



Date: 03 Dec 2021

Time: 1400 – 1500H

Meeting platform: Webex

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

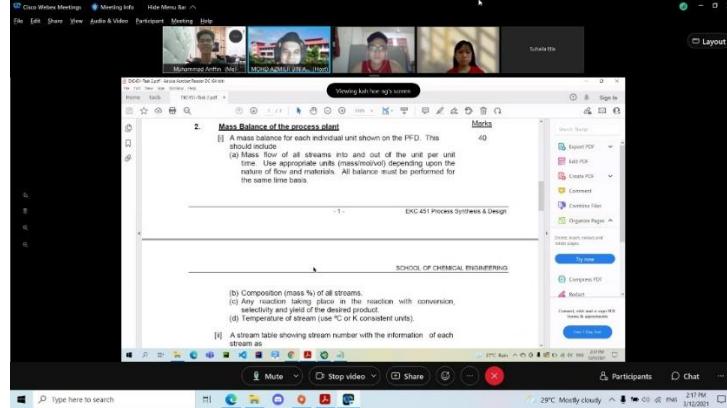
- Updated the work distribution
- Discussed the current progress of polymath and mass balance
- Discussed the selectivity of reactor
- Consulted with Prof regarding to the chosen site plant and its capacity
- Confirmation of the process block diagram and its operating condition

Prepared by,

Suhaila

Noor Suhaila binti Razaman

Meeting minute 8



Date: 08 Dec 2021

Time: 2030 – 21300H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

- Updated the current progress of part 2
- Discussed relevant temperature and pressure of each equipment

Prepared by,

MunCheng

(How Mun Cheng)

Meeting minute 9

The screenshot shows a Microsoft Excel spreadsheet titled "Mass Balance for distillation column 1 & purified". The spreadsheet contains a table with columns for Stream, Flow rate (kg/hr), and Mass (kg). The table includes rows for feed, overhead, and various components like Ethane, Propane, Butane, Isobutane, Methane, Ethane, Propane, and Isobutane. The total mass balance is shown as 3830.400 kg/hr. The participants in the meeting are Mun Cheng How and Ng Kah Hoe.

Date: 10 Dec 2021

Time: 0830 – 0900H

Meeting platform: Webex

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

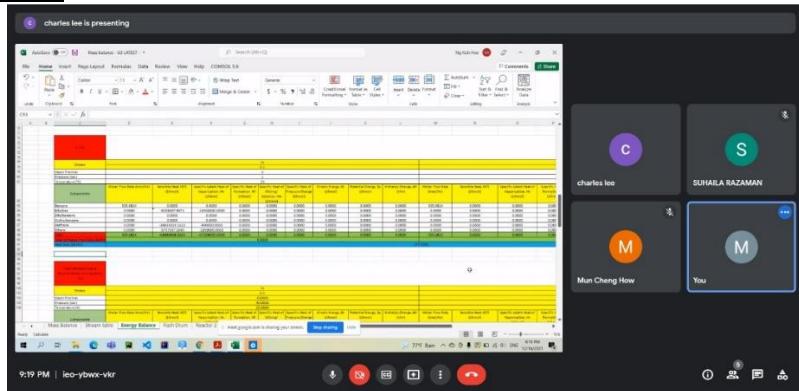
- Confirmation of vapor pressure calculation
- Reviewed the calculation for first reactor

Prepared by,

Ariffin

(Muhammad Ariffin bin Samsu)

Meeting minute 10



Date: 16 Dec 2021

Time: 2030 – 2130H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

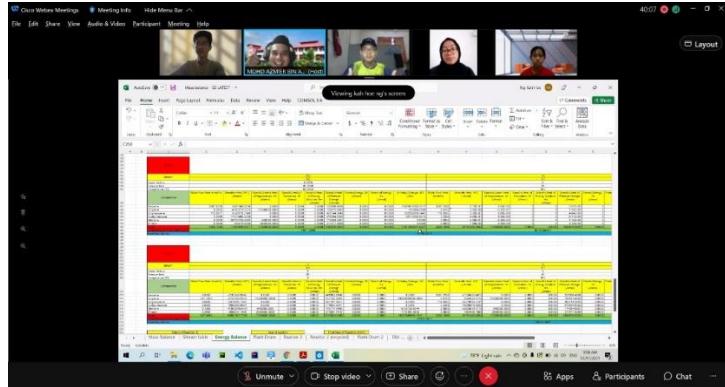
- Discussing outcome of each member's part
- Dividing task for energy balance

Prepared by,

Kah Hoe

Ng Kah Hoe

Meeting minute 11



Date: 17 Dec 2021

Time: 0830 – 090H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	How Mun Cheng
4	Muhammad Ariffin bin Samsu

Meeting agenda:

- Updated the progress with supervisor
- Proposed the calculation of energy to supervisor

Prepared by,

Suhaila

Noor Suhaila binti Razaman

Meeting minute 12

The screenshot shows a Google Meet interface. In the center is a Microsoft Excel spreadsheet titled "West End Energy Balance (S1-Q1) - Sheet1". The spreadsheet contains several tables of data, likely energy balance calculations. On the right side of the screen, there is a participant list with three participants: SUHAILA RAZAMAN (green circle), charles lee (purple circle), and You (blue circle). The meeting title is "charles lee is presenting". The bottom of the screen shows the Google Meet control bar with options like "New tab", "Share screen", "Energy Balance", "Hang Out", and "Switch 2". The status bar at the bottom left indicates "9:53 AM | bzq-zpyy-div".

Date: 22 Dec 2021

Time: 0900 – 1000H

Meeting platform: Google meet

Attendance:

No.	Name
1	Ng Kah Hoe
2	Noor Suhaila binti Razaman
3	Muhammad Ariffin bin Samsu

Meeting agenda:

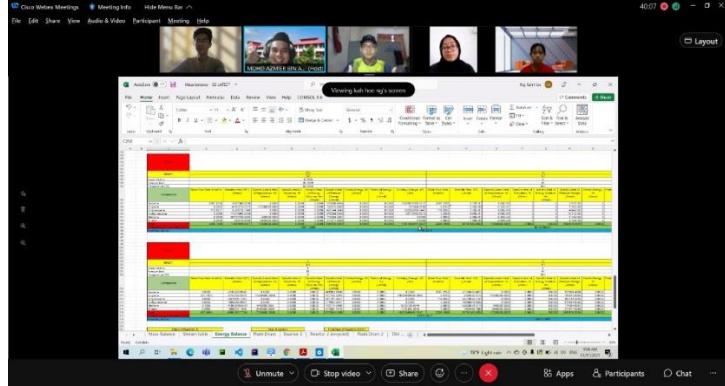
- Discussed the final part of energy balance
- Discussed the equipment to be added in the PFD

Prepared by,

Ariffin

(Muhammad Ariffin bin Samsu)

Meeting minute 13



Date: 31 Dec 2021

Time: 0815 – 0830H

Meeting platform: Google meet

Attendance:

No.	Name
1	Noor Suhaila binti Razaman
2	How Mun Cheng
3	Muhammad Ariffin bin Samsu

Meeting agenda:

- Discussed the comparison of mass and energy balance by using Aspen
- Discussed the final report

Prepared by,

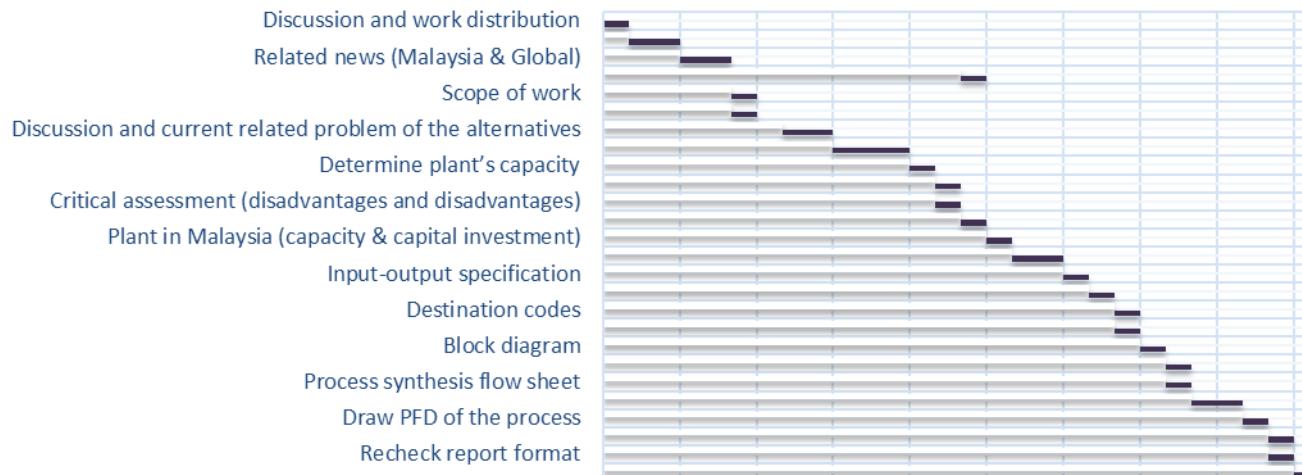
MunCheng

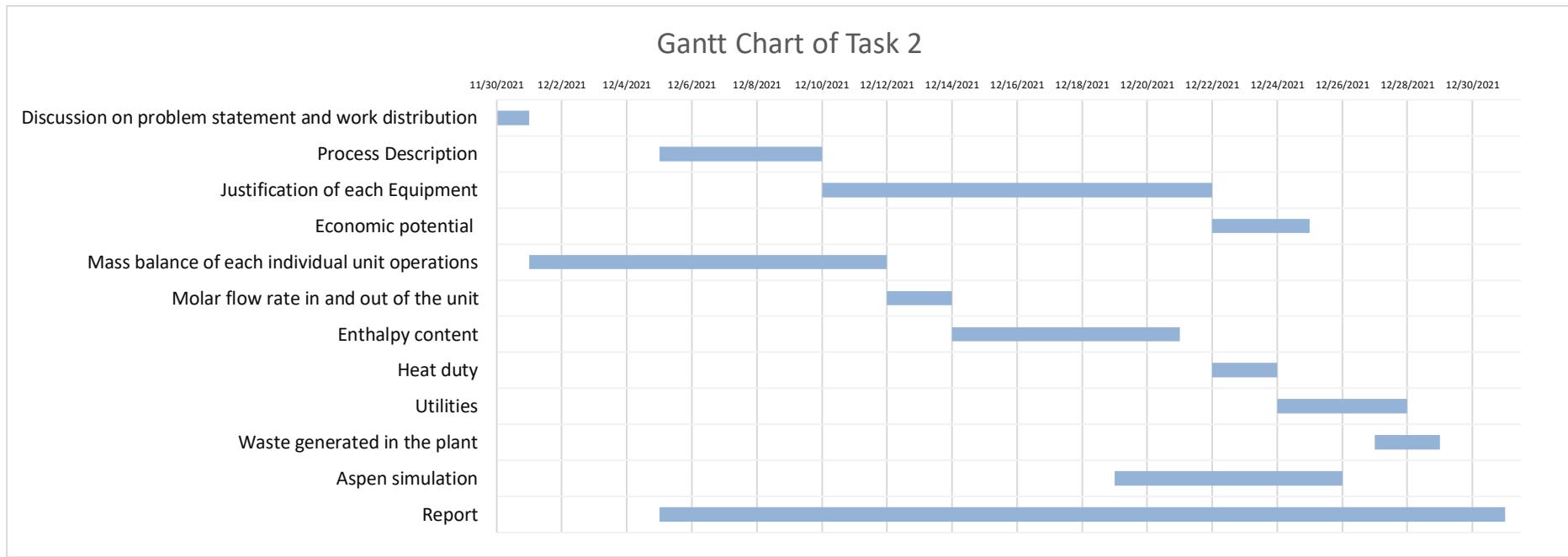
(How Mun Cheng)

APPENDIX I
==GANNT CHART

Gantt Chart Task 1

25/10/2021 26/10/2021 27/10/2021 28/10/2021 29/10/2021 30/10/2021 31/10/2021 01/11/2021 02/11/2021 03/11/2021 04/11/2021 05/11/2021 06/11/2021 07/11/2021 08/11/2021 09/11/2021 10/11/2021





Gantt Chart Task 3

