

Production of food grade CO₂ from HCl



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Certificate

This is to certify that the work in this thesis has been carried out by **Mr. Ali Adil, Mr. Shummas Humayun, and Mr. Qazi Abdullah Hassan** and completed under supervision of Dr. Muhammad Taqi Mehran in School of Chemical and Materials Engineering (SCME), National University of Sciences and Technology (NUST), H-12, Islamabad, Pakistan.

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Dedication

From the grace of Allah, this piece of work is dedicated to our teachers and parents, who were a source of constant support and have helped us in becoming the people we are today.

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We would like to acknowledge the efforts of the dedicated faculty at our School of Chemical and Materials Engineering (SCME NUST). In specific, we would like to thank **Principal SCME, Dr. Arshad Hussain** and **Head of Department, Dr. Bilal Khan Niazi**, who supported us throughout and provided us the resources at SCME that were necessary to carry this project out. Secondly, we would like to acknowledge the constant support of our dedicated project supervisor **Dr. Taqi Mehran** for being a beacon of light for us throughout the project, and for having a steadfast belief in our capabilities. In the end, to all our hardworking and dedicated teachers who pushed us to strive harder at every step, making us mentally competent enough to carry this project out successfully.

We also acknowledge the assistance and cooperation from our industrial supervisor, **M. Afzaal Azeem**, shift engineer, **Sitara Chemicals limited**, for providing us all the information necessary to proceed with our work.

Abstract

The prime aim of this project is to manufacture carbon dioxide through hydrochloric acid of such a purity that can be used in the food and beverage Industry. Currently, hydrochloric acid is produced in an excess amount as a byproduct in Sitara Chemicals Limited. The dumping of such a copious amount of hydrochloric acid is a big problem as it poses a number of environmental risks and hazards. A scheme to purify the carbon dioxide after its production is suggested, which involves a number of prominent chemical processes. The result is 99.8% pure carbon dioxide in a liquid form, which is stored in cryogenic tanks. This highly pure carbon dioxide is suitable enough to be used in a wide range of applications in the food industry, especially in the carbonation of soft drinks.

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Chapter 1: Introduction

1.1 Overview of the project

In Sitara Chemicals, hydrochloric acid is produced in an excess amount. Dumping of this hydrochloric acid is a huge problem as it poses a number of environmental risks and hazards. Rather than dumping this hydrochloric acid, Sitara Chemicals could react it with Calcium Carbonate to produce carbon dioxide with a purity of 99.8%. This pure carbon dioxide can then be sold to beverage and food industries, for food applications.

Our aim is to design an efficient plant for Sitara chemicals that is capable of achieving a carbon dioxide purity of 99.8%.

1.2 Background

Carbon dioxide (CO₂) is a highly abundant atmospheric gas, with content ranging from 350 to 600 parts per million (by volume). The exact carbon dioxide content in the air, however, depends on the location on Earth where it is measured. Nevertheless, one can safely consider it to be the 3rd most abundant atmospheric gas.

Carbon dioxide is highly crucial for the life cycle of plants and animals. The carbon dioxide which is naturally available is readily used by plants in photosynthesis. Similarly, when plants and other organic materials decay (a slow oxidation process), carbon dioxide is released into the atmosphere.

Respiration (breathing), of all humans and animals also gives off carbon dioxide during the exhalation. Similarly, plants also tend to release carbon dioxide as part of the respiration process.

In a similar fashion, volcanic eruptions are also known to release some amount of carbon dioxide into the atmosphere. Apart from the natural processes, industries also play a wide role in releasing carbon dioxide into the atmosphere as a byproduct of processes.

The carbon dioxide that is manufactured industrially is readily used in liquid, gas, solid, and other supercritical forms in a range of commercial processes. For instance, it is commonly used in beverage carbonation, food preservation, manufacturing of chemicals, greenhouses, rubber tumbling, pH depression of wastewater, therapy, medical applications, oil well secondary recovery, mining operations, and the preparation of foundry-mold.

Throughout history, carbon dioxide has avidly been used for the maintenance of value, shelf-life, and quality of vegetables, muscle foods, fruits, and grains.

Chapter 2: Literature review

2.1 The manufacturing of carbon dioxide

J. B. Van Helmont (1577 - 1644) was the first to observe that carbon dioxide was a major product formed as a result of fermentation and combustion processes. Today, we know that copious amounts of carbon dioxide gets produced when carbonaceous fuels are burned.

Similarly, when sugar gets converted into alcohol in the fermentation process, carbon dioxide evolves. Hence, industries readily capture carbon dioxide produced in the fermentation process, during the manufacturing of industrial alcohol. The gas collected from these fermentation vessels then undergoes a purification process for the removal of odors, before being compressed as carbon dioxide into the cylinders.

Carbon dioxide is also captured readily as a by-product in the manufacturing of synthetic ammonia. Other processes in which carbon dioxide is produced as a by-product and captured include decomposition of calcium carbonate to oxide in limekilns, reaction of a carbonaceous material with steam in hydrogen manufacturing, and reaction of phosphoric acid with sodium carbonate in sodium phosphate manufacturing. It is also widely captured from natural carbon dioxide gas wells.

In the industries, a major part of carbon dioxide in liquid form gets manufactured by burning coke. In this process, boilers are used, as a result of which compression of pure carbon dioxide is achieved. At the same time, the boilers furnish the powder and heat, which results in a separation of carbon dioxide from alkaline carbonate solutions. These alkaline carbonate solutions would otherwise absorb the carbon dioxide from the outgoing flue gases.

Since carbon dioxide is a constituent of the flue gases that are produced as a by-product in a range of different industrial chemical processes, it is often separated and retrieved in copious amounts through Stripping. In this process, the outgoing flue gas is dissolved with ethanolamine

(a solvent) within a temperature range of 25 - 65 degrees centigrade. The dissolved gas is then separated from the solvent and retrieved.

After its manufacturing, carbon dioxide is primarily transported in the following ways: rail tank cars with insulations, in insulated trailers as a low pressure liquid, in steel cylinders as a high pressure liquid, and in insulated trailers as ice.

2.2 The applications of carbon dioxide in the food industry

2.2.1 Carbonated beverages

Production of carbonated beverages and soft drinks is one of the oldest and most common modern applications of carbon dioxide. This usage of carbon dioxide is also extended to sparkling wine and beer to some extent, even though carbon dioxide is also produced in the fermentation of alcohol to some extent.

In the United States, about 90% of the carbon dioxide which produced during the 1920s was used in the carbonation of beverages. Since carbon dioxide results in stimulation of the gustatory and olfactory nerves, it results in a 'bite' and gives the beverage a unique pungent taste. At the same time, beverages are also carbonated so that molds do not grow. In some instances, carbonation may also be used to destroy existing bacteria and to inhibit its growth depending on the carbonation extent.

2.2.2 Meat industry

Carbon dioxide is commonly used in slaughterhouses, where animals that are to be slaughtered are driven through carbon dioxide tunnels in which the gas gets injected. On exposure to carbon dioxide the animals are rendered immobilized and their blood pressure increases. As a result of this, a greater amount of blood is recovered. Consequently, it improves the quality of the meat (slower pH decline rate). This method of slaughtering is preferred to

It was found that carbon dioxide results in a far improved meat quality, as compared to the alternate electrical stunning method.

Furthermore, carbon dioxide is also widely used to inhibit the bacteria growth in meat that occurs at a high storage temperature. For this purpose, carbon dioxide content of around 20% is considered to be highly effective. Around 42% of all meat produced in Denmark gets packed under a high carbon dioxide atmosphere. In the United Kingdom, around 29% of the meat produced is packed in this manner, whereas in France it is lower at 15% and in Germany, at 5%.

2.2.3 Monitoring of food quality

Apart from processing and preservation of the food products, carbon dioxide is also readily used to indicate changes of quality in food materials during storage and processing. By using the concentration change in carbon dioxide in grains storage containers, growth of microorganisms such as fungi and presence of insects/pests can be checked.

Similarly, the dry matter loss can also be quantified by measuring the concentration of carbon dioxide produced from in grains including wheat and corn. The extent of this carbon dioxide depends on the temperature, moisture, and mechanical damage.

As a result of this, carbon dioxide content is often related to the quality of the grain. This allows engineers to figure out the optimum conditions of temperature and moisture for storage, at which the quality of grains can be maintained and preserved.

2.2.4 Quick freezing in food industry

Quick frozen foods have been growing in popularity all over the globe. As a result of this, the industry has gone through a great amount of growth. Nowadays, frozen sea foods and meat is top on the list in global trade. It is followed by meals that are ready to eat, fruits, vegetables, and poultry.

The United States ranks at the top in the global frozen food trade. Similarly, European countries including the United Kingdom and Germany are also the prime contenders in this global trade.

2.2.5 Enzyme inactivation

Fatty foods often contains a number of lipolytic microorganisms that include psychotropic bacteria. These bacteria are responsible for the production of the lipase enzyme. The presence of the lipase enzyme could hinder the quality of food.

As an example, in case the lipase enzyme is present in a large amount, it could result in the rancidity of the fatty food. In this regard, carbon dioxide is used. This inactivates the activity of the lipase enzyme, as first tested by Erkmen and Fadilogu. In this test, more than 84% of the enzyme's initial activity was inactivated at a temperature of 50 degrees centigrade and a pH of 7.15, within the first five minutes.

Such treatment with carbon dioxide may be used under atmosphere pressure as a non-thermal liquid food preservation technique. Moreover, this process can also be a substitute for high pressure treatments that are carried out for enzyme inactivation.

In similar tests, the enzyme relates browning in peeled potatoes can also be inhibited by the perfusion of carbon dioxide via immersion water. One reason could be the increased levels of acidity in the water. Nevertheless, this method was developed to substitute the earlier sulfate treatment method for inhibiting the enzyme related browning of peeled potatoes.

2.2.6 Precipitation of protein

A continuous process for the precipitation of casein from milk was developed by Tomasula et al. (1997), through the use of carbon dioxide in a tubular reactor at a pressure less than 14 MPa.

The resulting casein product obtained had pressure and temperature conditions of 5.52 MPa and 38 degrees centigrade. This method has been preferred over other traditional methods including the use of lactic acids, primarily because it carries a number of advantages. Since the residual pH is relatively high at 6.0, the whey does not need a lot of pretreatment. At the same time, it rules out a lot of disposal problems as compared to the conventional methods in which whey with 4.6 pH was obtained.

Similarly, Soy protein can be precipitated by using high pressure carbon dioxide (Khorshid et al. 2007). It has been observed that by using 3.0 MPa of pressurized carbon dioxide around 68.2% of the soy protein precipitated at conditions of around 5.6 pH and 22 degrees centigrade. As compared with the conventional precipitation techniques that involve the use of mineral oil, pressurized carbon dioxide precipitation is more reliable. This is primarily because high pressure it results in food protein of high purity which does not require extensive further treatments for purifications. Apart from that, it is also a clean process.

2.2.7 Other miscellaneous applications of carbon dioxide

Carbon dioxide is very widely used as a reliable inert medium for the displacement of air from the bread manufacturing equipment. This eliminates the bacteria and dust that the air stream in the room often carries (Jones, 1923a).

Carbon dioxide is also commonly used in food packaging, as presence of carbon dioxide prevents odors from accumulating along with oxidation of flavors and vitamins. Similarly, introduction of carbon dioxide can prevent the oxidation in butter in case it is introduced while churning. As a result of this, the time that the butter takes to turn rancid can get delayed significantly. Moreover, carbon dioxide presence is also known to allow citrus fruits to become ripe faster.

Before beating the ice cream mixture, carbon dioxide is often used instead of air. Since ice cream has a greater solubility over air, beating it in the presence of carbon dioxide increases its mechanical strength. Moreover, carbon dioxide present also prevents the oxidation, and enhances the flavor through its bactericidal action on ice cream cones.

Similarly, structured extrudes can be produced when carbon dioxide is injected inside extrusion cookers. This is useful for mixtures of starch-sucrose under high moisture and low-temperature conditions. In similar tests, many industries make use of carbon dioxide with a pressure of 0.1 to 0.6 MPa in order to expand the extrudates of rice flour that has been gelatinized beforehand via twin-screw extrusion.

It has been observed that the bulk specific volume of dehydrated green bell peppers can be increased by puffing them using carbon dioxide at a pressure of around 6.48 MPa. This is also known to increase the rehydration ratio by 143% and 340 respectively, as compared to the use of air. Hence, can be seen that puffing in the presence of carbon dioxide results in a larger bulk specific volume, with a greater rehydration ratio as compared to the air-dried technique.

Moreover, carbon dioxide is also known to have the ability of reducing the pH of food products, and dissolving certain materials. This property of carbon dioxide is avidly used in order to increase the life of membranes in reverse osmosis.

Chapter 3: Proposed solution/Methodology

3.1 Process flow diagram

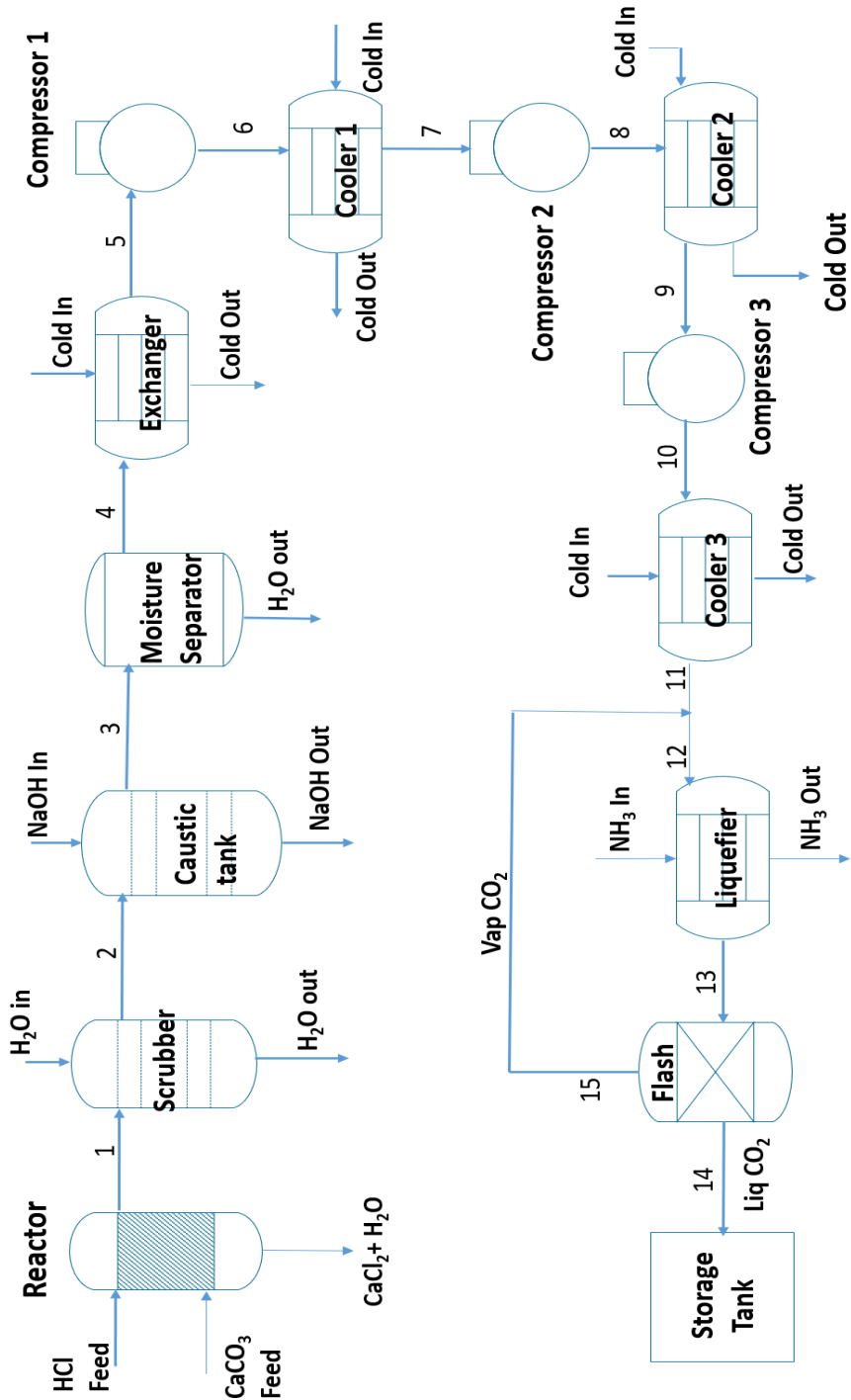


Figure 1.1 Process flow diagram

3.2 List of components

The process that we have proposed consists of the following components:

1. Reactor
2. Scrubber
3. Caustic tank
4. Moisture separator
5. Shell and tube heat exchanger
6. Triple effect compressor
7. Liquefier
8. Flash separator
9. Storage tank

3.3 Process description

The process begins with raw materials, CaCO_3 and hydrochloric acid entering into the reactor, where they react to form CO_2 , CaCl_2 , and H_2O that leave the reactor through. The H_2O and CaCl_2 produced in the reactor leave through an exit stream, and the CO_2 along with some traces of hydrochloric acid and water move into the scrubber.

The scrubber removes the traces of hydrochloric acid by using water, and then the stream moves on to the Caustic tank. The Caustic tank makes use of NaOH to neutralize the acidic CO_2 solution, raising its PH level from 3-4 to 7-8.

After neutralization in the caustic tower, the stream enters a moisture separator where moisture is removed and water leaves through an exit stream. Then, it enters a shell and tube heat exchanger where its temperature gets cooled down from 30 degrees centigrade to 10 – 15 degrees centigrade, at a pressure of 1 bar.

Then, it enters into the triple effect compressor. In the triple effect compressor, the pressure of the resultant stream increase from 1 bar to 6 bar after leaving compressor 1. At this point, the temperature of the stream rises to 150 degrees centigrade.

From here, the stream is sent into the first intercooler, which cools it down so that it is easier to compress it further. After leaving the first intercooler, the stream has a pressure of 6 bar and a temperature of 48 degrees centigrade.

Now, the stream enters the second compressor. After leaving it, its pressure rises to 12 bar and at the same time, temperature goes up to 180 degrees centigrade. Again, cooling is required so that the work requirements to compress it further are reduced.

Hence, the stream enters the second intercooler. After leaving the second intercooler, the stream has a pressure of 12 bar and a temperature of 40 – 45 degrees centigrade.

Now, the stream enters the third compressor where its pressure is raised from 12 bar to 24 bar. At the same time, the temperature increases to 130 degrees centigrade which is pretty high. Again, the stream is sent to an intercooler where the temperature is reduced to 40 – 45 degrees centigrade while the pressure remains high i.e. 24 bar.

After that, the stream enters a liquefier tank where the phase change of CO₂ from vapor to liquid occurs by cooling it down from 40 – 45 degrees Centigrade to -22 degrees Centigrade through a heat exchange process. In this heat exchange process, ammonia is used as a coolant.

After the stream leaves the liquefier, it enters a flash tank which primarily separates the vapor and liquid phases. The uncondensed vapor content from the flash tank is recycled back to the liquefier for further condensation, whereas the liquid phase moves forward and is stored into a storage tank at a pressure of 24 bar and temperature of -22 degrees Centigrade.

Chapter 4: Material balance

Throughout the material balance, we make use of the fundamental equation of conservation of mass on each stream.

Mass flow in = Mass flow out

Basis: 1 hour

Units: kmol/hr

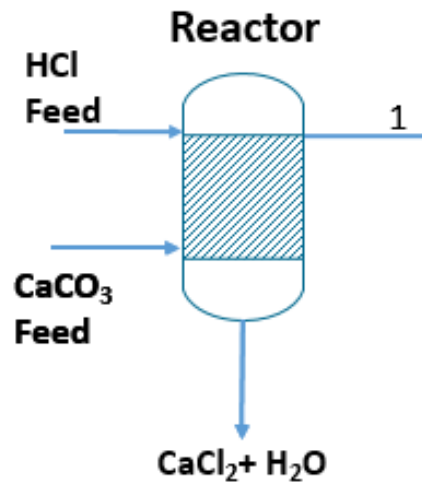


Figure 4.1 Reactor

R-100					
Components	HCl feed	CaCO ₃ Feed	1	CaCl ₂ + H ₂ O	CO ₂ Purity(%)
HCl	81.50	0.00	0.32	0.01	
CaCO ₃	0.00	50.00	0.00	9.41	
CO ₂	0.00	0.00	40.57	0.02	
CaCl ₂	0.00	0.00	0.00	40.59	
H ₂ O	0.00	0.00	6.02	34.61	
Total	81.50	50.00	46.91	84.64	86.48

Table 4.1 Reactor material balance

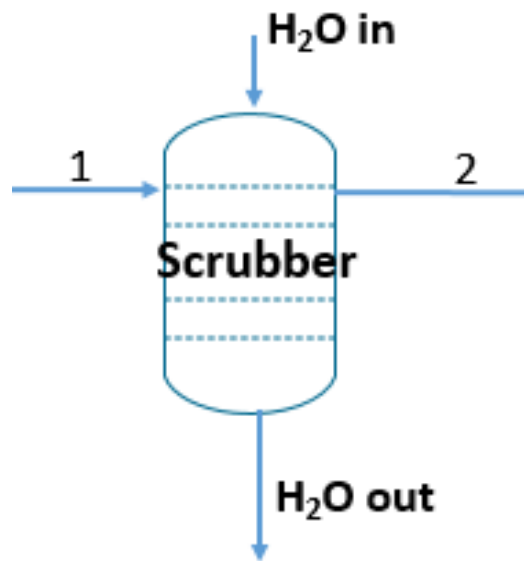


Figure 4.2 Scrubber

Scrubber					
Components	H2O in	1	2	H2O Out	CO2 Purity(%)
CaCO ₃	0.00	0.00	0.00	0.00	
CO ₂	0.00	40.57	40.53	0.04	
CaCl ₂	0.00	0.00	0.00	0.00	
H ₂ O	194.44	6.02	2.18	198.28	
HCl	0.00	0.32	0.22	0.10	
Total	194.44	46.91	42.93	198.42	94.41

Table 4.2 Scrubber material balance

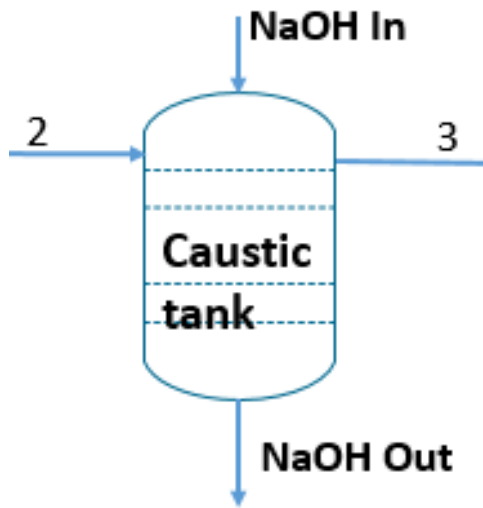


Figure 4.3 Caustic Tower

Caustic Tower					
Components	NaOH in	2	NaOH out	3	CO2 Purity(%)
HCl	0.00	0.22	0.17	0.05	
CaCO3	0.00	0.00	0.00	0.00	
CO2	0.00	40.53	0.00	40.53	
CaCl2	0.00	0.00	0.00	0.00	
H2O	3.40	2.18	3.40	2.18	
NaOH	1.60		1.60		
Total	5.00	42.93	5.17	42.76	94.78

Table 4.3 Caustic Tower material balance

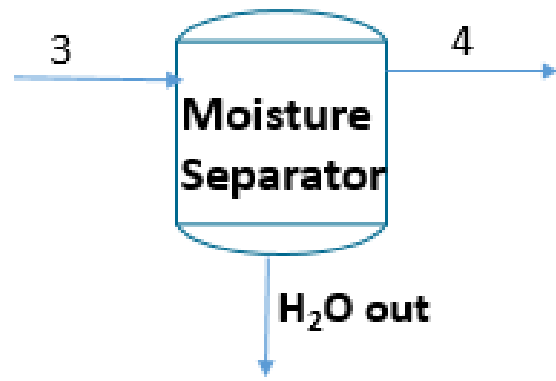


Figure 4.4 Moisture separator

Moisture Separator				
Components	3	4	H2O Out	CO2 Purity
HCl	0.05	0.05	0.00	
CaCO ₃	0.00	0.00	0.00	
CO ₂	40.53	40.53	0.00	
CaCl ₂	0.00	0.00	0.00	
H ₂ O	2.18	0.03	1.99	
Total	42.76	40.61	1.99	99.81

Table 4.4 Moisture separator

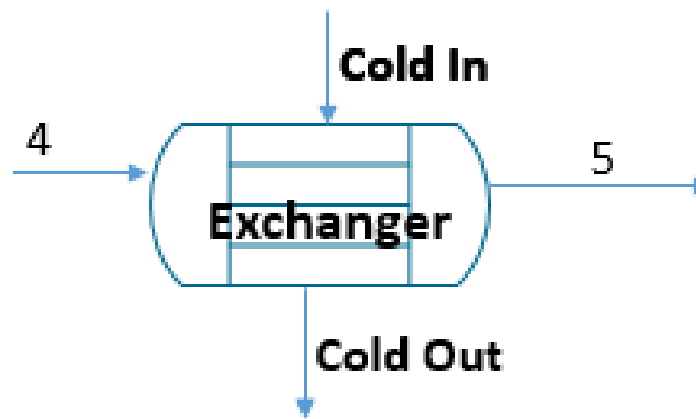


Figure 4.5 Heat exchanger

Exchanger				
Component	4	Cold In	5	Cold Out
HCl	0.05	0.00	0.05	0.00
CaCO ₃	0.00	0.00	0.00	0.00
CO ₂	40.53	0.00	40.53	0.00
CaCl ₂	0.00	0.00	0.00	0.00
H ₂ O	0.03	0.00	0.03	0.00
NH ₃	0.00	58.82	0.00	58.82
Total	40.61	58.82	40.61	58.82

Table 4.5 Heat exchanger material balance

Compressor 1

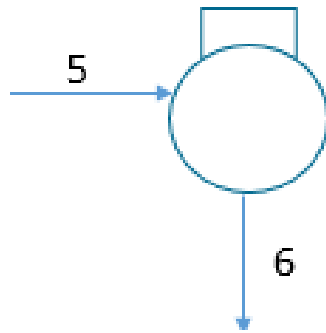


Figure 4.6 Compressor

Compressor (COMP 1)		
Components	5	6
HCl	0.05	0.05
CaCO ₃	0.00	0.00
CO ₂	40.53	40.53
CaCl ₂	0.00	0.00
H ₂ O	0.03	0.03
Total	40.61	40.61

Table 4.6 Compressor material balance

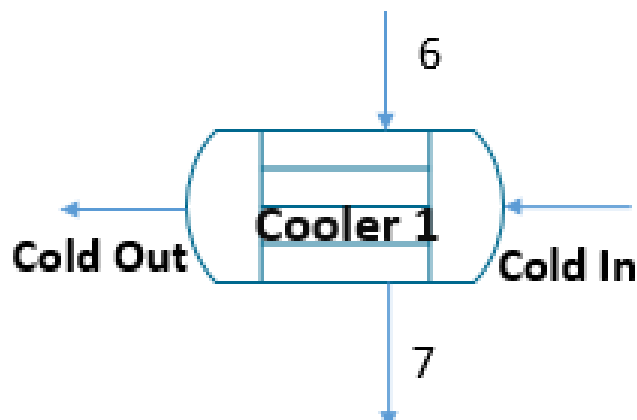


Figure 4.7 Cooler 1

COOLER 1					
Components	6	Cold in	7	Cold out	CO2 Purity
HCl	0.0521	0	0.0521	0	
CaCO3	0	0	0	0	
CO2	40.5267	0	40.5267	0	
CaCl2	0	0	0	0	
H2O	0.02655	352.941	0.02655	352.9411	
Total	40.60535	352.9411	40.60535	352.9411	99.80630631

Table 4.7 Cooler 1 material balance

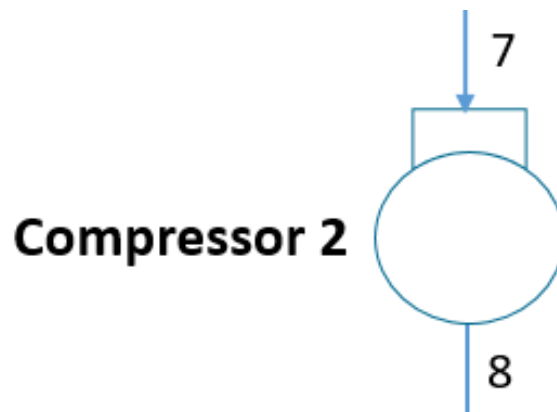


Figure 4.8 Compressor 2

Compressor (COMP 2)		
Components	7	8
HCl	0.05	0.05
CaCO ₃	0.00	0.00
CO ₂	40.53	40.53
CaCl ₂	0.00	0.00
H ₂ O	0.03	0.03
Total	40.61	40.61

Table 4.8 Compressor material balance

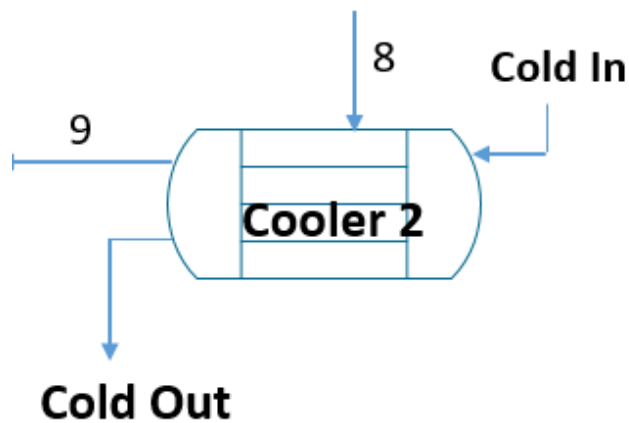


Figure 4.9 Cooler 2

COOLER2				
Components	8	H2O In	9	H2O Out
HCl	0.0521	0	0.0521	0
CaCO ₃	0	0	0	0
CO ₂	40.5267	0	40.5267	0
CaCl ₂	0	0	0	0
H ₂ O	0.02655	126.47	0.02655	126.47
Total	40.60535	0	40.60535	0

Table 4.9 Cooler 2 material balance

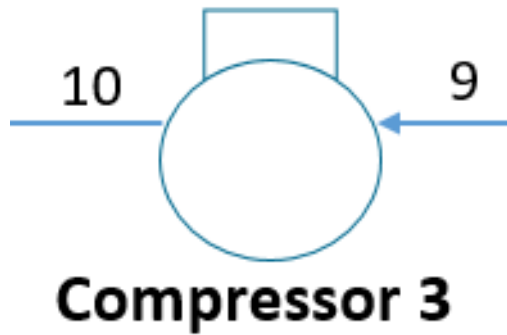


Figure 4.10 Compressor 3

Compressor (COMP 3)		
Components	9	10
HCl	0.05	0.05
CaCO ₃	0.00	0.00
CO ₂	40.53	40.53
CaCl ₂	0.00	0.00
H ₂ O	0.03	0.03
Total	40.61	40.61

Table 4.10 Compressor 3 material balance

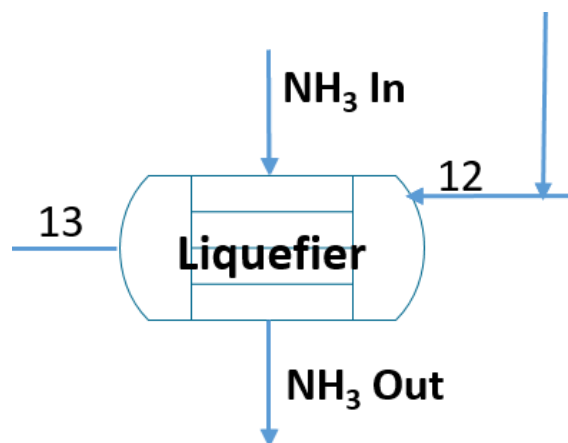


Figure 4.11 Liquefier

Liquifier					
Component	11	H2O In	13	H2O OUT	15
HCl	0.05	0.00	0.05	0.00	0.00
CaCO ₃	0.00	0.00	0.00	0.00	0.00
CO ₂	40.53	0.00	40.53	0.00	0.73
CaCl ₂	0.00	0.00	0.00	0.00	0.00
H ₂ O	0.03	0.00	0.03	0.00	0.01
NH ₃	0.00	88.24	0.00	88.24	0.00
Total	40.61	88.24	40.61	88.24	0.74

Table 4.11 Liquifier material balance

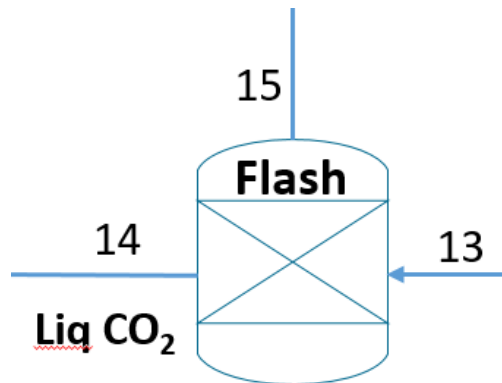


Figure 4.12 Flash vessel

Flash Vessel				
Component	13	14	15	CO ₂ Purity
HCl	0.05	0.05	0.00	
CaCO ₃	0.00	0.00	0.00	
CO ₂	40.53	39.80	0.73	
CaCl ₂	0.00	0.00	0.00	
H ₂ O	0.03	0.02	0.01	
Total	40.61	39.87	0.74	99.83

Table 4.12 Flash vessel material balance

Chapter 5: Energy balance

For the energy balance, we have used the equations:

$$Q = mc_p\Delta T$$

$$Q = \Delta H$$

$$\Delta H = 0$$

All units for enthalpy are kJ and J

Basis is 1 hour

Components on which energy balance has been applied include:

- Reactor
- Heat exchanger
- Compressor 1
- Cooler 1
- Compressor 2
- Cooler 2
- Compressor 3
- Cooler 3
- Liquefier
- Flash separator

5.1 Reactor

Components	Specific heats(kJ/kmol.K) - (cp) at 60C
CaCO3	76
HCl	29.15
CaCl2	74.077
CO2	37.3512
H2O	75.37

Components	Hf products
CaCO3	-1136149.1
HCl	-30093.06
CaCl2	-32178481.83
CO2	-15918737.18
H2O	-11493915.73

Components	Enthalpy of formation (kJ/kmol)
CaCO3	-120700
HCl	-92310
CaCl2	-795420
CO2	-393520
H2O	-285830

R-100		
	Reactants	Products
Molar flow(kmol/hr)	131.5	131.5
Enthalpy(kJ)	-13558265	-60757376.9
Temperature (C)	25	60
Heat released (J)	-47199111.9	

Table 5.1 Reactor energy balance

5.2 Heat exchanger

	NH3	5
Enthalpy of Product	-1755.6682	-16554236.54
Temp. C	25	20
Total	-16555992.2	

Component	Cp (KJ/Kmol.K)
NH3	80.05
CO2	36.88
CO2	37.37
H2O	75.3192
H2O	75.24
HCl	29.14
HCl	29.139

	NH3	4
Enthalpy of Reactant	-32308.1116	-16537641.99
Temp. C	15	30
Total	-16569950.11	

Exchanger	
Components	Hf reactants KJ
CaCO3	0
HCl	-4801.76003
CaCl2	0
CO2	-15957211.23
H2O	-575629.0059
Total	-16537641.99

Shell & Tube Exchanger		
	In	Out
Molar flow(kmol/hr)	80.80454	80.80454
Enthalpy(kJ)	-16569950.11	-16555992.2
Temperature (C)	30	15
Heat (Q)	13957.90292	

Table 5.3 Heat exchanger energy balance

5.3 Compressor 1

Compressor	
Components	Hf reactants KJ
CaCO3	0
HCl	-4771.387033
CaCl2	0
CO2	-15926009.46
H2O	-572589.7776
Total	-16503370.62

Compressor	
Components	Hf Products KJ
CaCO3	0
HCl	-4619.140413
CaCl2	0
CO2	-15751270.81
H2O	-556819.3761
Total	-16312709.33

1st Compressor		
	5	6
Molar flow(kmol/hr)	42.63784	42.63784
Enthalpy(kJ)	-16503370.62	-16312709.3
T(C) , P (bar)	50, 1	150,6
Work done (W)	190661.2921	

Table 5.3 Compressor 1 energy balance

5.4 Cooler 1

Cooler1	
Components	Hf reactants KJ
CaCO ₃	0
HCl	-4413.180829
CaCl ₂	0
CO ₂	-15481474.15
H ₂ O	-526115.2376
Total	-16012002.57

	Water	6
Enthalpy of Reactant	-71396904.04	-16012002.6
Temp. C	25	283
Total	-87408906.61	

Cooler1	
Components	Hf Products KJ
CaCO ₃	0
HCl	-4737.955968
CaCl ₂	0
CO ₂	-15890106.38
H ₂ O	-569230.5143
Total	-16464074.85

	Water	7
Enthalpy of Product	-71020638.38	-16464074.9
Temp. C	45	72
Total	-87484713.23	

1st Cooler		
	In	Out
Molar flow(kmol/hr)	292.42584	292.42584
Enthalpy(kJ)	-87408906.6	-87484713.23
T (C), P (bar)	150,6	48,6
Heat (Q)	-75806.62439	

Table 5.4 Cooler 1 energy balance

5.5 Compressor 2

Compressor2	
Components	Hf reactants KJ
CaCO3	0
HCl	-4774.425348
CaCl2	0
CO2	-15929182.01
H2O	-572893.9303
Total	-16506850.36

Compressor2	
Components	Hf Products KJ
CaCO3	0
HCl	-4573.215305
CaCl2	0
CO2	-15693486.07
H2O	-551582.573
Total	-16249641.86

2nd Compressor		
	In	Out
Molar flow(kmol/hr)	42.63784	42.63784
Enthalpy(kJ)	-16506850.36	-16249641.9
T (C), P (bar)	48,6	180,12
Work done (W)	257208.5034	

Table 5.5 Compressor 2 energy balance

5.6 Cooler 2

Cooler2	
Components	Hf reactants KJ
CaCO3	0
HCl	-4573.215305
CaCl2	0
CO2	-15693486.07
H2O	-551582.573
Total	-16249641.86

	Water	8
Enthalpy of Reactant	-26178855.29	-16249641.9
Temp. C	25	180
Total	-42428497.15	

Cooler2	
Components	Hf Products KJ
CaCO3	0
HCl	-4786.574964
CaCl2	0
CO2	-15941790.67
H2O	-574109.9463
Total	-16520687.19

	Water	9
Enthalpy of Product	-26040891.26	-16520687.2
Temp. C	45	40
Total	-42561578.46	

2nd Cooler		
	In	Out
Molar flow(kmol/hr)	134.22674	134.22674
Enthalpy(kJ)	-42428497.1	-42561578.46
T (C), P (bar)	150,12	45,12
Heat (Q)	-133081.3093	

Table 5.6 Cooler 2 energy balance

5.7 Compressor 3

Components	Hf reactants KJ
CaCO ₃	0
HCl	-4786.574964
CaCl ₂	0
CO ₂	-15941790.67
H ₂ O	-574109.9463
Total	-16520687.19

Components	Hf Products KJ
CaCO ₃	0
HCl	-4497.587205
CaCl ₂	0
CO ₂	-15607340.42
H ₂ O	-543911.6548
Total	-16155749.66

3rd Compressor		
	In	Out
Molar flow(kmol/hr)	42.63784	42.63784
Enthalpy(kJ)	-16520687.2	-16155749.66
T (C), P (bar)	45,12	130,24
Work done (W)	364937.5327	

Table 5.7 Compressor 3 energy balance

5.8 Cooler 3

Components	Hf reactants KJ
CaCO3	0
HCl	-4574.22891
CaCl2	0
CO2	-15781706.84
H2O	-559753.593
Total	-16346034.66

	Water	10
Enthalpy of Reactant	-23798977.54	-16346034.7
Temp. C	25	130
Total	-40145012.2	

Components	Hf Products KJ
CaCO3	0
HCl	-4786.574964
CaCl2	0
CO2	-15941790.67
H2O	-574011.3375
Total	-16520588.59

	Water	11
Enthalpy of Product	-23698635.46	-16520588.6
Temp. C	46	40
Total	-40219224.05	

3rd Cooler		
	In	Out
Molar flow(kmol/hr)	125.90054	125.90054
Enthalpy(kJ)	-40145012.2	-40219224.05
T (C), P (bar)	130,24	45,24
Heat (Q)	-74211.84446	

Table 5.8 Cooler 3

5.9 Liquefier

Components	Hf reactants KJ
CaCO ₃	0
HCl	-4801.76003
CaCl ₂	0
CO ₂	-15957211.23
H ₂ O	-5994.5298
Total	-15968007.52

	NH ₃	11
Enthalpy of Reactant	-607443.71	-15968007.52
Temp. C	-70	30
Total	-16575451.23	

Components	Hf Products KJ
CaCO ₃	0
HCl	-4880.706118
CaCl ₂	0
CO ₂	-16031154.19
H ₂ O	-6035.38593
Total	-16042070.29

	NH ₃	13
Enthalpy of Product	-434898.403	-16042070.29
Temp. C	-40	-22
Total	-16476968.69	

Liquefier		
	In	Out
Molar flow(kmol/hr)	128.8773	128.8773
Enthalpy(kJ)	-16575451.23	-16476968.7
Temperature	30	-22
Heat (Q)	98482.53943	

Table 5.9 Liquefier

5.10 Flash Separator

Components	Hf Products KJ	Hf SideStream KJ
CaCO3	0	0
HCl	-4524.723714	-350.778
CaCl2	0	0
CO2	-15731545.77	-302687.7136
H2O	-5295.485494	-771.741
Total	-15741365.98	-303810.2326

	13
Enthalpy of Reactant KJ	-16042156.3
Temp. C	-22
Total	-16042156.34

	14	15
Enthalpy of Product KJ	-15741365.98	-303810.233
Temp. C	-22	25
Total	-16045176.21	

Flash Separator		
	In	Out
Molar flow(kmol/hr)	40.64228	40.64228
Enthalpy(kJ)	-16042156.3	-16045176.21
Heat (Q)	-3019.86718	

Table 5.10 Flash separator energy balance

Chapter 6: Equipment design

6.1 Reactor design

For this process, we have chosen a packed bed reactor (PBR).



$$\text{Rate equation} = -r_A = kC_A C_B$$

$$= C_{B0}^2 \left(\frac{1}{M} - \frac{X_B}{2} \right) (1 - X_B)^2$$

$$M = \frac{C_{B0}}{C_{A0}}$$

6.1.1 Volume of reactor

Hydrochloric acid Conversion (X_B) = 99.6%

$$M = \frac{81.5}{50} = 1.63$$

$$F_{B0} = 81.5 \text{ kmol}$$

$$V/F_{B0} = \int_0^{X_B} \frac{1}{kC_{B0}^2} \times \frac{1}{\frac{1}{M} - \frac{X_B}{2}} dx$$

Put values in this equation to find V

$$\text{Volume} = 40 \text{ m}^3$$

6.1.2 Length of packing

Height to diameter ratio = 8:1

$$\text{Height} = 8D$$

Volume = Height x Area

$$40 = 8D \times \pi D^2/4$$

$$D = 1.85 \text{ m}$$

$$\text{Height} = 8 \times 1.85 = 14.83 \text{ m}$$

$$\text{Length of packing} = 14.83 \text{ m}$$

6.1.3 Calculating pressure drop

$$\text{Length of packing} = 14.83 \text{ m}$$

$$\text{Viscosity of hydrochloric acid } (\mu) = 2.1 \text{ mPa.s}$$

$$\text{Void fraction } (\epsilon) = 0.5$$

$$\text{Packing particle length} = 3 \text{ mm}$$

$$\text{Particle diameter } (D_p) = 1 \text{ mm}$$

$$\text{Liner velocity } (v_s) = 1.2 \text{ m/s}$$

$$\text{Packing density of material} = 0.62$$

Substituting these values in main equation of pressure drop

$$\Delta P = \frac{150 \mu L}{D_p^2} \frac{(1-\epsilon)^2}{\epsilon^3} v_s + \frac{1.75 L p}{D_p} \frac{(1-\epsilon)}{\epsilon^3} v_s |v_s|$$

$$\Delta P = 29647.5 \text{ Pa} = 4.3 \text{ psi}$$

6.2 Heat Exchanger Design

6.2.1 General Description

Shell and tube heat exchangers are considered to be one of the most common types of heat exchangers, primarily because it offers a great amount of flexibility to the designer for allowing a wide range of temperatures and pressures.

Shell and tube exchangers are generally divided into two main categories. These include:

- Heat exchangers in petrochemical industries that cover the TEMA (Tubular Exchanger Manufacturers Association) standards.
- The heat exchangers are employed in the power industry, such as power plant condensers and feed-water heaters.

There are a number of tubes that are mounted inside the cylindrical shell of a typical shell and tube heat exchanger. The figure below shows a typical shell and tube heat exchanger unit, commonly employed in petrochemical plants. This type of heat exchanger involves the use of two fluids that exchange heat among each other. One of these fluids flows through the outer part of the tubes whereas the other liquid flows inside the tube. These fluids may be two-phase fluids or single-phase fluids. Moreover, they can either flow in a counter/cross flow arrangement or a parallel arrangement.

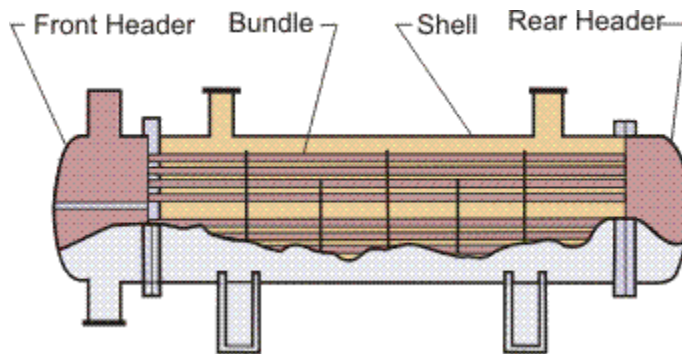


Figure 6.1 Shell and tube heat exchanger

There are four major parts of a heat exchanger. These include:

- The front header: the front header is the part of the heat exchanger through which the fluid enters into the tube side of the heat exchanger. The front header is also commonly known as ‘Stationary Header’.
- The rear header: the rear side is where the fluid in the tube side exists the heat exchanger.
- Shell: the shell is the area in which the tube bundle is contained.
- Tube bundle: the tube bundle contains the tube sheets, tie rods, baffles, and tubes. It primarily holds the entire bundle together.

The figures below show the main components of shell and tube heat exchangers.

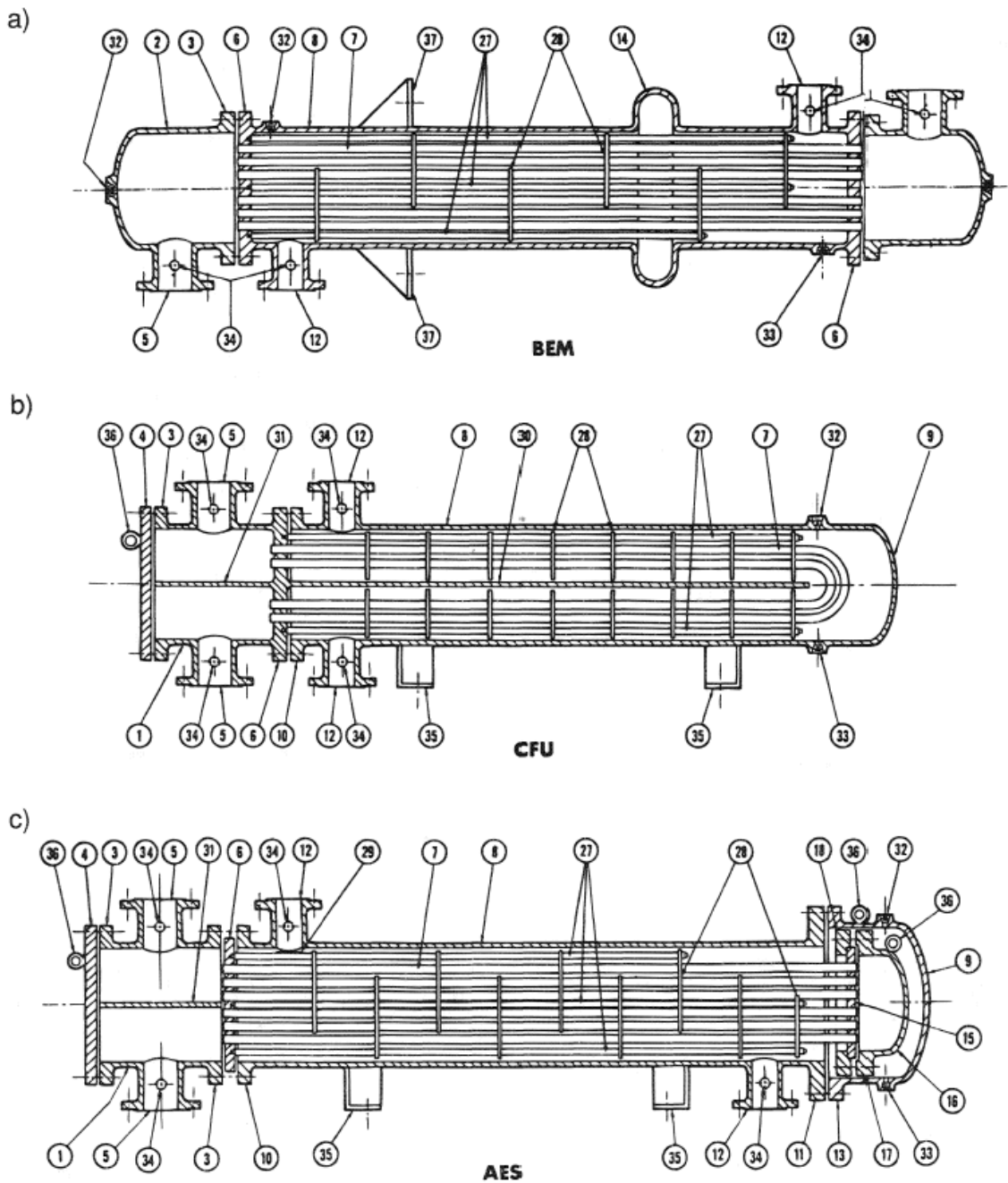


Figure 6.2 Types of shell and tube heat exchanger

- 1 Stationary (Front) Head—Channel 20 Slip-on Backing Flange
- 2 Stationary (Front) Head—Bonnet 21 Floating Tube sheet Skirt

3	Stationary (Front) Head Flange	22	Floating Tube sheet Skirt
4	Channel Cover	23	Packing Box Flange
5	Stationary Head Nozzle	24	Packing
6	Stationary Tube sheet	25	Packing Follower Ring
7	Tubes	26	Lantern Ring
8	Shell	27	Tie Rods and Spacers
9	Shell Cover	28	Transverse Baffles or Support Plates
10	Shell Flange—Stationary Head End	29	Impingement Baffle or Plate
11	Shell Flange—Rear Head End	30	Longitudinal Baffle
12	Shell Nozzle	31	Pass Partition
13	Shell Cover Flange	32	Vent Connection
14	Expansion Joint	33	Drain Connection
15	Floating Tube sheet	34	Instrument Connection
16	Floating Head Cover	35	Support Saddle
17	Floating Head Flange	36	Lifting Lug
18	Floating Head Backing Device	37	Support Bracket
19	Split Shear Ring		

6.2.2 Tema Designations

TEMA, which is an abbreviation for Tubular Exchanger Manufacturers Association has developed a standard nomenclature for the use and designation of shell and tube heat exchangers. This is primarily because they are very popular and are commonly employed in a range of industries. A number of diagrams and terms define this nomenclature. For instance, the front header type is defined by the first letter, whereas the second letter defines the type of shell and the third letter defines the type of rear header.

The figure below shows an illustration of the TEMA nomenclature. Whereas the figure above gives us examples of CFU, AES, and BEM heat exchangers.

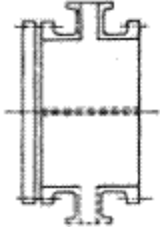

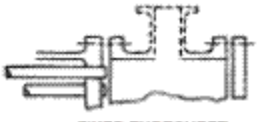
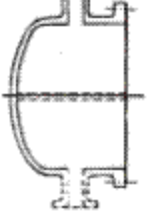

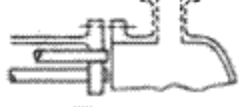
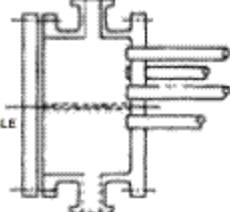
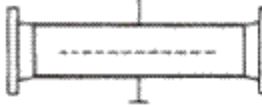

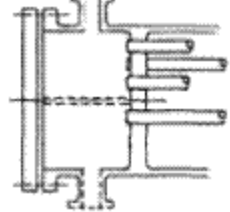
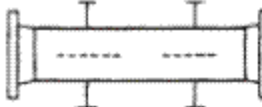
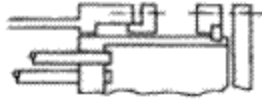
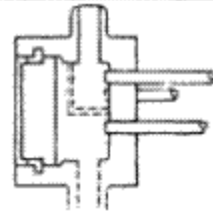


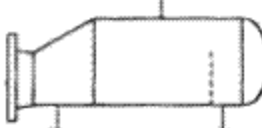
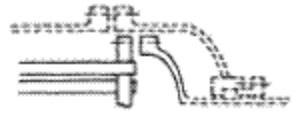
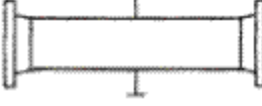
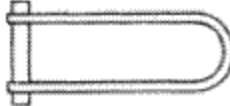

FRONT END STATIONARY HEAD TYPES		SHELL TYPES		READ END HEAD TYPES	
A	 CHANNEL AND REMOVABLE COVER	E	 ONE PASS SHELL	L	 FIXED TUBESHEET LIKE "A" STATIONARY HEAD
B	 BONNET (INTEGRAL COVER)	F	 TWO PASS SHELL WITH LONGITUDINAL BAFFLE	M	 FIXED TUBESHEET LIKE "B" STATIONARY HEAD
C	 REMOVABLE TUBE BUNDLE ONLY CHANNEL INTEGRAL WITH TUBESHEET AND REMOVABLE COVER	G	 SPLIT FLOW	N	 FIXED TUBESHEET LIKE "N" STATIONARY HEAD
N	 CHANNEL INTEGRAL WITH TUBESHEET AND REMOVABLE COVER	H	 DOUBLE SPLIT FLOW	P	 OUTSIDE PACKED FLOATING HEAD
D	 SPECIAL HIGH PRESSURE CLOSURE	J	 DIVIDED FLOW	S	 FLOATING HEAD WITH BASKING DEVICE
		K	 KETTLE TYPE REBOILER	T	 PULL THROUGH FLOATING HEAD
		X	 CROSS FLOW	U	 U-TUBE BUNDLE
				W	 EXTERNALLY SEALED FLOATING TUBESHEET

Figure 6.3 TEMA nomenclature

The table below tells us the most common combinations for E-type shells. However, industries also employ a number of other combinations.

Fixed tube sheet exchangers *U-tube exchangers* *Floating head exchangers*

AEL AEU AES

AEM CEU BES

AEN DEU

BEL

BEM

BEN

In general, there are three main combinations that are used. These include:

- *Fixed tube sheet exchangers*
- *U-tube exchangers*
- *Floating header exchangers*

6.2.3 Fixed Tube sheet Exchanger (L, M, and N Type Rear Headers)

A fixed tube sheet exchanger essentially involves a tube sheet welded on to a shell. As a result of this, a simple construction is obtained, which is not only economic but is also easy to be cleaned both chemically and mechanically. However, it is important to note that the outer surface of the tubes in this heat exchanger remain mechanically inaccessible. Hence, they can only be cleaned chemically.

If there is a big temperature difference between the materials in the tube and shell side, incorporation of expansion bellows will be necessary in the shell. This will remove the excessive stresses that may result from expansion.

6.2.4 U-Tube Exchangers

The rear header in a U-tube exchanger is usually an M-type header. As for the front header, any type can be used. Because of the U-tubes, unlimited amount of thermal expansion is possible. Moreover, it also allows the tube bundle to be removed and cleaned easily. However, it is difficult to clean the tubes internally through mechanical means. Hence, this type of exchanger is normally used in cases where the fluids in the tube side are relatively clean.

6.2.5 Floating Head Exchanger (P, S, T and W Type Rear Headers)

In a Floating Head Exchanger, there is no welding between the shell and the Rear header tube sheet. However, the tube sheet is allowed to float or move. The Front Header tube sheet at the same time, has a large diameter as compared to the shell, and is sealed similar to how it is sealed in a fixed tube sheet reactor design.

Moreover, the rear header tube sheet of the shell has a diameter that is a little smaller than the shell diameter. This allows the bundle to get pulled into the shell. Since a floating head is used, this means that thermal expansion can be accounted for, and tube bundles can be removed easily for cleaning purposes. While there are a number of header types that can be used, the S-type for the rear head is the most common and popular choice.

Floating head heat exchangers are primarily suitable when rigorous duties that are associated with pressures and temperatures. However, these heat exchangers tend to be more expensive as compared to the fixed tube sheet heat exchanger.

6.2.6 Design of Heat Exchanger

Cold fluid: NH₃

Inlet temperature of cold stream = $t_1 = 70\text{ }^\circ\text{C}$

Outlet temperature of cold stream = $t_2 = -40\text{ }^\circ\text{C}$

Inlet temperature of hot stream = $30\text{ }^\circ\text{C}$

Outlet temperature of hot stream = $-22\text{ }^\circ\text{C}$

Heat transfer for CO2

$$C_p = 36.087 \text{ kJ/kmol-K}$$

$$N = 40.89 \text{ kmol/hr}$$

$$\Delta T = - 52 \text{ }^\circ\text{C}$$

$$Q = 36.087 \times 40.89 \times (-52) \\ = - 76731.066 \text{ kJ/hr}$$

Heat transfer for Ammonia

$$N = Q / C_p (\Delta T)$$

$$= - 76721.066 / 73.552 \times 30 \\ = 34.77 \text{ kmol/hr}$$

Calculation of LMTD

$$\text{Hot fluid } T_1 = 30 \text{ }^\circ\text{C}$$

$$\text{Hot fluid } T_2 = - 22 \text{ }^\circ\text{C}$$

$$\text{Cold fluid } t_1 = - 70 \text{ }^\circ\text{C}$$

$$\text{Cold fluid } t_2 = - 40 \text{ }^\circ\text{C}$$

$$\text{LMTD} = 70 - 48 / \ln (70/48)$$

$$\text{LMTD} = 58.3 \text{ }^\circ\text{C}$$

$$R = 52 / 30 = 1.733$$

$$S = 30 / (30 + 70)$$

$$F_T = 0.95$$

$$\Delta T = 0.95 \times 58.3$$

$$\Delta T = 55.385 \text{ }^\circ\text{C}$$

$$\Delta t_c / \Delta t_h = 48 / 70 = 0.6857$$

16 BWG (Birmingham Wire Gauge)

$$\text{OD} = 0.0254 \text{ m}$$

$$\text{ID} = 0.0221 \text{ m}$$

$$\text{Pitch} = 0.03175 \text{ m}$$

$$\text{Tube spacing } C = 0.005$$

$$\text{Baffle spacing} = 0.14 \text{ m}$$

$$\text{Length of tube (l)} = 7.32 \text{ m}$$

$$\text{Area of one tube at} = \pi \times D \times l$$

$$\text{Area} = 3.14 \times 0.0254 \times 7.32 = 0.5838 \text{ m}^2$$

$$\text{Number of tubes} = 350$$

$$\text{Area} = 350 \times 7.32 \times 0.0254 \times \pi = 204.438 \text{ m}^2$$

$$\text{Tube side passes} = n = 2$$

Shell dimensions

$$D_b = \text{OD} (N_t / K_i)^{1/n}$$

$$K_i = 0.156$$

$$n = 2.291$$

$$N_t = 350$$

$$\text{Tube bundle diameter (D}_b\text{)} = 0.737$$

$$\text{Shell bundle clearance} = 11 \text{ mm} = 0.011 \text{ m}$$

$$\text{Shell diameter (D}_s\text{)} = 0.737 + 0.011 = 0.748 \text{ m}$$

$$D_e = 0.0252 \text{ m}$$

$$\text{Shell passes (n)} = 1$$

$$\text{Baffle spacing range is } 0.2 D_s \text{ to } 1 D_s$$

$$B = 0.4 D_s$$

$$= 0.1404 \text{ m}$$

Calculation for film coefficient

Shell side (cold fluid)

$$\text{Flow area in shell} = a_s = ID \times C \times B / P_1$$

$$= 0.1404 \times 0.0221 \times 0.011 / 0.03175$$

$$= 0.0107 \text{ m}^2$$

$$\text{Mass velocity} = G_s = m/a_s$$

$$= 591.1 / 0.0107$$

$$= 55242.99 \text{ kg} / \text{m}^2\text{-hr}$$

$$U = 320 \times 10^{-6} \times 3600$$

$$= 1.152 \text{ kg/m-hr}$$

$$\text{Reynold's number } (R_e) = D_e G_s / \mu$$

$$R_e = 0.0252 \times 55242.9 / 1.152 = 12084.4$$

Value of j_H from graph = 779

Outside film coefficient (K) for ammonia = 1.1436 kJ/m-hr-°C

$$C_p = 4.326 \text{ kJ} / \text{kg}^\circ\text{C}$$

$$J_H = 79$$

$$(\mu / \mu_w)^{0.14} = 1$$

$$h_o = j_H \times K/D \times (C\mu / K)^{1/3} \times (\mu / \mu_w)^{0.14}$$

$$h_o = 79 \times 45.38 \times 1.633$$

$$h_o = 1626.64 \text{ W/m}^2\text{-}^\circ\text{C}$$

Calculation for tube side film coefficients

Tube side (hot fluid)

$$a_t = N_t * a_t' / n$$

N_t = Number of tubes

n = number of passes

a_t' = inside tube area

$$a_t = (350 \times 0.000384) / 2$$

$$a_t = 0.0672$$

Mass velocity = $G_t = m/a_t$

$$\text{Flowrate of CO}_2 = 40.89 \times 44 = 1799.16 \text{ kg/hr}$$

Mass velocity = $G_t = m/a_t$

$$G_t = 1799.16 / 0.0672 = 267732.1 \text{ kg/m}^2$$

Reynolds number (Re) = $D_i \times G_t / \mu$

$$\mu = 0.0135 \text{ centipoise} = 0.0486 \text{ kg/m-hr}$$

Putting values in above equation of Reynolds number we have

$$\text{Re} = 12174.6$$

From the graph,

$$jH = 80$$

Inside film coefficient

$$k = 1.017 \text{ kJ/m-hr-}^\circ\text{C}$$

$$\mu = 0.0486 \text{ kg/m-hr}$$

$$C_p = 0.82 \text{ kJ/kg-}^\circ\text{C}$$

$$\begin{aligned} h_i &= j_H * \frac{k}{D} * \left(\frac{C\mu}{k}\right)^{1/3} * \left(\frac{\mu}{\mu_w}\right)^{0.14} \\ &= 80 * (1.017/0.0221) * ((0.82 * 0.0486) / 1.017)^{1/3} * 1 \\ &= 1250.44 \text{ kJ/m}^2\text{-hr} \end{aligned}$$

$$h_i = 347.34 \text{ W/m}^2\text{-}^\circ\text{C}$$

Calculation for h_{io}

$$h_{io} = h_i * ID/OD$$

$$= 347.34 * 0.0221/0.0254$$

$$h_{io} = 302.2 \text{ W/m}^2\text{-}^\circ\text{C}$$

Overall heat transfer coefficient

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

$$= (302.2 * 1626.64) / (302.2 + 1626.64)$$

$$U_c = 254.85 \text{ W/m}^2\text{-}^\circ\text{C}$$

$$R_d = 0.002$$

For calculating U_d

$$1/U_d = 1/U_c + R_d$$

$$U_d = 168.8 \text{ W/m}^2\text{-}^\circ\text{C}$$

Finding area

$$A = Q / U_d * \Delta T$$

$$= 76731.066 / 168.8 * 55.385$$

$$\text{Area} = 8.21 \text{ m}^2$$

$$R_d = (U_c - U_d) / (U_c * U_d)$$

$$= (254.85 - 168.8) / (254.85 * 168.8)$$

$$R_d = 0.002$$

Pressure Drop

On the shell side:

$$Re = 12084.4$$

$$\text{Friction factor (f)} = 0.0002 \text{ ft}^2/\text{in}^2$$

$$G_s = 55242.9 \text{ kg/m}^2\text{-hr} = 103146.48 \text{ lb/ft}^2$$

$$\text{Specific gravity} = 0.6826$$

$$\text{No. of crosses} = N+1 = L/B$$

$$= 7.32/0.14$$

$$\text{No. of crosses} = 52.14$$

$$\text{Equivalent diameter} = D_e = 0.0252 \text{ m} = 0.0827 \text{ ft}$$

Substituting these values in pressure drop equation=

$$\text{Pressure drop} = \frac{f * G_s^2 * D_s * (N+1) * 144}{5.22 * 10^{10} * D_e * s}$$

Pressure drop = $\Delta P_s = 13$ psi

On the tube side:

Reynolds number = 12174.6

Friction factor (f) = 0.0022

$G_t = 26773.21$ kg/m²-hr = 548673.4 lb/ft²-hr

Specific gravity = 1.5189

Length of tube = L = 7.32 m = 24 ft

Inside diameter of tube (Di) = 0.0221 m = 0.0725 ft

Number of passes (n) = 2

Putting these values in equation of pressure drop=

$$\text{Pressure drop} = \Delta P_t = \frac{f \times G_t^2 \times D_s \times L \times n}{5.22 \times 10^{10} \times D_i \times s}$$

Pressure drop = $\Delta P_t = 2.9$ psi

Return loss = $\Delta P_r = 0$

Total pressure drop = $\Delta P_t + \Delta P_r = 2.9$ psi

6.3 Triple Effect Compressor Design

6.3.1 Multi-Stage Compressors

Multi-stage compressors usually involve the use of reciprocating or piston type compressors. Both of these compressors make use of a cylinder that forces air inside a chamber. In this chamber, the air gets compressed which raises its pressure.

The simplest form of compressor features a single chamber/cylinder arrangement. While this setup may be straightforward and easy to use, it is highly limited in its capacity and efficiency to deliver large volumes of air at a high pressure.

This is where multistage compressors are used. The multi-stage compressors make use of a number of cylinder chambers. Multi-stage compressors tend to work far more efficiently as compared to single stage compressors.

6.3.2 The working of multi-stage compressors

Multi-stage compressors include a number of cylinder chambers, each of which may have a different diameter. In between every single stage, air goes through an intercooler which cools it down. As a result of this cooling, the amount of work that is required to compress the air further gets reduced.

What are the benefits of a multi-stage compressor?

Both the multi-stage and single-stage compressors carry their own benefits. The compressor that is to be chosen will depend on a number of factors and the application.

Typically, the specific advantages of triple-effect compressors over a two-stage compressor include:

- **Greater efficiency:** Multi-effect compressors tend to be more efficient as compared to a two-stage compressor. However, they tend to have higher costs.
- **Better reliability:** A triple-effect compressor reduces the probability of overheating, as a result of which greater productivity and a higher uptime is achieved.
- **Less buildup of moisture:** Cold air tends to have a lower level of moisture. Due to the presence of moisture in a compressed air, premature wear and equipment failure may

result. A three-stage compressor in this case, saves the equipment from getting damaged and the need for an external air dryer is removed. This in turn, saves a lot of costs.

- **Smaller footprint:** Triple effect compressors tend to deliver a higher air pressure as compared to two-stage compressors for applications that require a heavier duty.
- **Fewer requirements for maintenance:** Due to a cooler temperature of air, parts in a triple-effect compressor do not wear out very quickly. Hence, service and maintenance intervals tend to be long.

What are the applications of multi-stage compression?

There are a number of benefits of choosing a multi-stage compressor over a single or even a two-stage compressor. However, multi-stage compressors tend to be more expensive. As a result of this, they are not always the perfect choice for all applications.

In general, for light-duty applications that have a pressure requirement lower than 100 PSIG, single-stage compressors are used.

On the other hand, three-stage compressors provide a better reliability and value for continuous applications that include manufacturing and auto repair.

What are the advantages of multi-stage compression?

- Saves a lot of power as it reduces the work required in compressing the air further.
- Chances of mechanical problems are reduced as the temperature remains controlled.
- The delivery and suction valves are maintained in clean conditions primarily because the vaporization and temperature of the lubricating oil is not high.
- Multi-stage compressors tend to be more balanced and smaller in stature, as a result of which they can easily fit in compact spaces.
- Multi-stage compressors tend to handle the moisture effects far better, due to draining at every stage.
- The compression occurs near isothermal conditions.

- As compared to a single-stage compressor, the compression ratio in a multi-stage compression at every stage tends to be lower.
- The moving parts of a multi-stage compressor are usually lighter and are made of aluminum, as a result of which they are easier to maintain.

6.3.3 Design of a triple effect compressor

The inlet pressures are given as:

Compressor 1: 1 bar = (100000 N/m^2)

Compressor 2: 6 bar = (600000 N/m^2)

Compressor 3: 12 bar (1200000 N/m^2)

The inlet temperatures are given as:

Compressor 1: 50°C

Compressor 2: 48°C

Compressor 3: 45°C

The outlet pressures are given as:

Compressor 1: 6 bar = (600000 N/m^2)

Compressor 2: 12 bar = (1200000 N/m^2)

Compressor 3: 24 bar (2400000 N/m^2)

The outlet temperatures are given as:

Compressor 1: 150°C

Compressor 2: 180°C

Compressor 3: 220 °C

To calculate the intermediate pressure:

$$P_i = \sqrt{P_1 * P_2}$$

Intermediate pressures for each compressor are given as:

$$\text{Compressor 1: } 2.44949 \text{ bar} = 244949 \text{ N/m}^2$$

$$\text{Compressor 2: } 8.485281 \text{ bar} = 848528.1 \text{ N/m}^2$$

$$\text{Compressor 3: } 16.97056 \text{ bar} = 1697056 \text{ N/m}^2$$

Specific heat ratio (n) of $\text{CO}_2 = C_p/C_v = 1.289$

Take the inlet pressure $P_1 = 1 \text{ bar} = 100 \text{ kN/m}^2$, absolute.

Outlet pressure, $P_2 = 6 \text{ bar} = 600 + 100 = 700 \text{ kN/m}^2$, absolute.

For equal work in each stage the intermediate pressure, $P_i = \sqrt{(1 \times 10^5 \times 7 \times 10^5)} = 2.8495 \times 10^5 \text{ N/m}^2$

For air, take ratio of the specific heats γ to be 1.4.

Take the first inlet temperature to be 40 °C. At this temperature the specific volume is given by:

$$v_1 = 44/24.4 \times 323/273 = 2.32 \text{ m}^3/\text{kg}$$

$$v_2 = 44/24.4 \times 321/273 = 2.30 \text{ m}^3/\text{kg}$$

$$v_3 = 44/24.4 \times 318/273 = 2.28 \text{ m}^3/\text{kg}$$

Specific volumes in each compressor are given by:

Compressor 1: 2.324045 m³/kg

Compressor 2: 2.309655 m³/kg

Compressor 3: 2.288069 m³/kg

$$\text{Work done} = P_1 v_1 \times \frac{n}{n-1} [(P_2/P_1)^{(n-1)/n} - 1]$$

$$\text{Work done} = 1 \times 10^5 \times 2.324 \times \frac{1.4}{1.4-1} [(2.8495/1)^{(1.4-1)/1.4} - 1]$$

$$= 230.5899528 \text{ kJ/kg}$$

Work done for each compressor is given as:

Compressor 1: 230.5899 kJ/kg

Compressor 2: 499.4317 kJ/kg

Compressor 3: 989.528 kJ/kg

From the figure 6.4 below,

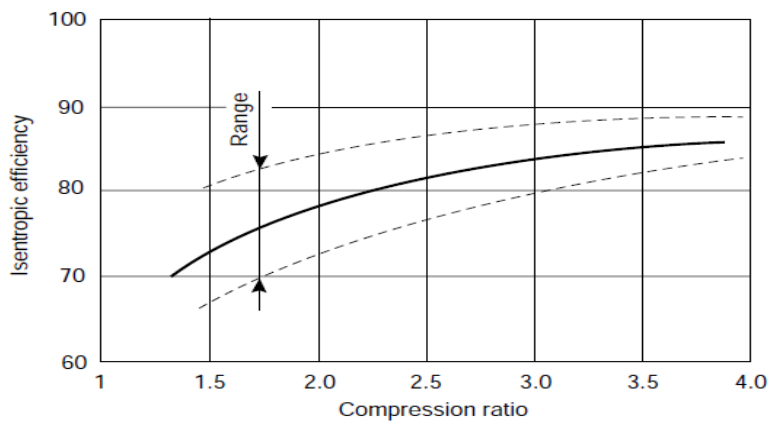


Figure 6.4 Isentropic efficiency vs Compression ratio for triple effect compressors

We can see that for a compression ratio of 2.85 the efficiency is approximately 84%.

So work required = $230.589/0.84 = 274.512$ kJ/kg

Work required for each stage is:

Stage 1: 274.512 kJ/kg

Stage 2: 594.562 kJ/kg

Stage 3: 1178.009 kJ/kg

Mass flow rate of CO₂ = $1800/3600 = 0.5$ kg/sec

So the power required is:

Stage 1 = $274.512 \times 0.5 = 137.256$ kW

Stage 2 = $594.562 \times 0.5 = 297.280$ kW

Stage 3 = $1178.009 \times 0.5 = 589.005$ kW

6.4 Flash Separator Design

A flash separator is a piece of equipment that is used in a number of industrial applications, for the separation of a liquid-vapor mixture. Flash separators are also referred to as vapor-liquid separators, break-pot, compressor suction drum, knock-out pot, and compressor inlet drum.

In cases where a flash separator is used for the removal of suspended droplets of water from a stream of air, it is also referred to as a demister.

6.4.1 Method of operation of Flash Separator

Commonly, liquid settles down below a vertical vessel due to the action of gravity, from where it gets withdrawn. In environments where the action of gravity is minimal such as in a space station, a normal flash separator may not work. This is primarily because gravity will not be present to facilitate the mechanism of separation. In such cases, centrifugal force will be required. This may be achieved through the use of a centrifugal separator which will drive the liquid towards the edges of the chamber. From here, the liquid will then get removed. At the same time, the gases migrate to the center of the chamber.

In both of the flash separator varieties, gas outlets are usually surrounding with a grating or a spinning mesh screen. So in case any liquid approaches the outlet, it strikes with the grating and it is accelerated in the opposite direction, hence being thrown away. At the same time, vapors pass through the outlets for gas with a design velocity that reduces the entrainment of the liquid in vapor, as the vapor passes through.

A liquid that is totally or partially flashed into a liquid and vapor upon entering may also be used as a feed to the flash separator.

6.4.2 The use cases of a Flash Separator

There are a wide number of industrial applications in which Flash Separators are used. These include the following:

Vapor–liquid separators are very widely used in a great many industries and applications, such as:

- Oil refineries
- Petrochemical and chemical plants
- Natural-gas processing plants (NGL)
- Refrigeration systems
- Compressor systems
- Air conditioning
- Gas pipelines
- Geothermal power plants
- Steam condensate flash drums
- Combined cycle power plants
- Soil vapor extraction
- Flare stacks
- Paper mills

6.4.3 Process Design of flash separator

The operating conditions are given as:

Operating temperature = - 24° C

Operating pressure = 24 bar

Liquid density = 771 kg/m³

Vapor density = 1.98 kg/m³

Volumetric flow rate of vapor = 0.00445 m³/sec

Volumetric flow rate of liquid = 0.000636 m³/sec

Vapor velocity is given as:

$$V_v = K_H [(\rho_L - \rho_v) / \rho V]^{0.5}$$

To find K_H we calculate vapor liquid separator factor =

$$\frac{W_l}{W_v} \sqrt{\rho_v / \rho_L} = 2.82$$

Where,

W_l = liquid flow rate

W_v = Vapor flowrate

ρ_L = Liquid density

ρ_v = vapor density

So,

We find value of K_H from graph by locating Vapor Liquid Separation Factor=

$$K_H = 0.1053$$

$$K_v = 1.25 * 0.1053 = 0.131625 \text{ m/sec}$$

Now put values to calculate Vapor Velocity =

$$V_v = 2.075 \text{ m/sec}$$

The minimum vessel cross sectional area is given as:

$$A_{\min} = Q_v / V_v$$

Where,

Q_v = Volumetric Flow rate of Vapor m^3/sec

V_v = Vapor Velocity = 2.075m/sec

Volumetric Flow rate of vapor can be found from:

$$Q_v = m_v/\rho_v = 0.00445 \text{ m}^3/\text{sec}$$

So,

$$A_{\min} = 0.216 \text{ m}^2$$

Calculating the vessel diameter:

$$D = (4A/\pi)^{0.5}$$

Solving this, we get

$$D = (4*0.216/\pi)^{0.5}$$

$$D = 0.137$$

For an increment of 6 inch or 0.1524 m:

$$D = 0.137 + 0.1524 = 0.290 \text{ m}$$

Calculating the hold-up time and hold-up volume:

$$V_H = T_H \times Q_L$$

Where,

T_H = Holdup time, in this case Holdup time from feed to column is around 5 minutes, from the graph

Q_L = Volumetric flowrate of liquid m^3/min

$$Q_L = 0.0382 \text{ m}^3/\text{min}$$

Put all values and calculate V_H

$$V_H = (5 \times 0.0382)$$

$$\text{So Hold up Volume} = 0.191 \text{ m}^3$$

Surge volume can be calculated as:Proc

$$V_s = T_s \times Q_L$$

Where,

T_s = Surge time, in our case surge time from feed to column is 3 minutes, as found from the graph

Q_L = Volumetric flowrate of liquid m^3/min (as calculated previously)

Now put all these and calculate V_s

$$V_s = 3 \times 0.0382$$

$$\text{So Surge volume} = V_s = 0.1145 \text{ m}^3$$

Vapor height can be calculated as:

$$h_v = 1.5D + 1.5$$

Where,

h_v = vapor height

D = vessel diameter

So,

$$h_v = (1.5 \times 0.205) + 1.5$$

$$h_v = 1.935 \text{ m}$$

Liquid height can be calculated as:

$$h_L = (V \times 4) / \pi D^2$$

$$V = Q_L \times \text{surge time} = 0.1146 \text{ m}^3$$

Where,

h_L = liquid height

D = vessel diameter

V = volume of vessel

Now,

$$h_L = (0.1146 \times 4) / \pi \times 0.29$$

$$h_L = 3.481 \text{ m}$$

Total length can be calculated as:

$$L = h_v + h_L$$

Now,

$$L = 1.935 + 3.481$$

$$\text{Total length} = 5.416 \text{ m}$$

$$L/D \text{ ratio} = 5.416 / 0.29 = 18.6$$

As this ratio is greater than five, this proves a satisfactory design and proves it is a horizontal separator.

6.4.4 Mechanical Design of Flash Separator

- Shell thickness
- Head selection

- Head thickness
- Material of construction
- Support selection

Thickness of the vessel

$$T = [PD_1 / (2 * FJ - P)] + Cc$$

Where,

T = thickness

P = Design pressure

F = Maximum allowable stress, kN/m²

J = Welding joint efficiency, 80-90 %

Cc = Corrosion allowance

Now,

$$P = 24 \text{ bar} = 2400 \text{ kN/m}^2$$

For stainless steel

$$Cc = 2 \text{ mm} = 0.002 \text{ m}$$

$$F = 162500 \text{ kN/m}^2$$

Substituting all values in above equation

$$T = 0.00454 \text{ m} = 4.54 \text{ mm}$$

Head Selection

Three types of head:

- Ellipsoidal

- Hemispherical
- Tori spherical

We have chosen Tori spherical head because at the given conditions it is cheaper to fabricate.

Thickness of head

The head thickness can be calculated as

$$T = [P \cdot R_c \cdot C_c / 2FJ + P (C_s - 0.2)]$$

Where,

T = thickness of Head, m

P = Design pressure, kN/m²

R_c = Crown radius

C_s = Stress concentration factor for Tori spherical head

$$C_s = 1/4 [3 + (R_c/R_k)^{0.5}]$$

R_k = knuckle radius

Since R_c/R_k should less than 0.06 to avoid buckling

Suppose,

$$R_c/R_k = 0.04$$

$$D = 0.29 \text{ m}$$

$$R_k = D/2 = 0.29/2 = 0.145 \text{ m}$$

$$R_c = 0.145 \times 0.04 = 0.0058 \text{ m}$$

Substituting R_c/R_k in equation we get,

$$C_s = 1/4 [3 + (0.04)^{0.5}]$$

$$C_s = 0.8$$

$$F = 162500 \text{ kN/m}^2$$

Substituting all values in equation we get,

$$T = 0.000041 \text{ m}$$

Corrosion allowance= 2mm

$$T = 0.000041 + 0.002 = 0.002041 \text{ m}$$

$$T = 2.041 \text{ m}$$

Material of construction

The construction material we used is stainless steel 316

- Comprises of high temperature strength
- Easy to clean
- Better resistance to corrosion and pitting
- Easy to fabricate
- Gives good mechanical properties in case of larger flow rates

Support

There are three types of supports available:

- Skirt type
- Bracket type
- Saddle type

For horizontal vessels, we have selected saddle type. For tall vessels, skirt type is used.

For vessels like vertical or cylindrical, we use bracket type.

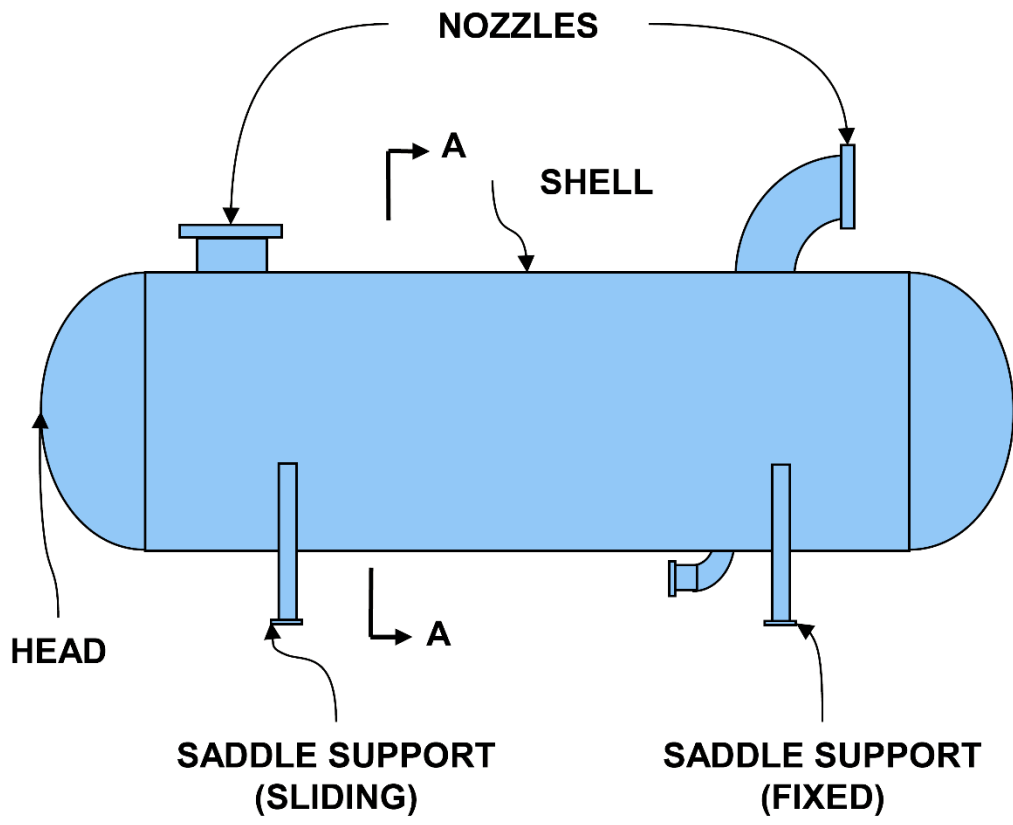


Figure 6.5 Flash separator diagram

Chapter 7: Simulation

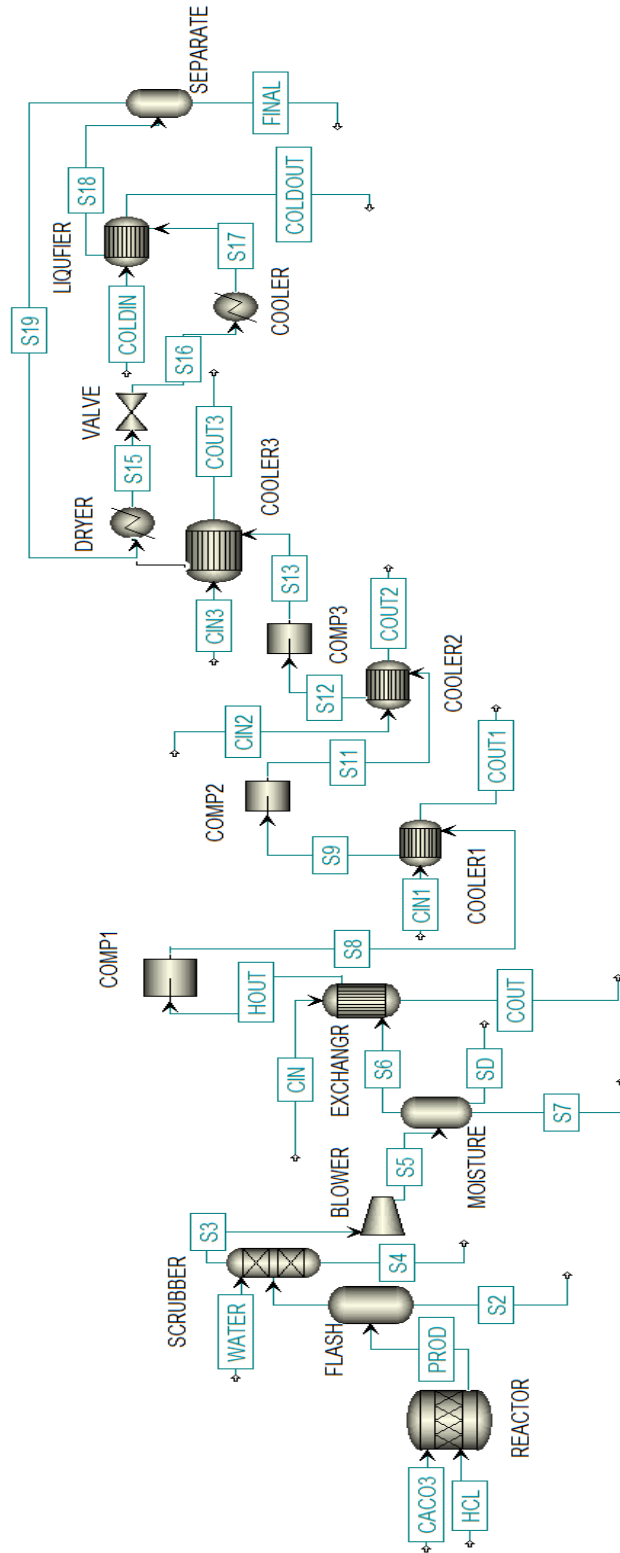


Figure 7 Simulation of the process

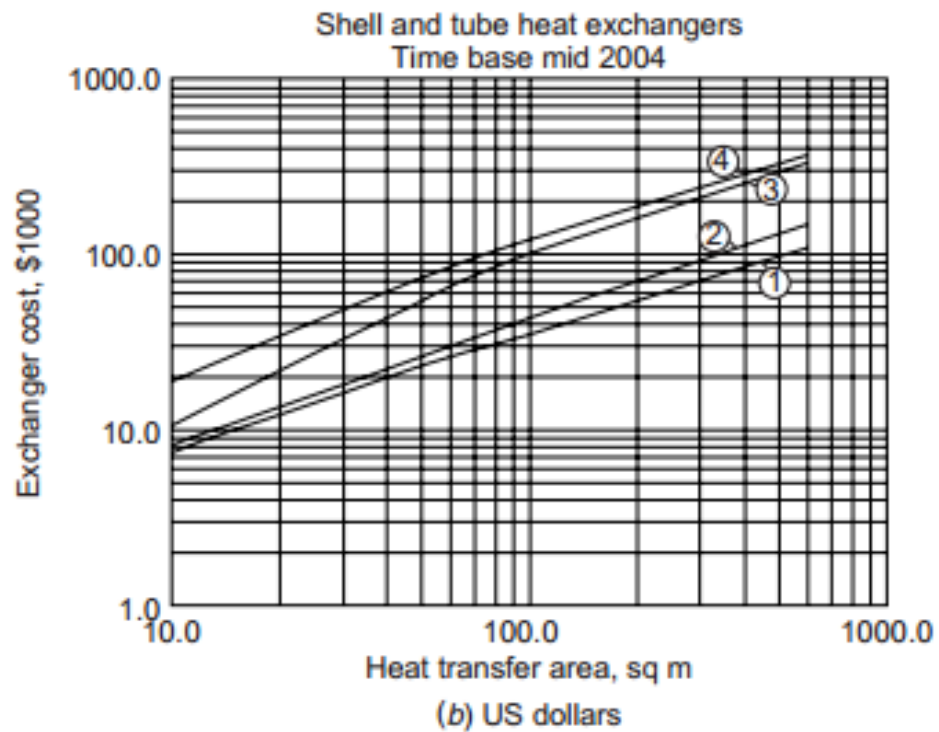
Chapter 8: Costing

8.1 Shell and Tube heat exchanger

The purchase cost for the heat exchanger is given by the following equation:

$$\text{Purchase cost} = \text{bare cost} \times \text{type factor} \times \text{pressure factor}$$

The bare cost is calculated from the figure below:



Materials		Pressure factors		Type factors	
Shell	Tubes				
① Carbon steel	Carbon steel	1–10 bar	× 1.0	Floating head	× 1.0
② C.S.	Brass	10–20	× 1.1	Fixed tube sheet	× 0.8
③ C.S.	Stainless steel	20–30	× 1.25	U tube	× 0.85
④ S.S.	S.S.	30–50	× 1.3	Kettle	× 1.3
		50–70	× 1.5		

Figure 8.1 Shell and tube heat exchangers time base mid 2004

The bare cost has been taken from the book, Coulson Richardson's Chemical Engineering Volume 6, along with the index.

The bare cost is \$7000 (from the figure).

For U-tube, the type factor is 0.85 (from the figure).

The heat transfer area is 8.21 m²

The pressure factor is 1.25 for a pressure of 24 bar (from the figure)

Purchase cost = bare cost x type factor x pressure factor

Purchase cost = 7000 x 1.25 x 0.85 = \$7437.5

8.2 Packed bed reactor

The purchased equipment cost for the packed bed reactor is given by the formula:

$$C_e = CS^n$$

Where C_e = the purchased cost of equipment

S = the characteristic size parameter (from the figure below)

C = cost constant (from the figure below)

n = index for the equipment

Equipment	Size unit, S	Size range	Constant		Index n	Comment
			C, £	C, \$		
<i>Agitators</i>						
Propeller	driver	5-75	1200	1900	0.5	
Turbine	power, kW		1800	3000	0.5	
<i>Boilers</i>						
Packaged						oil or gas fired
up to 10 bar	kg/h steam	$(5-50) \times 10^3$	70	120	0.8	
10 to 60 bar			60	100	0.8	
<i>Centrifuges</i>						
Horizontal basket	dia., m	0.5-1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	$\times 1.7$ for ss
<i>Compressors</i>						
Centrifugal	driver	20-500	1160	1920	0.8	electric,
	power, kW					max. press.
Reciprocating			1600	2700	0.8	50 bar
<i>Conveyors</i>						
Belt	length, m	2-40				
0.5 m wide			1200	1900	0.75	
1.0 m wide			1800	2900	0.75	
<i>Crushers</i>						
Cone	t/h	20-200	2300	3800	0.85	
Pulverisers	kg/h		2000	3400	0.35	
<i>Dryers</i>						
Rotary	area, m ²	5-30	21,000	35,000	0.45	direct
Pan		2-10	4700	7700	0.35	gas fired
<i>Evaporators</i>						
Vertical tube	area, m ²	10-100	12,000	20,000	0.53	carbon steel
Falling film			6500	10,000	0.52	
<i>Filters</i>						
Plate and frame	area, m ²	5-50	5400	8800	0.6	cast iron
Vacuum drum		1-10	21,000	34,000	0.6	carbon steel
<i>Furnaces</i>						
Process						
Cylindrical	heat abs, kW	10^3-10^4	330	540	0.77	carbon steel
Box		10^3-10^5	340	560	0.77	$\times 2.0$ ss
<i>Reactors</i>						
Jacketed, agitated	capacity, m ³	3-30	9300	15,000	0.40	carbon steel
			18,500	31,000	0.45	glass lined
<i>Tanks</i>						
Process	capacity, m ³					
vertical		1-50	1450	2400	0.6	atmos. press.
horizontal		10-100	1750	2900	0.6	carbon steel
Storage						
floating roof		50-8000	2500	4350	0.55	$\times 2$ for
cone roof		50-8000	1400	2300	0.55	stainless

Table 8.1 Index and constants of equipment

$$C_e = CS^n$$

$$\text{Index (n)} = 0.42$$

$$\text{Constant (C)} = \$22000$$

Type = Carbon Steel

$$\text{Size capacity (S)} = 40 \text{ m}^3$$

$$C_e = 22000 \times 40^{0.42} = \$103582.855$$

8.3 Triple effect compressor

The purchased equipment cost for the packed bed reactor is given by the formula:

$$C_e = CS^n$$

Where C_e = the purchased cost of equipment

S = the characteristic size parameter

C = cost constant

n = index for the equipment

Stage 1

Size Range (S) = 137 KW

Constant (C) = \$2700

Index (n) = 0.8

$$C_e = CS^n$$

$$C_e = 2700 \times 137^{0.8} = 138273.9018$$

Stage 2

Size Range (S) = 297 KW

Constant (C) = \$2700

Index (n) = 0.8

$$C_e = CS^n$$

$$C_e = 2700 \times 297^{0.8} = 256784.5699$$

Stage 3

Size Range (S) = 589 KW

Constant (C) = \$2700

Index (n) = 0.8 (from figure 6.2)

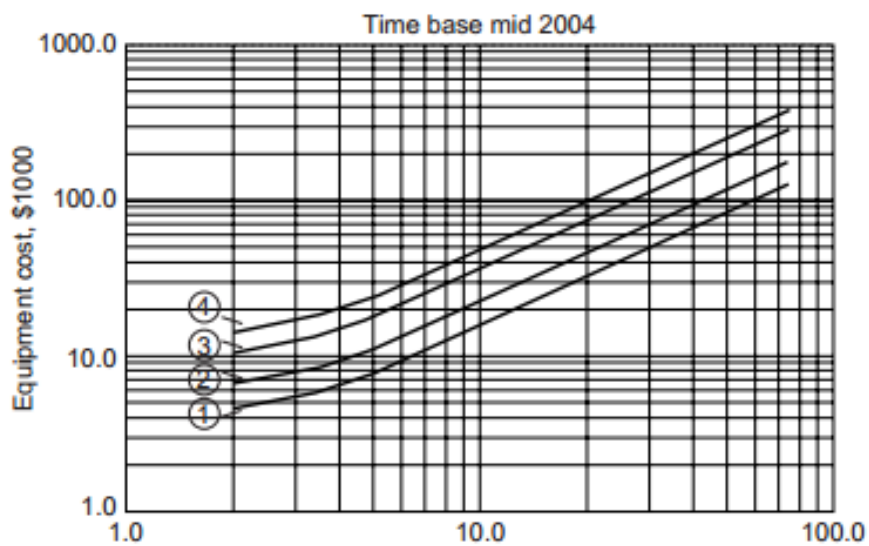
$$C_e = CS^n$$

$$C_e = 2700 \times 589^{0.8} = 444074.6682$$

8.4 Flash Vessel

The purchase cost for the flash vessel is given by the following equation:

Purchase cost = bare cost x type factor x pressure factor



(b) US dollars

Diameter, m		Material factors	Pressure factors
①—0.5	③—2.0	C.S. × 1.0	1–5 bar × 1.0
②—1.0	④—3.0	S.S. × 2.0	5–10 × 1.1
		Monel × 3.4	10–20 × 1.2
		S.S. clad × 1.5	20–30 × 1.4
		Monel × 2.1	30–40 × 1.6
		clad	40–50 × 1.8
			50–60 × 2.2

Temperature up to 300°C

Figure 8.2 Time base mid 2004 for flash vessel

Diameter = 0.2 m

Height = 4.2 m

Bare cost (from figure) = \$4000

Type factor for C.S = 1

Pressure factor for 20 - 30 bars = 1.4

The purchase cost is calculated to be = $4000 \times 1 \times 1.4 = 5600$

Chapter 9: HAZOP Analysis

9.1 HAZOP Analysis on Reactor

No.	Guide Word	Deviation	Consequences	Possible Causes	Action Required
1.	NO	No Flow	Excess calcium carbonate in reactor	Hydrochloric acid supply exhausted. Pipe bursts.	Automatic closure of valve on loss of flow from hydrochloric acid supply.
2.	LESS	Less Flow	Excess calcium carbonate released to work area. Team to calculate toxicity vs. flow	Partially closed valve. Partial plug or leak in pipe.	Calculate toxicity vs. flow reduction. Automatic closure of valve to reduce loss of flow of acid.
3.	MORE	More Flow	Excess hydrochloric acid degrades product	Negligence of machine operator.	
4.	PART OF	Normal Flow of decreased concentration of hydrochloric Acid	Excess calcium carbonate in reactor released, related to	Supply team deliver wrong concentration of material.	Check hydrochloric acid concentration

			quantitative reduction in supply	Error in charging hydrochloric acid supply tank.	after charging its tank.
5.	OTHER THAN	Material flow other than hydrochloric acid in stream	Depends on substitution. Members to test availability of other materials	Supply team wrong delivery. Wrong material chosen.	Plant procedures to provide check on material chosen before charging hydrochloric acid supply tank.

Table 9.1 Hazop Analysis on Reactor

Calcium carbonate reacts with hydrochloric acid to produce calcium chloride and carbon dioxide, results if hydrochloric acid reacts completely. If little hydrochloric acid is added then reaction is incomplete and an unreacted calcium carbonate is formed.

9.2 HAZOP Analysis on Shell & Tube Heat Exchanger (Liquefier)

Guide Word	Deviation	Causes	Consequences	Actions
NONE	No ammonia flow	Failure of inlet ammonia valve to open	carbon dioxide temperature is not lowered accordingly	Install low temperature indicators before and after carbon dioxide flow line
MORE	More ammonia flow	Failure of inlet ammonia valve to close	Output of carbon dioxide temperature is too low	Install low temperature alarm before and after process flow line
LESS	Less ammonia flow	Leakages in pipes	carbon dioxide temperature too low	Installation of flow meter
CONTAMINATION	carbon dioxide contamination	Contamination in ammonia flow	Outlet temperature becomes low	Proper maintenance and operator alert
MORE OF	More pressure on tube sides	Failure in carbon dioxide valve	Bursting of tubes	Installation of high pressure alarms

Table 9.1 Hazop Analysis on liquifier

In the liquefier part, ammonia is passed through shell whereas process fluid (carbon dioxide) passes through tubes. Due to cooling by ammonia, carbon dioxide is liquefied.

Chapter 10: Instrumentation and Process Control

Types of controllers

- **Proportional Controller (P):**
The output from the controller is proportional to error signal. The error signal is basically the difference between the process variable and set point.
- **Proportional Integral Controller (PI):**
This type of controller is used for non-integrating processes. This type of controller is used to remove the offset i.e. it returns back to same output eventually, given the same set of inputs.
- **Proportional Integral Differential Controller:** A continuous calculation of an error value occurs. This error value is the difference between measured process variable (PV) and set point (SP). A correction is applied on the error value based on proportional, integral and derivative terms. It reduces the oscillations in results.

Type of controller selected: We have selected the PI controller for our process and instrumentation control. This controller overshoots and returns back to same output eventually.

10.1 Process control applied over the Reactor

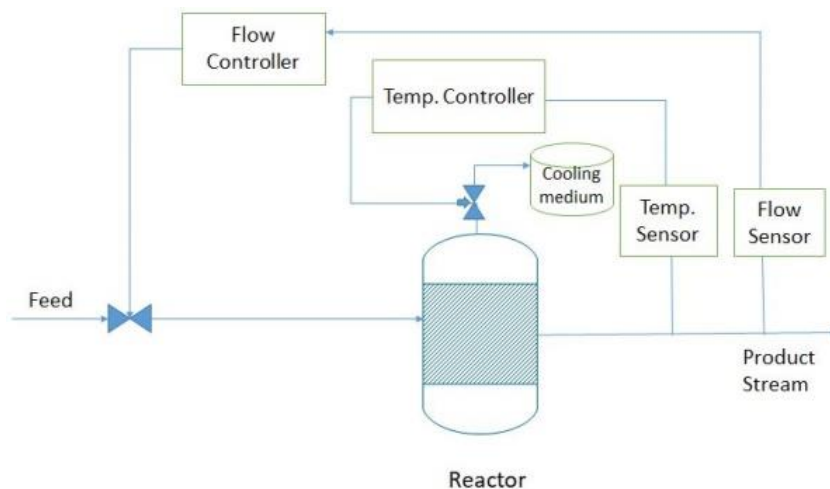


Figure 10.1 process control over reactor

Temperature Sensor:

The sensor will detect a change or increase in heat content or temperature of product stream. The controller will adjust amount of cooling water to cool or bring back the product to required temperature.

Flow sensor:

The sensor will detect a change or deduction in flow of product stream i.e. CO₂. The controller will adjust the flow of feed or raw materials into the reactor to enhance the flow or production of CO₂ as per requirement.

10.2 Process control applied over the heat exchanger

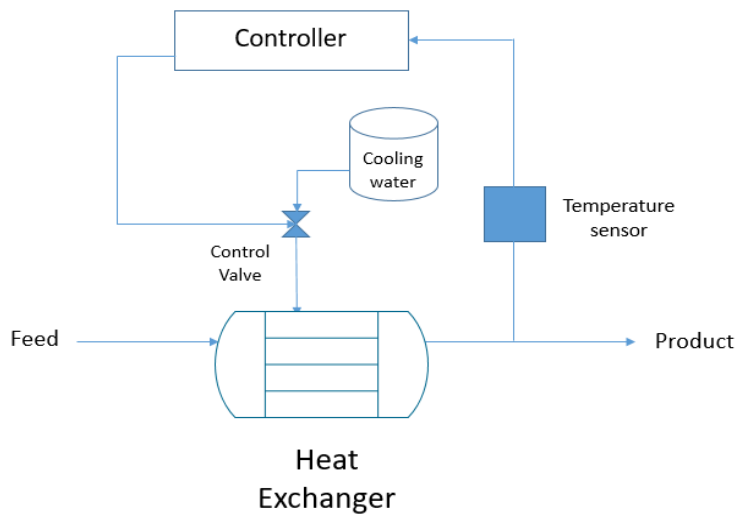


Figure 10.2 process control over heat exchanger

Temperature Sensor:

Here the phase change of CO₂ gas to liquid occurs at -24 °C in the product stream (that is to be maintained). The temperature sensor will detect any change or increase in temperature of product stream. The controller will adjust amount of coolant ammonia (in liquefier) or water (in intercoolers) to cool or bring back the product to required temperature.

Conclusion

We have achieved our desired goal i.e. purifying CO₂ up to a food grade level. We have come up with a purity of 99.8%. This makes our CO₂ product feasible to be used in food and beverage industries.

We have shown all the results in material balance. The purity of CO₂ achieved is shown after each equipment. Finally after the liquefaction and flash separation stage, we are able to store our product of 99.8% purity in cryogenic tanks that are to be supplied to food industries. The CO₂ is kept at -24°C temperature and 24 bar pressure.

The Sitara Chemical Industries proves out to be cheap suppliers of CO₂ to industries. The cost they offer lies around \$231/ton of CO₂.

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