DESIGN AND SIMULATION OF HIGH PRESSURE (HP) UREA SYNTHESIS LOOP

By

Muhammad Talha Tehseen
Sheikh Aliyan Asad
Abdul Moiz Faisal
Suman Tariq

School of Chemical and Materials Engineering

National University of Sciences and Technology

2024

DESIGN AND SIMULATION OF HIGH PRESSURE (HP) UREA SYNTHESIS LOOP

By

Leader – 332659 Muhammad Talha Tehseen
Member 1 – 339043 Sheikh Aliyan Asad
Member 2 – 342426 Abdul Moiz Faisal
Member 3 – 331888 Suman Tariq

A THESIS

Submitted to

National University of Sciences and Technology

in partial fulfilment of the requirements for the degree of

B.E. CHEMICAL ENGINEERING

School of Chemical and Materials Engineering (SCME)

National University of Sciences and Technology (NUST)

June, 2024

CERTIFICATE

This is to certify that work in this thesis has been completed by **Mr. Muhammad Talha Tehseen, Ms. Suman Tariq, Mr. Sheikh Allyan Asad** and **Mr. Abdul Moiz Faisal** under the supervision of Dr. Muhammad Ahsan Khan and Dr. Nouman Ahmed at the school of Chemical and Materials Engineering (SCME), National University of Science and Technology, H-12, Islamabad, Pakistan.

Dr Muhammad Ahsan
Associate Professor
Dept of Chemical Engineering
SCME, NUST H-12, Islamabad

Advisor:

Dr. Muhammad Ahsan

Department of Chemical Engineering
School of Chemical and Materials Engineering
National University of Sciences and Technology

Co-Advisor:

Dr. Nouman Ahmed

Department of Chemical Engineering
School of Chemical and Materials Engineering
National University of Sciences and Technology

Submitted Through:

HOD 5/6/24

Dr. Erum Pervaiz

Department of Materials Engineering
School of Chemical and Materials Engineering
National University of Sciences and Technology

5/6/24

Principal/Dean ....

Dr. Umair Manzoor

School of Chemical and Materials Engineering
National University of Sciences and Technology

DEDICATION

This thesis is dedicated to Allah Almighty for providing direction, strength, and intelligence; to our parents for their unwavering support and encouragement; and to our friends, without whose moral support, this would not have been possible.

ACKNOWLEDGEMENTS

Thank you, **Almighty Allah**, for His innumerable blessings and for providing us with the patience, strength, and drive to complete this project successfully.

A modest thank you to members of our faculty who have assisted us in some way with our issues.

We are really grateful to our supervisors, **Dr. Muhammad Ahsan Khan and Dr. Nouman Ahmed**, for their outstanding assistance with the technical aspects of the projects and for their guidance in solving many issues.

We would especially like to thank **Dr. Waheed Miran** for his assistance with various areas of our study.

Lastly, we would especially like to thank our parents and friends for supporting us throughout these trying times.

ABSTRACT

This thesis explores the design and simulation of a High-Pressure Urea Synthesis Loop employing the Stamicarbon Process. The report commences with a meticulous selection of technology through an extensive literature review, covering fundamental aspects of Urea synthesis and comparing available technologies, specifically Stamicarbon and Snamprogetti. The rationale behind choosing the Stamicarbon process is established, laying the foundation for the planned investigation and future project direction. The thesis outlines a comprehensive process flow diagram, detailing Urea production within the High-Pressure Loop. Key raw materials, including Ammonia and CO2, form the basis of the process, with additional components such as Water/Steam and Air also the part of the process. Detailed specifications of the critical equipment within the High-Pressure Loop are provided including, including the HP Reactor, HP Carbamate Condenser, HP Scrubber, and HP Stripper. Material and energy balances were carefully examined across the equipment. The High Pressure Urea synthesis loop is also simulated with the use of Aspen Plus. There was a strong emphasis on improving the economic aspects of this procedure. Designing and simulating a high pressure Urea synthesis loop requires selecting the optimal configuration and operating parameters to reduce overall annual costs.

TABLE OF CONTENTS

CHAPTER 1

CHAPTER 2

CHAPTER 3

CHAPTER 4

CHAPTER 5

CHAPTER 6

CHAPTER 7

CHAPTER 8

LIST OF TABLES

LIST OF FIGURES

NOMENCLATURE

NH3	Ammonia
C02	Carbon Dioxide
H_2NCONH_2	Urea
NH4CO2NH2	Ammonium Carbamte
O2	Oxygen
N2	Nitrogen
H2O	Water
MP	Medium Pressure
LP	Low Pressure
Cp	Specific Heat Capacity
V	Volume
F_{Ao}	Molar Flow
C_{Ao}	Initial Concentration
τ	Space Time
X_A	Conversion
r_A	Reaction Rate
R	Universal Gas Constant
LMTD	Log Mean Temperature Difference
Pr	Prandtl Number
F_P	Packing Factor

CHAPTER 1

INTRODUCTION

1.1 Project Description:

This thesis focuses on the design and simulation of a high-pressure urea synthesis loop using the Stamicarbon Process. In order to make urea synthesis more practical and feasible on an industrial scale, the initiative intends to take advantage of existing high-pressure infrastructure. Every piece of equipment has its design specifications completed, and the outcomes are displayed through simulations created with ASPEN Plus. Finally, the Economic Analysis and the HAZOP Analysis for the full section are completed efficiently.

1.2 Application of Urea in Industry:

Urea is a versatile compound with widespread applications across industries. In agriculture, it serves as a crucial component in fertilizers, promoting plant growth. The chemical industry utilizes urea in resins, plastics, and adhesives. Urea finds use in textile processing, pharmaceuticals, cosmetics, and as a food additive. Its role extends to de-icing agents, cleaning products, and water treatment. In laboratories, urea acts as a reagent, highlighting its diverse applications in addressing agricultural, industrial, and scientific needs, underlining its significance in various sectors. To sum up following are the uses of Urea in industries:

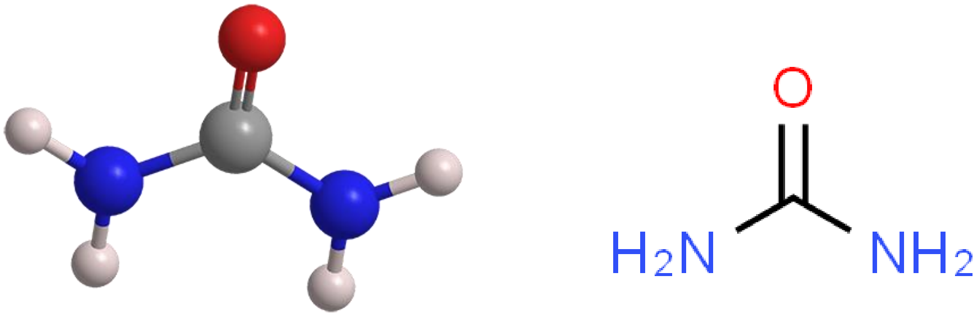


Figure 1: Structure of Urea

- Around 90% of the urea produced worldwide is intended for use as fertilizer.
- Specifically, formaldehyde resin, or urea, is a raw ingredient used in the production of plastics.
- A starting point for the production of several adhesives, such as urea-formaldehyde or urea-melamine-formaldehyde, the latter of which is waterproof and utilized to make marine plywood.

- A flame-proofing substance (such as urea potassium bicarbonate, which is frequently used in dry chemical fire extinguishers).
- Used in cold compressors for first aid due to its endothermic reaction with water.
- Cloud seeding agents and salts speed up the condensation of water in clouds, resulting in precipitation.
- Feedstock for ammonia's hydrolysis, which lowers emissions from combustion engines and power stations

1.3 Importance of High Pressure (HP) Synthesis Loop:

The High-Pressure (HP) urea synthesis loop holds significant importance in urea production, and is a critical section or the following reasons:

- **Efficiency:** The HP urea synthesis loop operates at elevated pressures and temperatures, typically ranging from 150 to 160 bar (2175 to 2320 psi) for pressure and 180 to 220 °C. These conditions crucial for promoting the urea synthesis reaction, as it helps to increase the equilibrium conversion of ammonia and carbon dioxide to urea. Higher pressures favor the formation of urea, leading to improved efficiency in the production process.

- **Yield:** The increased pressure in the HP urea synthesis loop enhances the yield of urea by driving the equilibrium of the reaction towards the formation of urea. This results in higher production rates and greater output of urea from the process.

- **Optimization:** The HP urea synthesis loop allows for the optimization of reaction conditions, such as temperature, pressure, and catalyst performance, to achieve the desired levels of urea production. Fine-tuning these parameters within the high-pressure environment helps to maximize the efficiency and yield of the urea synthesis process.

- **Economic Viability:** Operating at high pressure can be economically advantageous for urea production. While the equipment and infrastructure required for high-pressure operations may involve higher initial costs, the increased efficiency and yield achieved in the HP urea synthesis loop can lead to overall cost savings overall, thus also minimizing the need for extensive equipment modifications.

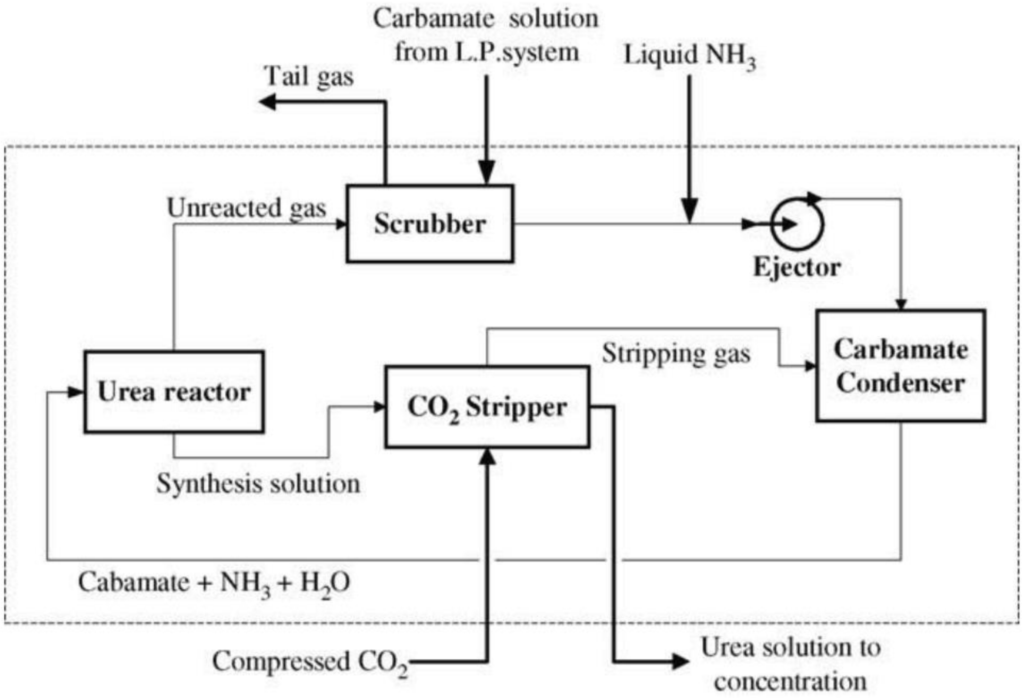


Figure 2: Process Flow Diagram

CHAPTER 2

LITERATURE REVIEW

2.1 Urea

Urea is an organic substance having the chemical formula (CO(NH2)2). The molecule consists of two functional groups connected by a carbonyl (C=O) functional group. Urea, scientifically known as Carbonyl diamide, is made of 45% nitrogen, 20% carbon, 26% oxygen, and 9% hydrogen. It is the most nitrogenous fertilizer in general usage, making it the favored nitrogen fertilizer worldwide. It is utilized in adhesives, formaldehyde resins, and solid and liquid fertilizers.

Urea was initially found in urine by Roulle in 1773. His discovery was succeeded by Whler's 1828 synthesis of urea from ammonia and cyanic acid, the first known synthesis of an organic chemical from an inorganic one. Bassarow conducted the first synthesis of urea by dehydration in 1870 by heating ammonium carbamate in a sealed tube. Globally, urea production is massive, with about 150 × 106 tons produced annually in 2010. Currently, the only industrial processes used to generate urea use NH_3 and CO_2 as the basic materials.

2.2 Physical Properties:

Urea is a white odorless solid. Due to extensive hydrogen bonding with water (up to six hydrogen bonds may form – two from the oxygen atom and one from each hydrogen) Urea is very soluble.

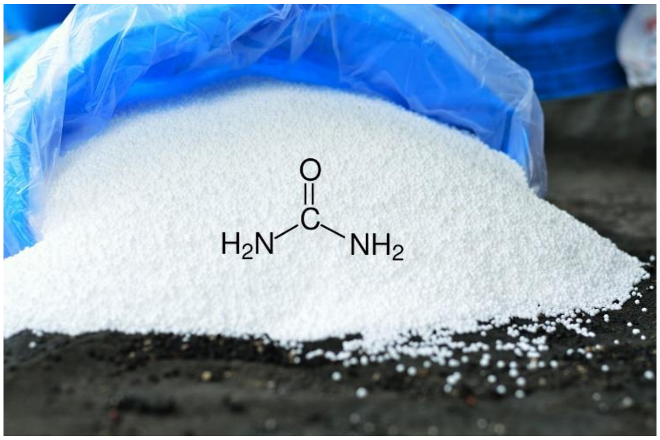


Figure 3: Urea

Table 1: Physical Properties of Urea

Property	Range
Cas Number	57-13-6
Molecular Weight	60.07
Melting Point (°C)	132.7
Boiling Point (°C)	135
Density (gm/cm^3), solid	1.335
Bulk density (gm/cm^3)	0.74
Viscosity, v^{20} (mPa.sec)	1.9
Heat of fusion (J/gm)	251
Heat of solution in water (J/gm)	243
Specific heat, S° (KJ/kg.°C)	1.439
Specific gravity (gm/cc)	1.335
Vapor pressure (Pa)	<10
Solubility in water (g/100ml)	108 (20°C) 167(40°C) 251 (60°C) 400 (80°C) 733(100°C)

2.3 Chemical Properties:

- When urea reaches its melting point and atmospheric pressure, it breaks down into ammonia, biuret, ammelide, and triuret.
- Urea combines with acids to generate salts by acting as a monobasic. Like when nitric acid is used to create urea nitrate $CO(NH_2)_2.HNO_3$.
- Urea interacts with NOx in the gas phase at 800-1150 °C and liquid phase at lower temperatures, producing N_2, CO_2, and H_2O.
- In an acidic environment, urea and formaldehyde react to produce methylene urea and its derivatives (such as trimethylene and dimethylene).
- If urea is diluted with acids, alkalis, or water vapor above 150°C, it will react similarly to amides.

$$\underset{\text{(Urea)}}{NH_2CONH_2} + H_2O \rightarrow 2NH_3 + CO_2$$

2.4 Environmental Effect:

One of the most significant factors in increasing agricultural productivity has been the use of chemical fertilizers; nevertheless, the breakdown of nitrogen fertilizers into nitrates, which are easily absorbed by the soil, has led to the release of ammonia, CO2, and urea into the atmosphere. in addition to their emissions to air and water, because it is soluble in water and can linger in groundwater for a considerable amount of time. Acid rain, contaminated groundwater, and ozone depletion are all caused by urea because the denitrification process releases nitrous oxide. Generally, there are four types of emissions estimating techniques (ETTs) that can be used to estimate emissions from the plant.

. The four types are:

1. Sampling or direct measurement
2. Mass balance
3. Fuel analysis or other engineering calculations
4. Emission factor

2.4.1 Elimination Methods:

Presently plants are equipped with the following features to keep the effluent and Emissions at extremely low levels:

1. N/C ratio meter
2. Waste water treatment section
3. Special operational facilities

N/C ratio meter in the synthesis section:

Instead of a spectrometer in the gas phase of the synthesis section, nitrogen/carbon (N/C) ratio meters are fitted in the liquid phase (reactor liquid outlet) of the urea synthesis section. With the help of this N/C ratio meter, the process may always be run at the ideal ratio to increase both reactor and energy efficiency. Utilizing certain protocols, emissions are removed upon startup.

Waste water treatment section:

Ammonia, carbon dioxide, and urea are removed from the condensate during the water treatment process. Usually, this water is released from the plant's urea concentration and evaporation portion. It might be challenging to eliminate ammonia and urea from wastewater when they are present because of this. The hydrolysis of urea to ammonium carbamate, which breaks down to NH_3 and CO_2, is one way to solve this issue. These gasses can then be eliminated from the wastewater. Depending on the necessary quality, this recovered water can be utilized for several purposes, including cooling water, etc.

2.5 Urea Production Methods:

The production of urea involves multiple steps. To get high efficiency, some of them use traditional methods, while others use contemporary ones. These processes offered several similar benefits and drawbacks in terms of investment costs, upkeep costs, energy costs, productivity, and product quality. Here are a few of the commonly used urea production methods.

2.5.1 **Haber-Bosch Process:**

This is the initial step in urea production. Nitrogen gas (N_2) is reacted with hydrogen gas (H_2) using an iron-based catalyst at elevated temperature and pressure to produce ammonia

$$\mathbf{3N_2 + 3H_2 \rightarrow 2NH_3}$$

2.5.2 Once-Through Urea Process:

It is a traditional method in which the unconverted carbamate (an intermediate component in the urea manufacturing process) is degraded to NH_3 and CO_2 by heating the urea synthesis reactant effluent mixture under low pressure. After being extracted from the urea solution, the NH_3 and CO_2 are absorbed to create ammonium salts.

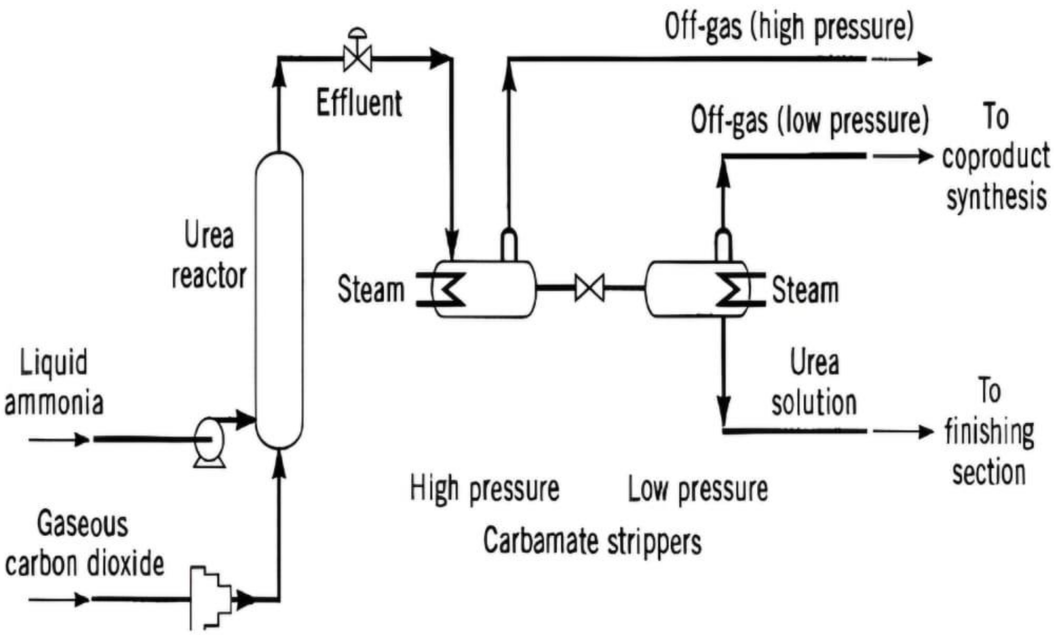


Figure 4: Typical Once-through Urea Process

2.5.3 Partial Recycle Process:

The Partial Recycle Process optimizes urea production by efficiently recycling unreacted ammonia and carbon dioxide. Initially, ammonia is synthesized through the Haber-Bosch process, usually derived from nitrogen and hydrogen. Carbon dioxide, obtained from diverse sources like industrial processes or combustion, is purified for use in urea synthesis. In the urea reactor, ammonia and carbon dioxide undergo a high-pressure, high-temperature reaction, often catalyzed, to form ammonium carbamate, which decomposes into urea. Partial recycling comes into play by reintroducing a portion of unreacted ammonia, carbon dioxide, and some urea back into the reactor, ensuring favorable reaction conditions for improved efficiency and yield. After separation and purification, where liquid urea is separated from gases, the recycled gases, along with unreacted ones, are compressed and returned to the reactor. This method enhances resource utilization, reaction kinetics, and energy efficiency, resulting in elevated production efficiency and reduced costs.

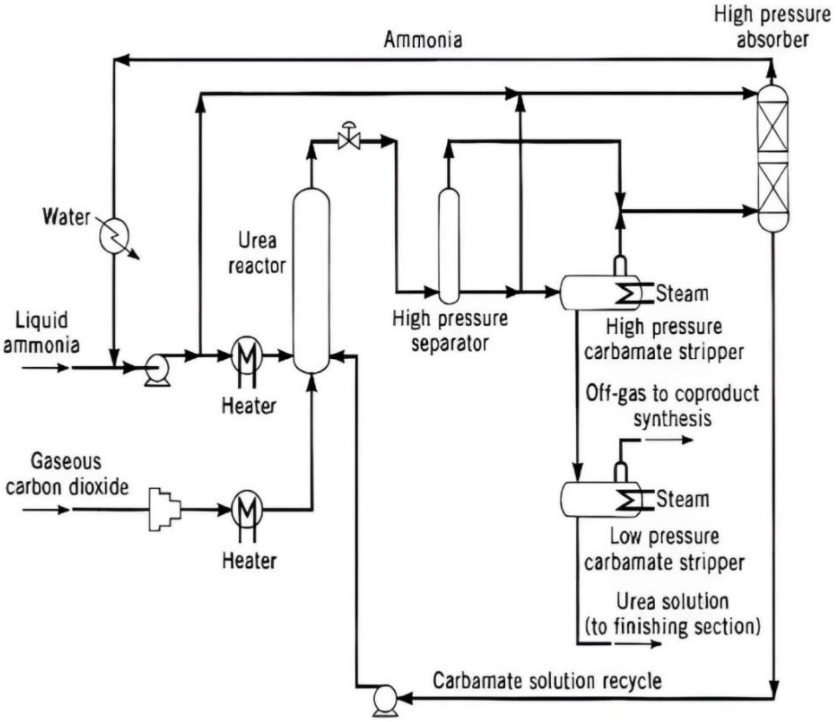


Figure 5: Typical Partial Recycle Process

2.5.4 Stripping Process Based Plants (Internal Carbamate recycle):

Instead of allowing the reactor effluent to drop to a significantly lower Pressure, gaseous CO_2 or NH_3 is used to remove the unreacted carbamate and excess ammonia from the urea Synthesis reactor effluent at the reactor pressure. Condensed and fed back into the reactor by gravity flow, the recovered NH_3 and CO_2 gas is recovered at reactor pressure.

2.5.4.1 Snamprogetti Process:

Urea Synthesis with Desorption:

The Snamprogetti process involves urea synthesis followed by a desorption step to remove excess ammonia. This method aims to improve urea concentration and purity. After the urea synthesis, the solution contains excess ammonia. During the desorption step, by incorporating a high pressure, excess ammonia is removed from the urea solution. This is typically done by applying heat, causing ammonia to be released from the solution. In both the Stamicarbon and Snamprogetti processes, Urea synthesis occurs in two steps. Following are the two reactions for the formation of Urea:

1. $\mathbf{2NH_3 + CO_2 \rightleftharpoons NH_2COONH_4}$
2. $\mathbf{2NH_3 + CO_2 \rightarrow NH_2CONH_2 + H_2O}$

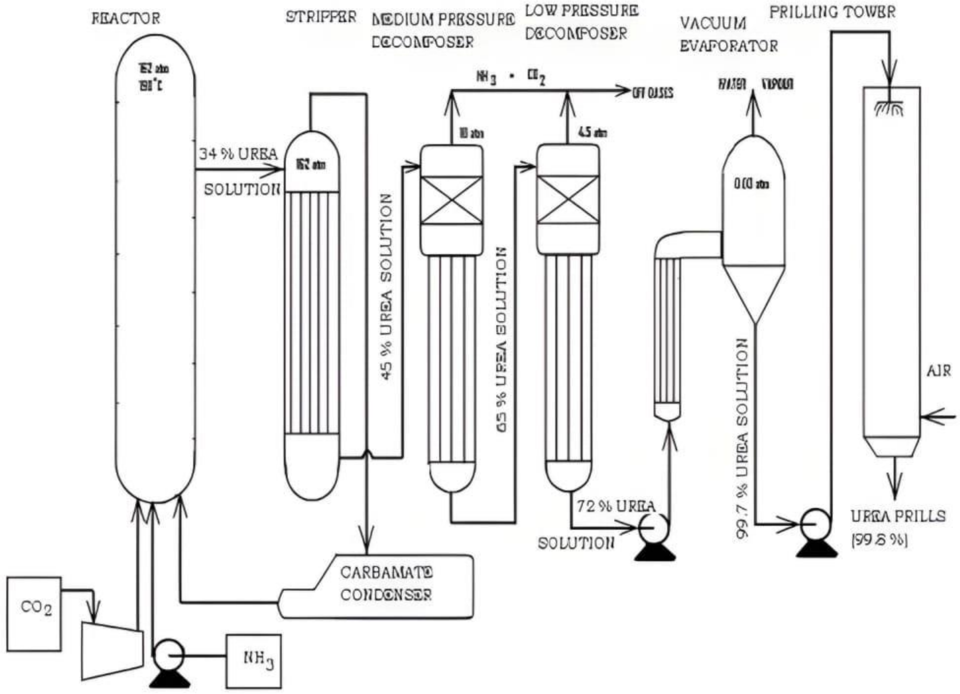


Figure 6: Snamprogetti Process Flow Diagram

2.5.4.2 Stamicarbon CO2 Stripping Process:

In this process, ammonia is reacted with carbon dioxide and the reaction produces urea and water. Developed by Stamicarbon, a Dutch company specializing in fertilizer technology, this process offers certain features that make it efficient and well-suited for large-scale urea production. One of those features is that the synthesis reaction takes place under high pressure and temperature conditions. The elevated pressure helps improve the conversion of ammonia and carbon dioxide into urea. The product of the synthesis reaction is typically a concentrated urea solution. Water is added to this solution to dissolve the urea, forming a liquid product that can be processed further. Moreover, the optional granulation step allows to produce Urea granules, which facilitates handling, storage, and application in the agricultural sector.

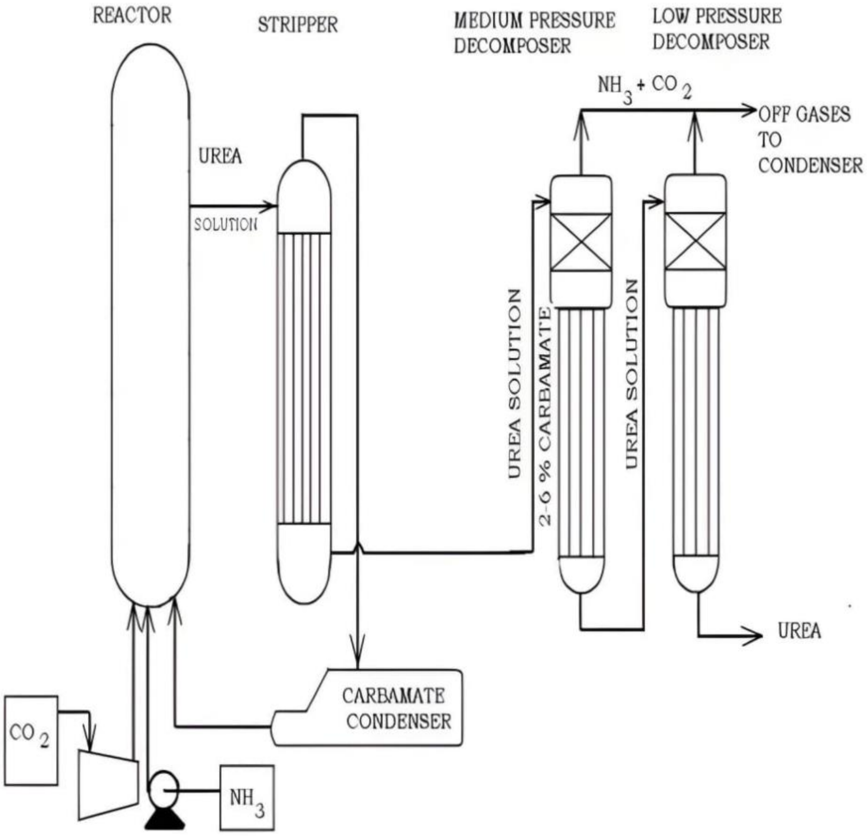


Figure 7: Stamicarbon Process Flow Diagram

2.5.4.3 ACES Process:

Toyo Engineering Corporation created the ACES (Advanced Process for Cost and Energy Saving) process. The reactor, stripper, two parallel carbamate condensers, and scrubber are all part of the synthesis section and are all run at 175 bar. The reactor is run at 190°C with a 4:1 molar feed ratio of NH_3 to CO_2. There are five primary sections in all. Sections 1 through 5 include:

1. Synthesis;

2. Purification;

3. Concentration and prilling;

4. Recovery; and

5. Process condensate treatment.

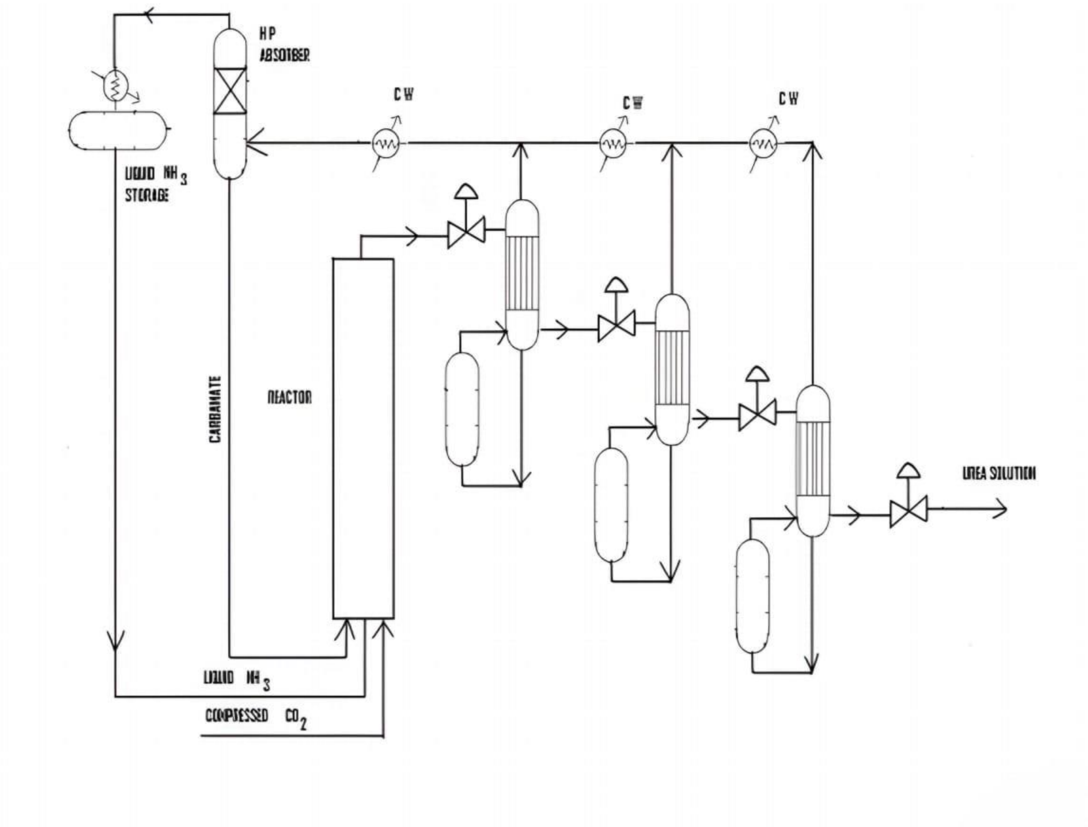


Figure 8: ACES Process Diagram

CHAPTER 3

PROCESS OVERVIEW

3.1 Selection of the Process:

The Stamicarbon urea synthesis process is chosen, wherein NH_3 and CO_2 are transformed into urea using ammonium carbamate at 140 bar of pressure, 180–185°C, and a 3:1 molar ratio. The majority of the unconverted carbamate is broken down in the Stripper, where CO_2 is used as a stripping agent to remove ammonia and carbon dioxide. Following their removal, the CO_2 and NH_3 are partially condensed and returned to the reactor. The heat released during this condensation is used to create 4.5 bar steam, some of which is utilized to heat the plant's downstream parts. During the bar breakdown step, the NH_3 and CO_2 in the stripper effluent evaporate and then condense to create a carbamate solution. In the evaporation section, where 99.7% of the urea melt is produced, the urea solution is further concentrated.

The Stamicarbon process stands out as a premier method for urea production, highly regarded for its efficiency, reliability, and technological advancement. Renowned for its high conversion rates of ammonia and carbon dioxide into urea, the Stamicarbon process optimizes energy usage through sophisticated engineering and control mechanisms. Its compact design not only minimizes the plant's footprint but also enhances operational flexibility and maintenance ease. Moreover, Stamicarbon plants boast exceptional reliability, thanks to advanced automation and control systems ensuring uninterrupted operation and minimal downtime. Offering versatility in feedstock selection and production capacity, the process accommodates various ammonia synthesis sources, making it adaptable to diverse market demands. Continual investment in research and development ensures Stamicarbon remains at the forefront of urea production technology, consistently delivering improved performance and competitiveness. These qualities collectively position the Stamicarbon process as the preferred choice in urea production, favored for its efficiency, reliability, flexibility, and innovative technology.

3.2 Process Flow Diagram:

The PFD illustrates the high-pressure Urea production loop by displaying unit operations and material flow. The PFD outlines major equipment and processes involved in producing urea.

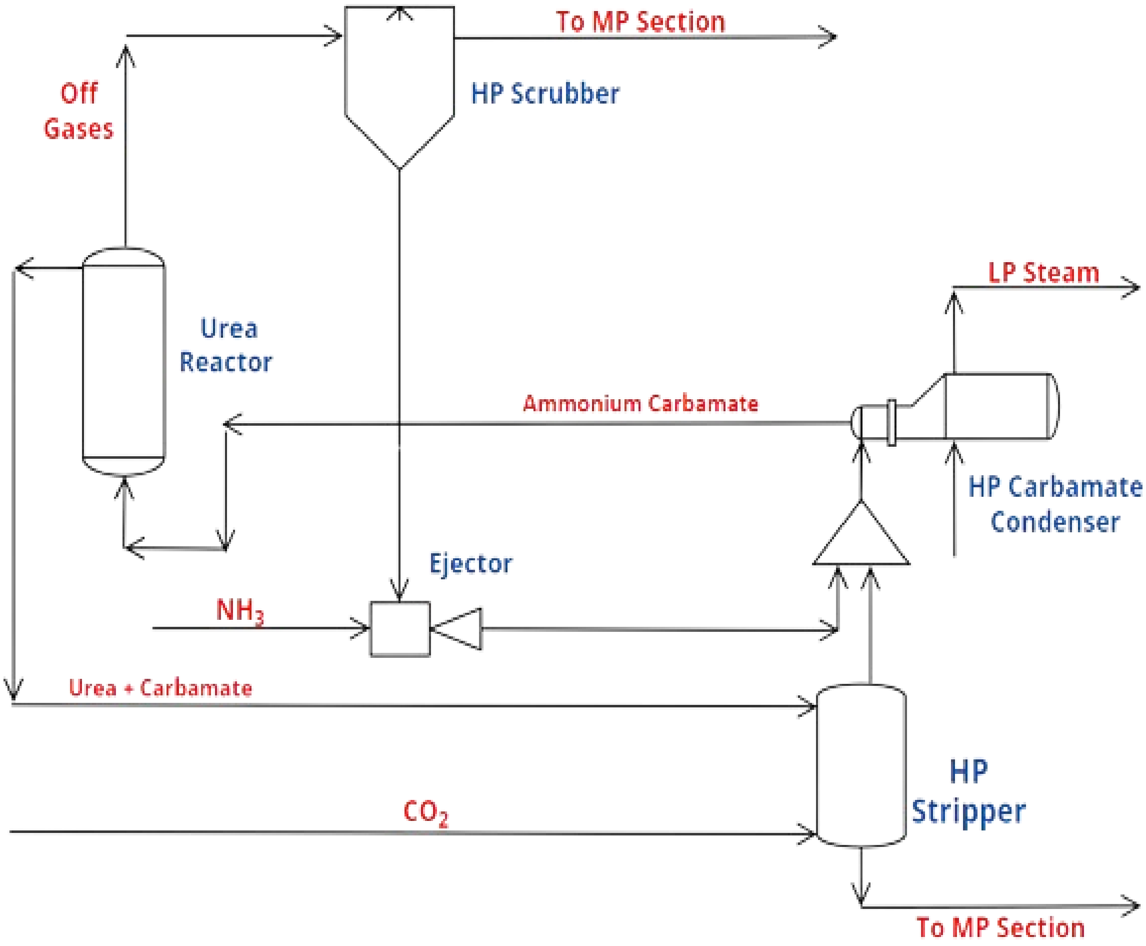


Figure 9: Process Flow Diagram

3.3 Process Description:

Carbon dioxide from the ammonia plant is compressed using staged compression. From where it enters the High pressure urea synthesis loop. Ammonia from the storage tank is pumped to the high pressure synthesis loop. There are four major components in this section. Namely:

3.3.1 Urea Reactor:

In the urea reactor, there are two reactions that take place since the process is a two stage reaction. First is the formation of an intermediate product called ammonium carbamate. Second is the decomposition of ammonium carbamate into urea and water. The reactor used is a plug flow reactor in which some residence time is given. Heat given off in the first reaction is absorbed by the carbamate formed to decompose into water and Urea. The downstream line of the plug flow reactor hence contains a mixture of urea, ammonium carbamate, carbon dioxide, ammonia and water. This mixture then flows to the high pressure stripper for decomposition of the carbamate formed into ammonia and carbon dioxide.

3.3.2 HP stripper:

HP stripper is a falling film type heat exchanger in which HP steam is introduced in the shell side and a solution of urea, carbamate, water, ammonia gas and carbon dioxide flows down the shell side counter-currently contacting with ammonia which acts as a stripping agent. The objective is the occurence of a reverse reaction by increasing the amount of one of the reactants i.e ammonia in the stream by introducing it from the other stream. This reverse reaction occurs on the basis of Le Chatelier's principle. Carbamate is broken down into ammonia and CO_2 by reducing the partial pressure of carbon dioxide. By doing this, the concentration of urea exiting the HP stripper increases.

3.3.3 HP Condenser:

The next component in line is the HP Condenser, which is an essential Shell and Tube Heat Exchanger. The primary function of the HP condenser is to condense the high-pressure steam into liquid form by transferring heat to a coolant, usually water. As the steam passes through the condenser tubes, it releases heat to the surrounding coolant, causing it to condense and form liquid water. Urea formation is not a single step reaction. It is in fact a two stage reaction in which ammonia and CO_2 react to form carbamate. This carbamate formation is achieved in the HP condenser. It is an exothermic reaction releasing 119 KJ/mol of heat.

3.3.4 HP Scrubber:

The HP scrubber is typically located downstream of the urea reactor and operates at high pressure, usually around 150 to 200 bar. It receives the synthesis gas mixture, which consists of ammonia, carbon dioxide, urea, and other by-products. The primary function of the HP scrubber is to remove unreacted ammonia and carbon dioxide from the synthesis gas. These components are recycled back to the synthesis loop to ensure optimal conditions for urea production. The scrubber achieves this by using an absorbent solution, often aqueous ammonia, which selectively absorbs ammonia and carbon dioxide from the gas stream. After passing through the HP scrubber, the gas stream is typically compressed before being returned to the synthesis loop. This compression increases the pressure of the recycled gases to match the operating pressure of the urea reactor, ensuring smooth integration into the synthesis process.The HP scrubber also helps maintain the equilibrium of the urea synthesis reaction. This equilibrium is critical for achieving high conversion rates and maximizing the yield of urea from the synthesis gas.

3.4: Raw Materials:

3.4.1 Ammonia (NH_3):

Ammonia is made up of nitrogen and hydrogen. In its aqueous state, it is known as ammonium hydroxide. There is a strong smell to this inorganic substance. It is hazardous and corrosive when concentrated. It is typically obtained from natural gas or other nitrogen-rich sources. Ammonia is frequently produced via the Haber-Bosch process, which involves reacting nitrogen and hydrogen at high temperatures and pressures.

3.4.2 Carbon Dioxide (CO_2):

Compressed Carbon dioxide is another raw material used in the manufacturing of urea. It can be found in nature either alone or in combination. It is a component of the atmosphere, accounting for around 1% of the volume of dry air. It results from the combustion of carbonaceous fuels such as coal, coke, fuel oil, gasoline, and cooking gas.

3.5 Intermediate Product:

3.5.1 Ammonium Carbamate (NH_2COONH_4)

Ammonium carbamate is a chemical compound formed during the synthesis of urea. It is an intermediate compound in the urea production process. Ammonium carbamate is produced when ammonia and carbon dioxide react under high pressure and temperature in the presence of a catalyst. The chemical formula for ammonium carbamate is NH_2COONH_4.

In the urea synthesis reaction, ammonia and carbon dioxide combine to form ammonium carbamate, which then undergoes further chemical transformations to yield urea **($CO(NH_2)_2$)**. Ammonium carbamate is unstable and decomposes readily into urea and water. This decomposition step is typically facilitated by heating or by lowering the pressure, allowing the production of urea.

CHAPTER 4

MATERIAL AND ENERGY BALANCE

4.1 Material Balance

Monitoring the amounts of carbon dioxide and ammonia that enter the system and contrasting them with the amounts of urea and byproducts generated constitutes the material balance. The following is an expression for the material balance equations, which are commonly based on the idea of conservation of mass:

General Material Balance Equation:

Mass In – Mass Out + Generation – Consumption = Accumulation

Units = Kg/hr

Incoming Mass = Outgoing Mass

4.1.1 Reactor

Steady State Operation

Mass In = Mass Out + Generation – Consumption

Reactions:

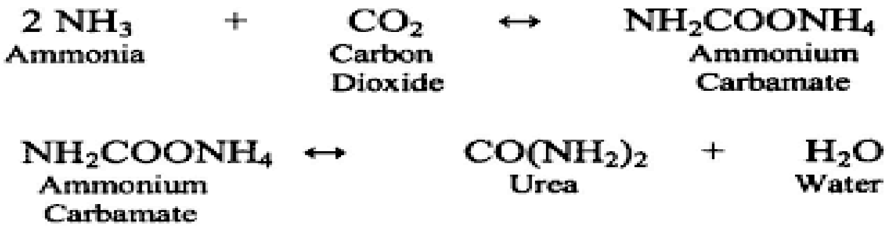


Table 2: Material Balance of Reactor

Component	Inlet (Kg/hr)	Consumption (Kg/hr)	Generation (Kg/hr)	Outlet (Kg/hr)
UREA	175.153	-	42571.25	42746.4
CARB	75715.2	39832.4	-	35882.8
CO_2	16374.1	8743.11	-	7630.99
NH_3	35028.1	6766.7	-	28261.4
H_2O	9882.69	-	12770.51	22653.2
N_2	1337.48	-	-	1337.48
O_2	228.096	-	-	228.096

4.1.2 Stripper

Mass In = Mass Out + Generation – Consumption

Reaction:

Table 3: Material Balance of Stripper

Component	Inlet (Kg/hr)		Consumption (Kg/hr)	Generation (Kg/hr)	Outlet (Kg/hr)	
	CO2	Reactor Bottom			Top	Bottom
UREA	-	42733.8	-	-	97.5488	42636.3
CARB	-	35880.7	25947.94	-	17.0597	9915.7
CO_2	31313	2124.47	-	14627.18	46432.2	1632.45
NH_3	-	22447.2	-	11320.65	31988.4	1779.45
H_2O	142.621	22250.5	-	-	2098.97	20294.1
N_2	1283.95	40.6483	-	-	1320.9	3.70302
O_2	199.993	19.7927	-	-	217.275	2.5102

4.1.3 Condensor

Mass In = Mass Out + Generation – Consumption

Reaction:

$$2NH_3 + CO_2 \rightarrow NH_4OCONH_2$$

Table 4: Material Balance of Condenser

Component	Inlet (Kg/hr)	Consumption (Kg/hr)	Generation (Kg/hr)	Outlet (Kg/hr)
UREA	175.153	-	-	175.153
CARB	21743.7	-	53971.5	75715.2
CO_2	46798.7	30,424.6	-	16374.1
NH_3	58575	23,546.9	-	35028.1
H_2O	9882.69	-	-	9882.69
N_2	1337.48	-	-	1337.48
O_2	228.096	-	-	228.096

4.1.4 Scrubber

Mass In = Mass Out

Table 5: Material Balance of Scrubber

Component	Inlet (Kg/hr)		Outlet (Kg/hr)	
	TOP	LP Section	TOP	BOTTOM
UREA	12.5462	65.0596	-	77.6057
CARB	2.08826	12807.2	-	21728.2
CO_2	5506.52	2.47835	113.935	367.355
NH_3	5814.23	517.935	8.53895	2432.46
H_2O	402.701	7384.76	3.81347	7783.65
N_2	1296.83	-	1280.25	16.5778

4.2 Energy Balance

The energy balance is calculated by measuring the energy inputs (such as heat and steam) and outputs (such as waste heat). The energy balance equations are based on the concept of energy conservation and take the following form:

Energy In = Energy Out

The energy balance equations account for the heat transfer that occurs within various unit activities, such as the stripper and condenser. In addition to accounting for the energy required for chemical reactions, the energy balance equations also consider the energy content of the feed and products.

The precise energy balance equations used in the UREA production process can change depending on the unit operations and overall process design. Among the equations that are commonly used are the heat transfer equations, enthalpy calculations, and reaction energy estimates pertinent to the chemical reactions involved in the synthesis of UREA.

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

$$\Delta H = A\left(T - T_{ref}\right) + B\frac{(T^2 - T_{ref}^2)}{2} + C\frac{(T^3 - T_{ref}^3)}{3} + D\frac{(T^4 - T_{ref}^4)}{4} + E\frac{(T^5 - T_{ref}^5)}{5}$$

$$E = Molar\ Flow \times Enthalpy$$

By conducting a complete material and energy balance, it is possible to assess the overall process efficiency, pinpoint areas for improvement, and optimize resource use in the UREA production process.

Table 6: Coefficient values for calculation of Enthalpy

	A	B	C	D	E
O_2	29.526	-0.0088999	0.000038083	-3.2629E-08	8.8607E-12
N_2	29.324	-0.0035395	0.000010076	-4.3116E-09	2.5935E-13
CO_2	27.437	0.042315	-0.000019555	-3.9968E-09	2.9872E-13
NH_3	33.573	-0.012581	0.000088906	-7.1783E-08	1.8569E-11
UREA	965.507	-5.0993	0.010028	-6.3799E-06	0
H_2O	33.933	-0.0084186	0.000029906	-1.7825E-08	3.6934E-12
H_2O(l)	92.053	-0.039953	-0.00021103	5.3469E-07	0
Carbamate	1	0.439932	0	0	0

4.2.1 Reactor

Inlet:

Temperature = 440K

Reference Temperature = 298K

Table 7: Inlet from Condensor

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	18988.64	2.91655	55381.32283
CARB	23193.56	969.7	22490792.16
CO_2	5701.79	372.055833	2121384.199
NH_3	5369.763	2056.77917	11044417.61
H_2O	8220.737	548.570833	4509656.676
N_2	4144.601	47.7441667	160311.5261
O_2	4255.42	7.12829167	24514.6055
		Total	**40406458.1**

Outlet:

Temperature = 456K

Reference Temperature = 298K

Table 8: Outlet of Reactor

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	20909.6	711.7875	14883194.33
CARB	26362.99	459.616667	12116869.36
CO_2	6375.734	173.392917	1105507.067
NH_3	6010.954	1,659.45	9974902.933
H_2O	12081.69	1,257.44	15192016.06
N_2	4614.736	47.7441667	220326.7366
O_2	4745.107	7.12829167	33824.50687
		Total	**53526641**

Moles of Urea Formed from Carbamate:

= Carbamate (in) – Carbamate (Out) = 510Kmol/hr

Heat of Reaction = 25650 KJ/Kmol

Heat Required = 510 x 25650 = 13083637.5 KJ/hr

Moles of Urea formed from reactants:

= Moles of Urea Out – Moles of Urea formed from CARB

= 201.704167 Kmol/hr

Heat of Reaction = 13400 KJ/Kmol

Heat Released = 201.704167 x (-13400) = 2702835.83 KJ/hr

Q = Energy In – Energy Out + Heat of Reaction + Heat Released

Q = 23500984.6 KJ/hr or 6528 KW

4.2.2 Stripper

Inlet:

Bottom:

Temperature = 373K

Reference Temperature = 298K

Table 9: CO_2 Bottom Inlet

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
CO_2	2945.584	711.5	2095783.325
N_2	2183.542	45.83	100071.7142
O_2	2228.403	6.25	13927.52076
$H_2O(l)$	5643.04	7.91666	44674.03155
		Total	**2254456.592**

Top:

Temperature = 456K

Reference Temperature = 298K

Table 10: Top Inlet from Reactor

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	20909.6	711.579	14878835
CARB	26362.99	459.5917	12116210
CO_2	6375.734	48.2725	307772.6
NH_3	6010.954	1318.054	7922763
$H_2O(l)$	12081.69	1235.088	14921940
N_2	4614.736	1.451025	6696.098
O_2	4745.107	0.58685	2784.666
		Total	**50157002**

Outlet:

Top:

Temperature = 414K

Reference Temperature = 298K

Table 11: Top Outlet

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	15871.19	1.624325	25779.978
CARB	18283.43	0.218515	3995.204116
CO_2	4619.216	1055.04167	4873465.531
NH_3	4344.305	1878.29583	8159890.233
H_2O	3943.604	116.510417	459470.9333
N_2	3382.203	47.1520833	159477.9129
O_2	3464.397	6.79008333	23523.54386
		Total	**13705603.34**

Bottom:

Temperature = 439K

Reference Temperature = 298K

Table 12: Bottom Outlet

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	18868.88	709.9542	13396040
CARB	22999.21	127.0088	2921101
CO_2	5659.861	37.09296	209941
NH_3	5329.948	104.4854	556901.8
$H_2O(l)$	10724.37	1126.496	12080957
N_2	4115.243	0.132187	543.9819
O_2	4224.889	0.078447	331.4284
		Total	**29165816**

Moles of water vaporized = 116.514167 Kmol/hr

Latent Heat = 34390 KJ/Kmol

Moles of Carbamate Decomposed = 332.364401 Kmol/hr

Heat of Reaction = 159550KJ/Kmol

Q = Energy out – Energy In + Heat of Reaction + Latent Heat of Vaporization

Q = 47495494.38 KJ/hr or 13193.192KW

4.2.3 Condenser:

Inlet:

Temperature = 413.64K

Reference Temperature = 298K

Table 13: Inlet of Condensor

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	15462.65	2.91655	45097.60306
CARB	18130.49	278.512083	5049559.812
CO_2	20746.85	1063.37083	22061590.93
NH_3	4311.666	3439.40833	14829579.37
H_2O	8220.737	548.570833	4509656.676
N_2	3357.72	47.7441667	160311.5261
O_2	3439.058	7.12829167	24514.6055
		Total	**46680310.52**

Outlet:

Temperature = 440K

Reference Temperature = 298K

Table 14: Outlet of Condensor

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	18988.64	2.91655	55381.32283
CARB	23193.56	969.7	22490792.16
CO_2	5701.79	372.06	2121384.199
NH_3	5369.763	2,056.78	11044417.61
H_2O	8220.737	548.570833	4509656.676
N_2	4144.601	47.7441667	197880.5129
O_2	4255.42	7.12829167	30333.87505
		Total	**40449846.36**

Moles of Water Condensed = 222.37 Kmol/hr

Latent Heat = 34390 KJ/Kmol

Moles of Carbamate formed = 691.19 Kmol/hr

Heat of Reaction = 159550 KJ/Kmol

Q = Energy Out – Energy In + Heat of Reaction + Latent Heat of vaporization

Q = 98830099.17 KJ/hr or 27452.10 KW

4.2.4 Scrubber

Inlet: (Top)

Temperature = 345.4K

Reference Temperature = 298K

Table 15: Top inlet of Scrubber

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	7166.284	1.083333	7763.474
CARB	6755.738	164.0454	1108248
CO_2	1843.469	0.056314	103.8127
NH_3	1732.067	30.41213	52675.84
H_2O	3565.38	409.9583	1461657
N_2	1378.794	0	0
O_2	1403.751	0	0
		Total	**2630448**

Bottom:

Temperature = 456K

Reference Temperature = 298K

Table 16: Bottom inlet of Scrubber

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	20909.6	0.20891125	4368.251383
CARB	26362.99	0.02674817	705.1616373
CO_2	6375.734	125.120417	797734.461
NH_3	6010.954	341.4	2052139.751
H_2O	12081.69	22.3533333	270065.9666
N_2	4614.736	46.2929167	213629.6006
O_2	4745.107	6.50970833	30889.26275
		Total	**3369532.455**

Outlet:

Top:

Temperature = 359K

Reference Temperature = 298K

Table 17: Top Outlet of Scrubber

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	-	-	-
CARB	-	-	-
CO_2	2390.536	2.588863	6188.77
NH_3	2245.77	0.501392	1126.01
H_2O	2068.008	0.21168	437.76
N_2	1779.918	45.70125	81344.46
O_2	1814.287	6.171625	11197.10
		Total	**100294.09**

Bottom:

Temperature = 427K

Reference Temperature = 298K

Table 18: Bottom outlet of Scrubber

Component	Enthalpy (KJ/Kmol)	Molar Flow (Kmol/hr)	Energy (KJ/hr)
UREA	17460.96	1.29224167	22563.77472
CARB	20746.85	278.312917	5774115.224
CO_2	5168.551	8.347125	43142.5422
NH_3	4864.017	142.412917	692698.8471
$H_2O(l)$	9799.992	432.058333	4234168.26
N_2	3770.233	0.59177917	2231.145452
O_2	3866.52	0.33809458	1307.249386
		Total	10770227.04

Q = Total Inlet – Total Outlet

Q = 4870540 KJ/hr or 1352.92 KW

CHAPTER 5

EQUIPMENT DESIGN

5.1 Reactor

5.1.1 Plug Flow Reactor:

In a plug flow reactor, the fluid composition varies throughout the flow channel, necessitating a material balance for each reaction component based on a volume differential (dV). Thus, given a reactant A, the mass balance is:

Input = output + accumulation + disappearance due to reaction

When accumulation is zero, the equation takes this form:

Input = Output + disappearance due to reaction

Reactor volume can be calculated using the following formula.

$$\frac{V}{F_{AO}} = \frac{\tau}{C_{Ao}} = \int_{0}^{X_{Af}} \frac{dX_A}{-r_A}$$

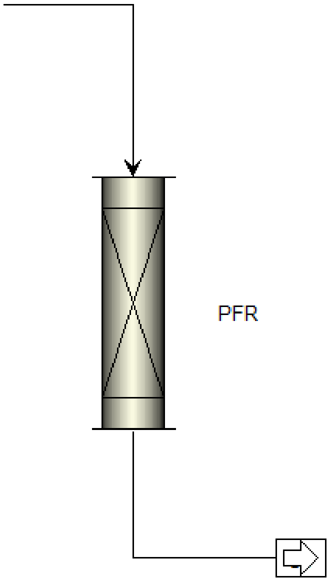


Figure 10: Plug Flow Reactor

5.1.2 Design of PFR using ASPEN Plus:

Reactions:

$$2NH_3 + CO_2 \rightarrow NH_4COONH_2 + H_20$$

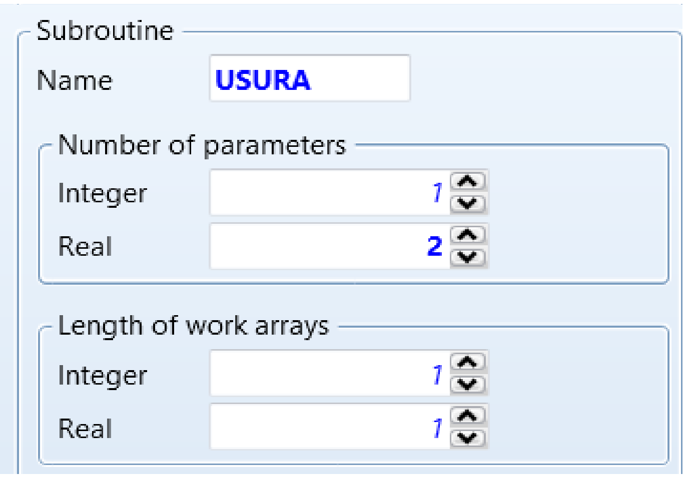
(Carbamate)

$$NH_4COONH_2 \rightarrow NH_2CONH_2 + H_20$$

(Urea)

Reaction Kinetics:

The kinetics of both of these reactions are adjusted within APSEN Plus through a user subroutine USURA.F, in which both the forward and reverse reactions were considered.



Subroutine

Name: USURA

Number of parameters

Integer: 1

Real: 2

Length of work arrays

Integer: 1

Real: 1

Figure 11: Subroutine in ASPEN Plus

The equilibrium constant for Reaction 1, in terms of mole fractions, is given as:

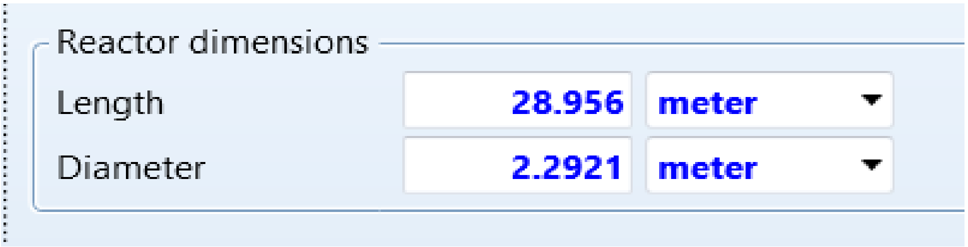
$$K_1 = \exp\left\{\frac{-\left(G^0_{CARB} - 2G^0_{NH3} - G^0_{CO2}\right)}{RT}\right\}\left(\frac{P}{P^0}\right)^2\left[\frac{\phi^2_{NH3}\phi_{CO2}}{\phi_{CARB}}\right]$$

The rates for reactions 1 and 2, in units of kmol/s/m^3 are:

$$Rate_1 = k_1\left\{x_{NH3}^2 x_{CO2} - \frac{x_{CARB}}{K_1}\right\} \quad , \quad Rate_2 = k_2\left\{x_{CARB} - \frac{x_{UREA}x_{H2O}}{K_2}\right\}$$

Design Specifications for PFR:

Following are the finalized dimensions of PFR to achieve the required percentage of Urea within the reactor effluent:



Reactor dimensions

Length 28.956 meter

Diameter 2.2921 meter

Figure 12: Dimensions of PFR

Table 19: Parameters and Design Specifications of PFR

Parameters	Value
Temperature	183 C
Pressure	141 kg/sqcm
Length	28.956 m
Diameter	2.2921 m
Residence Time	0.4446 hr
Volume	119 m^3

5.2 Stripper

“The separation column is a multi-staged countercurrent column that has a liquid feed at the top and a vapor feed at the bottom."

5.2.1 Stripping process:

Stripping is the process of transferring a solute (such as NH3 or CO2) from the liquid to gas phase.

In the stripper, ammonium carbamate decomposes, liberating more NH_3 and CO_2 to be stripped out. Heat is supplied on the shell side of tubes by condensing steam while the urea solution falls inside the tubes counter currently down past the rising CO_2 stripping gas. The outlet liquid solution from the stripper is rich in urea and goes to the downstream section for urea purification.

5.2.2 Stripping Agent:

Compressed Carbon Dioxide (CO2) gas is used as a stripping agent during high pressure Urea synthesis loop.

5.2.3 Choice between packed or plate column:

- Scale: for the diameter. Because small trays are more expensive to fabricate, towers with less than one meter of packing are preferable. Since there are issues with liquid distribution and the weight of a big volume of packing, huge column plate towers are used.

- Foaming (forth) is caused by vapor bubbling through the liquid, hence a packed column is recommended when using foaming substances.
- For fouling systems with suspended particles or sludge, plate towers are preferred.

- Corrosive system; as packed towers use corrosion-resistant ceramics, they are the preferred (less expensive) option.

- To remove heat from heat plate columns, use a cooling coil.

- Plate towers often have lower pressure drop (ΔP) due to fewer plates.

5.2.4 Physical Consideration:

- Maintenance, cleaning is easy in plate column, while in packet column packing must be remove.
- Weight, packed column are heavier and need heavy support and foundation.

5.2.5 Trays:

There are three common types of trays these are:

i) Bubble cup trays
ii) Sieve trays
iii) Valve trays

5.2.5 Our Selection:

We have used Sieve trays due to the following mentioned advantages:

- **Cost:** Among the three types of separation equipment, the sieve trays are the most basic and have the least number of components that move during their operation. This implies, that in the case of the trays themselves and perhaps the entire column, more reasonable initial cost investments may be required.

- **Fabrication:** They are also easy to fabricate since they are relatively simpler in design than the more complex ones. This can result in reduced lead time and perhaps lower fabrication costs compared to traditional methodologies.

- **Maintenance:** Sieve trays require low maintenance as there are no complicated accessories that would require replacement or repair constantly. This minimizes other operational costs incurred in carrying out different organizational functions.

- **Pressure Drop:** Sieve trays generally have the capability of bearing the least pressure drop across the tray when compared with Valve and Bubble cap trays. This can be useful when you are trying to strip a column where you wish to reduce the pressure you have to apply to force the vapor phase up to strip the component you require from the liquid.

- **Capacity:** Sieve trays offer more versatility in the rates of vapor and liquid compared to Valve trays though the latter has higher capacity when it comes to throughput rates.

5.2.6 Design using Aspen Plus:

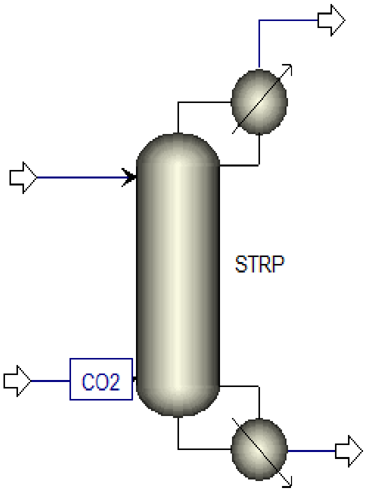
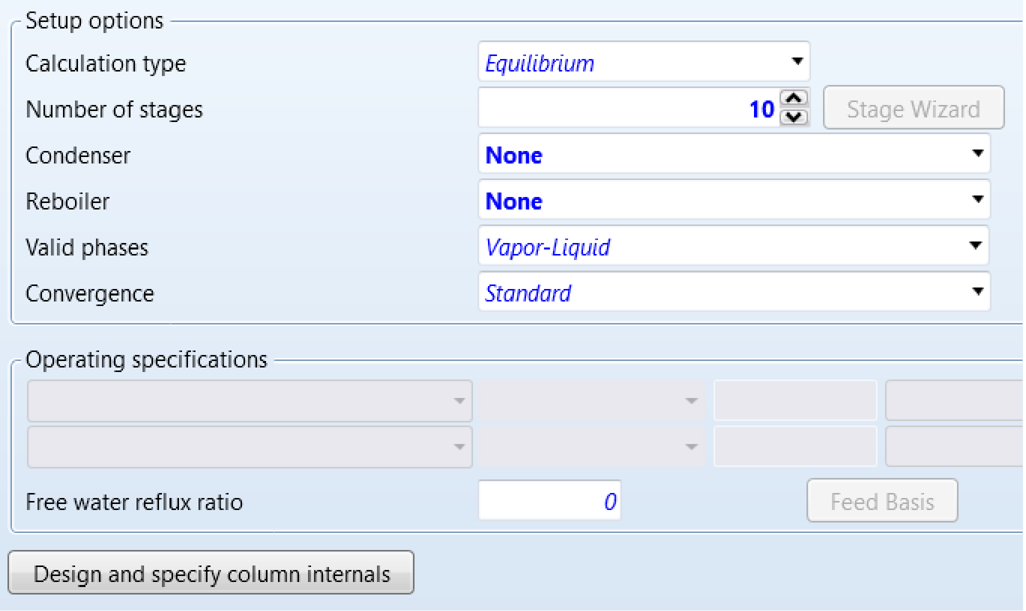


Figure 13: High Pressure Stripping Column

Number of Stages:

To achieve the required percentage of Urea, the first step is to calculate the number of stages which in our case is finalized as 10 as shown below:



Setup options

Calculation type	*Equilibrium*
Number of stages	**10**
Condenser	**None**
Reboiler	**None**
Valid phases	*Vapor-Liquid*
Convergence	*Standard*

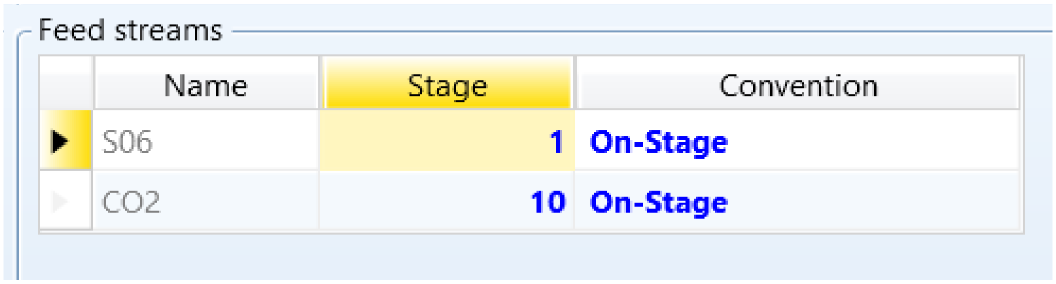
Operating specifications

Free water reflux ratio: *0*

Figure 14: Number of stages of Stripper

Feed:

- The reactor effluent which is in the liquid phase, enters the stripping column from the top and moves in the downward direction.
- Carbon Dioxide which is the gas phase, enters the stripping column from the bottom and movies in the upward direction such that, both feeds are in counter-current contact with each other.
- Steam is used to provide the required amount of heat to carry out the process of stripping.



Feed streams

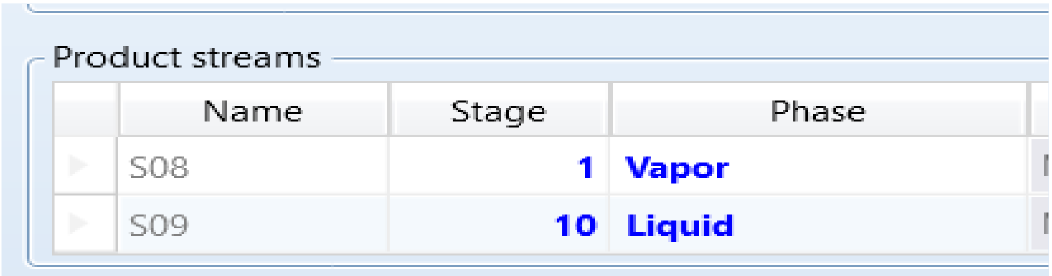
	Name	Stage	Convention
▶	S06	1	On-Stage
	CO2	10	On-Stage

Figure 15: Feed Streams of Stripper

Product:

With the use of the stripping agent, both unreacted Carbon Dioxide (CO2) and Ammonia (NH3) are stripped out of the reactor effluent and exit the stripping column from the top.

The concentrated form of Urea then exits the stripping column from the bottom stream and goes into the purification section.



Product streams

	Name	Stage	Phase
	S08	1	Vapor
	S09	10	Liquid

Figure 16: Product Streams of Stripper

Design Specifications:

Table 20: Design Specifications of HP Stripping Column

Parameters	**Value**
Temperature (Top, Bottom)	185˚C , 165˚C
Pressure	141 kg/cm^2
Tray Type	Sieve Trays
Tray Spacing	0.6096 m
Diameter	1.9833 m
Height	6.096 m

For columns with a diameter of about 1 m, tray spacing must be between 0.3 – 0.6 m.

5.3 Condenser

A condenser is a kind of heat exchanger that uses a coolant, such as water, to remove latent heat and transfer vapors into a liquid state. Condensers can be divided into two primary categories.

- Those where the condensate stream and coolant are separated by a solid surface, often a tube wall;
- Those where the coolant and condensing vapor are brought into direct touch.

5.3.1 Condenser Types

1. Double pipe and multiple pipe
2. Air-cooled condensers
3. Compact condensers
4. Shell and Tube

5.3.2 Assumptions:

- Ammonia, Carbon dioxide & water are mixed before entering the carbamate condenser to form Ammonium Carbamate.
- Ammonium Carbamate leaving the Condenser is at it's dew point
- Heat of the Reaction is completely absorbed by water to produce steam, therefore the temperature at the shell inlet is same as that of shell outlet.
- Inert gases are not taken into consideration.

5.3.3 Design Procedure

The selected type for this project is fixed shell and tube condenser:

(1 - Shell and 4 tube passes) in which Carbamate is in the shell side and cooled while Water in the tube side.

Shell Side Conditions:

T_1 = Inlet = 167°C

T_2 = Outlet = 167°C

Pressure at Inlet = Pressure at Outlet = 141.5 kg/cm^3

Mass Flow Rate = 138741 kg/hr

Carbamate physical properties at 167℃

Specific heat(Cp) =2.596 KJ/kg

Thermal conductivity (k)= 0.531 W/m K

Density= ρ =1600 kg/m^3

Viscosity = ɥ = 6×10^{-4} Pa. sec

Tube Side Conditions:

T_1 = Inlet = 25℃

T_2 = Outlet = 147℃

Pressure Inlet: 1.0135 bar (1atm)

Pressure at Outlet = 4.5 bar

Water Flow Rate:

Mass flow rate of carbamate= 138741.6 kg/hr =38.53 kg/sec

λ = Heat of Vaporization of carbamate = 180 KJ/kg

Q= 38.53 x 180 = 6935 KJ/sec

Q= mCpΔT + λ (for water), m= 6935/ (4.2 × (147−25) + 2200)

M= 2.55 kg/s

Water physical properties at 87°C

Specific heat (Cp) =4.2 KJ/kg

Thermal conductivity (k) = 0.746 W/m.°K

Density = ρ = 966 kg/m^3

Viscosity = ɥ = 3.2 x 10^{-4} Pa. sec

LMTD Calculation:

T1=T2= 167, t1=25, t2=147

$$\text{LMTD} = \frac{((T1-t2)-(T2-t1))}{\ln((T1-t2)/(T2-t1))} = 62°C$$

Ft Correction Factor:

For 1-Shell Pass and 4- Tube Pass, Ft correction factor will be

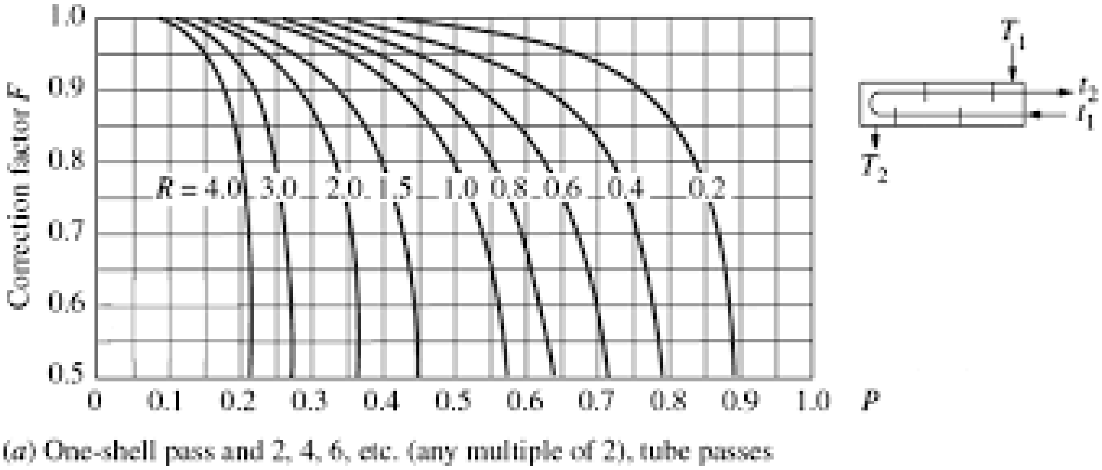


Figure 17: Correction Factor (F)

$\mathbf{P} = \frac{(t2 - t1)}{(T1 - t1)} = 0.88$ $\mathbf{R} = \frac{(T1 - T2)}{(t2 - t1)} = 0$

From the graph,

Ft =1

Since $\Delta Tm = LMTD \times Ft$

$\Delta Tm = 62°C$

Overall heat transfer coefficient assuming

Assuming $Uo = 600\ W/m^2\ °C$

Total area and number of tubes:

$$A = \frac{Q \times 1000}{Uo \times \Delta Tm}$$

$$A = \frac{6935 \times 1000}{600 \times 62°C} = 185.4\ m^2$$

Choose $d_o = 22$ mm, di= 17 mm L= 3.8 m

Area of one tube = 0.42 m^2

Number of tubes (Nt) = total area/area of one tube

= 185.4/0.42 = 440

Shell side diameter

For a triangular pitch (1 shell pass and 4 tube passes)

Pt =1.25 do, n=2.3, k= 0.175

$Db = do\ (\frac{Nt}{k})^{1/n}$

$22(440/0.175)^{1/2.3}$ =657.96 mm

From split ring floating head

C=61,

Ds= Db+ C,

Ds=718.96 mm

Tube side heat transfer coefficient (hi)

Tmean = 25+147/2 = 87 C

At = $4di^2 \times Nt/Np$, At= $4 \times (17\times0.001)^2 \times 440/4$ =0.025m^2

Gt=Wt/At, Gt= 2.55/0.025= 102 kg/m^2 sec

Ut =Gt/ρ, Ut=102/966=0.10559 m/s

hi=4200(1.35+0.02 tmean)Ut0.8/di 0.2 =1210 W/m^2

Shell side heat transfer coefficient (ho)

As =(pt−do)/pt × LB* Ds , pt=1.25 do , LB= Ds/5

As=0.02 m^2

Gs =Ws/As ,Gs=38.53/0.02=1926.5 kg/m2 sec

de=1.1/do (pt2 −0.917 do^2) =1.1/22× (1.25^2 −0.917×22^2)=15.8 mm

Re=Gs×de/ɥ = 50,718 kg

Pr= cp × ɥ/k = 2.596*1000*6*10-4 /0.531 =2.93

Jh =0.0033

h_o×de/k=jh×Re×$Pr^{0.33}$,

h_o=4990 W/m2

Dirt coefficients

h_{id}= 5000 W/m^2

h_{od}=5000 W/m^2

Calculated overall heat transfer coefficients (Uo)

$$\frac{1}{Uo} = \frac{1}{ho} + \frac{1}{hod} + \frac{do*\ln(\frac{do}{di})}{2*kw} + (\frac{1}{ho} + \frac{1}{hod})\frac{do}{di}$$

Kw=50 W/m K for Stainless Steel

1/Uo=0.0017

Uo =588.23 W/m^2

Ucal < Uassume

Tube side pressure drop

For Re=4858.824, Jf=5.9*10^{-3}

ΔPt= Np*(8*jf*(L/di) +2.5)* ρu^2 /2

$\Delta Pt= 4(8\times5.9\times10^{-3} \times (3.8*1000/17) +2.5) \times 966\times (0.100597)^2 /2$

$\Delta Pt=430.3384$ Pa =0.4303384 Kpa

Shell side pressure drop

For Re=50718, $jf=3.8*10^{-2}$

$\Delta Ps=8\times jf\times(L/LB)\times(Ds/de)\times(\rho u^{2} /2)$

$\Delta Ps=8\times4\times10-2 \times(3.8/0.140063)\times(718.96/15.8)\times(1600\times(0.937)2 /2)$

$\Delta Ps=386539$ Pa =386.539 kpa

Since the pressure drop of shell is too high it can be reduced by increasing the baffle pitch, tripling the pitch reducing the shell side velocity, which reduces the pressure drop by a factor of approximately $(1/3)^2$

$\Delta Ps=386.539/9=42.94878$ kpa

This will reduce the shell side heat transfer coefficient by a factor of $(1/3)^{0.8}$

$ho=4990.226 \times (1/3)^{0.8} =2887.403$ W/m2

This will give overall coefficient of 611 W/m^2 still above the assumed value of 600 W/m^2.

5.4 Scrubber

Particulate matter, volatile organic compounds (VOCs), odorous compounds (H2S), alkaline gases (NH3), acid gases (HCl, SO2, HF), and particulate matter are among the contaminants that scrubbers are employed to remove from industrial exhaust streams.

They function by successfully cleaning the gas stream by absorbing and neutralizing the contaminants with a liquid, commonly water or a caustic solution. Scrubbers may remove some pollutants with removal efficiency that are frequently over 95%.

5.4.1 Design Consideration:

Design considerations for a scrubber include:

1. **Pressure Drop:**

   One crucial aspect of the design is the pressure drop throughout the scrubber. It is the pressure differential between the scrubber's input and exit, and its packing, irrigation, and internal parts all have an impact on it. Because it impacts the scrubber's function and, if left unchecked, might result in decreased efficiency, the pressure drop is significant.

2. **Packing Material:**

   Performance of the scrubber is largely dependent on the packing material employed in it. To guarantee ideal gas-liquid contact and reduce pressure drops, packing material must be carefully chosen in terms of both kind and size as well as construction material. For instance, materials made of stainless steel perform well in hot conditions but poorly in hydrochloric acid.

3. **Collection And Holding Tank:**

   The scrubber system's collecting and storage tank is an essential part. It needs to be built to support both the amount of scrubbing liquid and any accumulated contaminants. The choice of scrubbing medium, such as caustic lye or water, is determined by the working conditions and the contaminants' solubility.

4. **Material Compatibility:**

   It is crucial that the materials used in the scrubber components be compatible with the contaminants and operating circumstances. This involves making certain that the components and packaging material can endure the corrosive effects of the contaminants and the operational environment.

5. **Operating Temperature:**

   It influences both the scrubber's performance and the solubility of the pollutants, the operating temperature of the scrubber is very important. For best results, the scrubber needs to be made to work at the designated temperature range.

5.4.2 Procedure for Scrubber Design Calculation:

1. Gas and Liquid Properties:

Table 21: Gas and Liquid Properties

Properties	Values
Gas Flowrate	13243.2 Kg/hr
Gas Density	1.9 Kg/m^3
Liquid Flowrate	20777.4 Kg/hr
Liquid Density	1141.1 Kg/m^3
Liquid Viscosity	0.3917cp

2. Selection of Solvent:

28% (v/v) Ammonium Carbamate is used as scrubbing agent. The stream is coming from the Low Pressure (LP) Section of Urea Production. Ammonium Carbamate Scrubs a large quantity of Ammonia from the stream. However it also proves to be a good scrubbing agent for Carbon Dioxide as it dissolves an appreciable quantity of CO^2 from the stream as well.

3. Selection of Column and Packing Material:

Packed bed columns is used because they offer a wide wetted surface area where the scrubbing liquid and contaminated air flows can come into contact. As a result, clean air is released into the atmosphere and pollutants in the air stream can be efficiently absorbed or reacted with. The scrubbing efficiency is increased by the packing material inside the column, such as Raschig rings or Pall rings, which enhance the surface area and encourage gas-liquid interaction. To further improve the removal of contaminants, the packed bed design also permits a countercurrent flow of gas and liquid.

Ceramic materials are so resistant to corrosion, they are employed in packing. This is especially crucial in situations where there are gasses that are either acidic or alkaline, as they can seriously harm other materials. Because ceramic materials, such as alumina, porcelain, or silicon carbide, are so resistant to heat shock and chemical corrosion, they can be used in hostile process conditions.

4. Operating Conditions:

Temperature = 456 K

Pressure = 138 bar

5. Calculating Columns diameter:

Table 22: Packing Properties

Factors	Value
Size of packing(mm)	51
Diameter of packing (D_p)	51
Bulk Density	609
Surface Area	108
Packing Factor (F_p)	130/m

Now Calculating Flow Factor:

$$F_{LV} = \frac{L_W^*}{V_W^*}\sqrt{\frac{\rho_V}{\rho_L}}$$

$F_{LV} = 0.06$

Table 23: Calculation of Percentage Flooding

Factors	Value
K_4	1.5
K'_4	4
Percentage Flooding	61.23
$\Delta \boldsymbol{P}_{\boldsymbol{Flooding}} = \mathbf{0.115}(\boldsymbol{F_P}^{0.7})$	1.521
Channeling (D_c/D_p)	49.04

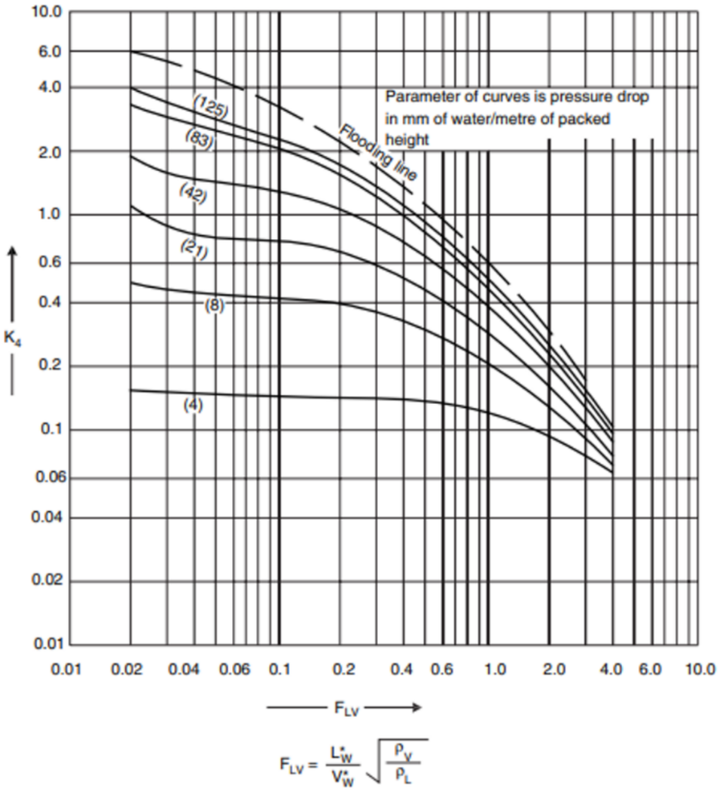


Figure 18: K4 vs Flow Factor

Table 24: Calculation of Column Diameter

Gas Mass velocity $V'_W = \sqrt{\frac{K_4\rho_V(\rho_L - \rho_V)}{13.1F_p(\frac{\mu_l}{\rho_l})^{0.1}}}$	0.78
Column Area (G/V_W*)	4.712
Column Diameter	2.45

6. Calculating Column Height:

For Calculating N_{OG}:

$$G_m(y_1 - y_2) = L_m(x_2 - x_1) \text{ ……(i)}$$

Moles fractions can be calculated from eq.(i). Using these mole fractions, N_{OG} can be calculated from the figure below:

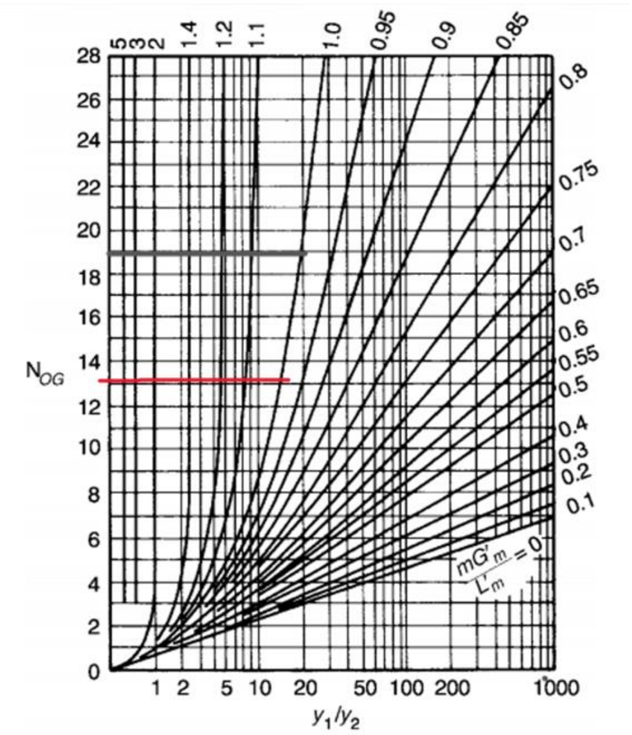


Figure 19: NOG vs y1/y2

N_{OG} = 13

For the calculation of K_G and K_L, which are mass transfer film coefficient for gas and liquid respectively. We will use the Onda's Method:

$$k_L\left(\frac{\rho_L}{\mu_L g}\right)^{1/3}=0.0051\left(\frac{L_w^*}{a_w\mu_L}\right)^{2/3}\left(\frac{\mu_L}{\rho_L D_L}\right)^{-1/2}(ad_p)^{0.4}$$

$$\frac{k_G}{a}\frac{RT}{D_v}=K_5\left(\frac{V_w^*}{a\mu_v}\right)^{0.7}\left(\frac{\mu_v}{\rho_v D_v}\right)^{1/3}(ad_p)^{-2.0}$$

K_G = 0.067

K_L = 0.085

Now for Determining H_G and H_L. We will use the following relation:

$$\mathbf{H}_G=\frac{G_m}{k_G a_w P}$$

$$\mathbf{H}_L=\frac{L_m}{k_L a_w C_t}$$

H_G = 0.1486

H_L = 0.2880

Table 25: Calculation of Column Height

Factors	***Value***
$\boldsymbol{H_{OG}=H_G+m\frac{G_m}{L_m}H_L}$	0.4251
$\boldsymbol{Z=\ N_{OG}\times H_{OG}}$	5.527m
Allowance for liquid distribution	0.5m
Allowance for liquid redistribution	0.5m
Total Height	6.527m

7. Pressure Drop:

Using the figure below, we will calculate the total pressure across the height of packed column.

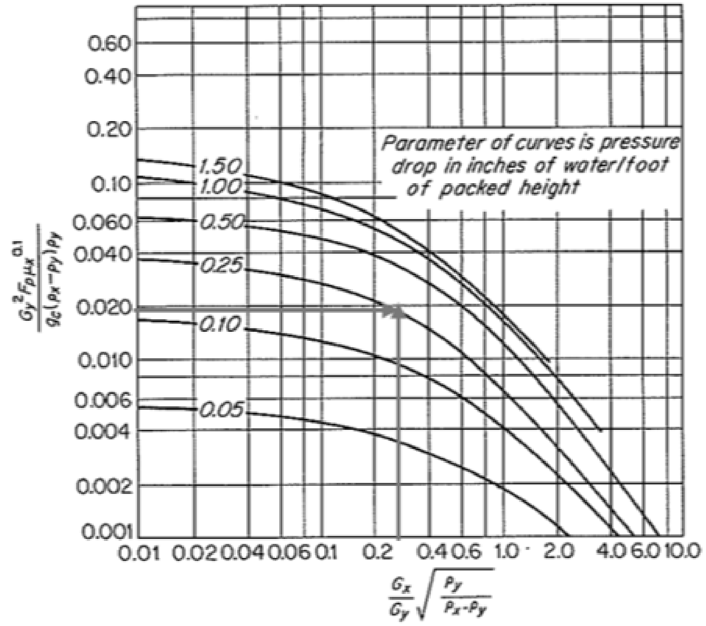


Figure 20: Pressure drop

Table 26: Calculation for Pressure drop

$\frac{G_x}{G_y}\sqrt{\frac{\rho_g}{\rho_L-\rho_g}}$	0.096
$\frac{G_y F_p \mu_L}{\rho_g\,(\rho_L-\rho_g) g_c}$	0.046
Pressure drop per packing (mmH2O/ft)	0.45
Total pressure drop	548pa

8. HETP Analysis:

Height Equivalent Theoretical Plate Analysis gives us the length of each theoretical plate for the scrubber. It is calculated using Norton Correlation:

$$lnHETP = n - 0.187ln\alpha + 0.283ln\mu$$

HETP = 0.94457

If we add 20% Safety factor:

HETP + 20% Safety Factor = 1.1335

Now using the formula for total number of Plates:

$$Number\ of\ plates = \frac{Z}{HETP}$$

Number of plates = 4.876

Therefore the total number of plates calculated to achieve the required scrubbing is 5.

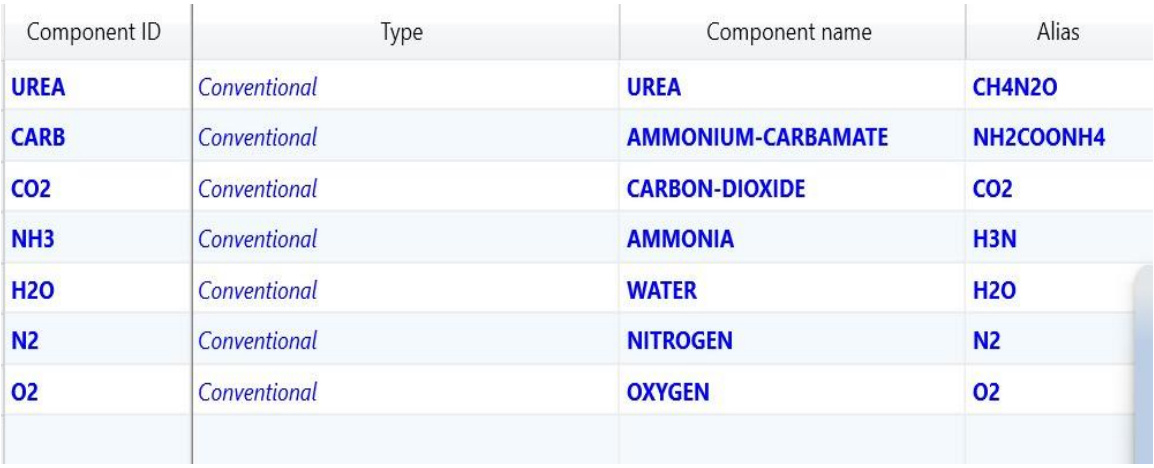
CHAPTER 6

PROCESS SIMULATION

6.1 ASPEN Plus

Simulation of our project in ASPEN Plus was done in order to check its feasibility. The reactor we used was a plug flow reactor. To model this reactor in ASPEN Plus we used RPLUG block. The reactions involved in our process were kinetic reactions. Their respective kinetics were adjusted using a developed subroutine. Component list was added via Aspen properties and fluid package was selected to be SR-POLAR because it accommodates all the required components. Simulation of our model is shown below:

Components:

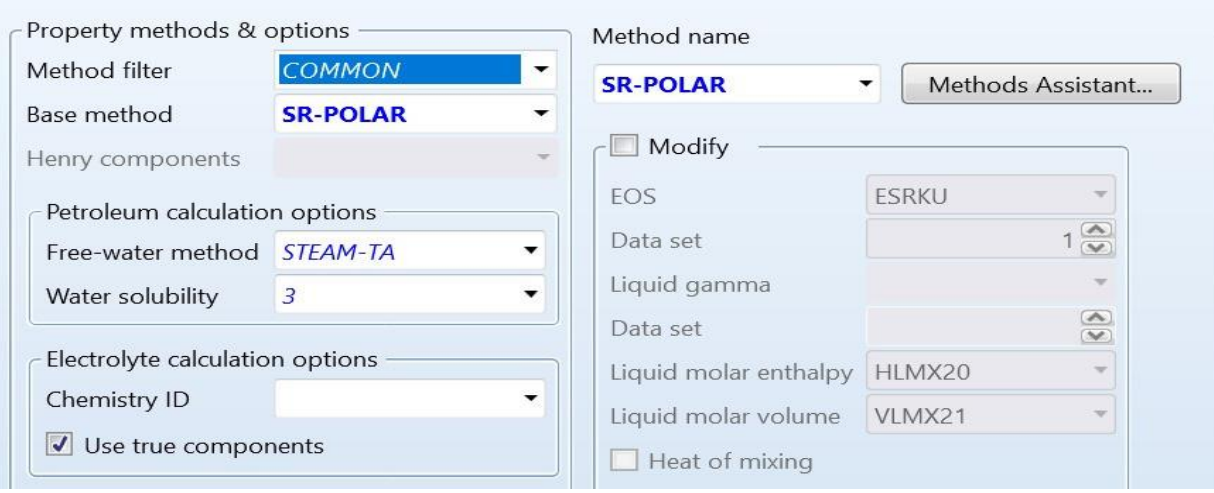


Component ID	Type	Component name	Alias
UREA	*Conventional*	**UREA**	**CH4N2O**
CARB	*Conventional*	**AMMONIUM-CARBAMATE**	**NH2COONH4**
CO2	*Conventional*	**CARBON-DIOXIDE**	**CO2**
NH3	*Conventional*	**AMMONIA**	**H3N**
H2O	*Conventional*	**WATER**	**H2O**
N2	*Conventional*	**NITROGEN**	**N2**
O2	*Conventional*	**OXYGEN**	**O2**

Figure 21: Components used for HP Loop

Property Package:

SR-POLAR is used as it is recommended for high temperature and pressure systems. Moreover, it can be used for mixtures of non-polar and polar compounds, in combination with light gases.



Property methods & options

Method filter: COMMON

Base method: SR-POLAR

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: SR-POLAR

☐ Modify

EOS: ESRKU

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX20

Liquid molar volume: VLMX21

☐ Heat of mixing

Figure 22: Fluid Package

Process Flow Diagram:

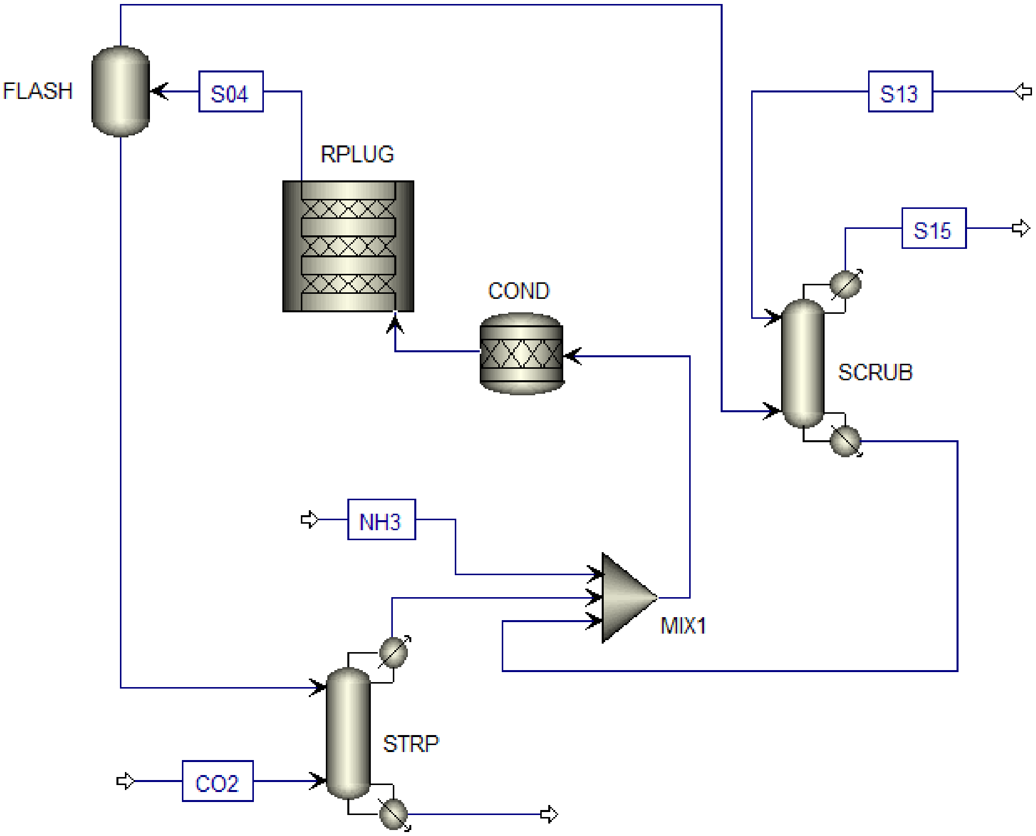
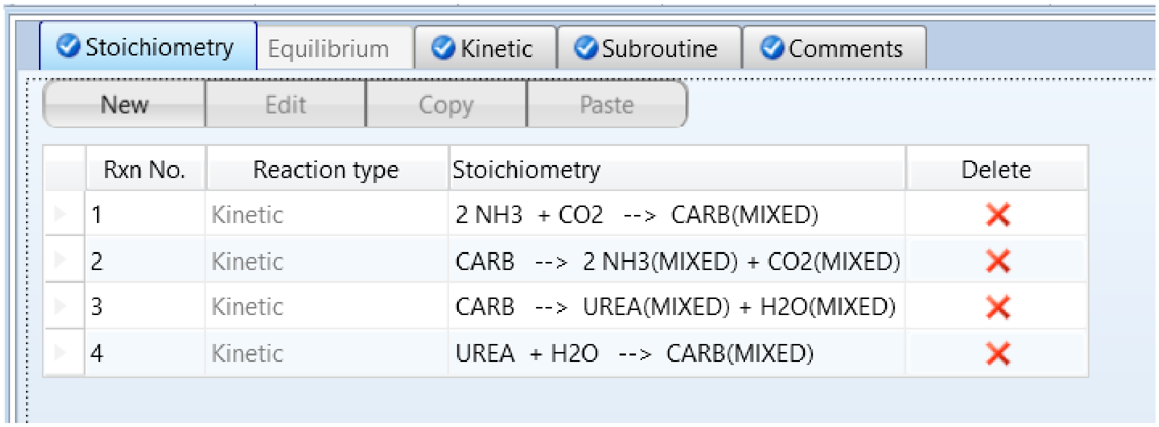


Figure 23: Main Flow Sheet

Reactions:

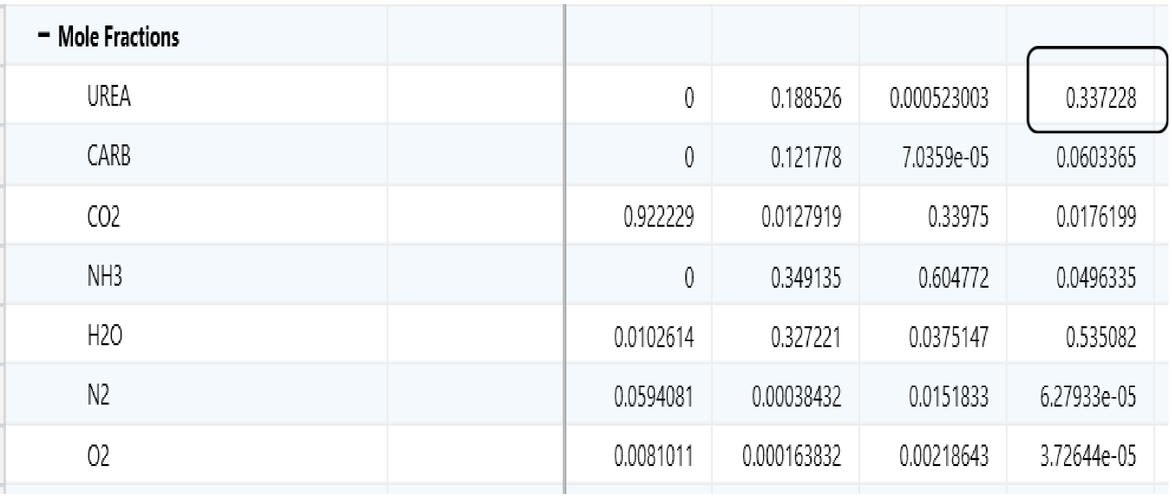


Rxn No.	Reaction type	Stoichiometry	Delete
1	Kinetic	2 NH3 + CO2 --> CARB(MIXED)	✕
2	Kinetic	CARB --> 2 NH3(MIXED) + CO2(MIXED)	✕
3	Kinetic	CARB --> UREA(MIXED) + H2O(MIXED)	✕
4	Kinetic	UREA + H2O --> CARB(MIXED)	✕

Figure 24: Reactions within the reactor

6.1.1 Reactor

Following are the obtained results after both the reactions have occurred within the PFR.

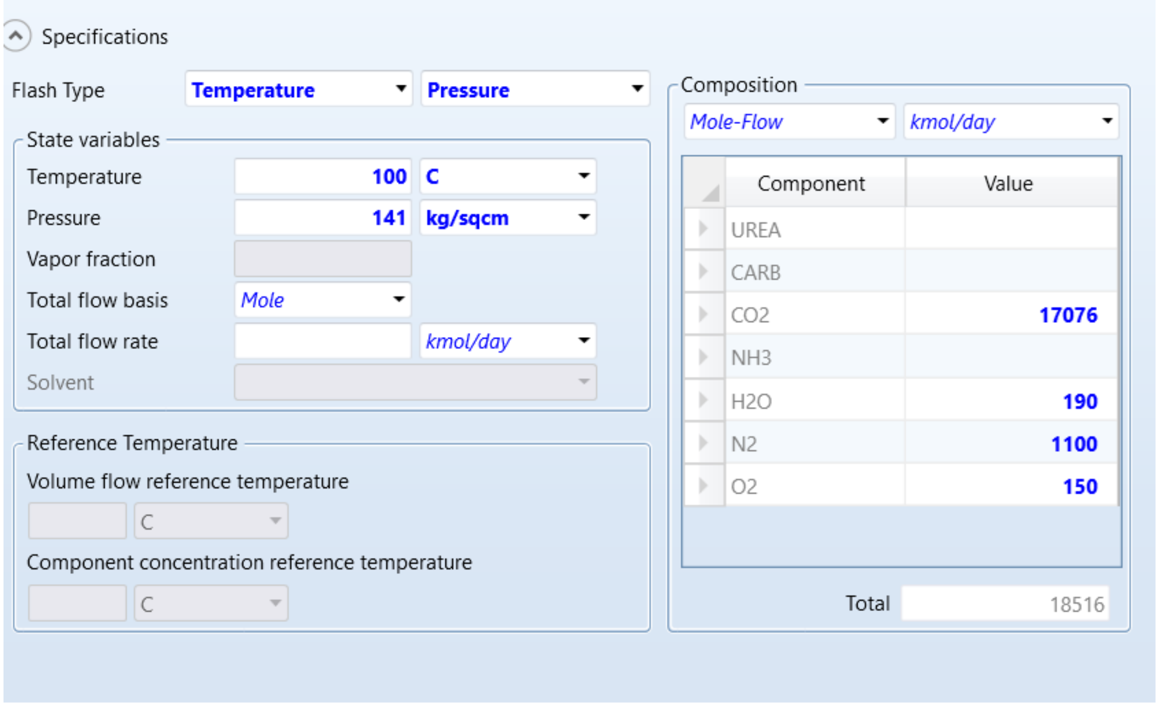


- Mole Fractions					
UREA		0	0.188526	0.000523003	0.337228
CARB		0	0.121778	7.0359e-05	0.0603365
CO2		0.922229	0.0127919	0.33975	0.0176199
NH3		0	0.349135	0.604772	0.0496335
H2O		0.0102614	0.327221	0.0375147	0.535082
N2		0.0594081	0.00038432	0.0151833	6.27933e-05
O2		0.0081011	0.000163832	0.00218643	3.72644e-05

Figure 25: Molar fractions of components

6.1.2 Stripper

Feed:



Flash Type: Temperature, Pressure

State variables

Temperature: 100 C

Pressure: 141 kg/sqcm

Vapor fraction:

Total flow basis: Mole

Total flow rate: kmol/day

Solvent:

Reference Temperature

Volume flow reference temperature: C

Component concentration reference temperature: C

Composition: Mole-Flow, kmol/day

Component	Value
UREA	
CARB	
CO2	17076
NH3	
H2O	190
N2	1100
O2	150

Total: 18516

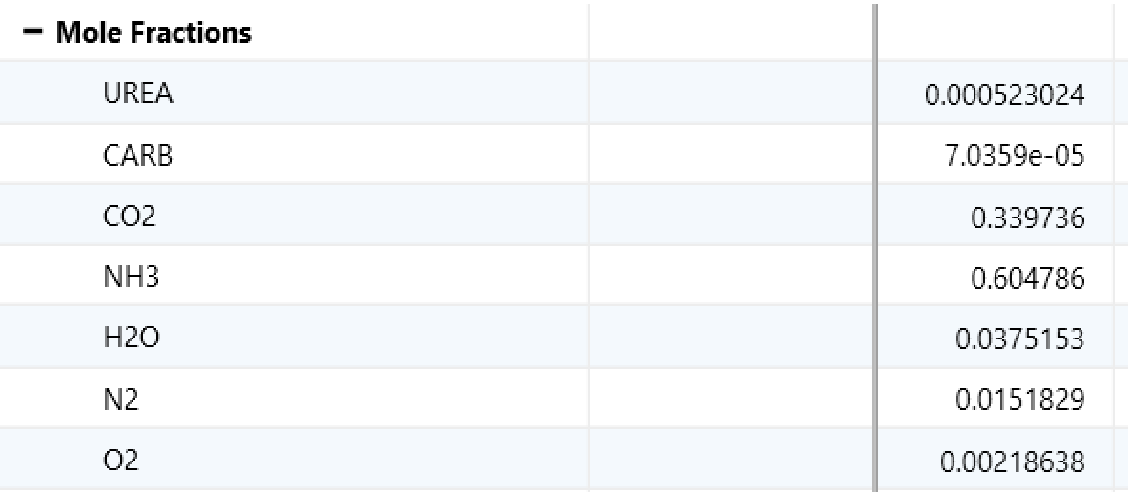
Figure 26: Feed conditions of Stripper

Outlet (Bottom):

− Mole Fractions		
UREA		0.497224
CARB		0
CO2		0
NH3		0
H2O		0.502628
N2		9.27322e-05
O2		5.50304e-05

Figure 27: Molar Fraction of Components

Outlet (Top):

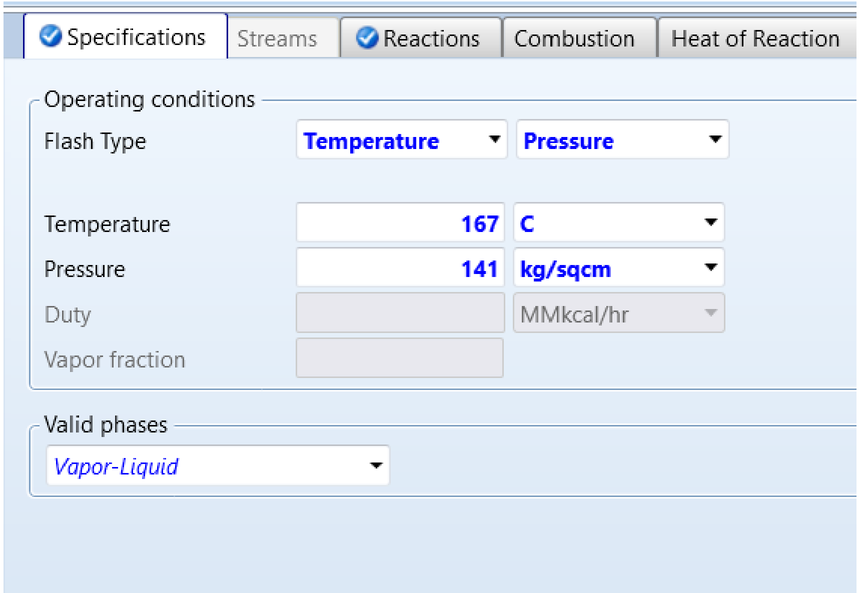


Mole Fractions	
UREA	0.000523024
CARB	7.0359e-05
CO2	0.339736
NH3	0.604786
H2O	0.0375153
N2	0.0151829
O2	0.00218638

Figure 28: Molar Fraction of Components

6.1.3 Condenser (RSTOIC)

Carbamate Condenser for the High pressure Urea synthesis Loop is modeled with an RSTOIC block as the formation of Carbamate occurs within the vessel hence a reactive system is required.



Operating conditions

Flash Type: Temperature, Pressure

Temperature: 167 C

Pressure: 141 kg/sqcm

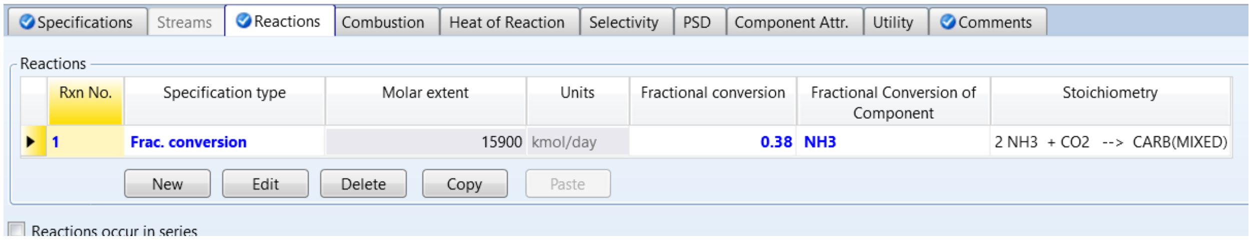
Duty: MMkcal/hr

Vapor fraction:

Valid phases: Vapor-Liquid

Figure 29: Inlet Conditions of RSTOIC

Carbamate Formation:



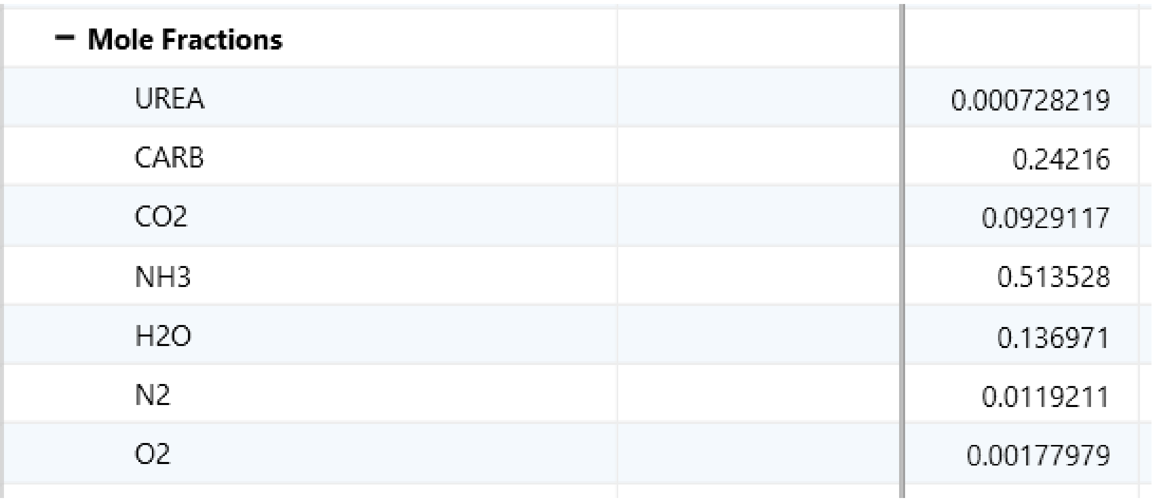
Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion	15900	kmol/day	0.38	NH3	2 NH3 + CO2 --> CARB(MIXED)

☐ Reactions occur in series

Figure 30: Fractional Conversion

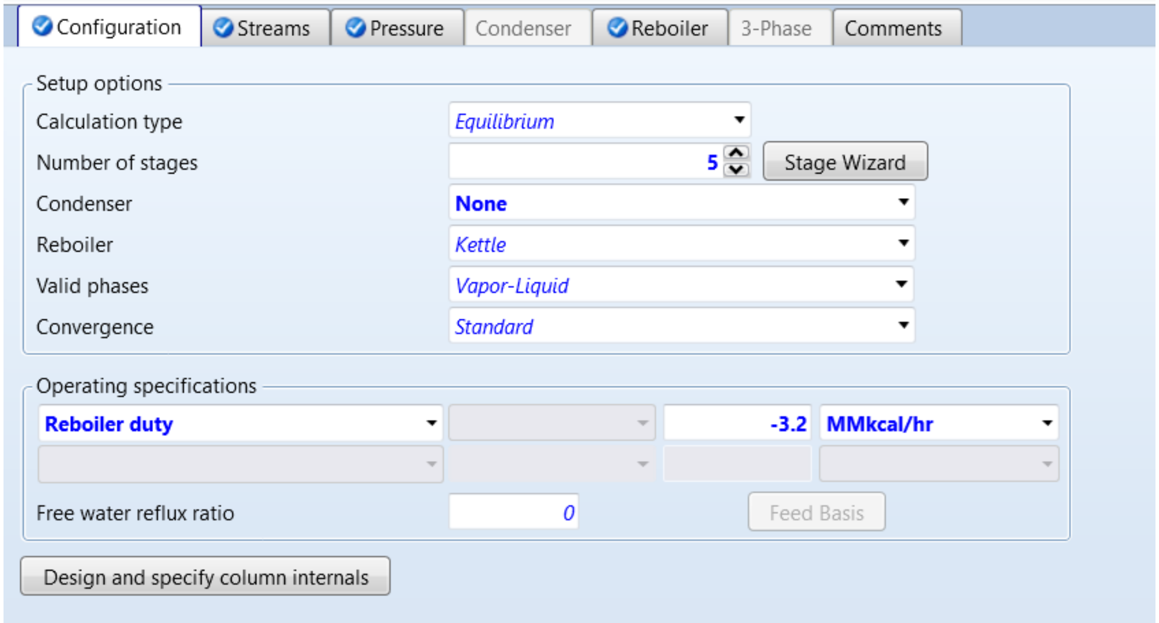
Results:



Mole Fractions	
UREA	0.000728219
CARB	0.24216
CO2	0.0929117
NH3	0.513528
H2O	0.136971
N2	0.0119211
O2	0.00177979

Figure 31: Molar Fractions of Components

6.1.4 Scrubber



Setup options

Calculation type: Equilibrium

Number of stages: 5

Condenser: None

Reboiler: Kettle

Valid phases: Vapor-Liquid

Convergence: Standard

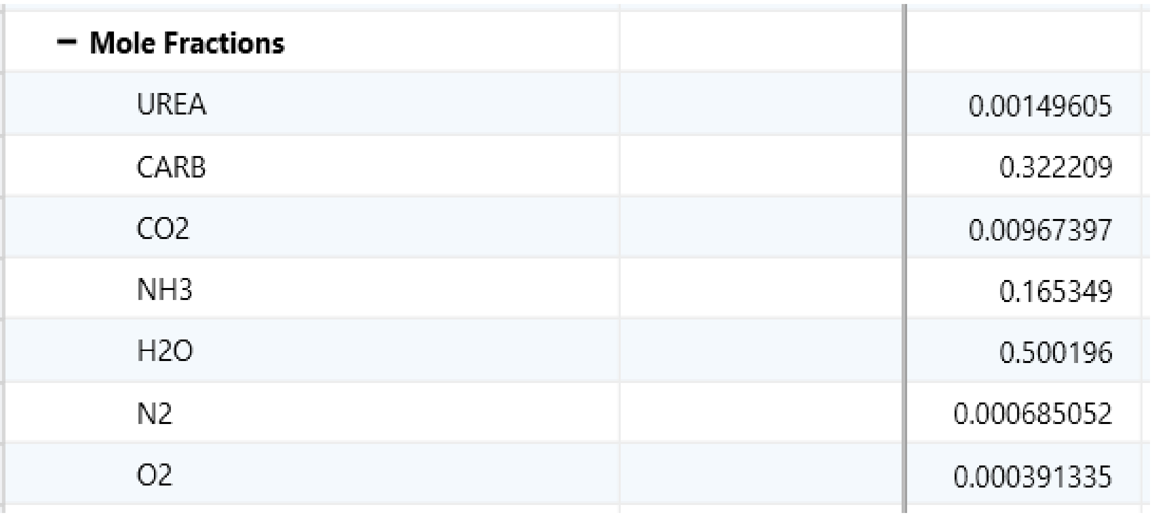
Operating specifications

Reboiler duty: -3.2 MMkcal/hr

Free water reflux ratio: 0

Figure 32: Inlet Conditions of Scrubber

Results:



Mole Fractions		
UREA		0.00149605
CARB		0.322209
CO2		0.00967397
NH3		0.165349
H2O		0.500196
N2		0.000685052
O2		0.000391335

Figure 33: Molar Fractions of Components

CHAPTER 7

COST ANALYSIS

A fixed capital investment, which is essentially the whole of all direct and indirect costs, comes first in the cost assessment process. Purchased items like pumps, heat exchangers, columns, etc. are included in the direct costs. Together with the aforementioned equipment, they also include buildings, sites, facilities, land, pipes, control, and instrumentation, electrical equipment. Indirect costs, on the other hand, consist of engineering and supervision, which includes administrative, design, and inspection. They also consist of start-up, contingency, contractor's fee, and building expenses.

Capital and operating costs are the most important concerns for anyone considering a fertilizer plant. The estimation of capital costs may be the cause of delayed decisions on several projects. This can be attributed to a variety of factors, including variations in the design, locations, market conditions, and attributes of the items and equipment. Then, estimating costs accurately becomes crucial to the startup of a factory. Though estimation errors may occur, depending on the level of engineering design, the margin might be drastically decreased. Estimators ought not to work alone at all.

Following are the purchased costs of equipment obtained from Apsen Plus.

Table 27: Purchased Cost of Equipment

Purchased Cost of Equipment	
Reactor	1209500
Stripper	220600
Condenser	337500
Scrubber	38100
Flash Vessel	233000
PCE = $ 2038700	

The following table helps in estimation of costs of Project Fixed Capital Costs

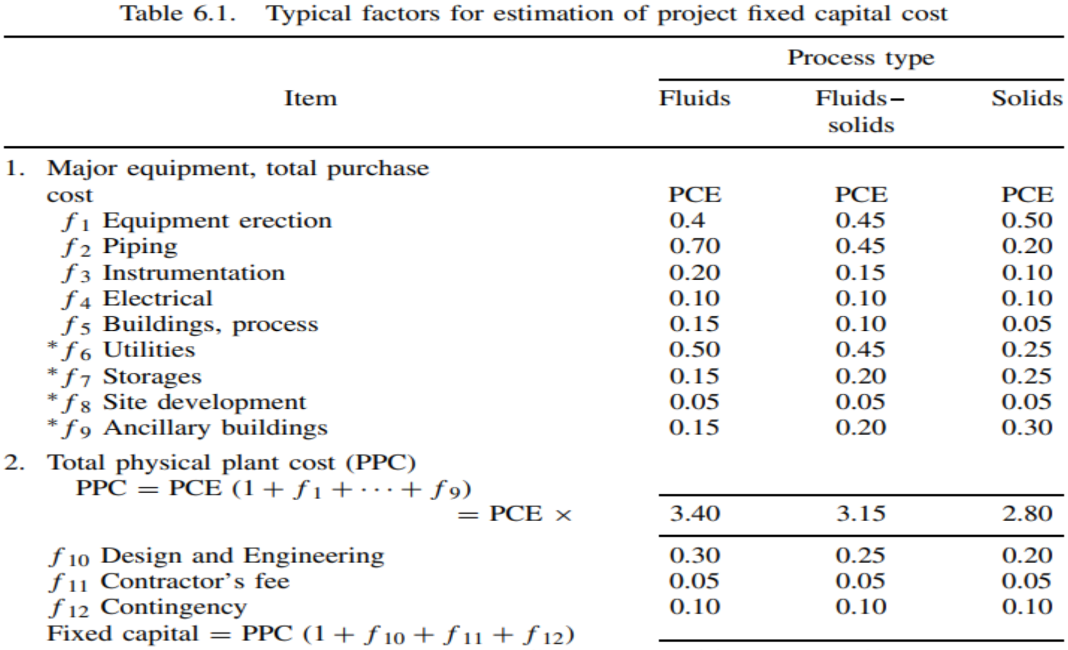


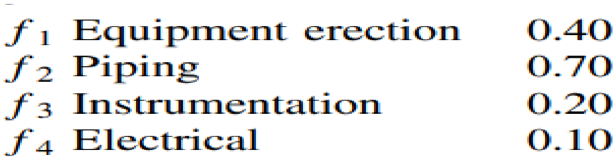
Table 6.1. Typical factors for estimation of project fixed capital cost

Item	Process type		
	Fluids	Fluids–solids	Solids
1. Major equipment, total purchase cost	PCE	PCE	PCE
f_1 Equipment erection	0.4	0.45	0.50
f_2 Piping	0.70	0.45	0.20
f_3 Instrumentation	0.20	0.15	0.10
f_4 Electrical	0.10	0.10	0.10
f_5 Buildings, process	0.15	0.10	0.05
* f_6 Utilities	0.50	0.45	0.25
* f_7 Storages	0.15	0.20	0.25
* f_8 Site development	0.05	0.05	0.05
* f_9 Ancillary buildings	0.15	0.20	0.30
2. Total physical plant cost (PPC) $\text{PPC} = \text{PCE}\,(1 + f_1 + \cdots + f_9)$ $= \text{PCE} \times$	3.40	3.15	2.80
f_{10} Design and Engineering	0.30	0.25	0.20
f_{11} Contractor's fee	0.05	0.05	0.05
f_{12} Contingency	0.10	0.10	0.10
Fixed capital $= \text{PPC}\,(1 + f_{10} + f_{11} + f_{12})$			

Figure 34: Cost Estimation Factors

Physical Plant Cost (PPC):

PPC = PCE × (1 + 0.4 + 0.7 + 0.2 + 0.1) = $ 4892880

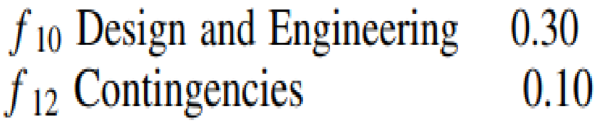


f_1 Equipment erection	0.40
f_2 Piping	0.70
f_3 Instrumentation	0.20
f_4 Electrical	0.10

Figure 35: Cost Estimation Factors

Fixed Capital Cost (FCC):

FCC = PPC × (1 + 0.3 + 0.1) = $ 6850032



f_{10} Design and Engineering	0.30
f_{12} Contingencies	0.10

Figure 36: Cost Estimation Factors

Working Capital is 5% of fixed capital cost.

Working Capital Cost = $ 342501.6

Total Investment required for project:

= Working Capital + Fixed Capital

= $ 342501.6 + $ 6850032

Total investment = $ 7192534

Table 28 Variable Costs

Variable Costs	
Raw materials	280195.7
Miscellaneous materials	34280.22
Utilities	660106.8
Sub-total A = $ 974582.7	

Table 29: Fixed Costs

Fixed Costs	
Maintenance	342802.1
Operating labor	37785.6
Laboratory costs	7557.12
Supervision	7557.12
Overheads	3778.56
Capital charges	685604.3
Insurance	68560.43
Local taxes	137120.9
Royalties	71988.46
Sub-total B = $ 1362755	

Sales Expense = $467467.5

Sub-total C = $467467.5

Annual Production Cost:

A + B + C = $2804805

Cost Inflation: 2004 → 2024

CPE Index = 1.79 (795.1/ 442.2)

Cost in year 2024 = 2804805 × 1.79 = $ 5020601

Annual Revenue = $ 166256640

Profit:

(Annual Revenue - Annual Production Cost)

Profit = $ 161236039.62

Payback Period:

(Initial Investment / Profit) = 7192534 / 161236039.62

Payback Period = **4.5 years**

CHAPTER 8

HAZOP ANALYSIS

8.1 HAZOP Study:

HAZOP, which is short for Hazard and Operability Study, is a safety procedure that is very important and practical to ensure the identification of possible hazards and related operational problems in a chemical process. It is a technique that is particularly used to identify deviations within a process from the plans that were initially designed that may result in accidents, harm, or harm to the environment.

8.1.1 Preparation:

- **Assemble a HAZOP Team:** Assemble a competent team of specialists in different disciplines to the process among them being chemical engineers and process safety specialists, operations officers, and maintenance technologists.
- **Gather Information:** Gather PFDs/PIDs, P&IDs, detailed process description, SDS for materials used, and current standard operating procedures.

8.1.2 Define the Scope:

- Be very precise whether the process being reviewed is an organizational, operational, management, or other type of process. This involves defining the beginning and end of a process segment being analyzed.

8.1.3 Node Selection and Data Review:

- **Analyze** the overall process and split it into segments, which can be reactors, storage tanks, heat exchangers, pipelines, etc.
- **Design intent:** What is the purpose of this node in the overall process and what do you need to accomplish here?

- **Process parameters:** Such variables as temperature and pressure, flow and level, and many others.
- **Operating conditions:** The average levels and variability of each parameter under routine conditions.

8.1.4 HAZOP Guidewords and Deviations:

At each node of the tree, use a predetermined set of questions or guidewords to look for potential ways that the design may have departed from the intended result. Common guidewords include:

- **No:** The cases in which a parameter is missing (the absence of a flow, for example)
- **More:** Going further than what the normal working range should be in some ways (e. g. more pressure)
- **Less:** Falling below the normal operating condition, for example, temperature.
- **As Well As:** Physical incorporation of an unforeseen element or state
- **Part of:** A subtle failure in a certain portion of the equipment (such as a leakage in a heat exchanger).

Analyze each process parameter at each node against the following guidewords to find out the potential deviations.

8.1.5 Cause and Consequence Analysis:

For each identified deviation, speculate on potential causes that may have led to the deviation. These may include equipment failure, operator or technical error, process disturbance or fluctuations, and other conditions. Scrutinize the possible implications of the deviation.

- Safety hazards: Fire, explosion, toxicity, personnel harm
- Environmental impact: Contamination, leaks
- Operational issues: Defect or quality of products, time loss, and other monetary losses.

8.1.6 Safeguards and Recommendations:

- Review existing measures that would have been put in place to help prevent or manage the identified hazards and operability problems. Such control measures may include alarms, interlocks, safety valves, or specific ways and methods of operating the plant.
- Where current measures are considered not enough, suggest other measures that could be taken. This may mean redesigning some structures, optimizing the process, or adding protective gear.

8.1.7 Documentation and Follow-Up:

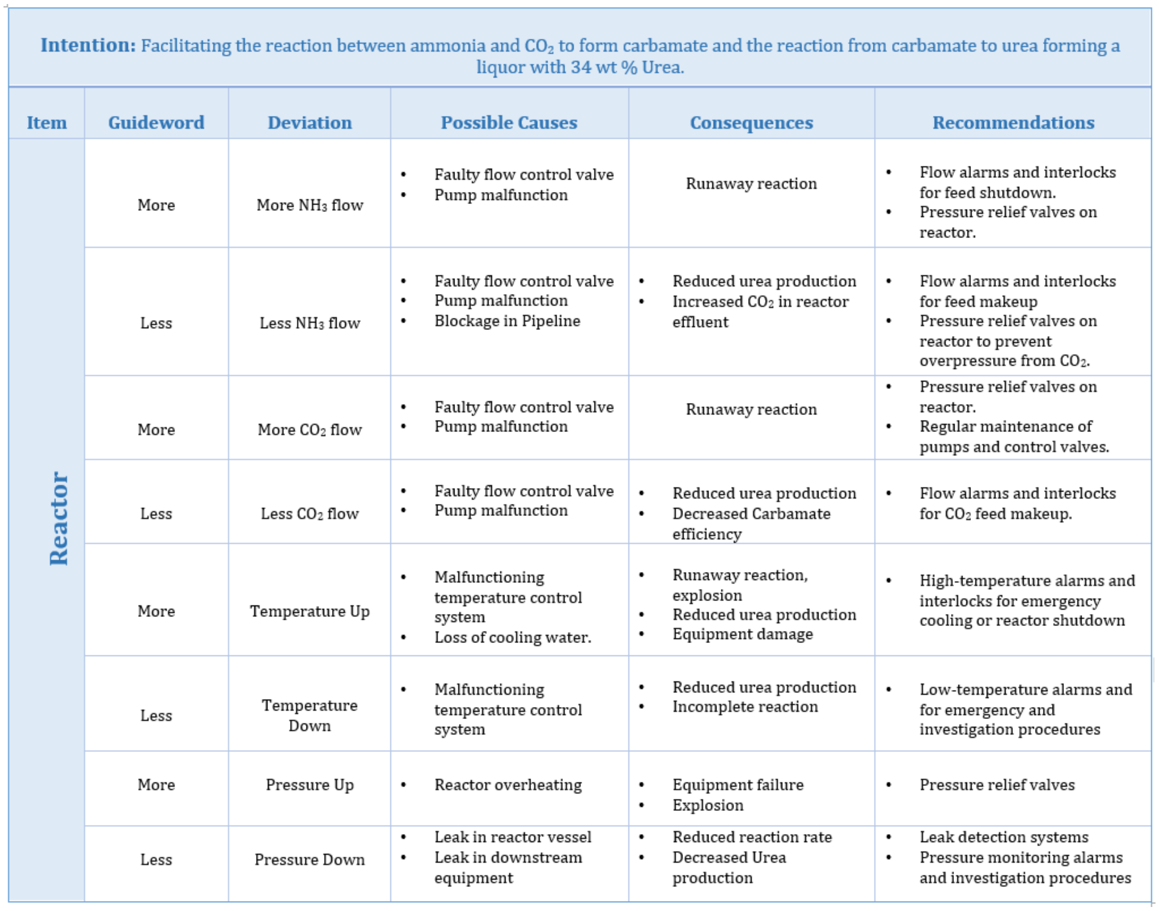
It will be necessary to develop a HAZOP report that will provide information about the entire study.

- Collect process information on each node
- Define deviations, explain their reasons, and outcomes
- The measures that are currently available and how effective they are
- Steps to be taken to increase effectiveness·

Ensure that the responsibility of putting into practice the recommended actions lies with someone responsible and set the cycle for follow-ups to ensure that remedial actions are carried out. Students should also be well-trained and experienced to conduct the HAZOP study to enhance its functionality. Moreover, to ensure optimal assessment of problems in the given field, the study has to preserve creativity and critical thinking during its process. HAZOP studies are repetitive; the sequential analyses may require additional studies after making changes based on previous recommendations or process variations. By the adoption of the above guideline, a HAZOP study can be a strong weapon in enhancing the safety and operability of the chemical processes, thus minimizing accident occurrences and optimizing the entire process flow.

HAZOP Analysis on Reactor:

Table 30: HAZOP on Reactor

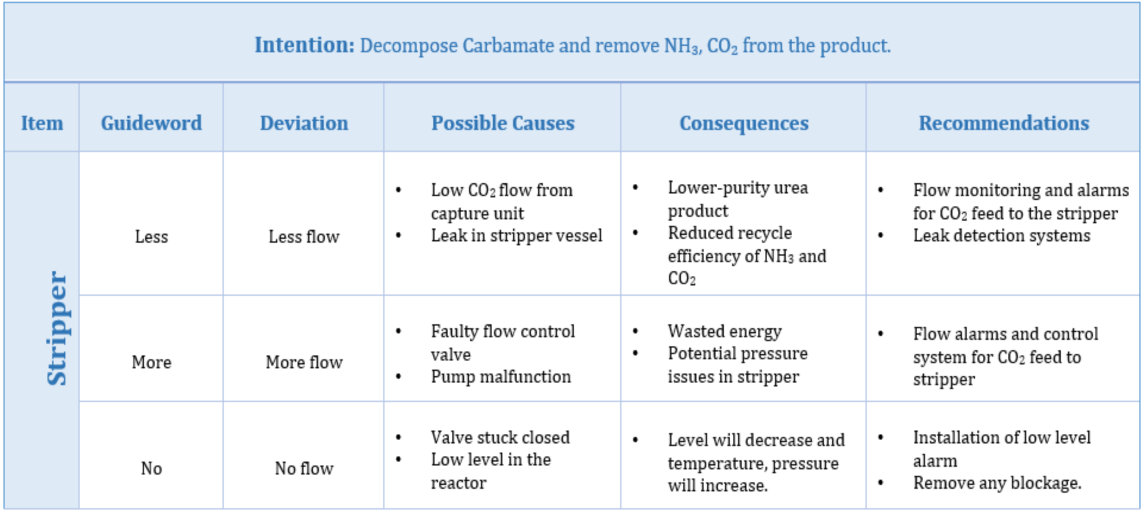


Intention: Facilitating the reaction between ammonia and CO_2 to form carbamate and the reaction from carbamate to urea forming a liquor with 34 wt % Urea.

Item	Guideword	Deviation	Possible Causes	Consequences	Recommendations
Reactor	More	More NH_3 flow	- Faulty flow control valve - Pump malfunction	Runaway reaction	- Flow alarms and interlocks for feed shutdown. - Pressure relief valves on reactor.
	Less	Less NH_3 flow	- Faulty flow control valve - Pump malfunction - Blockage in Pipeline	- Reduced urea production - Increased CO_2 in reactor effluent	- Flow alarms and interlocks for feed makeup - Pressure relief valves on reactor to prevent overpressure from CO_2.
	More	More CO_2 flow	- Faulty flow control valve - Pump malfunction	Runaway reaction	- Pressure relief valves on reactor. - Regular maintenance of pumps and control valves.
	Less	Less CO_2 flow	- Faulty flow control valve - Pump malfunction	- Reduced urea production - Decreased Carbamate efficiency	- Flow alarms and interlocks for CO_2 feed makeup.
	More	Temperature Up	- Malfunctioning temperature control system - Loss of cooling water.	- Runaway reaction, explosion - Reduced urea production - Equipment damage	- High-temperature alarms and interlocks for emergency cooling or reactor shutdown
	Less	Temperature Down	- Malfunctioning temperature control system	- Reduced urea production - Incomplete reaction	- Low-temperature alarms and for emergency and investigation procedures
	More	Pressure Up	- Reactor overheating	- Equipment failure - Explosion	- Pressure relief valves
	Less	Pressure Down	- Leak in reactor vessel - Leak in downstream equipment	- Reduced reaction rate - Decreased Urea production	- Leak detection systems - Pressure monitoring alarms and investigation procedures

HAZOP Analysis on Stripper:

Table 31: HAZOP on Stripper

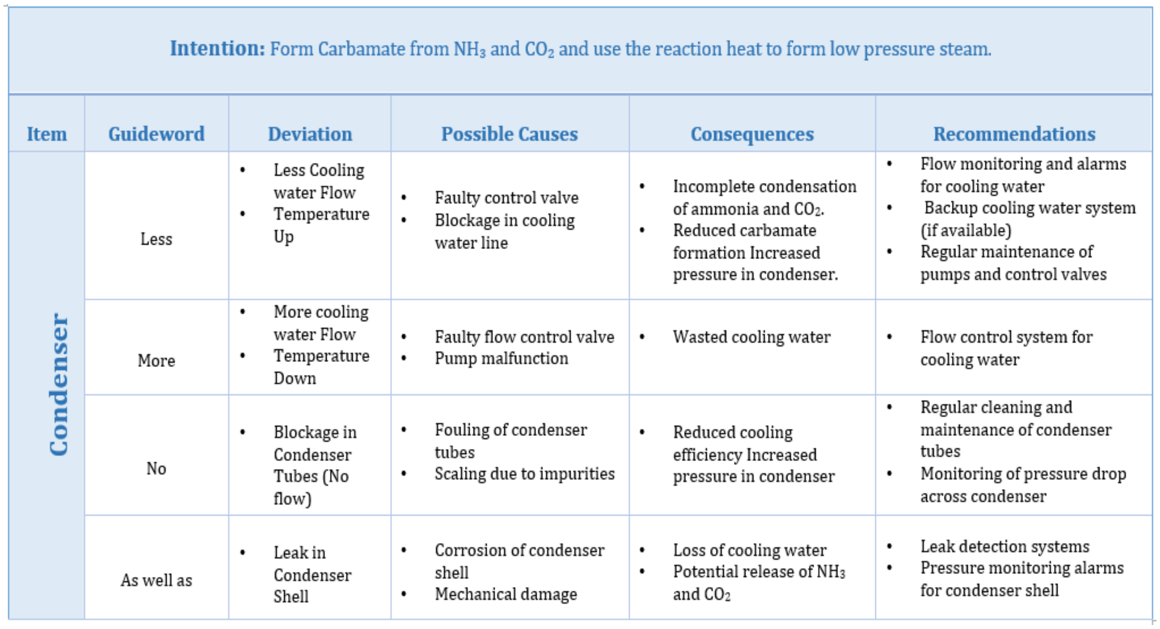


Intention: Decompose Carbamate and remove NH_3, CO_2 from the product.

Item	Guideword	Deviation	Possible Causes	Consequences	Recommendations
Stripper	Less	Less flow	- Low CO_2 flow from capture unit - Leak in stripper vessel	- Lower-purity urea product - Reduced recycle efficiency of NH_3 and CO_2	- Flow monitoring and alarms for CO_2 feed to the stripper - Leak detection systems
	More	More flow	- Faulty flow control valve - Pump malfunction	- Wasted energy - Potential pressure issues in stripper	- Flow alarms and control system for CO_2 feed to stripper
	No	No flow	- Valve stuck closed - Low level in the reactor	- Level will decrease and temperature, pressure will increase.	- Installation of low level alarm - Remove any blockage.

HAZOP Analysis on Condenser:

Table 32: HAZOP on Condenser

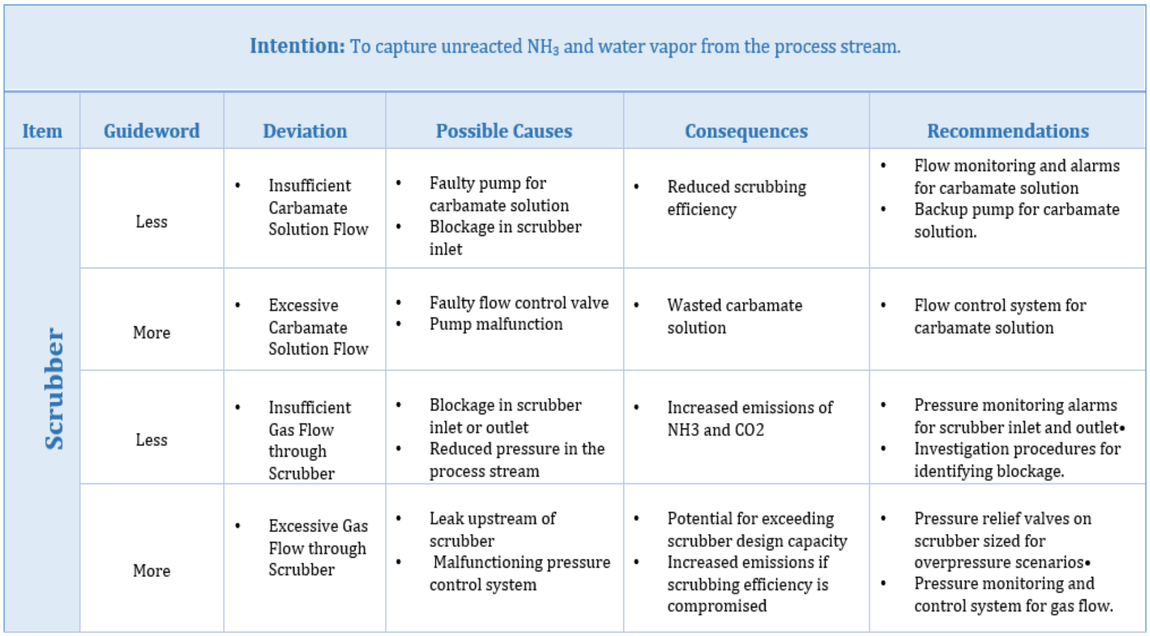


Intention: Form Carbamate from NH_3 and CO_2 and use the reaction heat to form low pressure steam.

Item	Guideword	Deviation	Possible Causes	Consequences	Recommendations
Condenser	Less	• Less Cooling water Flow • Temperature Up	• Faulty control valve • Blockage in cooling water line	• Incomplete condensation of ammonia and CO_2. • Reduced carbamate formation Increased pressure in condenser.	• Flow monitoring and alarms for cooling water • Backup cooling water system (if available) • Regular maintenance of pumps and control valves
	More	• More cooling water Flow • Temperature Down	• Faulty flow control valve • Pump malfunction	• Wasted cooling water	• Flow control system for cooling water
	No	• Blockage in Condenser Tubes (No flow)	• Fouling of condenser tubes • Scaling due to impurities	• Reduced cooling efficiency Increased pressure in condenser	• Regular cleaning and maintenance of condenser tubes • Monitoring of pressure drop across condenser
	As well as	• Leak in Condenser Shell	• Corrosion of condenser shell • Mechanical damage	• Loss of cooling water • Potential release of NH_3 and CO_2	• Leak detection systems • Pressure monitoring alarms for condenser shell

HAZOP Analysis on Scrubber:

Table 33: HAZOP on Scrubber



Intention: To capture unreacted NH_3 and water vapor from the process stream.

Item	Guideword	Deviation	Possible Causes	Consequences	Recommendations
Scrubber	Less	• Insufficient Carbamate Solution Flow	• Faulty pump for carbamate solution • Blockage in scrubber inlet	• Reduced scrubbing efficiency	• Flow monitoring and alarms for carbamate solution • Backup pump for carbamate solution.
	More	• Excessive Carbamate Solution Flow	• Faulty flow control valve • Pump malfunction	• Wasted carbamate solution	• Flow control system for carbamate solution
	Less	• Insufficient Gas Flow through Scrubber	• Blockage in scrubber inlet or outlet • Reduced pressure in the process stream	• Increased emissions of NH3 and CO2	• Pressure monitoring alarms for scrubber inlet and outlet• • Investigation procedures for identifying blockage.
	More	• Excessive Gas Flow through Scrubber	• Leak upstream of scrubber • Malfunctioning pressure control system	• Potential for exceeding scrubber design capacity • Increased emissions if scrubbing efficiency is compromised	• Pressure relief valves on scrubber sized for overpressure scenarios• • Pressure monitoring and control system for gas flow.

CONCLUSION

- The proposed process has been efficiently designed and simulated to meet the requirements i.e. the final product, Urea with a percentage of 49.7 % whereas keeping in view the obtained plant data, percentage of Urea obtained after the high pressure synthesis loop is 45 – 46%. Hence, the chosen operating parameters provided valuable insights into optimizing conversion efficiency, energy consumption, and overall process performance.
- The chosen thermodynamic model faithfully depicted the multiphase behavior of the vapor/liquid phase and the reaction kinetics within the chemical system under high pressure and temperature requirements.
- The results of the process simulation validated the calculations and design of the process and verified the operability of the process. The process is evaluated for a pay-out period of 4.5 years which indicate that the process is not only feasible but economically profitable as well.
- Hazop analysis of the process was also done in order to make sure that the possible hazards can be dealt efficiently while maintaining safe environment for the synthesis of Urea.
- The successful design of this HP loop has the potential to contribute to achieving Sustainable Development Goal (SDG) 2: For instance, on the issue of eliminating world hunger through enhanced crop production by using Haber's process, it supports Zero Hunger by enhancing the production of urea fertilizers thereby improving crop yields. However, social responsibility mechanisms and additional analysis are needed to decrease possible damage to the environment allied to elements of SDGs 3 and 12.

RECOMMENDATION FOR FUTURE RESEARCH

The following recommendations for future research are aimed at overcoming the shortcomings of the existing “High-pressure Urea Synthesis loop”. The industry would have an opportunity to have a more efficient, environment-friendly, and reliable method of manufacturing urea by focusing on efficiency, the possibility of sustainability, control, and safety issues.

10.1 Refined Thermodynamic Models:

Further improvement of the thermodynamic models for the multi-component system of ammonia, carbon dioxide, water, and urea is also required at high pressures and temperatures. This will allow for better analysis and optimization of the processes involved.

10.2 Machine Learning for Optimization:

Another recommendation includes optimization, as well as the prediction of equipment failures using machine learning. This could entail applying the sensor data toward detecting potential areas of poor productivity and potential equipment failure.

10.3 Improved Reactor Design:

Designing reactors that produce less undesired side products like biuret and carbamate and designing safety features to control some risks including the risk of uncontrolled exothermic reactions.

10.4 Advanced Materials for Equipment:

Exploring new materials of construction for equipment in the loop that performs well in the rigorous working environment with enhanced corrosion protection.

10.5 Risk Assessment and Mitigation Strategies:

Employing enhanced risk evaluation techniques to recognize safety risks and designing effective measures to avoid mishaps.

REFERENCES

1. Rozana. (2007). Title of dissertation Steady State Modeling of Urea Synthesis Loop. FGSGUGSU

2. Coulson, J. M., & Richardson, J. F. (1999). Coulson & Richardson's chemical engineering. Volume 1 : fluid flow, heat transfer and mass transfer. Butterworth-Heinemann.

3. Kern, D. Q. (2017). Process Heat Transfer.

4. Urea. (2021, January 11). American Chemical Society.

   https://www.acs.org/molecule-of-the-week/archive/u/urea.html

5. Green, D. W., & Southard, M. Z. (2019). *Perry's chemical engineers' handbook* (9th ed.). Mcgraw-Hill Education.

6. Jean. (2011). *Engineers Guide: Flow Diagram of Urea Production Process from Ammonia and Carbon-dioxide*. Engineers Guide. https://enggyd.blogspot.com/2010/09/flow-diagram-of-urea-production-process.html

7. Germany), D. C., University of Würzburg and IPA Group, Humboldt-Unversität zu Berlin, and KDE Group, University of Kassel, and L3S Research Center, Hanover.

8. (2013). *Modeling and simulation of high-pressure urea synthesis loop. | BibSonomy*.Www.bibsonomy.org. https://www.bibsonomy.org/bibtex/137568360681935be95806ea47cf507ba