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Design and Simulation of a 4,000-Metric Tons per Day Toyo ACES21 Urea Plant

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Abstract
This study presents the design and simulation of a 4,000 MTPD Urea plant in Aspen HYSYS. The plant was first designed through detailed material to get per day requirement of 3,256.887 Tons of CO2 and 2,266.80152 Tons for NH3 to get the 4,000TPD at 99% urea purity. Conclusive energy balance gave heat duties for the different units was done and the Urea Reactor design gave a volume of 396.991m^3 with a length of 80.86m. A simulation was developed for the high-pressure urea synthesis section of the plant. The validity of the simulation was demonstrated by comparing against plant data from the Indorama plant. The simulation results show that the simulation could predict the behaviour of the urea synthesis section. The effect of reactor inlet ratio (NH3/CO2) on Urea yield was studied to show that the yield drops gradually as the ratio increased. The CO2 conversion in the first equilibrium reactor is calculated by Aspen HYSYS to be approximately similar as found in the Indorama Plant; that is 60% with 5% error. The overall loop conversion of CO2 to urea in the high-pressure urea synthesis loop with the recycle stream is calculated by HYSYS to be approximately 89.73% which is 10% higher than is found in the Indorama plant. The study conducted showed that the simulation could be used to predict the CO2 conversion as well as Urea yield as throughput is varied within 10% error.

Keywords: *Aspen HYSYS Simulation, Toyo ACES21 Process, High-Pressure Urea Synthesis, Material and Energy Balance, Reactor Design, CO_2 Conversion Efficiency, NH_3/CO_2 Molar Ratio*

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I.INTRODUCTION

Urea is a widely used nitrogen fertilizer produced industrially through the Bosch–Meiser process, which involves the reaction of ammonia (NH_3) and carbon dioxide (CO_2) in a high-pressure synthesis loop. The process consists of integrated unit operations, including the reactor, high-pressure carbamate condenser (HPCC), stripper, and scrubber, designed to enhance conversion efficiency and recover unreacted materials. Urea formation occurs via two sequential reactions: the rapid, exothermic formation of ammonium carbamate, followed by a slower, reversible, endothermic dehydration to urea and water. Due to thermodynamic and kinetic limitations, per-pass conversion remains low, necessitating extensive recycling of reactants. High operating pressures (140–200 bar) and temperatures (170–200 °C) are employed to maximize yield, while auxiliary units such as the HPCC, stripper, and scrubber play critical roles in reactant recovery, emission control, and downstream product purity. The HPCC promotes additional carbamate formation through condensation, the stripper removes residual ammonia and carbamate from the urea solution, and the scrubber minimizes gaseous losses and environmental emissions. Process modelling and simulation are essential tools for optimizing the urea synthesis loop. Rigorous models based on mass and energy balances, reaction kinetics, and thermodynamic equilibrium enable evaluation of operating conditions, energy integration, and system behavior without costly plant trials. Modern simulation platforms support steady-state and dynamic analyses, facilitating process optimization, energy reduction, and environmental compliance. Overall, simulation-based analysis provides a robust framework for improving efficiency, sustainability, and economic performance in industrial urea production.

II.EXTENT OF PAST WORKS

Early kinetic studies, such as those by Hofmann & Lang (1983), provided empirical models describing the reaction rates of urea synthesis based on industrial data. These models focused on the two-step reaction pathway: the rapid formation of ammonium carbamate and its slower dehydration to urea. Subsequent research by Agarwal *et al.* (2008) applied differential equations to describe the rate of urea formation, integrating mass and energy balances under steady-state assumptions. While such models advanced the understanding of urea kinetics, most were built on ideal mixing assumptions and lacked consideration of phase behaviour or multi-phase flow, which are significant in high-pressure operations.

(Patel & Rao, 2020), Urea, chemically known as carbamide (NH_2CONH_2), is one of the most widely produced nitrogenous compounds in the world and serves as a crucial input in agriculture, chemical industries, and pharmaceuticals. It is primarily used as a nitrogen fertilizer due to its high nitrogen content (approximately 46% by weight), which makes it more efficient and cost-effective compared to other nitrogenous fertilizers like ammonium nitrate or ammonium sulfate.

Urea holds a significant place in the history of chemistry and industrial development, both as a naturally occurring compound and as the first organic molecule to be synthesized artificially. It will be first isolated in 1727 by Dutch chemist Herman Boerhaave from human urine, marking an early understanding of nitrogen metabolism in biological systems (Wöhler, 1828/1971). However, the true historical breakthrough came in 1828 when Friedrich Wöhler synthesized urea from an inorganic compound, ammonium cyanate. This marked a pivotal moment in the field of chemistry, as it disproved the prevailing theory of vitalism, which held that organic compounds could only be produced by living organisms (Ihde, 1964).

Wöhler's synthesis of urea is now widely recognized as the birth of modern organic chemistry. By demonstrating that an organic compound could be synthesized from inorganic precursors, Wöhler laid the foundation for later advances in synthetic chemistry, chemical engineering, and biotechnology. His work initiated a paradigm shift in how chemists understood and approached the study of organic matter (Todhunter, 2003).

The industrial production of urea began in earnest in the early 20th century, in conjunction with the development of large-scale ammonia synthesis via the Haber-Bosch process. The Bosch– Meiser process, developed in the 1920s, enabled the reaction of ammonia and carbon dioxide under high pressure and temperature to produce urea efficiently. This process remains the basis for modern urea production, with ongoing technological advancements focused on improving energy efficiency and conversion rates (Kumar & Bandyopadhyay, 2018).

During the mid-20th century, the importance of urea in agriculture increased rapidly due to its high nitrogen content and cost-effectiveness. Urea soon became the most widely used nitrogen fertilizer, especially in regions with intensive agricultural practices such as Asia and Latin America (FAO, 2021). Its role expanded further with its application in industrial sectors, including the production of resins, adhesives, plastics, and diesel exhaust fluids (DEF) for emissions control.

Today, urea is not only a staple in agricultural fertilizer markets but also a focal point in global discussions on carbon utilization and sustainable chemical production. The dual nature of its production, consuming CO_2 as a feedstock while potentially emitting it during inefficiencies makes it central to efforts aimed at decarbonizing industrial chemical processes (Nasr & Mokhtarani, 2015).

III.MATERIALS AND METHOD

2.1 Materials Used

The following materials were used in the course of this work

i. Data and Process Information:

- Plant Capacity: 4000 metric tons of urea per day
- Feedstock: Ammonia (NH_3) and Carbon dioxide (CO_2)
- Process Conditions: Typical Toyo ACES21 operating pressures (140–175 bar) and temperatures (170– 190°C).
- Thermophysical Properties: Density, specific heat, enthalpy of reaction, vapor-liquid equilibrium data for ammonia-CO_2-water-urea system.

ii. Software and Tools:

- Aspen HYSYS V11 for process modelling, material and energy balance development, and reactor simulation.
- Microsoft Excel – for manual calculations, tabulation of results, and preliminary mass and energy balance checks.
- Microsoft Word / PowerPoint – for documentation and report presentation.

iii. Reference Materials:

- Toyo ACES21 process literature and patents.

Textbooks on Chemical Process Design, Plant Design and Economics for Chemical Engineers, and Urea

Technology.

2.2 Method used

This study was conducted using a computational approach to simulate the high-pressure synthesis loop of an industrial urea production process. The simulation was designed to meet the objectives and comply with the scope by focusing on component-level modelling of the reactor, high-pressure carbamate condenser (HPCC), stripper, and scrubber under steady-state, hypothetical conditions. The steps followed are detailed in equations.

2.2.1 MASS BALANCE CALCULATION

The General Material Balance Equation States that:

$$\begin{pmatrix}\text{Rate of accumulation of}\\ \text{Products within the}\\ \text{reactor volume per time}\end{pmatrix} = \begin{pmatrix}\text{Rate of input of}\\ \text{Feed into the}\\ \text{reactor volume per time}\end{pmatrix} + \begin{pmatrix}\text{Rate of generation of}\\ \text{Products within the}\\ \text{reactor volume per time}\end{pmatrix} - \begin{pmatrix}\text{Rate of output of}\\ \text{Materials out of the}\\ \text{reactor volume per time}\end{pmatrix} - \begin{pmatrix}\text{Rate of depletion of}\\ \text{Feed within the}\\ \text{reactor volume per time}\end{pmatrix}$$

(1)

Urea production per day = 4000.0 Tons CO_2 conversion = 63.00 %
CO_2 requirement per day = 3,256.887 Tons NH_3 requirement per day = 2,266.80152 Tons

Table 1: Chemical formula and Molecular weight of components

COMPONENT	CHEMICAL FORMULA	MOLECULAR WEIGHT
Ammonia	NH_3	17
Carbon Dioxide	CO_2	44
Urea	NH_2CONH_2	60
Water	H_2O	18
Biuret	$NH_2CONHCONH_2$	103
Ammonium Carbamate	NH_2COONH_4	78

Input ratio to reactor NH_3:CO_2 Molar ratio 4 : 1
Weight ratio 68 : 44
Reactions involved in the process
$2NH_3 + CO_2 \leftrightarrow NH_2COONH_4$ + heat

Sch 2 1 1

Mass 34 44 78

M.F. 0.4359 0.5641 1.000

NH_2COONH_4 + heat $\leftrightarrow NH_2CONH_2 + H_2O$

Sch 1 1 1

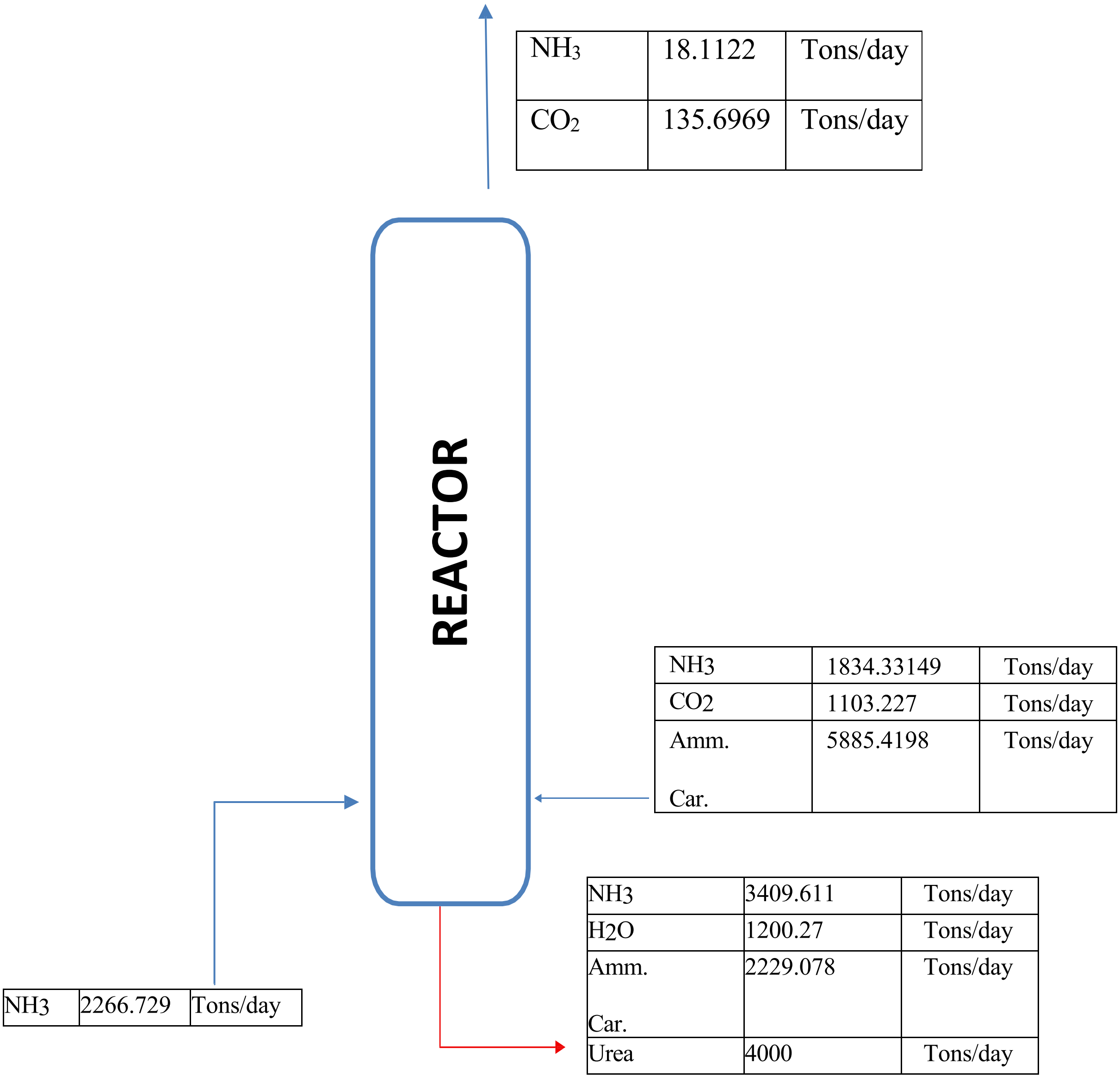
Mass	78		60 18
Wt%	1.000	0.7692	0.2308

$2NH_3 + CO_2 \leftrightarrow NH_2CONH_2 + H_2O$

Sch	2	1	1	1
Mass	34	44	60	18
Wt%	0.4359	0.5641	0.7692	0.2308

2.2.2 REACTOR

BASIS: Taking 4000tons/day of Urea production



NH_3	18.1122	Tons/day
CO_2	135.6969	Tons/day

NH3	1834.33149	Tons/day
CO2	1103.227	Tons/day
Amm. Car.	5885.4198	Tons/day

NH3	3409.611	Tons/day
H2O	1200.27	Tons/day
Amm. Car.	2229.078	Tons/day
Urea	4000	Tons/day

NH3	2266.729	Tons/day

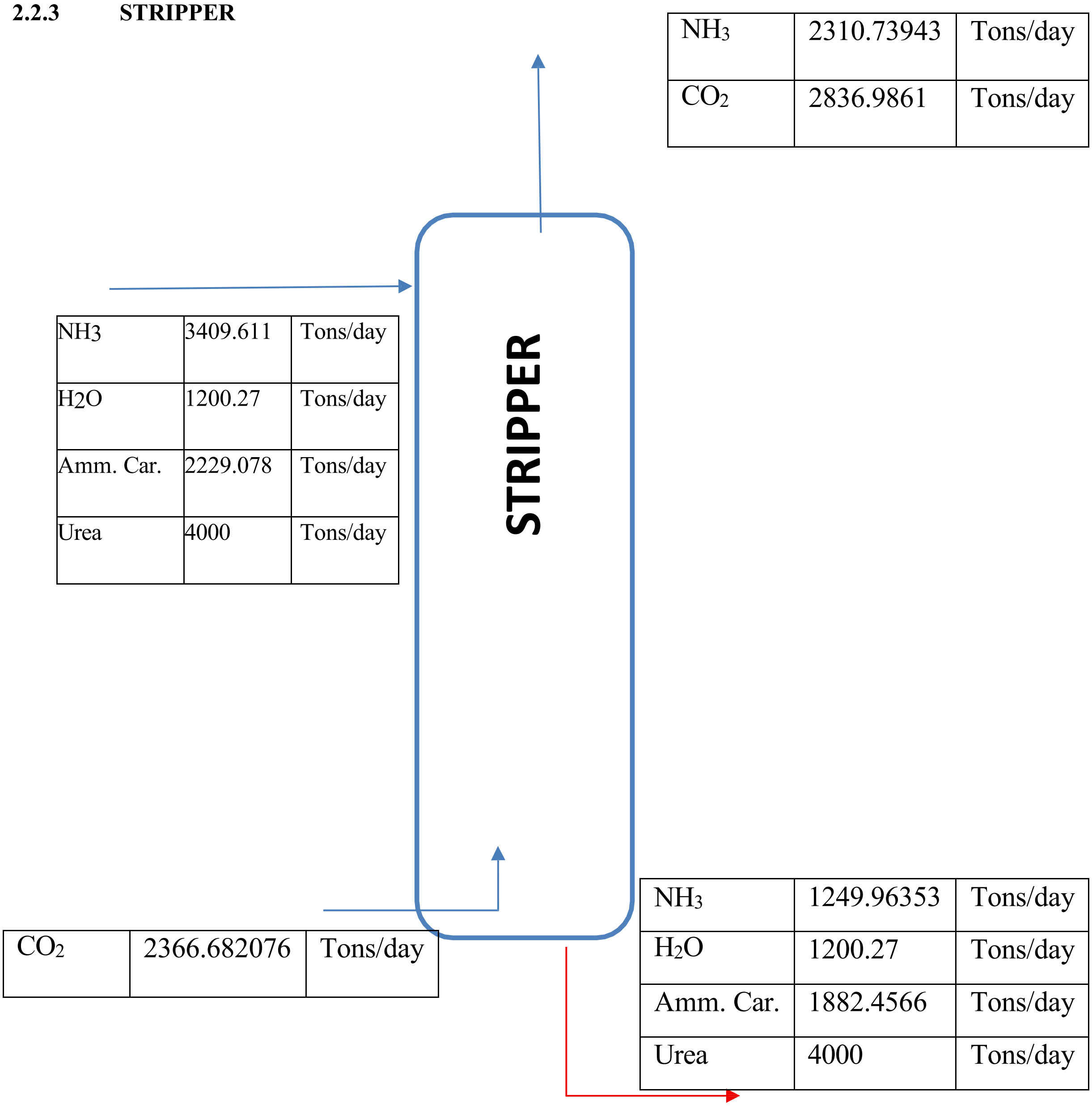
Figure 1: Mass balance in the Reactor

Conversion of Carbon dioxide to ammonium carbamate is complete but, the conversion of Ammonium Carbamate to urea is 63%. Based on stoichiometry, we are getting

Table 2: Mass Balance in the Reactor

COMPONENT	INLET(TONS/DAY)	OUTLET(TONS/DAY)
Ammonia (NH_3)	3409.611	3560.70296
Carbon Dioxide (CO_2)	1103.227	135.6969
Ammonium Carbamate (NH_2COONH_4)	5885.4198	2229.078
Urea (NH_2CONH_2)	0.00	4000.00
Water (H_2O)	0.00	1200.27
Biuret ($NH_2CONHCONH_2$)	0.00	0.00
Total	11125.74786	11125.74786

2.2.3 STRIPPER



NH_3	2310.73943	Tons/day
CO_2	2836.9861	Tons/day

NH3	3409.611	Tons/day
H2O	1200.27	Tons/day
Amm. Car.	2229.078	Tons/day
Urea	4000	Tons/day

CO_2	2366.682076	Tons/day

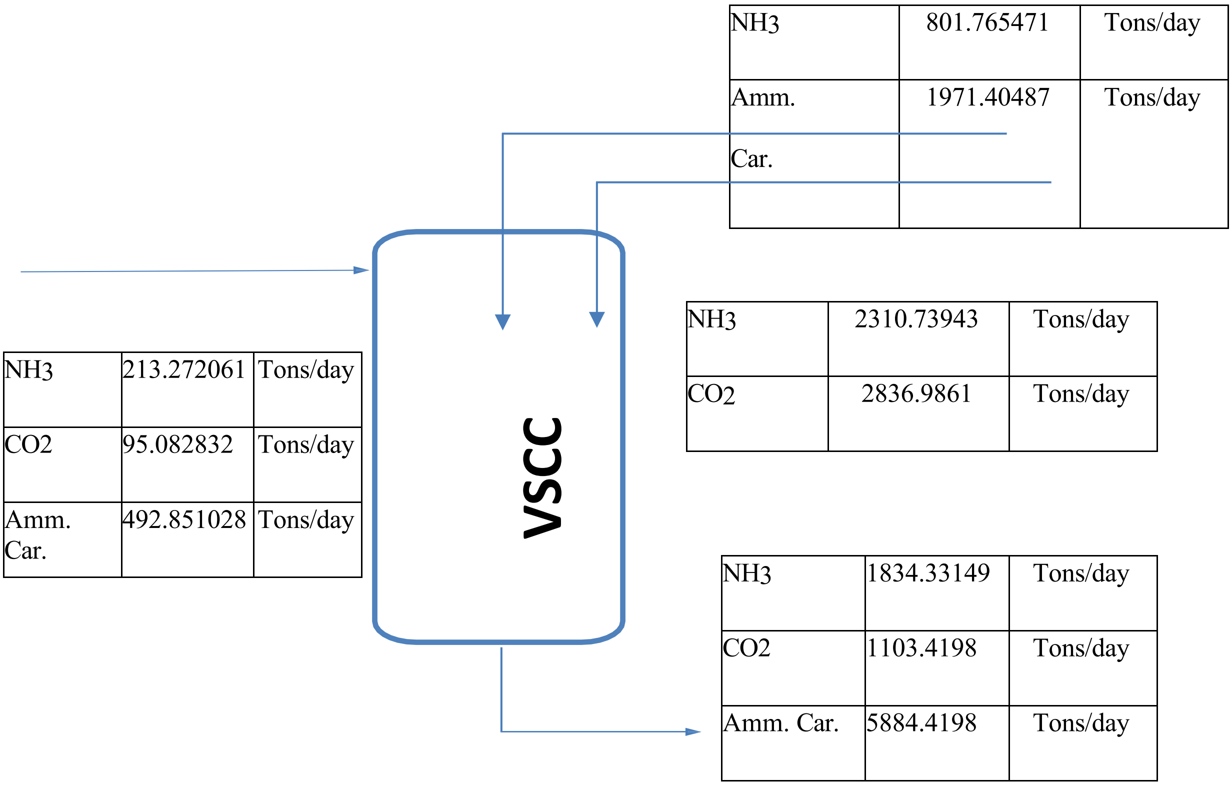
NH_3	1249.96353	Tons/day
H_2O	1200.27	Tons/day
Amm. Car.	1882.4566	Tons/day
Urea	4000	Tons/day

Figure 2: Mass balance in the Stripper

Table 3: Mass Balance in the Stripper

COMPONENT	**INLET(TONS/DAY)**	**OUTLET(TONS/DAY)**
Ammonia (NH_3)	4101.06049	3427.7232
Carbon Dioxide (CO_2)	2366.682076	2836.9861
Ammonium Carbamate (NH_2COONH_4)	2229.078	1882.4566
Urea (NH_2CONH_2)	4000.00	4000.00
Water (H_2O)	1200.27	1200.27
Biuret ($NH_2CONHCONH_2$)	0.00	0.00
Total	11089.70729	11089.70729

2.2.4 Vertically Submerged Carbamate Condenser (VSCC)



NH_3	801.765471	Tons/day
Amm. Car.	1971.40487	Tons/day

NH_3	213.272061	Tons/day
CO_2	95.082832	Tons/day
Amm. Car.	492.851028	Tons/day

NH_3	2310.73943	Tons/day
CO_2	2836.9861	Tons/day

NH_3	1834.33149	Tons/day
CO_2	1103.4198	Tons/day
Amm. Car.	5884.4198	Tons/day

Figure 3: Mass balance in the Carbamate Condenser

Table 4: Mass Balance in the Carbamate condenser

COMPONENT	INLET(TONS/DAY)	OUTLET(TONS/DAY)
Ammonia (NH_3)	3325.776962	1834.33149
Carbon Dioxide (CO_2)	2932.068932	1103.4198
Ammonium Carbamate (NH_2COONH_4)	2464.255898	5884.4198
Urea (NH_2CONH_2)	0.00	0.00
Water (H_2O)	0.00	0.00
Biuret ($NH_2CONHCONH_2$)	0.00	0.00
Total	8822.17109	8822.17109

IV.RESULTS AND DISCUSSION

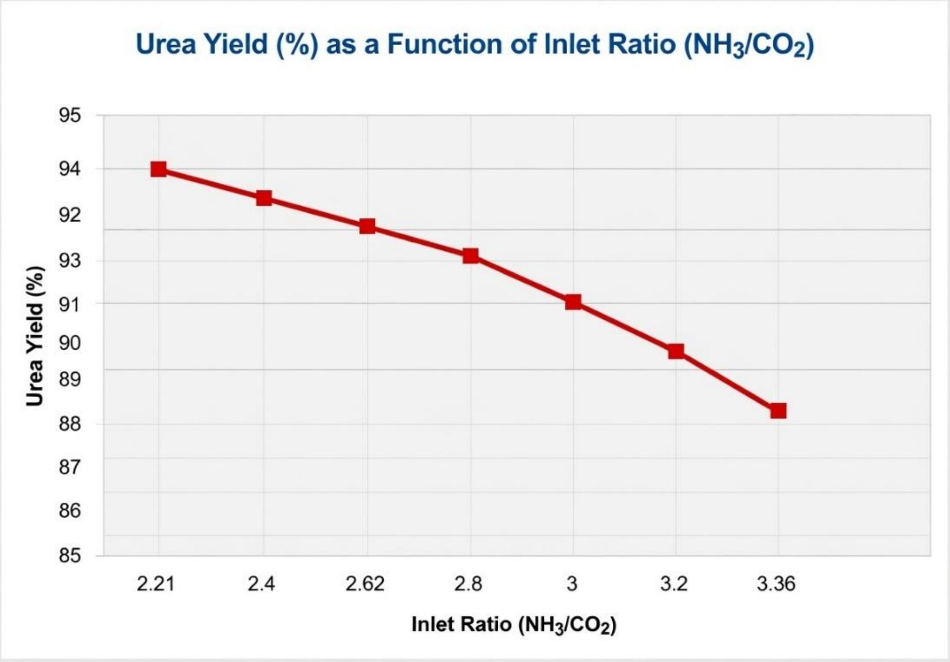


Fig. 4 Urea Yield (%) as a function of inlet Ratio NH_3/CO_2 into the Reactor

Figure 4 shows the relationship between the urea yields (%) with the inlet ratio NH_3/CO_2 into the reactor. From figure 4, it shows that the urea yield decreasing while the inlet ratio is increased.

Hence, the urea yielded is also increased while the inlet ratio into the reactor is decreased. As can be seen from this figure, for the inlet ratio of 2.21 the maximum possible yield is 93.74% which results 3% more yield compared to the base case. And again, the cost of raw material can be further reduced since it requires lower inlet ratio to gain the same amount of urea capacity.

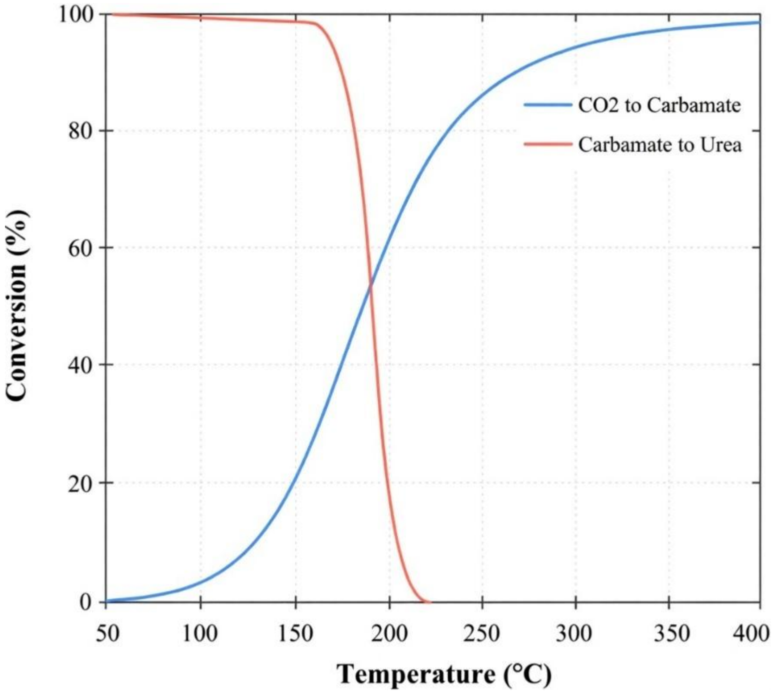


Fig. 5. Effect of temperature on the equilibrium conversion of CO_2 to ammonium carbamate and conversion of ammonium carbamate to urea.

Figure 5. shows the effects of temperature on the equilibrium conversion of CO_2 to ammonium carbamate and conversion of ammonium carbamate to urea for a typical condition. The heat exchanged between shell and tube influences the amount of carbon dioxide converted to ammonium carbamate. In a real plant, the amount of gas entered to the urea reactor is controlled by the pressure of saturated stream in the shell side of the carbamate condenser. Higher steam pressure corresponds to smaller temperature difference between the cooling and process sides, i.e., lower heat flux.

Since increasing the pressure in the shell of the carbamate condenser results in increasing its temperature, it is necessary to investigate the effect of the temperature on the conversion of the two main reactions occurring in the urea reactor, i.e., ammonium carbamate and urea formation. Effect of temperature on the equilibrium conversion of ammonium carbamate formation and urea formation are shown in figure 4.2. Since formation of ammonium carbamate is an exothermic reaction, increasing the temperature beyond 170°C causes decreasing the formation of ammonium carbamate, as seen in figure 4.2. On the other hand, it is shown in the same figure that conversion to urea through an endothermic reaction increases when the temperature is increased. Thus, due to the opposite effect of temperature on these reactions occurring in the reactor, there exists an optimum value for the temperature of the inlet of the reactor at which the formation of ammonium carbamate would be at its maximum value. From figure 4.2, it shows that when the inlet temperature is approximately 274.2°C, the corresponding conversion of ammonium carbamate to urea is found to be 92%.

Table 5: Comparison of Equilibrium conversion between Aspen HYSYS results, Indorama Plant Data and Literature

	Reactor Inlet T(ºC)	Reactor Outlet T (ºC)	Equilibrium Conversion(%)
Indorama Plant	180	182	63
Literature	183	183	60.7
Aspen HYSYS	226.9	274.2	60

Table 5 shows the comparison on equilibrium conversion of carbon dioxide to ammonium carbamate calculated by Aspen HYSYS with Indorama Plant data and literature. From the table, it can be seen that the conversion calculated by HYSYS at inlet temperature equals to 226.9 °C agrees with the results obtained by HYSYS as well as the plant and literature data. HYSYS calculated the equilibrium conversion to be approximately 60% in the urea reactor which agrees with the Indorama plant data and literature value. From this thesis, the comparison is only made on the results that obtained from the overall simulation result excluding the insight of the reactor itself. It is strongly recommended to further the study to explore reactor insight so that variation of variables such as temperature and pressure along the reactor can be studied.

IV. CONCLUSION

This research successfully achieved its objective of developing a complete material and energy balance, reactor design, and Aspen HYSYS simulation for a 4000 MTPD Toyo ACES21 Urea Plant.

From the analysis and results obtained, the following key conclusions can be drawn:

The material balance confirmed that maintaining an optimal NH_3/CO_2 molar ratio (3.7) ensures high conversion efficiency and stable operation, with minimal unreacted components.

The energy balance demonstrated that the Toyo ACES21 process effectively integrates heat recovery within its synthesis and decomposition sections, significantly reducing steam consumption and improving thermal efficiency compared to conventional urea processes.

The study provides the following contributions to knowledge:

i. The research provides a complete and rigorously calibrated Aspen HYSYS simulation of a 4,000 ton/day ACES21 urea plant. Existing literature often focuses on the Stamicarbon and Snamprogetti provides partial simulations or focuses only on the synthesis loop; this work integrates HP, LP, recovery, recycle, and evaporation sections into a single unified model.

ii. By tuning equilibrium constants, reaction conversions, and stripping efficiencies to match ACES21 operating envelopes, the research quantifies the impacts of NH_3/CO_2 ratio, stripper duty, HP pressure, and carbamate recycle rates on per-pass and overall urea conversion. These findings provide engineers with practical guidance for debottlenecking, design, and startup optimization.

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