Modeling and simulation of automotive urea production in Peru

Nestor Tamayo[1] , Suemy Castro[2] , Teodoro Patiño-Chiri[3] , Williams Ramos, MSc[4] and Francisco Tarazona-Vasquez, Ph.D[5]

[1,2,3,4,5,] Universidad de Ingenieria y Tecnologia - UTEC, Peru, nestor.tamayo@utec.edu.pe, suemy.castro@utec.edu.pe, teodoro.patino@utec.edu.pe, wramosv@utec.edu.pe, ftarazona@utec.edu.pe

Abstract .- Air quality concerns in Peru have prompted the implementation of EURO 4 regulations in 2018, with a planned upgrade to EURO 6 in 2026. These regulations seek to reduce nitrogen oxide (NO_x) emissions from diesel vehicles. Selective Catalytic Reduction (SCR) technology employing automotive urea (AdBlue®), offers a highly effective solution by reducing NO_x emissions by at least 90%. However, Peru does not produce automotive urea, and there is a lack of technical research on manufacturing. This study addresses this gap by focusing on modeling and simulating an automotive urea production plant in Peru using the process simulation software ProMax 6.0. The design and parameters were based on information from a BR&E document and from the Stamicarbon patent. Thermodynamic models were selected, considering the most suitable for each stage of the process. Pure water, dry air, and dry natural gas from Camisea, Peru, were considered as raw materials. Additionally, a net profit margin analysis was conducted to assess the operational profitability of the process. An alternative scenario involving the sale of CO_2 purified was also considered. The model predicts that 10.01 MMSCFD of natural gas are required to produce 528,000 L/year of AdBlue®, with a composition of 32.66% urea by weight. Regarding energy requirements, the study found that 1.582 kWh/kg of AdBlue® is needed for heating, 2.397 kWh/kg for cooling, and 0.486 kWh/kg for electricity. The natural gas requirement and the CO_2 intensity of the overall process are 0.137 kg of natural gas per kg of AdBlue and 0.336 kg of CO_2 per kg of AdBlue, respectively. Finally, the alternative scenario with CO_2 process purification resulted in a higher net profit margin (37.74%) compared to the non-CO_2 process purification scenario (34.75%).

Keywords – Modeling and Simulation, Natural Gas, Stamicarbon, Automotive Urea, ProMax

I. Introduction

Automotive urea is an aqueous solution composed of 67.5% by mass of demineralized water (H_2O) and 32.5% by mass of urea ($CO(NH_2)_2$) [1]. This is a nitrogenous chemical compound synthesized through ammonia (NH_3) and carbon dioxide (CO_2). Automotive urea is utilized as an additive for diesel vehicles to mitigate nitrogen oxide (NO_x) emissions [2].

In 2021 and 2022, Peru had the worst air quality in Latin America [3]. The main sources of air pollution are vehicular traffic, the industrial sector, and gas stations, as they produce nitrogen oxide (NO_x), sulfur dioxide (SO_2), and particulates matter (PM) [4]. In response to this issue, the Peruvian government issued a Supreme Decree establishing the maximum permissible limits for pollutant emissions from motor vehicles, along with the implementation of Euro 4 and Euro 6 standards in 2018 and 2026, respectively [5] [6].

There are various alternatives to reduce pollution generated by internal combustion engine (ICE) vehicles. One of them is to use cleaner fuels such as CNG or LPG, as their NO_x emissions are lower compared to diesel [7]. However, CNG and LPG vehicles generally have lower power than vehicles using diesel and gasoline [8]. Therefore, it is important to employ technologies to decrease the emission of toxic gasses from ICE vehicles. Another alternative is Selective Catalytic Reduction (SCR) technology, which utilizes automotive urea and has demonstrated a reduction of over 90% in NO_x emissions from diesel engines [9].

In this context, the importance of automotive urea production in the country lies in its ability to significantly reduce vehicle NO_x emissions through SCR technology, which is already implemented in the country [2]. However, in Peru, this product is entirely imported, and research on automotive urea focuses mainly on the business aspect rather than technical aspects. In Iparraguirre's study [1], a business plan was developed for the importation and commercialization of automotive urea, indicating that the annual consumption of automotive urea in the country exceeds 14 million liters. Additionally, another research effort [2] formulated a business plan for the manufacture and commercialization of automotive urea in Arequipa. According to the authors, an annual production capacity of 528 thousand liters of automotive urea would be suitable for the plant. On the other hand, in Bolivia, an experimental analysis of automotive urea synthesis was conducted using granulated urea from the country's petrochemical plant [10]. It was reported that the obtained product complied with ISO 22241 and Euro 6 standards. This highlights the lack of academic research in Latin America regarding the analysis of urea synthesis processes on an industrial scale.

The main objective of this research work is to model and simulate the production of automotive urea using Peruvian natural gas as the raw material. The secondary objectives of the project are to compare the properties of the urea obtained in the simulation with the technical specifications of the product, to perform material and energy balances, to conduct an economic analysis of the plant, and to compare two scenarios within the economic analysis. The plant's capacity to be simulated will be 528,000 liters annually, utilizing ProMax 6.0 software and Stamicarbon technology for urea

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synthesis. Secondary objectives of the research include conducting material and energy balances, determining the efficiency and performance of the process, as well as performing a preliminary economic analysis.

II. MATERIALS AND METHODS

The simulated automotive urea production plant consists of six stages: Reforming Unit, Water Gas Shift (WGS) Unit, CO_2 Removal Unit, Methanation Unit, Ammonia Unit, and Urea Unit. The simulation design and parameters were based on an official document from BRE ProMax [11] and the patent of the conventional Stamicarbon process [12]. Figure 1 presents the overall process flow diagram of the simulated automotive urea production.
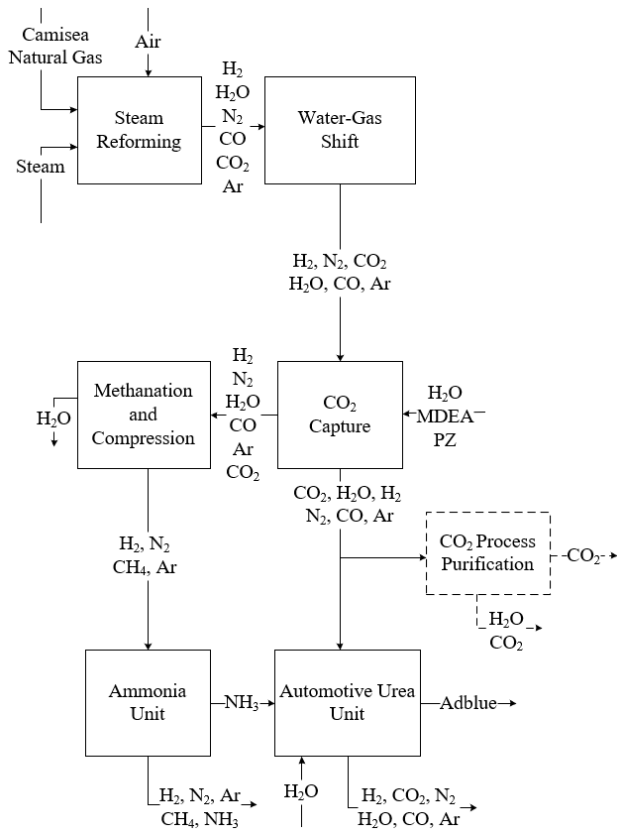

Fig. 1. Automotive urea (AdBlue®) production process flow chart.

A. Model Considerations

The thermodynamic models employed, as implemented in BR&E Promax 6.0, were "Amine Sweetening - Peng Robinson," "Amine Sweetening - SRK," and "SRK Polar" for the CO_2 Capture stage, the Ammonia Unit, and the Urea Unit, respectively. For the stages not mentioned, the Peng Robinson model was used. Additionally, the *biuret* component was not considered in the model due to its small quantities during urea production [13].

The raw materials used in the production process are as follows: 100% pure water; dry air composed of argon (1%), oxygen (21%), and nitrogen (78%); and Peruvian dry natural gas from Camisea with the composition described in Table I.

TABLE I

COMPOSITION OF PERUVIAN DRY NATURAL GAS FROM CAMISEA

Compounds	% molar
Methane (CH_4)	88.54
Ethane (C_2H_6)	10.32
Propane (C_3H_8)	0.02
Nitrogen (N_2)	0.54
Carbon Dioxide (CO_2)	0.58

Adapted from [33]

B. Steam Reforming and Water Gas Shift - Gas (WGS)

Natural gas and steam are preheated with the combustion gas from a burner before entering the primary and secondary reforming. This combustion gas also provides energy to the first reformer. Additionally, air is directly introduced into the second reformer. Reactors in this stage were modeled as Gibbs Minimization type. The gas obtained in the previous stage contains carbon monoxide, so it is directed to the Water Gas Shift (WGS) stage to convert it into carbon dioxide through two reactors modeled as Equilibrium type. The equilibrium constants used were based on literature [14].

C. Carbon Dioxide Removal

Subsequently, the syngas obtained in the WGS stage is fed to a CO_2 capture unit with the purpose of obtaining a treated gas with a molar concentration of CO_2 not exceeding 0.01%. This unit utilizes the "Heat and Mass Transfer" model for the absorption column of the "TSWEET Absorber/Stripper" type. For the recovery column, the "Ideal Stage" model of the "TSWEET Stripper" type is used. For this simulation, CO_2 capture worked with the MEA solvent due to its effectiveness in minimizing the energy consumption of the absorption process [15]. The capture solution in this simulation consists of 30% by weight of MEA, this solution enters the absorber.

D. Alternative Scenario: Carbon Dioxide Process Purification

The implementation of this stage represents the alternative scenario proposed for the sale of pure CO_2 as cylinder refills.

As shown in Figure 1, after capturing the CO_2, a portion is sent to the automotive urea unit, while the remainder, instead of being purged as in the base scenario, undergoes a purification process to meet the technical specifications required for sale: 99.9% mass purity, -20 degrees Celsius, and 17 bars of pressure [354]. This process involves a separation system that includes compressors, heat exchangers, and two-phase separators.

E. Methanation and Compression

The treated synthesis gas stream, leaving the CO_2 capture unit, rich in hydrogen and nitrogen, undergoes methanation to completely remove any remaining carbon monoxide and dioxide. Subsequently, before entering the synthesis stage, the stream passes through a compression system consisting of pumps, liquid-vapor separators, and molecular sieves. The latter equipment aims to selectively retain water molecules and is modeled with a component splitter [11].

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F. Ammonia Synthesis Unit

The Ammonia Synthesis Unit was simulated based on the loop model for ammonia synthesis described in the Ullman's Encyclopedia of Industrial Chemistry [16]. This stage comprises a section for ammonia synthesis followed by a separation section.

The first part of the process involves three beds, which were modeled using Gibbs Minimization reactors. The reactions in these beds were specified by the authors Čejka and Burr [11].

In the second part of the process, separation of the aqueous solution takes place using a condenser at a temperature of -20.6 °C, with a refrigerant R134-a at -34.44 °C. This separation results in two streams: a liquid stream rich in NH_3, which undergoes a purification process, and a gas stream with high contents of H_2 and N_2. The latter stream is recirculated back to the unit with a prior purge. To carry out the purification of the liquid stream, two flash separators are used. The two outgoing streams of inert gasses from the purification separators are considered as purges. Thus, a total of three purges are observed in the ammonia unit.

G. Automotive Urea Unit with Stamicarbon Technology

Stamicarbon technology is widely employed for urea production. It is distinguished by its efficiency, profitability, and environmental sustainability through the reduction of greenhouse gas emissions and the minimization of energy consumption compared to other urea production technologies [17].

The process model of Stamicarbon's conventional technology was based on its patent. The document specifies that the process, consisting of a synthesis section and a recovery section, produces concentrated liquid urea but not the commercial product AdBlue®. To obtain AdBlue®, an additional section needs to be implemented. Due to the high pressures involved in this process, the SRK-Polar thermodynamic model is recommended in the literature for accurate simulation [18].
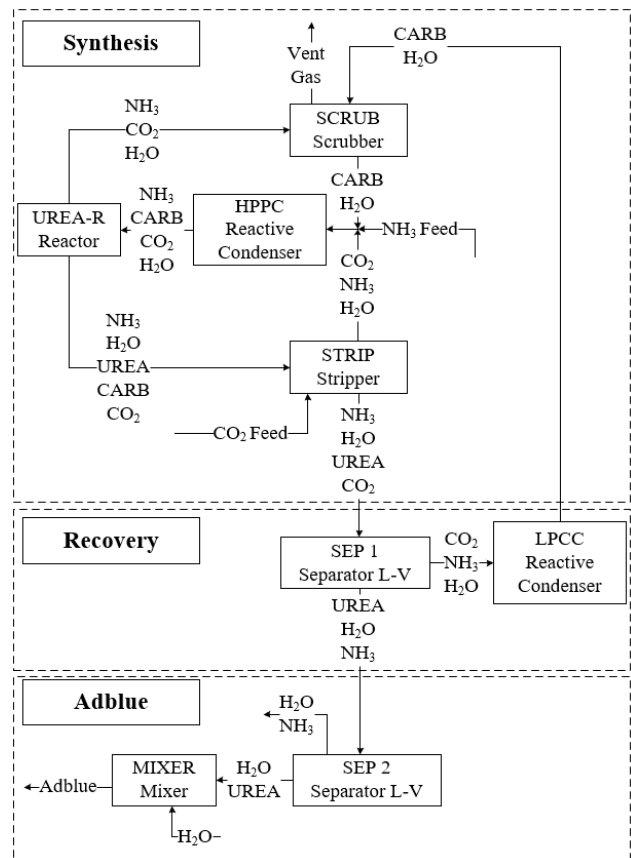

Fig. 2. Flowchart of Automotive Urea Unit.

The urea synthesis section can be observed in Figure 2. The process flow diagram comprises several units, such as the synthesis reactor (UREA-R), the stripper (STRIP), the high-pressure condenser (HPCC unit), and the scrubber (SCRUB). These operate at a pressure range of 12 to 18 MPa. The reactions occurring in this stage involve the condensation of ammonium carbamate and the urea synthesis according to the following equations:

$$CO_2 + NH_3 \leftrightarrow (NH_4)_2CO_3 \qquad (1)$$
$$(NH_4)_2CO_3 \leftrightarrow CH_4N_2O + H_2O \qquad (2)$$
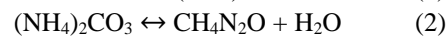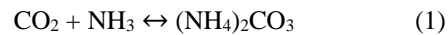
In this work, it was chosen to model the stripper and the scrubber as two multiphase conversion reactors instead of reactive columns. In the current simulation, using ProMax, this selection proves to be more advantageous as it enables the connection of an energy stream, which is crucial for determining the amount of energy consumed or released in the reactions.

The reactions represented by Equations (1) and (2) are reversible; however, typical results of the conversion percentage for Stamicarbon technology reactors under process conditions have been reported. Therefore, the simulation was adjusted to these parameters. In the HPCC unit, reaction (1) occurs with a 58% conversion of carbon dioxide, and in the UREA-R unit, reaction (2) takes place with an 85% conversion of ammonium carbamate [18].

In the synthesis section, the carbon dioxide fed to the STRIP unit recovers unconsumed ammonia and carbon dioxide. The gas leaving the STRIP unit mixes with fresh ammonia and reflux previously processed by the absorber in the recovery section. This mixture is sent to the HPCC unit

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where ammonium carbamate is formed. The formed solution is sent to the UREA-R unit to produce urea. The product has two outlets: on one side, the gases not converted in the UREA-R unit go to the SCRUB unit, and on the other side, the aqueous solution goes to the STRIP unit, where the decomposition of ammonium carbamate occurs. In the SCRUB unit, reaction (1) takes place with a 99.5% conversion of CO_2. Thus, from the bottom of the SCRUB unit exits ammonium carbamate and it is recirculated to the process as reflux, specifically at the mixing point observed in Figure 2. Meanwhile, the purge gas from the SCRUB, primarily composed of H_2, N_2, CO, CO_2, and Ar, is vented.

In the recovery section, a separator (SEP1) and a low-pressure reactive condenser (HPLC) are used. The outgoing urea solution from the STRIP unit expands at a pressure between 0.2 and 0.5 MPa and passes through a heater before entering the SEP 1 and SEP 2, where the concentrated urea solution is sent to the AdBlue® formulation section. On the other hand, the vapor containing CO_2 and NH_3 is sent to the LPCC unit to form aqueous ammonium carbamate, which is recirculated to the SCRUB. In this reactor (LPCC), only reaction (1) was considered with a conversion of 56%.

The AdBlue® formulation section is not described in the patent but is detailed on its official page [19]. The process consists of a separator (SEP2) and a mixer (MIXER) where the dilution of the concentrated urea solution with demineralized water occurs [20]. The concentrated urea solution, from the SEP 1, passes through a valve and then through a separator (SEP 2) to achieve ambient pressure and eliminate impurities, primarily NH_3. Finally, the urea solution is diluted with water to obtain the AdBlue® product with the required specifications [21].

H. Operational Profitability Analysis

This section assesses the operational profitability of both the base scenario and the alternative scenario (implementing the CO_2 purification process). Furthermore, all monetary values and calculations were expressed in US dollars, considering an exchange rate of 3.865 soles per dollar [22].

The operational profitability analysis focuses on calculating the net profit margin, derived by dividing the net profit by the revenue and expressing the result as a percentage [23, 24, 25], as shown in equation 3.

$$Net\ Profit\ Margin = \frac{Net\ Utility}{Net\ Sales}\ x\ 100\%\ (3)$$

In the base scenario, Net Sales only include revenue from the sale of automotive urea, while in the alternative scenario, revenue from the sale of pure carbon dioxide used for cylinder refills is added.

The Net Utility is calculated by applying a 29.5% income tax rate to the gross profit [26].

Gross profit is derived by subtracting the total income from the total product cost (TPC), which includes manufacturing costs and overhead expenses. These overhead expenses encompass administrative, distribution and sales, research and development costs, as well as financial interest. It is estimated that these overhead expenses represent 20% of the TPC, according to Peters' recommendations [27].

TABLE II.
CONSIDERATIONS TO CALCULATE DIRECT COSTS

Direct costs	Considerations
Raw material	Market unit price
Services	Market unit price
Labor	15% TPC
Supervision	3% TPC
Maintenance	6306 USD
Operational supplies	15% Maintenance
Laboratory charges	1.5% TPC
Patents and royalties	3% TPC

On the other hand, manufacturing costs incorporate direct costs, fixed charges, and plant overhead costs. Fixed charges and plant overhead costs, established at 15% and 5% of the TPC respectively, along with detailed direct production costs outlined in Table II, align with Peters' recommendations [27]. The maintenance cost was set at 24000 soles (6297 USD) annually, and is determined based on Condori and Mendoza's reference for an automotive urea plant with the same capacity [2].

TABLE III
CONSIDERATIONS FOR CALCULATING RAW MATERIALS AND UTILITY

Raw material and utility	Unit cost
Natural gas	4.0 USD / MMBTU
Electricity	0.09 USD /kWh
Steam at 450 psig	5.5 USD / 1000 lb
Steam at 150 psig	4.0 USD / 1000 lb
Distilled Process Water	4.0 USD / 1000 gal
Process Air	0.2 USD / 1000 ft³
River cooling water	0.2 USD / 1000 ft³
City Process Water	1.5 USD / 1000 gal

Table III details the unit cost of material and utility. According to the report on the natural gas sector in Peru, the tariff from the natural gas distributor Cálidda for an industrial category and supply is 4.012 USD/MMBTU excluding VAT [28]. Likewise, the electricity cost was based on the industrial sector rate in Peru [29], considering an operation of 330 days per year. The unit prices for steam in the heating service were extracted from Seider et al.[32], while the remaining unit prices were obtained from Peters [27], specifically opting for the highest unit prices from each respective source.

The unit price of automotive urea varies depending on the product's presentation. However, the average price per liter is estimated at S/ 3.00, a figure suggested by a market

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study in Peru. [2]. It is also noteworthy that taxes without Value Added Tax (VAT) were taken into account in the total sales price.

When considering an alternative scenario in which carbon dioxide is stored and sold as a byproduct, the market price of $0.4/kg CO_2 is considered [36]. It is also important to note that VAT was subtracted from the total CO_2 sales price.

III. RESULTS

A. Steam Reforming and Water Gas Shift - Gas (WGS)

In Table IV, the 4392 kmol/year of natural gas used as feed in the reformers is equivalent to 10.01 MSCFD. It is important to note that additionally, 2621 kmol/year (6.01 MSCFD) of natural gas and 26214 kmol/year of air were used in the burner. The purpose of the burner is to produce the combustion gas, used for the heating service for the reformers.

TABLE IV
MOLAR FLOW OF RAW MATERIALS USED IN REFORMERS

Raw material	Molar flow (kmol/year)
Natural gas	4,392.0
Water	11,666.0
Air	6,588.0

The molar flow of combustible natural gas represents 60% of the molar flow of the natural gas feed used in the reformers. This provides the necessary energy to achieve high hydrocarbon conversion in the reforming reaction. Additionally, the excess air percentage used in the burner is 0.5%. After steam reforming, the flow goes through the Water-Gas Shift stage, where a 3.78% mol and 0.36% mol of CO were achieved at the exit of the first and second reactors, respectively.

B. Carbon Dioxide Removal

In this stage, a stream enters the absorption column with a mass flow of 384,351 kg/year. A recirculation of 822,564 kg/year of MEA is required. Additionally, a makeup stream of MEA absorbent of 42.99 kg/year is needed.

Table V shows the composition and total molar flow of the outlet streams from the stage. It is noteworthy that the captured carbon dioxide undergoes a purification process, resulting in a purity level of up to 99.84%.

TABLE V
COMPOSITION AND TOTAL MOLAR FLOW OF TREATED GAS AND CAPTURED CARBON DIOXIDE FROM THE CO_2 CAPTURE STAGE.

Compound	Treated gas (% molar)	Captured CO_2 (% molar)
CH_4	0.010	0.000
C_2H_6	0.000	0.000
N_2	19.801	0.069
H_2	60.796	0.354
CO	0.422	0.002
CO_2	18.052	98.397
Ar	0.253	0.001
H_2O	0.668	1.174
Molar flow (kmol/year)	21,462.5	4,777.9

C. Alternative Scenario: Carbon Dioxide Process Purification

For this stage, a purified CO_2 flow rate of 60,922 kg/year and an acidic water stream of 300 kg/year containing 2.33% CO_2 were obtained. Chilled water and cooling water are required at mass flow rates of 25.7 kg/h and 7.1 kg/h respectively. Additionally, the compressors require a total power consumption of 0.17 kW.

D. Methanation and Compression

TABLE VI
COMPOSITION AND TOTAL MOLAR FLOW OF THE INPUT AND OUTPUT OF THE METHANATION AND COMPRESSION STAGES

Compuesto	Inlet (% molar)	Outlet (% molar)
CH_4	0.010	0.569
C_2H_6	0.000	0.000
N_2	24.037	24.772
H_2	73.772	74.341
CO	0.512	0.000
CO_2	0.023	0.000
Ar	0.307	0.316
H_2O	1.336	0.000
Molar flow (kmol/year)	21,462.6	20825.1

In Table VI, the composition and molar flow of the inlet and outlet streams of the methanation and compression unit are observed. The outlet stream from the methanation stage goes through a compression system and molecular sieves where its pressure is increased to 105 bar, and the contained

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water is removed. Under these conditions, the flow is ready to enter the ammonia synthesis unit.

E. Ammonia Synthesis Unit

The reactors achieve a nitrogen conversion of 25% to 30% mol at an inlet temperature of 275 °C [11]. In Table VII, the composition and molar flow of the inlet and outlet streams of the ammonia unit can be observed. It is also noted that the total molar flow of the three purges from the ammonia unit is 1073.99 kmol/year (equivalent to 16.2 tons/year of mass flow), of which 497.1 kmol/year corresponds to the amount of NH_3 present in the stream.

TABLE VII
COMPOSITION AND TOTAL MOLAR FLOW OF THE INLET AND OUTLET OF THE AMMONIA UNIT

Compound	Inlet (% molar)	Outlet (% molar)
CH_4	0.569	0.001
C_2H_6	0.000	0.000
N_2	24.772	0.000
H_2	74.341	0.000
CO	0.000	0.000
CO_2	0.000	0.000
Ar	0.316	0.000
H_2O	0.000	0.000
NH_3	0.000	99.999
Molar flow (kmol/year)	20825.1	9,634.5

F. Automotive Urea Unit with Stamicarbon Technology

The 9,634.5 kmol/year of ammonia product and 3345.27 kmol/year of captured CO_2 were used in the urea unit as feed streams to produce 528,000 L/year of automotive urea at 25 °C and 1 bar. Table VIII shows the composition and mass flow of the AdBlue® product and the purge gas from the urea unit. Table IX presents the composition and physical properties predicted by the simulation model for the AdBlue® product.

TABLE VIII
COMPOSITION AND MASS FLOW OF THE ADBLUE® PRODUCT AND THE PURGE GAS OF THE UREA UNIT STAGE

Compound	AdBlue® (% mass)	Purge gas % molar)
CH_4	0.000	0.034
C_2H_6	0.000	0.000
N_2	0.000	1.116
H_2	0.000	0.407
CO	0.000	0.032
CO_2	0.000	98.306
Ar	0.000	0.035
H_2O	66.767	0.068
NH_3	0.108	0.000
CH_4NO	33.045	0.000
CH_6N_2O	0.076	0.000
Mass flow (kg/year)	558,519.7	5,855.0

TABLE IX
COMPOSITION AND PHYSICAL PROPERTIES OF AUTOMOTIVE LIQUID UREA.

Property	Automotive urea obtained
Urea (% mass)	33.045
Ammonia(% mass)	0.108
Density(20 °C, g/cm³)	1.059
Dynamic Viscosity (25 °C, cP)	1.428
Thermal Conductivity (25 °C, W/mK)	0.477
Superficial Tension (20 °C, mN/m)	70.380

F. Global Process

The utility requirements for the production process are listed in Table X.

Additionally, Table XI shows the results of the calculation of natural gas (NG) requirements and the CO_2 intensity of the process. The first indicator describes the kilograms of natural gas (NG) needed to produce 1 kg of AdBlue®. The second indicator measures the amount of CO_2 produced per 1 kg of AdBlue®.

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TABLE X
ENERGY REQUIREMENTS OF THE PROCESS

Utility	Power (kWh/kg automotive urea)
Heating	1.582
Cooling	2.397
Electricity	0.486

TABLE XI
GLOBAL PROCESS INDICATORS

Indicator	Value
GN required (kg GN / kg automotive urea)	0.219
CO_2 intensity (kg CO_2 / kg automotive urea)	0.336

Fig. 3. Raw material cost distribution

G. Operational Profitability Analysis

The financial analysis of the project yielded the following results, as summarized in Table XIII. After considering income tax, the net profit was calculated to be $121,630 annually. The net profit margin, calculated as a percentage of revenue, was found to be 34.75%.

TABLE XII.
SUMMARY OF FINANCIAL RESULTS

Financial Metric	Value
Annual Revenue (1000 USD)	350.03
Total Annual Product Cost (1000 USD)	177.51
Gross Profit (1000 USD)	172.52
Income Tax (1000 USD)	50.89
Net Profit (1000 USD)	121.63
Net Profit Margin (%)	34.75

Figures 3 and 4 depict the percentage distribution of raw material and process service costs in the overall process, derived from the mass and energy balance results of the simulated process.
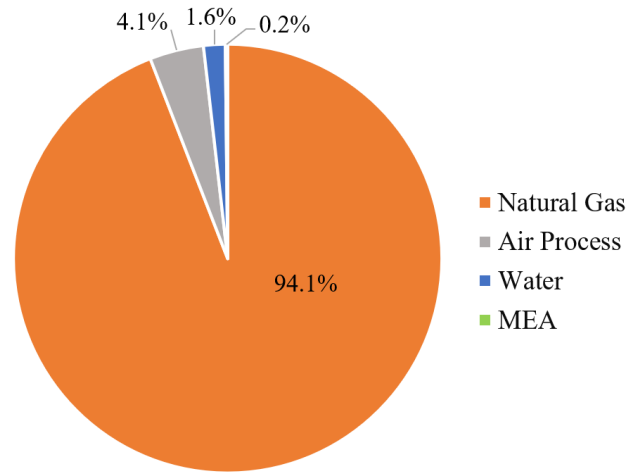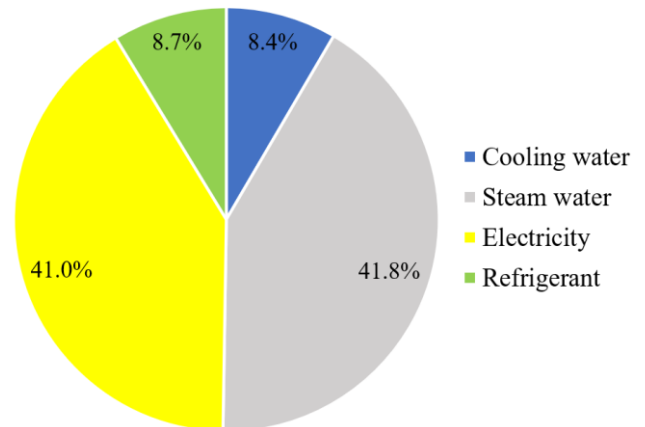

Fig. 4. Process services cost distribution

Additionally, an evaluation of an alternative scenario where the by-product carbon dioxide is sold revealed a substantial increase in profit margin by 2.99 percentage points compared to the baseline scenario without the sale of pure CO_2.

IV. DISCUSSION OF RESULTS

A. Steam Reforming and Water Gas Shift - Gas (WGS)

The conventional ammonia production process begins with a desulfurization stage [30]. However, as observed in Fig. 1, in the current process, the raw material is directed straight to the steam reforming stage. This design is specifically due to the absence of sulfur in the Peruvian natural gas from Camisea, as shown in Table I. The steam reforming and WGS (water-gas shift) processes are the stages with the greatest influence on hydrogen formation due to the occurring reactions. Therefore, during the simulation, the flow of air and natural gas were continuously adjusted until achieving a molar ratio of $H_2:N_2$ of 3.09; subsequently, in the

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methanation stage, there is a slight consumption of H_2 that brings it closer to the target value of 3.

B. Methanation and Compression

In Table IV, it can be observed that the molar ratio of $H_2:N_2$ in the outlet stream of the methanation and compression stage is 3.02. It is crucial to maintain this parameter in order to achieve efficient NH_3 production [11].

C. Ammonia Synthesis Unit

In Table V, it is observed that the ammonia product (outlet stream) has a purity of 99.999% in molar percentage. The predicted mass concentration percentage of ammonia in the simulation is also 99.999%. This result complies with the minimum required purity of 99.5% by mass. In the industrially obtained ammonia product by Fertiberia, a company, a purity of 99.9% is reported [3129].

D. Automotive Urea Unit with Stamicarbon Technology

The Stamicarbon technology patent stipulates that a recovery section is required if the concentration of urea in the solution exiting the STRIP unit desorber is at least 50% by weight. Due to the high conversion of ammonium carbamate in the STRIP unit, the model predicts a substantial desorption of the raw material and a concentration of 55.5% by weight of urea in the solution exiting the STRIP unit. For this reason, the production process only included a recovery section.

In the simulation, it was necessary to adjust the molar ratio of the two feed streams NH_3/CO_2 in order to achieve a NH_3/CO_2 molar ratio of approximately 2 in the gaseous product of the UREA-R unit. This ratio is the stoichiometric ratio for the reaction described by Equation (1) that occurs in the SCRUB unit; getting close to this value implies a higher recovery of the raw material in the form of ammonium carbamate. In this regard, it was determined that the molar ratio of the feed streams NH_3/CO_2 at 2.88 is the most favorable parameter, as it minimizes the amount of fresh NH3 used while simultaneously reducing CO_2 emissions. It is worth noting that this value falls within the recommended optimal range of 2 - 3.5 NH_3/CO_2 [18].

As seen in Table VI, the purge gas contains 39.4% CO_2. In the research conducted by Koohestanian [21], where the Stamicarbon technology process was simulated using Aspen Plus software, a CO_2 percentage of 61.0% was achieved in the purge gas. On the other hand, the concentration was 83.46% by mass for the concentrated urea solution, which is close to the estimated percentage of 80% in the production of AdBlue® by the company Fertiberia [20]. The concentrated urea solution is then diluted to obtain the final product (AdBlue®).

The information presented in Table XIII reveals that the simulation has successfully predicted the dynamic viscosity, surface tension, mass percentage of urea and ammonia in automotive urea within the established ranges for commercialization [21]. However, it is observed that both thermal conductivity and density exhibit values slightly different from the required ones. As a result, it has been determined that the average error of the simulation is 3.18% in relation to the technical specifications.

These limitations can be attributed to the use of 100% pure water during the simulation. In the industry, demineralized water is used, which still contains minimal levels of minerals such as calcium, phosphate, iron, copper, chromium, zinc, nickel, chromium, potassium, and aluminum [19]. Therefore, these minerals could have a slight influence on increasing the solution's density and its thermal conductivity.

TABLE XIII.
COMPARISON OF THE PROPERTIES OF SIMULATED ADBLUE® WITH THE RANGE OF TECHNICAL SPECIFICATIONS OF THE PRODUCT ACCORDING TO ISO 22241.

Property	Simulated AdBlue®	Range of technical specifications	Error (%)
Urea (% mass)	33.045	31.8 - 33.2	0.00
Ammonia(% mass)	0.108	Max. 0.2	0.00
Density(20 °C, g/cm³)	1.059	1.085 - 1.093	2.75
Dynamic Viscosity (25 °C, cP)	1.428	Approx 1.4	0.00
Thermal Conductivity (25 °C, W/mK)	0.477	Approx 0.570	16.32
Surface Tension (20 °C, mN/m)	70.380	Min. 65	0.00

Adapted from [20].

E. Global Process

In Tables VIII and XI, the energy requirements and ratios describing the efficiency of the simulated process are presented. These results can be used as benchmark indicators in future simulation studies related to the automotive urea production process. It was determined that to produce 1 kg of AdBlue®, it is necessary to use 0.137 kg of Peruvian natural gas. It is worth noting that only the natural gas used as raw material in the reforming process was considered. If the natural gas used in the burner, where combustion occurs to produce the combustion gasses serving as heating service for the reformers, is included, the overall process's natural gas requirement increases by 0.219 kg of natural gas per kilogram of automotive urea.

The CO_2 intensity of the process can be described as follows: to produce 1 kg of AdBlue®, 0.366 kg of pure CO_2 are released into the atmosphere. The considered carbon dioxide includes that released by combustion in the reforming stage, unused captured gas, and purge gases from the urea unit. It would be necessary to study the implementation of additional CO_2 capture and storage to determine its profitability and environmental impact.

Analyzing the scenario of selling CO_2, we find that to produce 1 kg of AdBlue®, 0.032 kg of pure CO_2 is released into the atmosphere. This amount is determined because the excess CO_2 from the capture process is no longer released if it is sold, and the CO_2 originates solely from the AdBlue® synthesis stage. Therefore, in terms of environmental friendliness, it is preferable to sell the CO_2 rather than releasing it as in the initial case.

F. Operational Profitability Analysis

The net profit result, which reaches 34.75%, indicates that the automotive urea production company with an annual plant capacity of 528,000 liters has a satisfactory profitability

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in Peru. This is due to the fact that a net profit margin exceeding 20% is regarded as high-quality profit [3~~4~~3].

Moreover, the cost analysis, based on Table 3 and Table 4, reveals a significant distribution in process services. electricity and steam water account for 41.0% and 41.8%, respectively, while refrigerant and cooling water represent smaller proportions, at 8.7% and 8.4%, respectively. Regarding raw material costs, natural gas comprises the majority at 94.1%, indicating its substantial impact. Water represents 1.6%, while process air and MEA are minor contributors at 4.1% and 0.2%, respectively.

This breakdown underscores the importance of efficient service management, particularly in electricity and steam water, and the optimization of gas natural use. Strategies aimed at reducing electricity and steam water consumption, along with improving gas natural efficiency, could significantly reduce overall process costs.

On the other hand, the strategy of selling the byproduct of pure carbon dioxide as a refill in cylinders has shown a slight positive effect on the profit margin. This outcome underscores the feasibility of implementing this alternative in terms of operational profitability.

However, it is essential to consider the cost associated with the necessary capital investment to implement this system. Installing a carbon dioxide purification system involves acquiring equipment and establishing wastewater treatment facilities. This initial cost must be carefully evaluated, as it directly impacts the long-term viability of this initiative.

V. CONCLUSIONS AND FUTURE WORK

It is possible to simulate the synthesis of automotive urea using Peruvian natural gas from Camisea as the raw material in ProMax 6.0 software. As a result of the simulation, a urea solution was obtained that meets the technical specifications for the commercialization of automotive urea.

The average error in the simulation is 3.18% compared to the specified technical requirements. The simulated plant has a production capacity of 528,000 L/year of automotive urea, which satisfies the necessary demand for a profitable industrial process according to the market analysis mentioned earlier, covering approximately 3.79% of the national demand.

Regarding the operational profitability analysis, it was calculated that the total revenues of the production plant amount to 350,032.04 USD, and the total production costs are 177,513.09 USD. Therefore, a positive profitability of 34.75% was determined, taking into account the sale without VAT and with income tax for profit.

Analyzing the scenario of selling CO_2, it becomes evident that producing 1 kg of AdBlue® results in the release of 0.032 kg of pure CO_2 into the atmosphere. This calculation is based on the fact that excess CO_2 from the capture process is no longer emitted if it is sold, and the CO_2 originates solely from the AdBlue® synthesis stage. Consequently, from an environmental standpoint, opting to sell the CO_2 rather than releasing it, as in the initial case, is preferable. This approach not only mitigates atmospheric CO_2 emissions but also aligns with sustainability objectives by effectively utilizing captured carbon dioxide.

In order to enhance the impact of these findings and address the identified limitations in the course of this research, certain recommendations are put forth. Firstly, optimizing the process conditions using advanced simulation tools such as ProMax 6.0 is suggested to improve efficiency and reduce operational costs. Secondly, conducting a more detailed economic analysis that includes evaluating key financial parameters such as Capital Expenditure (CAPEX), Net Present Value (NPV), and Internal Rate of Return (IRR) is recommended to provide a more comprehensive view of the financial viability of the process. Thirdly, there is a need to investigate and compare different alternative technologies for automotive urea production, considering aspects such as energy efficiency, environmental sustainability, and economic profitability.

Finally, it is suggested to conduct a more thorough analysis of the profitability of incorporating a residual carbon dioxide purification process. This will allow for a more comprehensive evaluation of the economic viability of this proposal, complementing the operational profitability analysis conducted in this study.

VI. ACKNOWLEDGMENT

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