4-27-2020

Modular Distributed Ammonia Production Proposal

Lauren Nicole Garner

Follow this and additional works at: https://louis.uah.edu/honors-capstones

Recommended Citation
https://louis.uah.edu/honors-capstones/349

This Thesis is brought to you for free and open access by the Honors College at LOUIS. It has been accepted for inclusion in Honors Capstone Projects and Theses by an authorized administrator of LOUIS.
Modular Distributed Ammonia Production Proposal

by

Lauren Nicole Garner

An Honors Capstone

submitted in partial fulfillment of the requirements

for the Honors Diploma

to

The Honors College

of

The University of Alabama in Huntsville

27 April 2020

Honors Capstone Director: Mr. Ralph Quigley

Instructor of Chemical Engineering

_____________________________________________________

Student Date 4/27/20

______________________________

Director Date

______________________________

Department Chair Date

______________________________

Honors College Dean Date
Honors Thesis Copyright Permission

This form must be signed by the student and submitted as a bound part of the thesis.

In presenting this thesis in partial fulfillment of the requirements for Honors Diploma or Certificate from The University of Alabama in Huntsville, I agree that the Library of this University shall make it freely available for inspection. I further agree that permission for extensive copying for scholarly purposes may be granted by my advisor or, in his/her absence, by the Chair of the Department, Director of the Program, or the Dean of the Honors College. It is also understood that due recognition shall be given to me and to The University of Alabama in Huntsville in any scholarly use which may be made of any material in this thesis.

____________________________
Student Signature

4/27/20

Date
Modular Distributed Ammonia Synthesis Proposal

Lauren Garner
Team Members:
Alyssa Lollar
Michael Garvey
Table of Contents

Abstract \hfill 3
Introduction \hfill 4
Process Flow Diagram and Material Balances \hfill 5
Process Description \hfill 7
Energy Balance and Utility Requirement \hfill 8
Equipment List and Unit Descriptions \hfill 9
Equipment Specification Sheets \hfill 10
Equipment Cost Summary \hfill 14
Fixed Capital Investment Summary \hfill 15
Safety, Health, and Environmental Considerations \hfill 16
Process Safety Considerations \hfill 20
Other Important Considerations \hfill 21
Manufacturing/Operation Costs \hfill 22
Economic Analysis \hfill 22
Conclusion and Recommendations \hfill 23
Bibliography \hfill 24
Appendix \hfill 25
Abstract

Ammonia is one of the leading synthetic chemicals produced in the world. One of its main applications is in the production of fertilizer. This plant will be located in Minnesota, near the corn fields where the fertilizer will be utilized. By adapting the traditional Haber-Bosch process, carbon emissions during the production of ammonia can be reduced. Nitrogen and hydrogen gas are needed to make ammonia in the Haber-Bosch process. The Haber-Bosch process normally produces greenhouse gas emissions during the synthesis of hydrogen gas through steam methane reforming. The steam methane reforming process will be replaced by emission-free water electrolysis. Because the plant will be built in the Minnesota Valley where wind and sun are abundant, a wind/solar energy alternative may be available to power the ammonia plant. An economic analysis of capital investment and profitability for this ammonia production plant was made.
Introduction

Ammonia is one of the largest volume synthetic chemicals produced in the world. In 2014, around 176 million metric tons were produced. It is critical in the manufacturing of fertilizers and is often used as a refrigerant. Without ammonia fertilizers, the crop yield would not be able to sustain the current population.

Ammonia as a chemical has been around for over 200 years. It was first isolated in its gaseous form in 1774. The first method of producing ammonia was discovered in 1898. This early method involved fixing nitrogen gas by calcium carbide to form calcium cyanamide, which was then hydrolyzed with water to form ammonia. This process did not result in significant quantities until early in the 20th century. A downside to this process was that it required high amounts of energy.

Fritz Haber, working with a student at the University of Karlsruhe, synthesized ammonia from hydrogen and nitrogen gas in the laboratory. Walther Nernst was also developing a process to make ammonia from N2 and H2. His process involved passing a mixture of these gases across an iron catalyst at 1000 degrees celsius and a pressure of 75 barg. With this process he was able to produce larger amounts of ammonia, but did not think the high pressures needed were feasible for industrial applications. They explored this high pressure route for ammonia synthesis and worked to create a commercially viable process. This process used a recycle stream to increase overall yield. BASF purchased the patents and developed equipment that could withstand the required high temperatures and pressure.¹

The Haber-Bosch process, as it has come to be known, produces enough ammonia to be turned into fertilizers to feed the world population. The traditional Haber-Bosch process was revolutionary, but also energy intensive, due to the high temperature and pressures, and has a high carbon footprint due to its use of methane as the source for hydrogen.¹

One of the methods being looked at to reduce the carbon footprint of ammonia synthesis is by using the electrolysis of water instead of methane as a hydrogen source. Water electrolysis is the decomposition of water into hydrogen and oxygen gases due to the passage of an electric current. The electrolytic cell is composed of a pair of metal electrodes immersed in water and an electrolyte that has been added to the water.² If the electricity that is used comes from a green source, such as wind energy, the carbon printfoot can be reduced even more.
Process Flow Diagram and Material Balances
### Overall Mass Balance (kg)

<table>
<thead>
<tr>
<th></th>
<th>H₂O</th>
<th>O₂</th>
<th>H₂</th>
<th>N₂</th>
<th>Air</th>
<th>NH₃</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>In</strong></td>
<td>79144</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>54078</td>
<td>0</td>
</tr>
<tr>
<td><strong>Intermediate</strong></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>41099</td>
<td>0</td>
</tr>
<tr>
<td><strong>Out</strong></td>
<td>0</td>
<td>81628</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>50000</td>
</tr>
</tbody>
</table>

Table 1: Total Mass Balance
Process Description

Nitrogen generation via pressure-swing adsorption

Air is cycled through a two-tower pressure-swing adsorption system. Two tower PSA units are typical in industry. From the air the PSA unit removes oxygen which is dispersed to the atmosphere as a nontoxic gas, while pure nitrogen continues through the ammonia production process.

Hydrogen production via alkaline water electrolysis

A nickel anode and cathode are immersed in an alkaline solution and separated by a hydroxide-permeable membrane. Electric current flows from the anode to the cathode where electrons convert water into hydrogen and hydroxide. From the cathode, hydroxide ions flow through the membrane to the anode where the conversion of hydroxide to water and oxygen occurs. A compressor transfers the hydrogen to a storage tank, and the oxygen is released to the atmosphere. A steady supply of alkaline water must be pumped through both electrode compartments to replace the water lost at the cathode and hydroxide lost at the anode.

Ammonia production via Haber-Bosch method

Nitrogen and hydrogen gas flow from their respective buffer tanks to a mixer where they are combined to form a single stream. The stream is compressed and heated before entering a packed-bed reactor. The ammonia in the reactor exit-stream is condensed after flowing through a heat exchanger and a condenser. The liquid ammonia is collected using a vertical-gravity separator and deposited into a refrigerated storage tank. Any unconverted nitrogen and hydrogen is recycled back through the process.
Energy Balance and Utility Requirement

PSA: 93 kilowatts for 12 hours needs 1116 kW*hr
Electrolysis: 443595 kW*hrs because a 70% efficiency with an energy requirement of 50 kW-hrs/kg.
Heat exchanger: 5610510 kJ/hr is needed to heat the gas mixture to the necessary temperature.

We will use electricity and corn ethanol as energy sources. Priority will be placed on green energy sources.
- Flow Rates included on the PFD and the P&ID located in the appendix
- Power, steam, cooling water, process water, boiler water, air, refrigeration, fuel gas

Electricity:
Monthly power rate without demand meter - $12 service charge + 10.204¢/kWh
Monthly power rate demand meter - $12 service charge + $6.50 demand charge for all kW + 7.619¢/kWh
For 13,000 V or higher, discount of $2.00/kW

Water:
Up to 26000 gallons - $2.46/1000 gallons
Over 26000 gallons - $3.27/1000 gallons
Equipment List and Unit Descriptions

- **N₂ PSA Unit**
  Air Compressor
  Adsorber
  Nitrogen Buffer Tank
  Temperature/Pressure Instruments
  Valves

- **Haber-Bosch Unit**
  H₂/N₂ Compressor
  Heat Exchanger
  Refrigerated Storage Tank
  PBR
  Condenser
  Separator
  Temperature/Pressure Instruments
  Valves

- **H₂ Electrolysis Unit**
  Electrolysis Unit
  Hydrogen Compressor
  Hydrogen Storage Tank
  Temperature/Pressure Instruments
  Valves
Equipment Specification Sheets

**Fixed-Bed Reactor**

Temp:
Reactor Press: Max: 250 atm
Bed height: 8.23 m
Inner diameter: 1.73 m
Volume: 28.66 L
Catalyst density: 116 lb/ft\(^3\)
Inner Shell MOC: Stainless Steel (SA 240 type 316)
Outer Shell MOC: Carbon Steel (SA 204 grade A)

**PSA Specification**

Service: Atmospheric Air
Type: Generon 10xNS-36-56
Quantity: 1
Disch. Molar Flow: Max: 250 kgmol/hr N\(_2\)
Disch Temp: Max: 300 K
Disch Press: Max: 1 atm

**Compressor Specification**

Service: Nitrogen/Hydrogen
Type: QGS-100 Rotary Screw
Mass Flow: Max: 1,000 kgmol/hr
Standard Vol Flow: Max: 24,000 slph Min: 6,000 slph
Inlet Temp: Max: 550 K
Inlet Press: Max: 20 bar
Disch Temp: Max: 600 K
Disch Press: Max: 150 bar
Heat-Exchanger Unit Specification

Service: Ammonia
Size: 10,000 L
Total surface area: 10 m²
Number of shells: 10
Surface area per shell: 1 m²
Number of passes: 1

<table>
<thead>
<tr>
<th>Shell</th>
<th>Tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream components:</td>
<td>Steam</td>
</tr>
<tr>
<td>Vapor: Steam</td>
<td>700 K</td>
</tr>
<tr>
<td>Temperature in:</td>
<td>400 K</td>
</tr>
<tr>
<td>Operating pressure: Max: 35 bar</td>
<td></td>
</tr>
<tr>
<td>Operating heat transfer rate: 160 W/m²</td>
<td></td>
</tr>
<tr>
<td>Heat exchanger material details: Stainless Steel</td>
<td></td>
</tr>
</tbody>
</table>

Buffer Tank Specification

Service: Nitrogen
Capacity: 10,000 L
Rating: 50 bar
Oper temp: 310 K
Oper press: 15 bar

Refrigerated Storage Tank Specification

Service: Liquid Ammonia
Capacity: 10,000 L
Rating: 50 bar
Oper temp: 235 K
Oper pressure: 1 atm

Separator Specification
Service: Ammonia/Nitrogen/Hydrogen
Type: Vertical Gravity Separator
Size: 10,000 L
Gas: Nitrogen/Hydrogen
Liquid: Ammonia
Oper press: 150 bar
Oper temp: 150 bar

Condenser Specification
Service: Ammonia
Type: Air Cooled Condenser
Size: 10,000 L
Inlet vol flow gas/vapor: 250 kgmol/hr
Outlet vol flow liquid: 250 kgmol/hr
Inlet temp: 650 K
Inlet press: 200 bar
Outlet temp: 350 K
Outlet press: 200 bar
Rating: 250 bar

Electrolysis Unit Specification
Size: 20 MW, 4,000,000 slph capacity
Inlet water temp: 300 K
Outlet \( \text{H}_2 \) vol flow: Max: 22,400 slph
Outlet \( \text{H}_2 \) molar flow: Max: 750 kgmol/h
Outlet \( \text{H}_2 \) press: 1 atm
Outlet \( \text{H}_2 \) temp: 360 K
**Piping Specification**

Pipe 101
Service: Nitrogen
Nominal Pipe Size: 3”
Schedule: 80
MOC: 316 SS

Pipe 102
Service: Hydrogen
Nominal Pipe Size: 3”
Schedule: 80
MOC: 316 SS

Pipe 103
Service: Nitrogen/Hydrogen
Nominal Pipe Size: 3.5”
Schedule: 80
MOC: 316 SS

Pipe 104
Service: Anhydrous Ammonia
Nominal Pipe Size: 1.5”
Schedule: 80
MOC: 316 SS
Equipment Cost Summary

The following estimated prices were inspired by prices observed for similar equipment.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Quantity</th>
<th>Price ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PSA</td>
<td>1</td>
<td>150000</td>
</tr>
<tr>
<td>Electrolyzer</td>
<td>1</td>
<td>150000</td>
</tr>
<tr>
<td>Reactor</td>
<td>1</td>
<td>255000</td>
</tr>
<tr>
<td>Heat Exchangers</td>
<td>2</td>
<td>1250</td>
</tr>
<tr>
<td>Compressor</td>
<td>1</td>
<td>4500</td>
</tr>
<tr>
<td>Separator</td>
<td>1</td>
<td>6000</td>
</tr>
<tr>
<td>Refrigeration Tank</td>
<td>1</td>
<td>8638</td>
</tr>
</tbody>
</table>
Fixed capital investment refers to the sum of the cost of land, construction, engineering, and initial equipment. The equipment includes all modules, piping, compressors, structural supports, etc. The land bought for the new plant will need to be sized sufficiently for the process and equipment. Estimation factors based on process equipment are often necessary to include engineering and construction prices. Our process equipment estimates were drawn from actual prices found on the internet. An investment is normally made in trust, and for this proposal requires confirmation that an environmentally friendly innovation does not negatively affect profitability. Banks charge interest for loans, so a business must first be deemed probably profitable before the loan is given. The type of interest buildup depends on the magnitude of risks and amounts of money being invested. A desired output of 50 mtpd requires millions of dollars in investment, and so compounded interest plans would probably be required by the banks. Profitability estimates must also take into account factors for inflation and plant depreciation, which both occur naturally. Also, an investment has a better chance to be financially supported if the land being considered to be bought by the company is desirably located, because land has the potential to increase in value. Investments also take into account the material of the initial plant constructions as well as services needed such as maintenance, utilities, construction to start up the plant until revenues begin to be generated. Investments are always made on the basis that over a period of time money will be made, even after taxes, inflation, depreciation, and unforeseen contingencies, so extremely conservative estimations are often necessary.¹

<table>
<thead>
<tr>
<th>Factor</th>
<th>Cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 Major Equipment</td>
<td>719235</td>
</tr>
<tr>
<td>10 Minor Equipment</td>
<td>359617.5</td>
</tr>
<tr>
<td>10 Installation</td>
<td>359617.5</td>
</tr>
<tr>
<td>15 Instruments &amp; Control System</td>
<td>539426.25</td>
</tr>
<tr>
<td>15 Piping, Installed</td>
<td>539426.25</td>
</tr>
<tr>
<td>10 Foundation &amp; Structures</td>
<td>359617.5</td>
</tr>
<tr>
<td>10 Utilities</td>
<td>359617.5</td>
</tr>
<tr>
<td>5 Land &amp; Grade Improvements</td>
<td>179808.75</td>
</tr>
<tr>
<td>5 Engineering Design</td>
<td>179808.75</td>
</tr>
<tr>
<td>Contingency</td>
<td>25%</td>
</tr>
<tr>
<td>Capital Cost</td>
<td>3596175</td>
</tr>
</tbody>
</table>
Safety, Health, and Environmental Considerations

**Ammonia: Safety, Health, and Environmental**

**Appearance**
Clear colorless gas, or a clear colorless liquid under pressure.

**Description**
Ammonia is a toxic gas or liquid that is corrosive to liquids. Ammonia is fatal if exposed to sufficient quantities.

**Routes of Exposure**
The routes of exposure ammonia can be absorbed into the body by inhalation, ingestion, eye contact, and skin contact. It is uncommon to be exposed to ammonia through ingestion.

**Personal Protection Equipment**
Persons working with ammonia should wear ammonia resistant protective gloves, eye or face protection, and appropriate chemical resistant clothing based on the task being performed. If inhalation is possible, wear an appropriately resistant respirator according to the manufacturer's parameters.

**Chemical Dangers**
Ammonia in contact with water produces a poisonous, visible vapor cloud. Ammonia forms ammonium hydroxide, which is a corrosive, alkaline solution, by dissolving in water producing heat. Ammonia forms shock sensitive compounds with mercury, silver, and gold oxides. It also reacts violently with strong oxidants, acids, halogen, and many heavy metals. It is corrosive to copper and galvanized surfaces. Ammonia will emit toxic fumes and nitrogen oxide if heated to decompositions. Liquid ammonia will attack some forms of plastics, rubber, and coatings.

**Explosion Hazard**
Ammonia forms an explosive mixture with air. Its lower explosive limit in air is 15%. Its upper explosive limit in air is 28%. Containers of ammonia may explode when heated and ruptured cylinders may rocket.

**Physical Dangers**
Ammonia gas is lighter than air. Under certain conditions, compressed liquified ammonia gas can escape its cylinder and forms an ammonia fog when in contact with moisture. Dangerous concentrations will occur in enclosed or poorly ventilated spaces quickly.

**NFPA Signal**
Health: 3
Flammability: 1
Reactivity: 0
Special:

Signs and Symptoms
Effects of Short Term Exposure
Short term exposure is considered as less than eight hours. Ammonia is a severe irritant of the eyes, respiratory tract, gastrointestinal tract, and skin. It reacts with the moisture in the body to produce ammonium hydroxide. The concentration of the gas or liquid will contribute to the extent of injury.

Long Term Implications
Severe ammonia inhalation injury survivors may suffer residual chronic lung disease. Cataracts and glaucoma have been reported in people who have had acute exposures to high concentration ammonia. Bleeding, rupture, scarring, or abnormal narrowing are possible permanent effects of ammonia ingestion. There is inconclusive evidence regarding ammonia’s potential as a carcinogen, developmental toxin, or reproductive toxin. Chronic or repeated exposure may cause chronic respiratory tract irritation, chronic cough, asthma, lung fibrosis, headaches, and chronic eye irritation.

Occupational Exposure Limits
NIOSH REL:
- TWA (10-hour): 25 ppm (18 mg/m³)
- STEL (15-minute): 35 ppm (27 mg/m³)

OSHA PEL:
- TWA (8-hour): 50 ppm (35 mg/m³)

ACGIH TLV:
- TWA (8-hour): 25 ppm
- STEL (15-minute): 35 ppm
- NIOSH IDLH: 300 ppm

DOE TEEL:
- TEEL-0: 15 mg/m³
- TEEL-1: 20.9 mg/m³
- TEEL-2: 111 mg/m³
- TEEL-3: 766 mg/m³

AIHA ERPG:
- ERPG-1: 25 ppm
- ERPG-2: 150 ppm
- ERPG-3: 750 ppm
Acute Exposure Guidelines

<table>
<thead>
<tr>
<th>AEGL 1</th>
<th>10 min</th>
<th>30 min</th>
<th>60 min</th>
<th>4 hr</th>
<th>8 hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>(discomfort, non-disabling)-ppm</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AEGL 2</th>
<th>10 min</th>
<th>30 min</th>
<th>60 min</th>
<th>4 hr</th>
<th>8 hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>(irreversible or other serious, long lasting effects or impaired ability to escape)-ppm</td>
<td>220</td>
<td>220</td>
<td>160</td>
<td>110</td>
<td>110</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AEGL 3</th>
<th>10 min</th>
<th>30 min</th>
<th>60 min</th>
<th>4 hr</th>
<th>8 hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>(life threatening effects or death)-ppm</td>
<td>2700</td>
<td>1600</td>
<td>1100</td>
<td>550</td>
<td>390</td>
</tr>
</tbody>
</table>

Environmental Concerns

Ammonia can harm aquatic life if it contaminates surface water. Surface water contamination can be direct or if water is used to depress an ammonia vapor cloud and it runs into surface water. Small amounts of ammonia will not negatively affect soil and plants, but larger amounts may. The best way to deal with a gas leak is to wet it down, properly containing the runoff if possible.

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Result</th>
<th>Species</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>ammonia</td>
<td>Acute EC50 20.8 mg/l Marine water</td>
<td>Algae - Ulva fasciata - Zoea</td>
<td>96 hours</td>
</tr>
<tr>
<td></td>
<td>Acute LC50 2080 µg/l Fresh water</td>
<td>Crustaceans - Gammarus pulex</td>
<td>48 hours</td>
</tr>
<tr>
<td></td>
<td>Acute LC50 0.53 ppm Fresh water</td>
<td>Daphnia - Daphnia magna</td>
<td>48 hours</td>
</tr>
<tr>
<td></td>
<td>Acute LC50 300 µg/l Fresh water</td>
<td>Fish - Hypophthalmichthys nobilis</td>
<td>96 hours</td>
</tr>
<tr>
<td></td>
<td>Chronic NOEC 0.204 mg/l Marine water</td>
<td>Fish - Dicentrarchus labrax</td>
<td>62 days</td>
</tr>
</tbody>
</table>

Nitrogen Gas: Safety, Health, and Environmental

Nitrogen is a colorless odorless gas with a vapor density of 0.967 compared to air with a vapor density of 1. It is chemically stable and hazardous reactions will not occur under normal conditions of storage and use. Typically stored as a compressed gas, which can cause explosions if heated. It may displace oxygen and cause rapid suffocation. Use only with adequate ventilation. Do not enter storage areas and confined spaces unless adequately ventilated. If inhalation does occur, remove the victim to fresh air and keep at rest in a position comfortable for breathing. The rescuer should wear an appropriate mask or self-contained breathing apparatus if fumes are suspected to still be present. If the victim is not breathing, breathing irregularly, or if respiratory arrest occurs, provide artificial respiration or oxygen by a trained professional, as it may be dangerous to give mouth-to-mouth resuscitation. If unconscious, place the victim in recovery position and get medical attention immediately. If the nitrogen gas makes contact with eyes, immediately flush with plenty of water, occasionally lifting the upper and lower eyelids for at least 10 minutes. If skin contact occurs, flush contaminated skin with plenty of water and remove
contaminated clothing to wash before reuse. Contact with rapidly expanding gas may cause burns or frostbite. Appropriate safety eyewear should be worn. Chemical-resistant, impervious gloves should be worn when handling. Appropriate footwear should be worn. Wear a respirator that meets the appropriate standard for oxygen displacement. A self contained breathing apparatus may be needed. There is no specific data available on its toxicology. There are no known significant ecological effects or critical hazards. In the NFPA diamond, it has a 0 for health, 0 for flammability, 0 for reactivity, and a special warning SA for simple asphyxiant.

Hydrogen Gas: Safety, Health, and Environmental

Hydrogen is a colorless, odorless gas that is extremely flammable. It has no toxic effects on the human body, but it can displace air to cause asphyxiation. Hydrogen has a wide explosive/flammability range (4%-74% in air). Hydrogen is very light and will rise quickly. It also can make certain metals brittle after prolonged use, so metal equipment needs to be checked regularly. When handling hydrogen, keep away from heat, sparks, and open flame, if stored in compressed cylinders, protect cylinders from damage. Hydrogen is the lightest known gas so it may leak out of systems that are airtight for other gases. All piped hydrogen systems and associated equipment must be grounded, with the electrical equipment being non-sparking or explosion proof. Hydrogen gas should be stored and used with adequate ventilation. It should be separated from oxidizers to prevent combustion. No smoking or open flames signs should be posted.

Process Safety Considerations

Waste Streams and BACT Treatment

- Air Out from PSA
  - Can be released to atmosphere
- O2 Out
  - Can be released to atmosphere
- Water from heat exchanger out
  - To water treatment plant
- Water from condenser out
  - To water treatment plant
Health Risks and Mitigation Techniques

<table>
<thead>
<tr>
<th>Health Risk</th>
<th>Mitigation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2 asphyxiation - oxygen displacement</td>
<td>To combat the risk of asphyxiation from nitrogen gas, proper signage, ventilation, confined space permits, and breathing apparatuses will be used.</td>
</tr>
<tr>
<td>Ammonia Exposure</td>
<td>Ammonia resistant gloves, clothing, and ventilators will be provided. This is in addition to the proper engineering and management controls.</td>
</tr>
<tr>
<td>Burns</td>
<td>Protective insulation on equipment</td>
</tr>
<tr>
<td>Hydrogen gas explosions</td>
<td>Store in approved containers</td>
</tr>
</tbody>
</table>

Lessons Learned From Industry

Many of the incidents regarding anhydrous ammonia originate from some form of failure in the refrigeration units. It is important to have backup systems, training, and emergency shut downs.
Other Important Considerations

A strong safety culture must be promoted by the company, not only to mitigate safety risks but also to communicate about and reinforce the importance of protecting our environment. For example, a no smoking policy on the premises should be followed by employees and visitors in order to mitigate risk of explosion. A no smoking policy would also have health benefits for the employees and is beneficial for the environment, as smoking is a leading cause of preventable deaths and litter from cigarette butts would be prevented. Due to the chances of a gas leak or explosion, the plant should make the surrounding people, companies, and first responders aware of what they should do if something were to happen.
Manufacturing/Operation Costs

The manufacturing costs can be broken into 3 parts: direct material costs, direct labor costs, and manufacturing overhead. For this plant, we are expected to produce about 50 tons per day which amounts to 18250 tons per year. This will require about 1.26 million kg of nitrogen and 270 thousand kg of hydrogen. If the nitrogen is produced from atmospheric air, there will be no costs associated with the direct purchase of raw material for the production of nitrogen. Hydrogen will be made from water via electrolysis. If the electrolysis unit consumes 1 liter of water per Nm$^3$ H$_2$ produced, about 4135776 gallons of water will be consumed per day. At $3.27 per 1000 gallons, it will cost about $13,600 per year to supply water to produce the desired amount of hydrogen.

Direct labor costs can be estimated by multiplying the direct labor hourly rate by the time required to produce one unit. If we consider one unit to be 50 metric tons, each unit requires 12 hours of production. An average chemical technician in Minnesota makes about $23.50/hr and we can assume to have about 25 employees. So the direct labor costs for one year would roughly be about $2,600,000.

The manufacturing overhead is all of the indirect costs incurred during the production process. This usually includes the depreciation of equipment used in the production process. We can assume a straight-line depreciation over 20 years on all material goods which means we will have a net loss of about $126,000 per year. We can also give an estimate of indirect cost/miscellaneous expenses to be about $15,000. The price of electricity for the year has been calculated to be around $45,000. Therefore the total operational costs will be approximately $2,900,000 per year.
Economic Analysis

\[
ROI = \frac{Net \ Profit}{Total \ Investment} \times 100
\]

\[
Net \ Profit = 7331859.69 \ $/year
\]

\[
Total \ Investment = 3596175 \ $
\]

\[
ROI = 203\%
\]

\[
NPV = \sum_{t=1}^{n} \frac{R_t}{(1 + i)^t} = 61,866,728.56
\]

For the net present value we used the time period of 20 years and a discount rate of 8%.
Conclusion and Recommendations

For this plant producing 50 mtpd of ammonia located in Minnesota we chose to adapt the traditional haber-bosch process to be more environmentally friendly. This was done through obtaining nitrogen from pressure swing absorption and hydrogen from water electrolysis. The electricity for the water electrolysis unit will be provided by windmills, which are abundant in the american midwest. This will lower the carbon emissions from the traditional Haber-Bosch process.

The economic analysis shows that this is a viable process. There were several estimates made on pricing due to lack of availability of pricing data. Even when that is acknowledged, the process demonstrates profitability.

We recommend additional research into electrolysis as it is the most novel aspect of our process in an industrial setting. Further research into a catalyst that allows for this reaction to occur at lower temperatures and pressures would also be beneficial.
Bibliography

Appendix
### Molar kmol Components

<table>
<thead>
<tr>
<th>Streams</th>
<th>N2</th>
<th>H2</th>
<th>NH3</th>
<th>Conv</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1467.136</td>
<td>4401.408</td>
<td>0</td>
<td>0.15</td>
</tr>
<tr>
<td>2</td>
<td>1247.096</td>
<td>3741.197</td>
<td>440.1408</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2934.272</td>
</tr>
<tr>
<td>4</td>
<td>1247.096</td>
<td>3741.197</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

### Mass kg Components

<table>
<thead>
<tr>
<th>Streams</th>
<th>N2</th>
<th>H2</th>
<th>NH3</th>
<th>tot</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>41099</td>
<td>8872</td>
<td>0</td>
<td>49971</td>
</tr>
<tr>
<td>2</td>
<td>34935</td>
<td>7541</td>
<td>7500</td>
<td>49976</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>50000</td>
<td>50000</td>
</tr>
<tr>
<td>4</td>
<td>34935</td>
<td>7541</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

### Reaction

\[
2\text{H}_2\text{O} \rightarrow \text{2H}_2 + \text{O}_2
\]

### Mole H2 O2 H2O

<table>
<thead>
<tr>
<th></th>
<th>H2</th>
<th>O2</th>
<th>H2O</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>4391.996</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>2195.998</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>4391.996</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Mass H2 O2 H2O

<table>
<thead>
<tr>
<th></th>
<th>H2</th>
<th>O2</th>
<th>H2O</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td>79143.76</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>70271.93</td>
</tr>
<tr>
<td>3</td>
<td>8871.831</td>
<td></td>
<td>79143.76</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Air vol% wt%

<table>
<thead>
<tr>
<th></th>
<th>vol%</th>
<th>wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2</td>
<td>78</td>
<td>76</td>
</tr>
<tr>
<td>O2</td>
<td>21</td>
<td>23</td>
</tr>
<tr>
<td>Ar</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

### N2 O2 Air

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>54078.25</td>
</tr>
<tr>
<td>2</td>
<td>41099.47</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>11356.43</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>-------------</td>
<td>----------------</td>
</tr>
<tr>
<td><strong>H2O</strong></td>
<td><strong>→</strong></td>
<td><strong>H2</strong> +</td>
</tr>
<tr>
<td><strong>Anode</strong></td>
<td><strong>6H2O</strong></td>
<td><strong>→</strong></td>
</tr>
<tr>
<td><strong>Cathode</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Overall</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>efficiency</td>
<td><strong>0.7</strong></td>
<td></td>
</tr>
<tr>
<td>energy</td>
<td><strong>50 kW-hrs/kg</strong></td>
<td></td>
</tr>
<tr>
<td><strong>8871.831</strong></td>
<td></td>
<td><strong>44359.5 kW-hrs</strong></td>
</tr>
</tbody>
</table>

**Assuming 12 hr work day**

<table>
<thead>
<tr>
<th><strong>m</strong></th>
<th><strong>P</strong></th>
<th><strong>r</strong></th>
<th><strong>mw</strong></th>
<th><strong>t</strong></th>
<th><strong>z</strong></th>
<th><strong>Q</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>57.0826</td>
<td>125</td>
<td>1514</td>
<td>28</td>
<td>537</td>
<td>0.99</td>
<td>91.16089</td>
</tr>
</tbody>
</table>

|              |        |       |        |       |       |
|              |        |       |        |       |       |
|              |        |       |        |       |       |
|              |        |       |        |       |       |
|              |        |       | 93     | kW    | 12 hr |
|              |        |       | 1116   | kWh   |        |

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Chemical Info</td>
<td>MW (kg/kmol)</td>
<td>conv</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Ammonia</td>
<td>17.031</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>N2</td>
<td>28.013</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Air</td>
<td>28.965</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Water</td>
<td>18.015</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Hydrogen</td>
<td>1.008</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Desired Ammonia</td>
<td>Ideal Needed N2</td>
<td>Ideal Needed H2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>50 tons/day</td>
<td>122325.9546 gmol/hr</td>
<td>366977.8639 gmol/hr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>50000 kg/day</td>
<td>3426716.967 g/hr</td>
<td>739827.3736 g/hr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>2935.822911 kgmol/day</td>
<td>156659.4368 gmol of air/hr</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>244651.9093 gmols/hr</td>
<td>3511364.616 Nm3 air/hr</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>12 hr/day</td>
<td>2741813.947 Nm3 N2/hr</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J</td>
<td>K</td>
<td>L</td>
<td>M</td>
<td>N</td>
<td>O</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Haber Bosch</td>
<td>T</td>
<td>700</td>
<td>alpha</td>
<td>beta</td>
<td>desired gas veloci</td>
</tr>
<tr>
<td>P</td>
<td>140</td>
<td>ammonia</td>
<td>4.225</td>
<td>0.0371</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>9.66799332 L</td>
<td>nitrogen</td>
<td>1.37</td>
<td>0.0387</td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>0.008314472 L\text{bar}/\text{mol}</td>
<td>hydrogen</td>
<td>0.3476</td>
<td>0.02661</td>
<td></td>
</tr>
<tr>
<td>nRT</td>
<td>1423906.915</td>
<td>n2 and h2</td>
<td>0.966813157</td>
<td>0.171525078</td>
<td></td>
</tr>
<tr>
<td>ammonia van der Waals</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>293.15 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>9240.87188 L</td>
<td>Gas Ammonia</td>
<td>337.8992428</td>
<td>0.09384979</td>
<td>162.1724365</td>
</tr>
<tr>
<td>R</td>
<td>0.006314472 L\text{bar}/\text{mol}</td>
<td>Nitrogen</td>
<td>3263.286644</td>
<td>0.966468254</td>
<td>1566.377109</td>
</tr>
<tr>
<td>nRT</td>
<td>299155.7487</td>
<td>Hydrogen</td>
<td>1566.01361</td>
<td>0.440291281</td>
<td>766.806029</td>
</tr>
<tr>
<td>nitrogen van der Waals</td>
<td>2.10205E-05</td>
<td>N and H in</td>
<td>2126.882256</td>
<td>0.590600527</td>
<td>1020.903483</td>
</tr>
<tr>
<td>PSA</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>363.15 K</td>
<td>air in</td>
<td>15714.55028</td>
<td>3.809597299</td>
<td>6582.984133</td>
</tr>
<tr>
<td>P</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>44482.51963 L</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>0.008314472 L\text{bar}/\text{mol}</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>nRT</td>
<td>110805.148</td>
<td>T</td>
<td>300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>hydrogen van der Waals</td>
<td>2.30052E-08</td>
<td>P</td>
<td>20.365</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>V</td>
<td>60236.5419 L</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>R</td>
<td>0.008314472 L\text{bar}/\text{mol}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Thank you, Ralph, for leading these efforts. I think in the future these AIChE contests will continue to make good Capstone projects for Honors Chemical engineers; especially if they did this well during these very unusual circumstances.

Bill

On Mon, May 4, 2020 at 1:34 PM Ralph Quigley <raq0002@uah.edu> wrote:

Dean Wilkerson, I am not sure what the protocol for assigning the remainder of the grades for the Honors Capstone Project but here are the grades as I evaluated the students’ performances:

Lauren Garner - Team Lead, completed the AIChE National Contest Project. Although her team report was not as detailed and thorough as the other teams’ reports she did complete a respectable report with a "challenging" team composition. Lauren did not prepare the report in time for the AIChE submission so she was asked to research and present a slide-show on Modular Industrial Plant Design; one of the fundamental concepts required in the AIChE Project. Here scores are recorded on Canvas as:

- Project Report, 95
- Modular Presentation, 91
  - Overall Score 93.

Caleb and Shela worked together with 2 other seniors to prepare a project report that will be sent to AIChE for the competition. This was a herculean task especially given the end of the semester crisis. I expect their report to be above average as compared to the other reports submitted. I was not able to record their grades on Canvas but are as follows:

- Caleb Jacobs, 96
- Shela Joyce, 94

John Mark Morris worked with another team led by Cameron Sawyer. Their team did not submit their report in time for the AIChE submission but submitted it in time for the final CHE448 Course Project. John Mark’s score was not posted on Canvas.

- John Mark Morris, 90.

All four students performed well during the adverse conditions.

--

Ralph Quigley, PE
Instructor
Chemical & Materials Engineering
Engineering Building ENG 117
T: 256-824-6810
F: 256-824-6839