Ammonia Reactor Design

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Abstract

In our design plan of an ammonia plant producing 100,000 tons of ammonia per year, we determined that the most cost-effective optimization of the process involves building a 142 ft³ reactor and operating the condenser at 6.7 °C, which results in an annual system cost of $219 million. The unknowns for this design problem are the amount of material in the feed stream fed into the process, the amount purged from the system, the amount in the recycle stream, and the operating temperature of the condenser that separates ammonia from the rest of the reactor effluent. To calculate the optimal process parameters, we established the bases as the process feed stream flow rate and the process's effective conversion of feed N_2 and H_2 into NH_3 product. The key tools we used in our calculations are molar balances and thermodynamic relations, involving Raoult's Law and Antoine's Equation. Upon finding the system flow rates, we scaled up the system to determine the optimal condenser temperature and minimum operating cost.

Introduction

We are optimizing the design of an ammonia plant that uses the Haber-Bosch process to produce ammonia at 100,000 ton/yr, using the chemical reaction $N_2 + 3H_2 \rightarrow 2NH_3$. The vapor feed stream entering the process was previously processed such that there is a stoichiometric 3:1 ratio of H_2 to N_2, and the mole fraction of argon is 0.0029. The feed stream is combined with a recycle stream, with a recycle ratio of 4:1, and feeds into a plug flow reactor with a promoted iron catalyst. The reactor has a single pass conversion of 0.20. The reaction occurs at a very high pressure of 300 bar, which shifts the reaction towards the products by Le Chatelier's principle, as the products contain fewer moles of gas than the reactants. The reaction is run at high temperature of 482°C, despite the reaction being exothermic. This makes the reaction thermodynamically unfavored, as demonstrated by the poor single pass conversion of 20%. However, the high temperature is required to produce ammonia at a practical rate. The reactor effluent is sent to a gas-liquid condenser, where most of the ammonia is condensed into a liquid and released as a product stream. The condenser vapor effluent is recycled back into the reactor, with a small amount purged from the system to prevent accumulation.

The goal of our analysis is to find the condenser temperature that minimizes the operating cost of the process while meeting the production demand. The total annual operating cost is the sum of the reactor volume cost and the condenser cooling cost. The reactor volume cost is directly proportional to the reactor's volume, which depends on the flow rate and composition of the feed. The condenser cooling cost is proportional to the molar flow rate into the condenser and the temperature difference between the reactor and the condenser. In all, the design requirements cause the system to have only one degree of freedom, so all of the other variables can be determined from the condenser temperature. Therefore, this is a complex optimization problem in which compromises must be made between reactor size and condenser temperature to minimize cost and meet production demand.

Design Approach

We centered our design by setting our independent variable as X_{eff}, the "effective conversion" of N_2 in the feed stream, F_1, to the amount of pure liquid NH_3 in the product stream, F_4. We also used a feed basis of 1 lbmol/hr (Equation 1).

$$X_{eff} = \frac{F_{4,NH_3}}{2F_{1,N_2}}$$

(1)

We chose to make our flow rate calculations in terms of the effective conversion instead of condenser temperature because effective conversion allows us to set a basis for both the feed stream and the product stream, significantly simplifying the algebra involved in solving for the flow rates. Because the entire system has only one degree of freedom, each effective conversion value corresponds to only one condenser temperature. Once we calculate the optimal effective conversion for the process, we know the vapor mole fraction of ammonia in the condenser, which we can subsequently use to condenser temperature.

With these parameters, we were able to solve for the flow rates of the components in each stream in terms of the variables y_{N2}, y_{NH3}, and F_4 by using mole balances. y_{N2} and y_{NH3} are the gaseous mole fractions while F_4 is the pure liquid ammonia product stream. Throughout our calculations, we established each unit in the process as an individual control volume and found the flow rates in and out of each unit using mole balances. For streams entering a unit that is not

a reactor, we applied conservation of moles to solve the mole balance because the inlet molar flow rate must equal that of the effluent for a steady state process. For the reactor feed stream, F_2, our mole balance calculations are written based on the reactor's single-pass conversion of 20%. A detailed calculation of the ammonia reactor plant and description of variable assignments can be found in Appendix A.1.

In addition to molar balances, we also used several thermodynamic concepts in the calculations involving the condenser. After solving for y_{NH3} from the system of mole balances, we used Raoult's Law and Antoine's Equation to determine the required operating temperature of the condenser for the X_{eff} chosen.

We used Raoult's Law (Equation 2), to relate the composition of ammonia in the vapor stream leaving the condenser, y_{NH3}, to the saturated pressure of ammonia, P_{NH3}^{sat}. We made the key assumption that a negligible amount of N_2, H_2, and argon condenses, so the liquid stream is pure ammonia.

$$y_{NH3}P = X_{NH3}P_{NH3}^{sat} \tag{2}$$

Thus, under this assumption, $X_{NH3} = 1$, there is a linear relationship between y_{NH3} and P_{NH3}^{sat}. By rearranging Antoine's equation and Antoine constants for ammonia, the temperature of the condenser, $T_{condenser}$, can be found (Equation 3).

$$\log(P_{NH3}^{sat}) = A - \frac{B}{T+C} \tag{3}$$

$$T_{condenser} = \frac{B}{A - \log(P_{NH3}^{sat})} - C \tag{3a}$$

The rearranged form of Equation 3 allows us to solve for temperature, where P [=] mmHg and T [=] °C. A, B, and C are Antoine constants for ammonia (Table 1).

To find the optimal operating conditions, we calculated the cost of the system at temperatures from -65 to 60 °C. We examined how the different operating temperatures would affect the cooling cost, the cost to condense ammonia into liquid, and the reactor cost, the cost to operate the reactor.

The cost of the condenser is dependent on the molar flow rate in and $T_{condenser}$, both specified at a given X_{eff}.

$$Cost_{condenser} = \frac{\$0.0002}{Btu}FC_p(T_{reactor} - T_{condenser}) \tag{4}$$

Where F [=] $\frac{lbmol}{hr}$ is the molar flow rate into the condenser, $C_p = 17.74 \frac{Btu}{lbmol\,K}$ is the mean molar heat capacity of reactor product stream, and T [=] K is temperature. Thus, the flow rate of the stream entering the condenser (F3) must be calculated from the condenser temperature, then the cooling cost for the stream can be calculated by plugging in the flow rate and the temperature.

The cost of the reactor is directly proportional to the volume of the reactor, which depends on the molar flow rate and the composition of the reactor feed stream. For the reactor volume calculation, the molar flow rates had to be scaled up from a 1 lbmol/hr basis to a flow rate that satisfies the 100,000 ton/year requirement.

The flow rate of F1 was scaled up according to this equation in terms of X_{eff}:

$$F_1 = \frac{F_4}{2*0.249*X_{eff}} \tag{7}$$

where F_{4NH3} [=] lbmol/hr is the desired amount of liquid ammonia product, the 2 is the stoichiometric ratio of ammonia to nitrogen, and 0.249275 is the mole fraction of nitrogen in the feed. F_1 is in pound moles per hour. This new F_1 value was then used to calculate the flow rates of the other streams in the process, which are necessary for the reactor volume calculation.

We modified the plug-flow reactor design equation by substituting in the component flow rates of stream 2, which allowed us to find the volume for any effective conversion. The derivation for this modified equation can be found in Appendix A.2.

$$\frac{dV}{dX_{N2}} = \frac{F_{2,N2}[(\frac{F_{2,NH3}+X_{N2}F_{2,N2}}{F_2})(\frac{F_{2,H2}-3X_{N2}F_{2,H2}}{F_2})^{1/2}+\beta(\frac{F_{2,H2}-3X_{N2}F_{2,H2}}{F_2})^2]^{3/2}}{k_1[(\frac{F_{2,N2}-X_{N2}F_{2,N2}}{F_2})(\frac{F_{2,H2}-3X_{N2}F_{2,H2}}{F_2})^3-(\frac{F_{2,NH3}+X_{N2}F_{2,N2}}{F_2})/(K^2P^2)]} \tag{5}$$

where $k_1 = 1.20$ $lbmol/ft^3\,hr$, K = 4.67 x 10^{-3}, $\beta = 0.00140$, and P = 300 bar. The initial value is $V(X_{N2} = 0) = 0$, and X_{N2} ranges from 0 to 0.2.

We then used the Runge-Kutta method to numerically solve the differential equation, which yielded the volume of the reactor. The reactor cost is then calculated by multiplying the reactor volume by $\$200,000/ft^3 yr$ (Equation 6).

$$\text{Cost}_{reactor} = V(X_{N2} = 0.2) * \$200,000/ft^3.yr \tag{6}$$

The total cost was calculated by summing the cooling cost and the reactor cost for every effective conversion value between 0.2 and 1. Then, we picked the minimum total cost from

these total cost values. The effective conversion that corresponded to this minimum total cost is the optimal effective conversion for the process. This effective conversion was then converted to the condenser temperature by taking the mole fraction of ammonia in the condenser vapor effluent and solving for the temperature using Antoine's equation, as described in Equations 2 and 3. This temperature is the optimal temperature of the condenser that minimizes overall operating costs.

Results and Discussion

Through our methodology of solving for the costs of both the reactor and condenser at a range of X_{eff}, we can conclude that the most cost-effective condition for the system is to run the condenser at 6.7 ℃ (Figure 2), with a reactor size of 142 ft^3 (Figure 5). The total cost is the sum of the cooling cost and the volume cost, and the minimum annual cost of the reactor is $219 million. Although our computations were made over the range of X_{eff} values, we choose to analyze our system parameters with respect to condenser temperature because temperature is the variable that is controlled during plant operation.
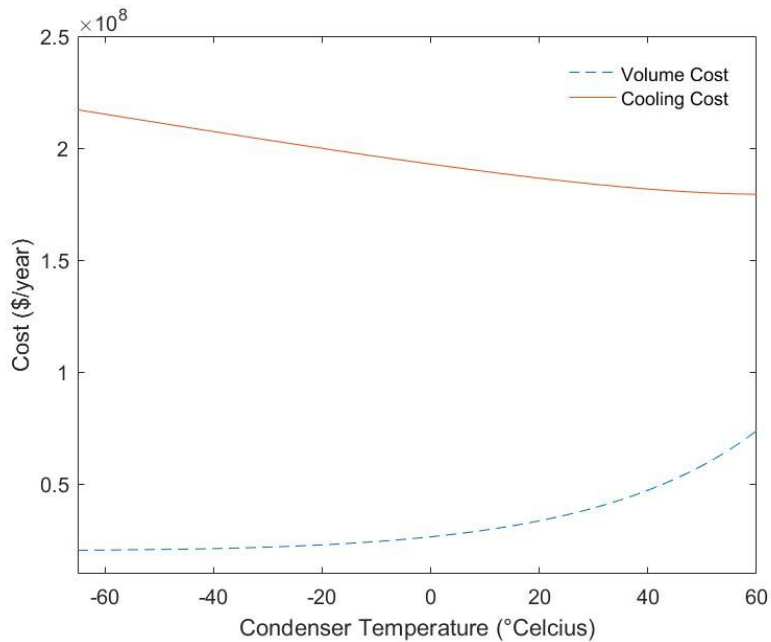
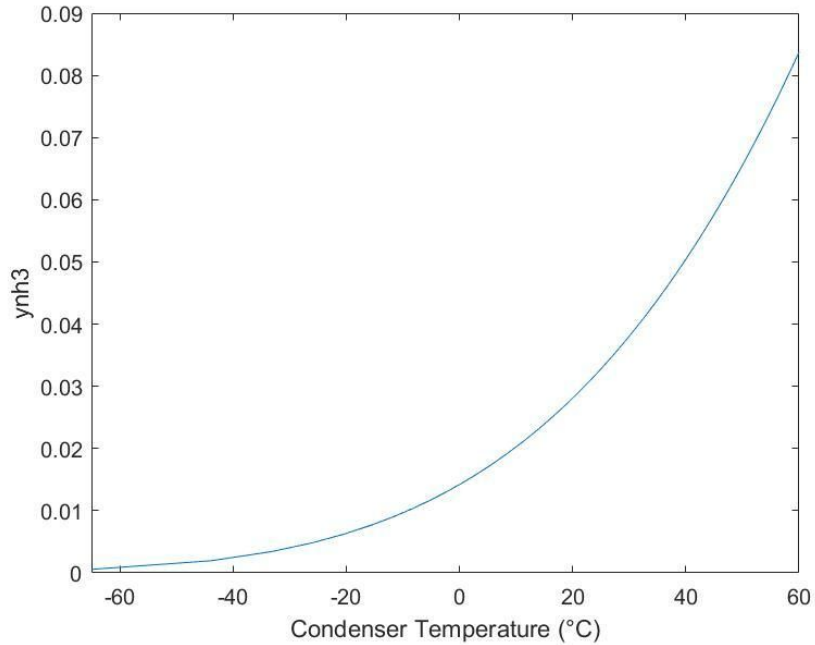**Figure 1.** Relationship between between both reactor cost and cooling cost versus condenser temperature.
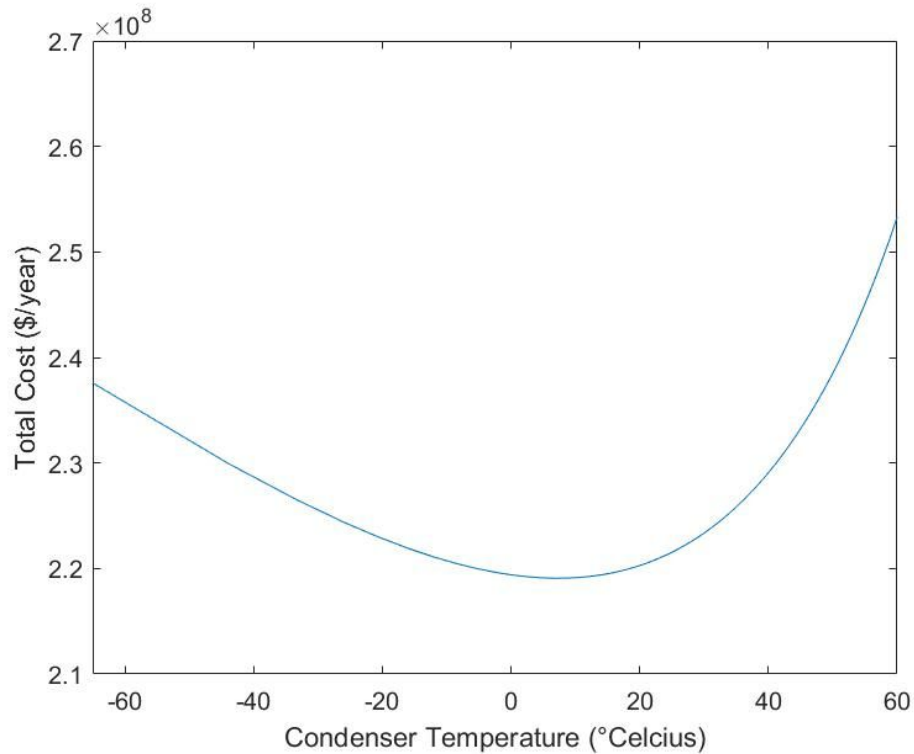
Figure 2. Relationship between the total system cost and condenser temperature. The minimum cost at 6.7℃ shows that 6.7℃ is the optimal condenser temperature.

The overall cost of the ammonia plant follows a parabolic trend (Figure 2). In the lower range of temperatures from -65 to 6.7 ℃, the term that dominates the trend of the total cost is the heat exchanger cooling cost. Since the heat exchanger cooling cost is linearly proportional to the temperature difference between the reactor (482 ℃) and the condenser, the cooling cost decreases linearly as condenser temperature increases closer to the reactor temperature. In this temperature range, volume increases slowly with respect to temperature, and thus the reactor size does not significantly affect overall cost. However, at temperatures above 0 ℃, the volume cost increases rapidly with temperature, causing the overall cost to increase rapidly as well (Figure 1).

The reactor volume increases with an exponential trend with condenser temperature (Figure 5), and this trend primarily drives the increase in total process cost as temperature increases. The reason behind this trend lies in the effect that temperature has on the mole fraction of ammonia in the condenser's vapor effluent (y_{NH3}). The equilibrium y_{NH3} increases with

temperature (Figure 3) by Antoine's Equation (Equation 3), because vapor pressure increases with temperature. The trend of increasing y_{NH3} means there is greater buildup of ammonia throughout the system, accounting for the increase in reactor volume. Furthermore, this increase in y_{NH3} leads to a rapidly increasing purge ratio of the condenser vapor effluent (Figure 4).
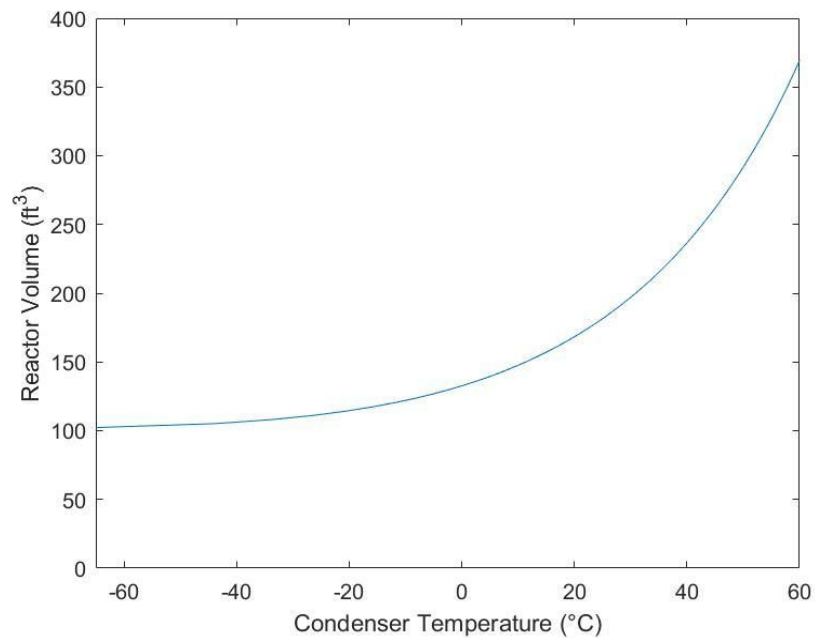

Figure 3. Relationship between ammonia mole fraction and condenser temperature. This relationship is derived from Antoine's equation.
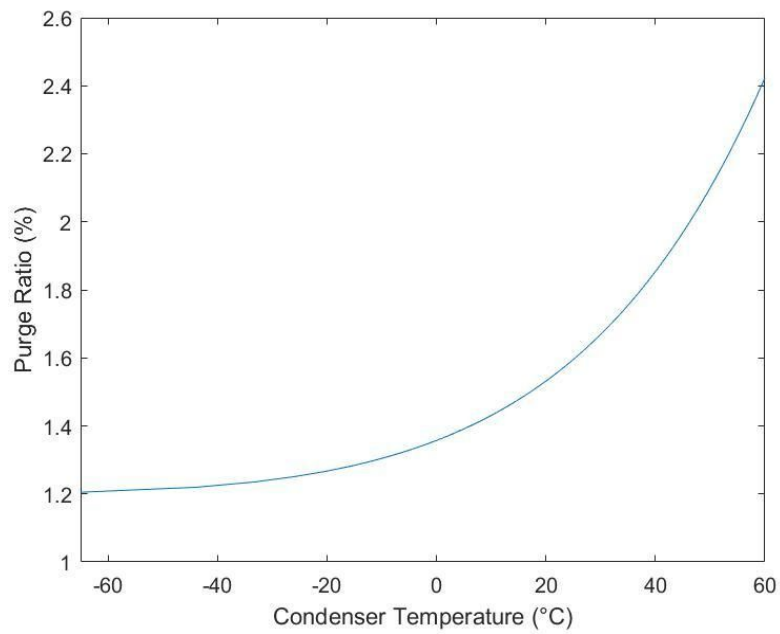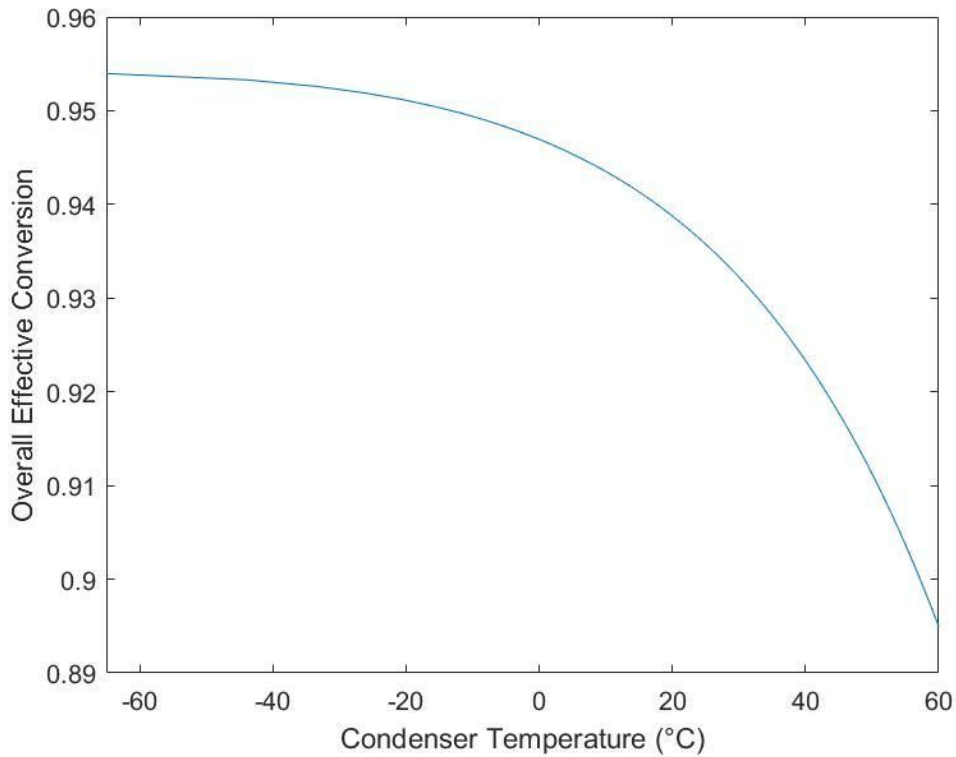
Figure 4. Relationship between condenser temperature and purge ratio. Purge ratio is defined as the ratio of condenser vapor effluent purged to condenser effluent recycled.

Figure 5. Relationship between reactor volume and condenser temperature.

This trend results from the requirement of maintaining the recycle ratio of 4. Since this is a steady state process, an increase in purge stream flow rate would require an increase in the system feed flow rate and subsequently the reactor volume. Additionally, a larger purge stream decreases overall conversion (X_{eff}) because more of the ammonia is exiting the system in this purge. This is why X_{eff} decays rapidly as condenser temperature increases (Figure 6). All in all, this analysis verifies that there exists a specific condenser temperature that minimizes total system cost.

Figure 6. Relationship between overall effective conversion, X_{eff}, and condenser temperature. For the temperature range within the Antoine's Equation parameters, the minimum X_{eff} is 0.895 and the maximum is 0.954.

Conclusion & Recommended Design

In conclusion, the condenser temperature at which the annual production cost is minimized is 6.7 ℃. At this temperature, the reactor volume must be 142 ft^3 to fulfill the production demand of 100,000 tons of ammonia. At this temperature, the reactor operating cost is $28.5 million and the condenser cooling cost is $190 million, for a total annual operating cost of $219 million. To arrive at our values, we make the key assumptions that N_2, H_2, and Ar do not condense into the liquid ammonia stream. With a more rigorous analysis, calculations with Henry's Law would take this phenomenon into account. Furthermore, a more rigorous cost analysis would take into account the cost of the feed stream because wasted feed could also be factored into overall cost.

Appendix A - Calculations and Derivations

Appendix A.1 - Solving The Process Flow Diagram

The calculations in Appendix A.1 details the equations used to solve the process flow diagram using a basis of 1 mole per hour feed.
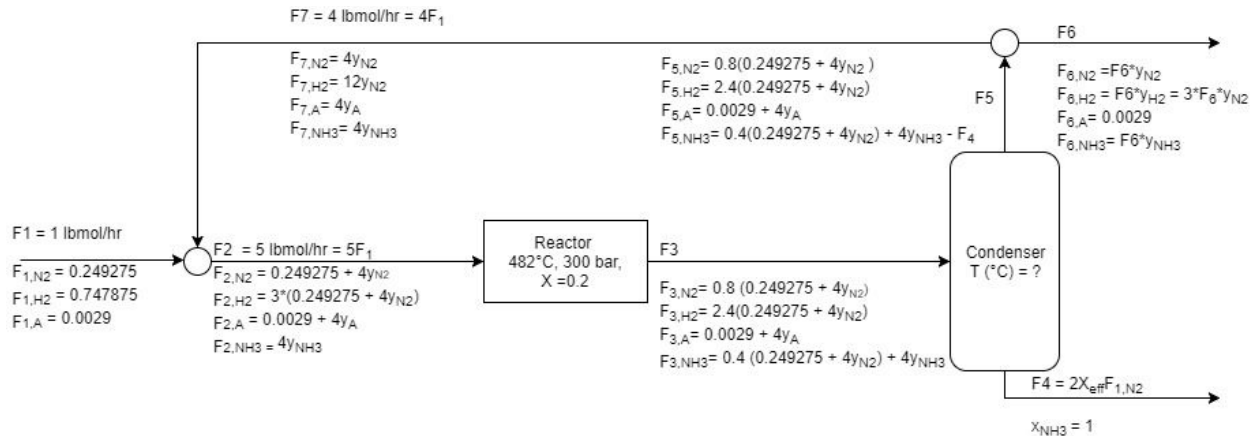
Figure 7. Process Flow Diagram of the Ammonia Reactor. Design specifications of this ammonia reactor are a fresh feed, F1, of fixed composition of N_2, H_2, and A, a recycle ratio of F_7: F_1 of 4:1, and a single pass conversion of the reactor at 0.2.

$F_{L,w} \rightarrow$ The subscript "L" indicates the stream and the subscript, "w." indicates the compound. If there is only subscript, "L," it indicates the total stream, the summation of all the compounds. Each stream in this PFD are in units of lbmol/hr.

$y_i \rightarrow$ "y" represents the vapor/gas molar composition of the compound "i" in a stream. In this PFD, y_i is referring to only streams F_5, F_6, and F_7; Since F_6 and F_7 is formed from splitting F_5, all three streams have the same molar composition.

Variable assignments:

F_1: Fresh feed stream into the system

F_2: Feed stream into the reactor

F_3: Feed stream into condenser

F_4: Liquid Ammonia Product Stream

F_5: Vapor stream leaving the condenser

F_6: Purge Stream

F_7: Recycle Stream

Subscripts assignments:

NH3: Ammonia

N2: Nitrogen gas

H2: Hydrogen gas

A: Argon and other inert gases

X_{eff} is the amount of N_2 in F_1 that is converted into NH_3 in F4.

X_{eff}

$$F_{1,N2\ Reacted} * \frac{2\ NH3}{1N2} = F_{4,NH3}$$
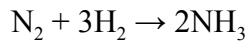
$$X_{eff} = \frac{F_{1,N2\ Reacted}}{F_{1,N_2}}$$

$$X_{eff} = \frac{0.5*F_{4,NH_3}}{F_{1,N_2}} \tag{1}$$

Molar Conversion out of the Reactor

The governing principle is that the molar flow rate out is equal to the molar flow rate in along with the generation or consumption of that stream.

$$F_{out} = F_{in} \pm XF_{in}$$

X represents the conversion.

$$N_2 + 3H_2 \rightarrow 2NH_3$$

For every one mole of N_2 consumed, two moles of NH_3 are produced. Therefore, the generated NH_3 out of the reactor can be written as

$$generated\ NH_3 = XF_{N2,in}$$

The conversion, X, will determined the amount of N_2 consumed and is defined as a value from 0 to 1.

Calculation of y_{NH3} from conservation around a splitter

Around a splitter, moles and molar compositions are conserved.

NH3 Balance:

$F_{5,NH3} = F_{6,NH3} + F_{7,NH3}$

$4y_{NH3} + 0.4(0.249275 + 4y_{N2}) - F_4 = F_6 y_{NH3} + 4y_{NH3}$

$0.4(0.249275 + 4y_{N2}) - F_4 = F_6 y_{NH3}$

$$0.09971 + 1.6y_{N2} - F_4 = F_6 y_{NH3} \tag{8}$$

N2 Balance:

$F_{5,N2} = F_{6,N2} + F_{7,N2}$

$0.8(0.249275 + 4y_{N2}) = F6 y_{N2} + 4y_{N2}$

$$0.199420 - 0.8y_{N2} = F_6 y_{N2} \tag{9}$$

Overall Splitter Balance:

$F_6 + 4 = 3.6(0.249275 + 4y_{N2}) + 4y_{NH3} + 0.0029 + 4y_A - F_4$

$y_A = 1 - 4y_{N2} - 1y_{NH3}$

$F_6 + 4 = 3.6(0.249275 + 4y_{N2}) + 0.0029 + 4 - 16y_{N2} - 4y_{NH3} + 4y_{NH3} - F_4$

$$F_6 = 0.90029 - 1.6y_{N2} - F_4 \tag{10}$$

Substitute (10) into (9)

$0.199420 - 0.8y_{N2} = (0.90029 - 1.6y_{N2} - F_4)y_{N2}$

$0.199420 - 0.8y_{N2} = (0.90029 - F4)y_{N2} - 1.6y_{N2}^2$

$$1.6y_{N2}^2 + (-1.70029 + F_4)y_{N2} + 0.199420 = 0 \tag{11}$$

→ solve for y_{N2} using fsolve in MATLAB

Using y_{N2} from (11), plug into (10) to find F_6

Now F6 and y_{N2} are known, they can be plugged into (8) to find y_{NH3}

$y_{NH3} = (0.09971 + 1.6y_{N2} - F_4)/F_6$

Using $\Sigma y_i = 1$, the other molar compositions can be found.

To scale the flow rates of the streams within Figure 7, the Equation 7 is used

$$F_1 = \frac{F_{4,NH_3}}{2*0.249275*X_{effective}} \tag{7}$$

This scales the process through the selection of how much liquid ammonia is produced, F_4, at a given overall effective conversion, X_{eff}.

Appendix A.2 - Cost Calculations

Annual Cooling Cost

The annual cooling cost of the condenser is a function of the flow rate into the condenser and the temperature of the condenser. The temperature of the reactor is set at 755.4 K.

$$Cost_{condenser} = \frac{\$0.0002}{Btu} F\ C_p (T_{reactor} - T_{condenser}) * \frac{8700\ hr}{1\ yr} \tag{12}$$

Where $F\ [=]\ \frac{lbmol}{hr}$ is the molar flow rate into the condenser, $C_p = 17.74\ \frac{Btu}{lbmol\ K}$ is the mean molar heat capacity of reactor product stream, and $T\ [=]\ K$ is temperature.

The flow rate into the condenser, F_3, can be derived by adding the components in F_3 seen in Figure 1.

$F_3 = F_{3,NH3} + F_{3,N2} + F_{3,H2} + F_{3,A}$

$F_3 = F_1(0.4(0.249275 + 4y_{N2}) + 4y_{NH3} + 0.8(0.249275 + 4y_{N2}) + 2.4(0.249275 + 4y_{N2}) + 0.0029 + 4y_A)$

$F_3 = F_1 (3.6(0.249275 + 4y_{N2}) + 4y_{NH3} + 0.0029 + 4(1 - y_{NH3} - 4y_{N2}))$

$$F_3 = F_1(12.9768 - 1.6y_{N2}) \tag{13}$$

Where y_{N2} is the molar composition found in (11) and F_1 is the fresh feed needed to produce 100,000 tons of ammonia (7).

$T_{condenser}$ can be found using Equation 3a using y_{NH3} derived in Appendix A.1.

Using y_{NH3}, P_{NH3}^{sat} can be found by Raoult's law

$y_{NH3}P^{system} = X_{NH3}P_{NH3}^{sat}$

In this conditions, we assume that N_2 and O_2 are negligibly soluble in ammonia, and so $X_{NH3} = 1$.

Using Antoine's equation, $T_{condenser}$ can be calculated

$$T_{condenser} = \frac{B}{A - log(P_{NH3}^{sat})} - C \tag{3a}$$

Where A,B, and C are the constants found in Table 1.

Table 1. Antoine parameters for ammonia: pressure in mmHg, temperature in °C.

14

	A	B	C	T_{min} (°C)	T_{max} (°C)
NH_3	7.36050	926.132	240.17	-83	60

At our optimum situation where $T_{condenser}$ is 6.7 °C and F is 12901 lbmol/hr, the resulting cooling cost is $190 million.

Reactor Size Cost

For a plug flow reactor (PFR), the conversion of a reactant changes over the volume of the reactor. Its differential change can be written as a function of the rate of reaction over the flow rate in.

$$\frac{dX_{N2}}{dV} = -\frac{r_{N2}}{F_{N2}} \tag{14}$$

The rate of reaction, r_{N2}, of ammonia over a promoted iron catalyst is

$$\frac{-k_1[y_{N2}y_{H2}^3 - y_{NH3}^2/K^2P^2]}{[y_{NH3}y_{H2}^{1/2} + \beta y_{H2}^2]^{3/2}} \tag{15}$$

Where k_1 = 1.20 $lbmol/ft^3\ hr$, K = 4.67 x 10^{-3}, β = 0.00140, P = 300 bar, and y_i is the molar composition of a compound i.

r_{N2} can be rewritten as a function of X_{N2} and the stream into the reactor, F_2.

$$\frac{-k_1[\frac{F_{2,N2} - X_{N2}F_{2,N2}}{F_2}(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^3 - (\frac{F_{2,NH3} + X_{N2}F_{N2}}{F_2})/K^2P^2]}{[\frac{F_{2,NH3} + X_{N2}F_{N2}}{F_2}(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^{1/2} + \beta(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^2]^{3/2}} \tag{16}$$

To find the reactor volume, equation (16) is substituted into equation (14).

$$\frac{dV}{dX_{N2}} = \frac{F_{2,N2}[(\frac{F_{2,NH3} + X_{N2}F_{N2}}{F_2})(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^{1/2} + \beta(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^2]^{3/2}}{k_1[(\frac{F_{2,N2} - X_{N2}F_{2,N2}}{F_2})(\frac{F_{2,H2} - 3X_{N2}F_{2,H2}}{F_2})^3 - (\frac{F_{2,NH3} + X_{N2}F_{N2}}{F_2})/(K^2P^2)]} \tag{17}$$

The flow rates within the equation can be solved as a function of F_1, y_{NH3}, and y_{N2} (Appendix A.1).

$$F_{2,N2} = 0.249275F_1 + y_{NH2}4F_1$$

$$F_{2,NH3} = y_{NH3}4F_1$$

$$F_{2,H2} = 3F_{2,N2}$$

To calculate the reactor sized need to meet the production need of 100,000 tons of ammonia per year, the variable F_1 was scaled up (7) and substituted into components of F_2.

This differential equation is solved using Matlab's ode45 with an initial value $V(X_{N2} = 0) = 0$ and boundaries on X_{N2} from 0 to 0.2. The volume of the reactor will be the volume at $X_{N2} = 0.2$. The reactor cost will be

$$\text{Cost}_{reactor} = V(X_{N2} = 0.2) * \$200,000/ft^3 * yr \tag{6}$$

In our optimum situation, the reactor volume is 412 ft³, costing $28.5 million annually.

Appendix B - MATLAB Code

Appendix B.1 - Minimum cost due to $T_{condenser}$ and Reactor Volume

We calculated the minimal cost of the reactor and the optimal condenser temperature using the Matlab code shown below. The function takes an input of a selected range of X_{eff} values and solves for the corresponding cost and $T_{condenser}$ values. The minimum and indexing built in Matlab functions are used to find the minimum cost and the corresponding $T_{condenser}$. These values are calculated using subfunctions created using the equations listed in Appendix A.

```
function [Condenser_temperature, Minimum_cost] = CBE140_Design_Project()
%Calculates the optimal operating temperature (in C) of condenser to minimize
%annual cost of producing ammonia using a process that follows the design specs.

X_effective_vector = linspace(.6,.954,500);
Cost_vector = zeros(1,500);
Temperature_vector = zeros(1,500);

%Setting up for loop to loop through entire range of X_effective
for i = 1:500
    Volume_cost = Volume_cost_from_X_effective(X_effective_vector(i));
    Cooling_cost = Cooling_cost_from_X_effective(X_effective_vector(i));
    Cost_vector(i) = Volume_cost + Cooling_cost;
    Temperature_vector(i) = T_from_X_effective(X_effective_vector(i));
end

%Finding the minimum cost and the temperature associated with minimum cost:
```

```matlab
[Minimum_cost, index] = min(Cost_vector);
Condenser_temperature = Temperature_vector(index);

%Plotting total cost versus condenser temperature:
plot(Temperature_vector, Cost_vector);
title('Total Cost versus Condenser Temperature')
xlabel('Condenser Temperature (°Celcius)')
ylabel('Total Cost ($/year)')
axis([-83 60 2.1e8 2.7e8])
End
```

Appendix B.2 - Volume Cost from X_{eff}

```matlab
function [Volume_cost] = Volume_cost_from_X_effective(X_effective)
%Calculates the annual cost of operating a reactor from X_effective

%Finding Volume of reactor
V = Volume_from_X_effective(X_effective);

%Finding annual cost from given price $200000/ft^3
Volume_cost = 200000.*V;
end


function [V] = Volume_from_X_effective(X_effective)
%Gives volume of the reactor from the overall conversion and gas mole
%fractions in stream 5.

%Finding gas mole fractions in stream 7:
[yN2,~,~,yNH3] = y_from_X_effective(X_effective);

%Finding F1 and F2:
F1 = 2.69221e3./X_effective;
F2 = 5.*F1;
F7 = 4.*F1;

%Define moles of each N2, H2, NH3 going into rxr (stream 2):
nN2 = .249275.*F1 + yN2.*F7;
nH2 = 3.*nN2;
nNH3 = yNH3.*F7;


%Define the mol fractions of gases as function of single-pass conversion
%varies (X_s = single-pass conversion):
xN2 = @(X_s) (nN2 - X_s.*nN2)./F2;
xH2 = @(X_s) (nH2 - X_s.*nH2)./F2;
xNH3 = @(X_s) (nNH3 + 2.*X_s.*nN2)./F2;

%Define constants necessary for r_N2:
k1 = 1.2;
K = 4.67e-3;
P = 300; %bar
```

```matlab
beta = .00140;

%Define r_N2:
r_N2            =            @(X_s)            -k1.*(xN2(X_s).*xH2(X_s).^3            -
xNH3(X_s).^3./(K^2*P^2))./(xNH3(X_s).*xH2(X_s).^(1/2) + beta*xH2(X_s).^2).^(3/2);

%Define differential equation using PFR design equation dX/dV = -r/n_in
%(where n_in = nN2):
dVdX_s = @(X_s, V) nN2./-r_N2(X_s);

%Specifying initial condition and X_s boundaries:
initial_V = 0;
X_s_boundaries = [0,.2];

%Using ode45 to solve diff eq:
[~, Volume_range] = ode45(dVdX_s, X_s_boundaries, initial_V);

%Volume of reactor is the V at X_2 = .2, which is the last value in the
%table:
V = Volume_range(end);
end
```

Appendix B.3 - Determination of y_{NH3} from X_{eff}

```matlab
function [yN2, yH2, yA, yNH3] = y_from_X_effective(X_effective)
%Calculates vapor mole fractions in the condenser from X_effective
%final temp should be 279.6K (+/- 20K is fine)
F4 = X_effective.*2*.249275;
f = @(y) 1.6.*y.^2 + (-1.7003 + F4).*y + .19942;
yN2 = fsolve(f,.1);
F6 = (.9003 - F4) - 1.6.*yN2;
yH2 = 3.*yN2;
yA = .0029./F6;
yNH3 = ((.4*.249275) - F4 + 1.6.*yN2)./F6;
end
```

Appendix B.4 - Determination of Cooling Cost from X_{eff}

```matlab
function [Cooling_cost] = Cooling_cost_from_X_effective(X_effective)
%Calculates the annual cooling cost from the X_effective and F3 (F3 is
%lbmol/hr)

%Finding F3:
F3 = F3_from_X_effective(X_effective);

%Finding total lbmol that flows through F3 per year:
F3_year = F3*24*365;

%Finding temperature that condenser is operating at:
T_condenser = T_from_X_effective(X_effective);

%Defining  molar  heat  capacity  of  the  gas  stream  out  of  reactor  and  reactor
```

```matlab
temperature:
Cp = 17.74; %(units = Btu/(lbmol*K)
T_reactor = (900 - 32)*(5/9); %have to convert from 900F to C

%Using given cooling cost equation to find BTU used annually:
Q = F3_year*Cp*(T_reactor - T_condenser);

%Calculating cost from given price $.0002/Btu
Cooling_cost = .0002*Q;
end


function [F3] = F3_from_X_effective(X_effective)
%Calculates the molar flow rate of stream 3 given X_effective

%Finding the vapor mole fractions in F5,F6,F7:
[yN2,~, yA, yNH3] = y_from_X_effective(X_effective);

%Finding F1,F7:
F1 = 2.69221e3./X_effective;
F7 = 4.*F1;

%Finding molar flow rates of each component in F2:
n2N2 = .249275.*F1 + yN2.*F7;
n2H2 = 3.*n2N2;
n2A = .0029*F1 + yA*F7;
n2NH3 = yNH3.*F7;

%Using 20% single-pass conversion to calculate component flow rates in F3:
n3N2 = .8*n2N2;
n3H2 = .8*n2H2;
n3A = n2A;
n3NH3 = n2NH3 + 2*.2*n2N2;

%Summing components to calculate total F3 flow rate (in lbmol/hr)
F3 = n3N2 + n3H2 + n3A + n3NH3;
end


function [T_condenser] = T_from_X_effective(X_effective)
%Calculates condenser temperature given X_effective

%Calculating vapor mole fraction of ammonia in condenser:
[~,~,~, yNH3] = y_from_X_effective(X_effective);

%Using vapor mole fraction to calculate condenser temperature:
T_condenser = T_from_yNH3(yNH3);
end


function [T] = T_from_yNH3(yNH3)
%This function takes the mole fraction of ammonia and gives the temperature
%of the condenser in Celsius.
```

```matlab
% Establishing Antoine Constants:
A = 7.36050;
B = 926.132;
C = 240.17;
%Putting system pressure in mmHg:
P = 300 * 760 / 1.01325;
%Using rearranged Antoine equation to find T:
T = (B / (A - log10(yNH3.*P))) - C;
end
```