Energy Balances and Numerical Methods
Design Project

Ammonia Production

Your assignment is to continue to evaluate the feasibility of a process to produce 50,000 tonne/y of ammonia from syngas.

A suggested process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point. Your assignment is to develop a “best” case, where “best” is dependent upon economic considerations, *i.e.*, EAOC. In reporting your best case, clearly indicate any modifications to the PFD and state the operating conditions for the modified process and the corresponding EAOC.

Chemical Reaction

Syngas is available from a pipeline at 1000 kPa and 200°C. It is compressed, mixed with a recycle stream, and heated or cooled to 350°C to be fed to the reactor. The reactor operates adiabatically. The reactor effluent is cooled, the pressure is reduced by a valve, and the stream partially condensed, producing an ammonia-rich stream. The ammonia liquid product is in Stream 8. Some of Stream 9 is recycled and some is purged. Depending on the pressure of the flash separator, V-601, the recycle stream may need to be compressed up the pressure of Stream 2.

The reaction that occurs in the reactor is reversible

$$N_2 + 3H_2 = 2NH_3 \qquad (1)$$

This is an equilibrium reaction, and the equilibrium constant over a wide range of temperatures is given by

$$K = 3.29\times10^{-12}\exp\left[\frac{11{,}806}{T}\right] \qquad (2)$$

In the reactor, 90% of the equilibrium conversion is obtained.

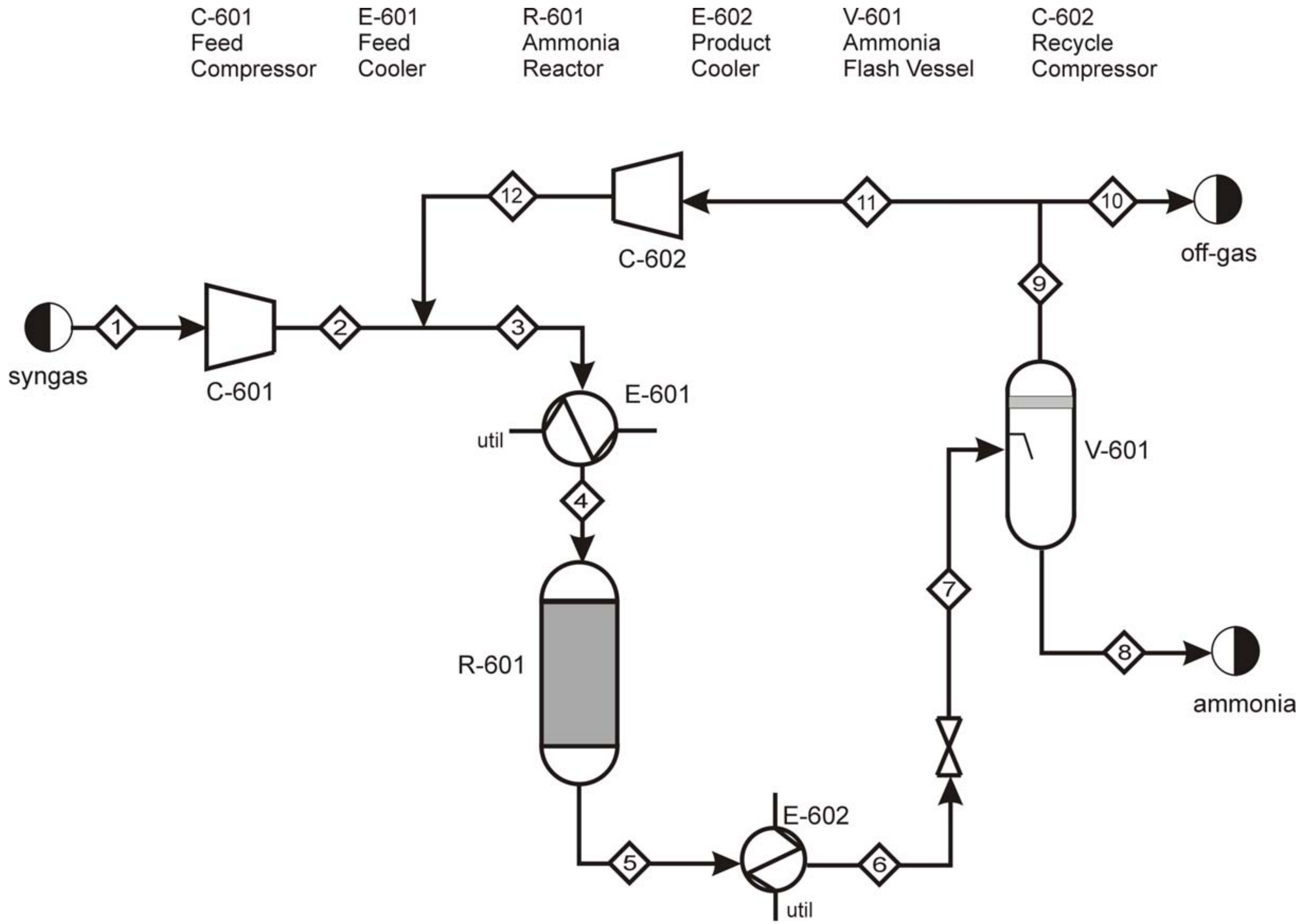

Figure 1: Ammonia Synthesis Loop

Process Details

Streams and Equipment Details

Stream 1: syngas – at 200°C and 1000 kPa – contains 72 mol% H_2, 24 mol% N_2, and 4 mol% CH_4

Stream 8: ammonia product – 50,000 tonne/y – a year is 8000 hours

Stream 10: purge used as fuel-gas to furnace – may take credit for lower heating value

Streams 9-11: unreacted syngas and ammonia not in the product stream are recycled – the recycle split is a potential decision variable

Equipment Information

Compressor (C-201)

The compressor increases the pressure of the feed stream to the pressure of the reactor. The compressor may be assumed to be adiabatic. In that case, the compressor power $\dot{W}_s$ (kW) may be calculated as

$$\dot{W}_s\,(\text{kW}) = 20{,}000\dot{m}(\text{kmol/s})\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.286} - 1\right] \tag{3}$$

where $\dot{m}$ (kmol/s) is the total molar flowrate of Stream 1. Equation 3 includes the compressor efficiency. The cost of electricity to run the compressor is a utility cost. The compressor increases the temperature of the stream being compressed according to

$$\frac{T_{out}}{T_{in}} = \left(\frac{P_{out}}{P_{in}}\right)^{0.286} \tag{4}$$

where T is absolute temperature.

In general, the ratio of outlet to inlet pressure in a compressor is between 3 and 5. If a compression ratio greater than 5 is needed, compressors are usually staged with cooling in between the compressor stages, but not after the last stage. If you choose to do this, the compression ratio for each stage should be identical, and the "intercooling" should be to 50°C. The process-flow diagram should accurately represent the chosen compressor configuration.

Heat Exchanger (E-601)

The reactor feed is cooled to T = 350°C using a cold utility. In any heat exchanger, the process stream may not be cooled below the temperature of the utility plus 10°C. The 10°C allowance is for design purposes as you will learn next year.

Reactor (R-601)

This is an adiabatic reactor. It is essentially a large pipe packed with catalyst. The equilibrium conversion can be calculated based on a choice of the operating pressure and the outlet temperature. These are decision variables that you are expected to manipulate to find optimum values. The reactor may operate at pressures of 500 kPa ≤ P ≤ 20,000 kPa and at any temperature above 350°C. The actual conversion in the reactor is 90% of the equilibrium conversion. You will find the conversions to be low, requiring a large recycle stream. An alternative reactor configuration that can increase the conversion is to stage several adiabatic reactors with a heat exchanger between the stages to reduce the inlet temperature to each subsequent reactor. The number of reactor stages is determined by the economics. The temperature of the "intercooled" stream is a potential decision variable. The process-flow diagram should represent the chosen reactor configuration.

Heat Exchanger (E-602) and Vessel (V-601)

This heat exchanger cools and partially condenses the reactor effluent to a temperature that condenses ammonia. The subsequent valve reduces the pressure to the desired pressure for the separator. Equation 4 is used to determine the outlet temperature of the valve for a chosen pressure. This vessel allows the vapor and liquid produced in E-602 to be separated. The vapor exits in the top stream, and the liquid exits in the bottom stream. Stream 9 contains all of the light gases in Stream 7 plus some ammonia. Stream 8 contains only ammonia, and the ammonia split must be calculated for the chosen temperature and pressure.. E-602, the valve, and V-601 may all be treated together for computational purposes as a flash operation at the chosen temperature and pressure. The temperature and pressure of this flash are potential decision variables. The appropriate utility must be used in E-602, and the appropriate utility depends on the temperature chosen for the separation. In any heat exchanger, the process stream may not be cooled below the temperature of the utility plus 10°C. The 10°C allowance is for design purposes as you will learn next year.

Compressor (C-602)

The compressor increases the pressure of the recycle stream to the pressure of the stream with which it is mixed. The compressor may be assumed to be adiabatic. In that case, the compressor power $\dot{W}_s$ (kW) may be calculated as

$$\dot{W}_s\,(\text{kW}) = 10{,}000\,\dot{m}(\text{kmol/s})\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.286} - 1\right] \qquad (5)$$

where $\dot{m}$ (kmol/s) is the total molar flowrate of Stream 11. Equation 3 includes the compressor efficiency. The cost of electricity to run the compressor is a utility cost. The compressor increases the temperature of the stream being compressed according to Equation 4.

In general, the ratio of outlet to inlet pressure in a compressor is between 3 and 5. If a compression ratio greater than 5 is needed, compressors are usually staged with cooling in between the compressor stages, but not after the last stage. If you choose to do this, the compression ratio for each stage should be identical, and the "intercooling" should be to 50°C. The process-flow diagram should represent the chosen compressor configuration.

Economic Analysis

When evaluating alternative cases, the objective function to be used is the Equivalent Annual Operating Cost (EAOC), defined as

EAOC = -(product value - feed cost – utility costs – waste treatment cost - capital cost annuity)

A negative value of EAOC means there is a profit. It is desirable to minimize EAOC; *i.e.*, a large negative value of EAOC is very desirable.

Utility costs are those for steam, cooling water, refrigerated water, refrigeration, boiler-feed water, electricity, and waste treatment.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed capital cost of plant construction and installation.

The capital cost annuity is defined as follows:

$$capital\ cost\ annuity = FCI\,\frac{i(1+i)^n}{(1+i)^n - 1} \qquad (6)$$

where *FCI* is the installed cost of all equipment; *i* is the interest rate; and *n* is the plant life, in [y]. For accounting purposes, take $i = 0.15$ and $n = 10$.

Optimization

You will learn optimization methods in ChE 230. The objective function (EAOC) is defined above. You should consider both topological and parametric optimization.

Topological optimization involves considering different process configurations (such location of process equipment, whether or not to add or remove equipment). You may alter the process configuration in any way that improves the economic performance as long as it does not violate the laws of nature. Determining the optimum number of staged reactors with intercooling is an example of a topological optimization.

Parametric optimization involves determining the best operating parameters for the chosen process topology. It is your responsibility to define appropriate decision variables. It is suggested that you look carefully at the efficient use of raw materials and the purge/recycle ratio for Stream 9 as well as the reactor temperature and pressure. If there are too many decision variables to do a reasonable parametric optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function. Then you should focus on only those decision variables. This is called a Pareto analysis.

Data

All of the required data, other than the heat capacity of liquid ammonia, may be found in the appendix of your textbook [1]. For this project, ***and for this project only***, you may use data that are outside the range of applicability, if necessary. It is suggested that you clearly state this assumption in your written report.

The heat capacity of liquid ammonia is [2]:

$$C_p = 3.0094 - 4.3692 \times 10^{-2} T + 2.4114 \times 10^{-4} T^2 - 5.856 \times 10^{-7} T^3 + 5.2953 \times 10^{-10} T^4 \quad (7)$$

where the temperature is in Kelvin and the heat capacity units are kJ/mol K.

Equipment Costs

The equipment costs for the ethanol plant are given in Table 1. Each cost is for an individual piece of equipment, including installation.

Table 1: Equipment Costs

Equipment	Installed Cost in \$thousands (in \$ for fired heater)
Reactor, per stage	500
Vessel, V-601	100
Any heat exchanger	200
Any pump	40
Any compressor	$0.0189\left(\dot{W}_s[\mathrm{W}]\right)^{0.8}$
Fired Heater	11×10^{x} where $x = 2.5 + 0.8\log_{10} Q$ where Q is the heat duty in kW

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit) $13.28/GJ

Medium-Pressure Steam (1135 kPa, saturated, cost or credit) $14.19/GJ

High-Pressure Steam (4237 kPa, saturated, cost or credit) $17.70/GJ

Natural Gas or Fuel Gas (446 kPa, 25°C)
cost $11.00/GJ
credit $9.00/GJ

Electricity $0.06/kWh

Boiler Feed Water (at 549 kPa, 90°C) $2.45/1000 kg
(There is a cost for boiler feed water only if the steam produced enters process streams. If, on the other hand, the steam produced is subsequently condensed, it can be made into steam again. In that case, there is no net cost for boiler feed water.)

Cooling Water $0.354/GJ
available at 516 kPa and 30°C, return pressure ≥ 308 kPa
return temperature should be no more than 15°C above the inlet temperature

Refrigerated Water $4.43/GJ
available at 516 kPa and 5°C, return pressure ≥ 308 kPa
return temperature should be no higher than 15°C

Low-temperature Refrigerant $7.89/GJ
available at -20°C

Very low-temperature Refrigerant $13.11/GJ
available at -50°C

Process (Deionized) Water $0.067/1000 kg
available at desired pressure and 30°C

Waste Water Treatment $56/1000 m^3
based on total volume treated

Raw Material Costs/Product Value

Raw Material or Product	price
syngas	$0.10/kg
ammonia	$500/tonne

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shutdown and maintenance.

Deliverables

Each group must deliver a word-processed report. It should be clear, concise and adhere to the prescribed format. The format is explained in the written report guidelines, provided in a separate document. Reports not adhering to the prescribed format will receive significant deductions and will have to be rewritten. When presenting results for different cases, graphs are superior to tables. The body of the report should be short, emphasizing only the results and explaining why the results presented are optimal. The report appendix should contain details of calculations that are easy to follow. Calculations that cannot be followed easily will lose credit. Computer output without detailed explanations is not appropriate; neatly hand-written calculations are best.

The written report is due on Friday, April 24, 2009, by 3:00 pm. Late reports may be submitted by Monday, April 27, 2009, at the beginning of class, but they will receive an automatic two-letter-grade deduction. There will be oral presentations of project results in CHE 202 class on Monday, April 27, 2009. Oral presentations will continue on April 29, 2009, since we will probably be unable to complete all presentations on April 27, 2009. Oral presentation guidelines will be provided in a separate document. There will be a project review in CHE 230 class on Thursday, April 30, 2009.

Anyone not participating in this project will automatically receive an F for both ChE 202 and ChE 230, regardless of other grades earned in these classes.

Grading

The report grade for each class will be based on the technical content pertinent to that class, which includes the response to questions during the oral presentation (50%); the overall technical content, including that pertinent to the other class (10%); the oral presentation (20%); and the written report (20%). The grades for the oral presentation and written report will include the quality of the writing or the oral presentation and the adherence to the prescribed format. The grades for the oral presentation and written report will be composite grades for the entire team. Therefore, group preparation and feedback are recommended.

The documents on the following web site provide an indication of the expected attributes of a written design report and oral presentation.

http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php

Groups

You will work on this project in groups of 3 or 4. More details of group formation and peer evaluation will be discussed in class.

Revisions

As with any open-ended problem, *i.e.*, a problem with no single correct answer, the problem statement above is deliberately vague. The possibility exists that, as you work on this problem, your questions will require revisions and/or clarifications. You should be aware that these revisions/clarifications may be forthcoming.

References

1. Felder, R. M. and R. W. Rousseau, *Elementary Principles of Chemical Processes (3rd ed.)*, Wiley, New York, 2005.

2. Chemcad Data Base, Chemcad 6.1, Chemstations, Inc., Houston, TX.