Fluid Mechanics, Heat Transfer, Thermodynamics

Design Project

Production of Ammonia

Your assignment is to continue evaluating the details of a process to produce 50,000 tonne/y of ammonia from a syngas feed. This is the amount of ammonia in the product stream, not the total mass of the product stream.

A base-case process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point. Your assignment is to complete the mini-designs described later in this document.

Chemical Reaction

Syngas is available from a pipeline at 1000 kPa and 200°C. It is mixed with a recycle stream, compressed, 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, resulting in partial condensation, producing an ammonia-rich liquid stream. The ammonia liquid product is in Stream 10. Some of Stream 11 is recycled and some is purged.

The reaction that occurs in the reactor is reversible

$$N_2 + 3H_2 = 2NH_3 \tag{1}$$

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

$$K = 3.29 \times 10^{-12} \exp\left[\frac{11{,}806}{T}\right] \tag{2}$$

The units of K are atm^{-2}. In the reactor, there is a 10°C approach to equilibrium.

Process Details

Feed Stream and Effluent Streams

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

Stream 10: ammonia product – 50,000 tonne/y – a year is 8000 hours

Stream 12: purge used as fuel-gas to furnace – there is no credit for this stream

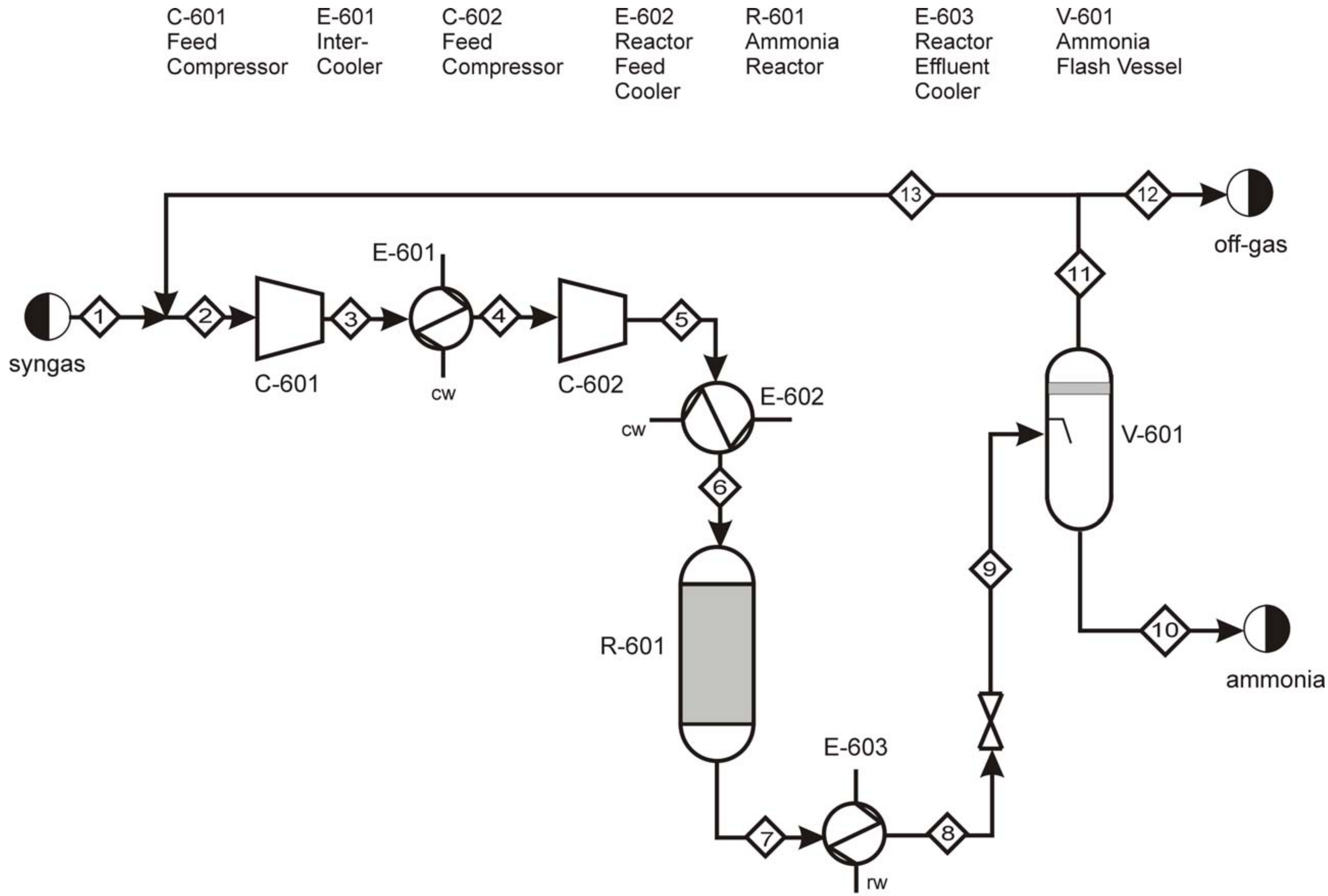

Figure 1: Ammonia Synthesis Loop

Base-Case Equipment Information

Compressors (C-601/C-602)

These compress the feed to a sufficient pressure so that the reactor inlet is at 15,000 kPa. The compressor consists of two stages with identical compression ratios. The compressors are adiabatic with a 65% efficiency.

Heat Exchanger (E-601)

This is an intercooler, cooling the feed stream to 50°C using cooling water. The pressure drop is 35 kPa. Since compressors do not get along well with liquids, both the feed and exit of this heat exchanger must be 100% vapor.

Heat Exchanger (E-602)

This heat exchanger heats or cools the reactor feed to 350°C. The pressure drop is 35 kPa.

Reactor (R-601)

This is an adiabatic, packed bed reactor. The inlet pressure is 15,000 kPa. This reactor should be simulated on Chemcad using the equilibrium reactor module. The pressure unit must be specified as atm. The approach to equilibrium is 10°C, and the pressure drop is 50 kPa.

Heat Exchanger (E-603)

This heat exchanger cools and partially condenses the reactor effluent. The base-case effluent temperature is 15°C, and refrigerated water is used. The pressure drop is 35 kPa. The subsequent valve reduces the pressure entering the flash to 1050 kPa.

Vessel (V-601)

This vessel separates the light gases from ammonia at the conditions of Stream 9. The pressure drop across the vessel is 25 kPa, which allows an additional 25 kPa of pressure drop for the recycle stream. This vessel should be simulated on Chemcad as a flash separator with mode zero. The vapor exits in the top stream, and the liquid exits in the bottom stream. Assume a 10-minute liquid residence time for sizing considerations. This means that the flowrate of the liquid stream exiting in Stream 10 is used to calculate a volume. Then, this volume is doubled to allow space for the vapor to disengage from the liquid. If you need to determine the cost of this vessel, assume it is a vertical vessel. The subsequent recycle/purge ratio is 9/1 in the base case.

Assignment

The assignment consists of the following "mini-designs."

1. Fluid Mechanics and Thermodynamics – (ChE 310 and ChE 320)

Design Problem

You are to optimize the design of the feed section of the process, which includes the feed compressors, the intercooler, and Streams 1-5. The stream conditions should be taken from the base-case simulation performed in Section 5. For exchanger E-601, a detailed design is required (Mini-Design #2). For the optimization portion, heat transfer areas (and subsequently costs) may be estimated using an overall heat transfer coefficient of 60 $W/m^{2\circ}C$.

For the final, detailed design of the heat exchanger (E-601), Mini-Design #2, heat transfer coefficients must be calculated.

The objective function for the optimization should be the Equivalent Annual Operating Cost (*EAOC*, \$/y) for this section only, that is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \tag{2}$$

where *CAP* (\$) is the capital investment for the compressors, the heat exchanger, and the piping, *AOC* (\$/y) is the annual operating cost, which includes utility costs for heat exchanger and compressors, and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{3}$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life).

The costs for the piping components and heat exchanger are given in the Appendix. The optimal pipe diameter and schedule number of each stream, the heat exchanger area, the heat exchanger tube size/pitch, and the compressor duty that minimizes the EAOC must be determined. For streams with no phase change, the pressure drops for each exchanger may be estimated from:

15 kPa for the shell-side fluid if 1 inch 16 BWG tubes at 1.25 in square pitch
35 kPa for the tube-side fluid if 1 inch 16 BWG tubes

For other configurations, the pressure drops can be obtained by the scaling methods illustrated in CHE 310 class.

For E-601, which will be designed in detail, the approximate pressure drops may be used in the calculations to determine optimal pipe diameter. However, in the detailed heat exchanger design, the pressure drops must be calculated using the appropriate relationships.

In order to evaluate the amount and cost of piping required for the mini-design, it may be assumed that C-601, E-601, and C-602 are at grade (ground level). C-601 is located 3 m of equivalent length from the mixing point for Streams 1 and 13 with the mixing point 1 m above grade. The suction line for each compressor is 0.5 m above grade, and the discharge line for each compressor is 1.5 m above grade. The equivalent length of the pipe for Stream 2 is 3 m, the equivalent length of the pipe for Stream 3 is 4 m, the equivalent length of the pipe for Stream 4 is 2 m, and the equivalent length of Stream 5 is 3 m. For this mini-design only, both E-601 and E-602 may be assumed to be horizontal, 1-2 exchangers, with the feed 1.5 m above grade and the discharge 0.5 m above grade

2. Heat Transfer – (ChE 311)

Design of Heat Exchanger, E-601

A detailed design of E-601 is required for base-case conditions. It should be assumed that cooling water is available at the conditions specified in the Appendix of this problem statement. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix to the mini-design.

3. Thermodynamics – (ChE 320)

You are to optimize the flash and recycle system, which includes Streams 8, 9, 11, 12, and 13 along with C-601/602, E-601, and V-601. The objective function for the optimization should be the Equivalent Annual Operating Cost (*EAOC*, \$/y) for this section only, that is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \qquad (2)$$

where *CAP* ($) is the capital investment for the equipment (includes compressors, heat exchangers, vessel, etc.), *AOC* ($/y) is the annual operating cost (includes utility costs for compressor as well as the reactant feed cost), and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \qquad (3)$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life). Optimization variables can include, but are not limited to the vessel pressure and temperature, and the recycle-to-purge ratio. The equipment and raw material costs, product value, and equipment efficiencies are found in the Appendix.

Additionally, the thermodynamics of the ammonia-nitrogen-hydrogen-methane mixture that enters the flash vessel must be modeled accurately. Inaccuracies in the thermodynamics of the vapor-liquid equilibrium of this mixture can lead to inaccurate calculations of the phase separation and the overall cost of the plant. Justify your choice of thermodynamics package based on an examination of the *T-xy* diagrams of the pairs of components at a variety of possible operating pressures.

4. Safety Analysis Report

When designing a chemical process, it is important to know the properties of the chemicals being consumed and produced in the process as well as the impact of any extreme process conditions. There is significant documentation of safety practices in ammonia plants. The purpose of the safety analysis report is to make management aware of risks to personnel due to extreme operating conditions as well as the flammability and toxicity of all chemicals consumed or produced in the process. As a minimum, the MSDS (material and safety data sheets) for all these chemicals should be provided in an appendix, and a brief discussion of the major concerns for each chemical should be given as a separate section of the report. This discussion should include general concerns and concerns that are specific to the operating conditions in this process. In addition, a brief discussion of possible safety hazards for each piece of equipment in your process should be provided. Finally, a feature of your process design that addresses one of these concerns should be explained.

5. Chemcad/Process Improvements

A Chemcad simulation of the base case of the process shown in Figure 1 should be provided. Process improvements that do not violate the laws of physics may be suggested. An explanation of the rationale for such process improvements should be provided, including an economic analysis, if possible. Since there is no reactor cost available at this time, it may be omitted from any economic analysis. Since the reactor is effectively a constant, the optimum is not affected, but the EAOC is off by a constant value.

Other Information

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

Suggested Plan of Attack

The safety analysis can begin as soon as the project is distributed. A good place to find MSDS sheets is http://siri.org. The Chemcad simulation can also be done immediately. Once the Chemcad simulation is done, the heat exchanger can be designed. The fluid mechanics/thermodynamics design and the thermodynamics design can be completed next. The vapor-liquid equilibrium analysis should not be attempted until that material is covered in thermodynamics class.

Deliverables

Written Reports

Each group must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor. The written project reports for all groups, regardless of presentation date, are due by 11:00 a.m. Thursday, December 3, 2009. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *Written Design Reports*. The report must contain a labeled process flow diagram (PFD) and a stream table, each in the appropriate format. The preferred software for preparing PFDs is Corel Draw. A PFD from Chemcad is unacceptable; however, it should be included in the appendix along with a Chemcad report for the base case. Figure 1 should be used as a template for your PFD. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each "mini-project." These may be hand written if done neatly. Alternatively, Excel spreadsheets may be included, but these must be well documented so that the reader can interpret the results. Calculations that cannot be easily followed and that are not explained will lose credit.

Since this project involves "mini-designs," it is suggested that the report be organized as follows. There should be a general abstract, which summarizes the results of your work, emphasizing what you found, not what you did. There should also be an introduction, which orients the reader to the problem. Then, there should be a results section followed by a discussion section for each "mini-design." General conclusion and recommendation sections should follow. At a minimum, there should be one appendix for each of the "mini-designs" with detailed calculations that are clearly written and easy to follow.

In order to evaluate each group member's writing skills, the results and discussion sections for each mini-design should be written by a different group member. The authorship of each of these mini-reports should be clearly specified in the report. Although the individual written portions of the reports must be authored by a single group member, it is the intent of the instructors that group members should help each other in writing different sections. To this end, we recommend that you seek input, such as proofreading and critiques, from other members of your group.

The reports will be evaluated as follows:

- course-specific technical content – 50%
- oral presentation – 20%
- written report – 20%
- technical quality of general sections (safety, simulation, etc.) – 10%

For a more detailed set of evaluation criteria that we will use, see the following web site (design project assessment, oral report assessment, written report assessment):
http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php

Each report will be assessed separately by each of the three instructors. A historical account of what each group did is neither required nor wanted. Results and explanations should be those needed to justify your choices, not a litany of everything that was tried. Each mini-report should be limited to 4-5 double space pages plus figures and tables.

Oral Reports

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak. Each group member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be Thursday, December 3, 2008, from 11:00 a.m. to 2:00 p.m. and on Friday, December 4, 2009, from 11:00 a.m. to 1:00 p.m. Attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the computer room). ***Failure to attend any of the above-required sessions will result in a decrease of one-letter-grade (per occurrence) from your project grade in ChE 310, ChE 311, and ChE 320. Anyone failing to present with his or her group is subject to a minimum one-letter-grade deduction from the project grade.***

Project Review

There will be a project review at 11:00 a.m. on Friday, December 11, 2009. Attendance is expected.

Teams

This project will be completed in teams 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 the project proceeds, questions from the class will require revisions and/or clarifications. It is important to be aware that these revisions/clarifications may be forthcoming.

Appendix
Economic Data

Equipment Costs (Purchased)

Note: The numbers following the attribute are the minimum and maximum values for that attribute. For a piece of equipment with a lower attribute value than the minimum, the minimum attribute value should be used to compute the cost. For a piece of equipment with a larger attribute value, extrapolation is possible, but inaccurate. To err on the side of caution, the price for multiple, identical, smaller pieces of equipment should be used.

Pumps

$$\log_{10}(\text{purchased cost}) = 3.4 + 0.05\log_{10} W + 0.15[\log_{10} W]^2$$

W = power (kW, 1, 300)
assume 80% efficiency

Heat Exchangers

$$\log_{10}(\text{purchased cost}) = 4.6 - 0.8\log_{10} A + 0.3[\log_{10} A]^2$$

A = heat exchange area (m^2, 20, 1000)

Compressors

$$\log_{10}(\text{purchased cost}) = 2.3 + 1.4\log_{10} W - 0.1[\log_{10} W]^2$$

W = power (kW, 450, no limit)
assume 65% efficiency

Compressor Drive

$$\log_{10}(\text{purchased cost}) = 2.5 + 1.4\log_{10} W - 0.18[\log_{10} W]^2$$

W = power (kW, 75, 2600)

Turbine

$$\log_{10}(\text{purchased cost}) = 2.5 + 1.45\log_{10} W - 0.17[\log_{10} W]^2$$

W = power (kW, 100, 4000)
assume 65% efficiency

Fired Heater

$$\log_{10}(\text{purchased cost}) = 3.0 + 0.66\log_{10} Q + 0.02[\log_{10} Q]^2$$

Q = duty (kW, 3000, 100,000)
assume 80% thermal efficiency
assume can be designed to use any organic compound as a fuel

Vertical Vessel

$$\log_{10}(\text{purchased cost}) = 3.5 + 0.45\log_{10} V + 0.11[\log_{10} V]^2$$

V = volume of vessel (m^3, 0.3, 520)

Horizontal Vessel

$$\log_{10}(\text{purchased cost}) = 3.5 + 0.38\log_{10} V + 0.09[\log_{10} V]^2$$

V = volume of vessel (m^3, 0.1, 628)

Storage Tanks

$$\log_{10}(\text{purchased cost}) = 4.85 - 0.397\log_{10} V + 0.145[\log_{10} V]^2$$

V = volume of tank (m^3, 90, 30000)

Additional Cost Information

Piping straight pipe: $\$/m = 5.0$ (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$
sch = schedule number for pipe
use the same schedule number for fittings and valves

Fittings (except valves) $\$/\text{fitting} = 50.0$ (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$

Valves
for gate (isolation) valves $\$100$ (nominal pipe diameter, in)$^{0.8}$ $(1+(\text{sch }\#)/20)^{0.25}$
for control valve use $\$1000$ (nominal pipe diameter, in)$^{0.8}$$(1+(\text{sch }\#)/20)^{0.25}$

Utility Costs

Low-Pressure Steam (618 kPa saturated)	$13.28/GJ
Medium-Pressure Steam (1135 kPa saturated)	$14.19/GJ
High-Pressure Steam (4237 kPa saturated)	$17.70/GJ
Natural Gas (446 kPa, 25°C)	$11.00/GJ
Fuel Gas Credit	none, but there is no treatment cost
Electricity	$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	$2.45/1000 kg
Cooling Water	$0.354/GJ

Cooling Water
available at 516 kPa and 30°C
return pressure ≥ 308 kPa
return temperature is no more than 15°C above the inlet temperature

Refrigerated Water $4.43/GJ
available at 516 kPa and 10°C
return pressure ≥ 308 kPa
return temperature is no higher than 20°C

Deionized Water $1.00/1000 kg
available at 5 bar and 30°C

Waste Treatment of Off-Gas incinerated – zero cost

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

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

Wastewater Treatment — $56/1000 m^3

Raw Material Costs/Product Value

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

Equipment Cost Factors

Total Installed Cost = Purchased Cost (4 + material factor (MF) + pressure factor (PF))

Pressure (absolute)
- < 10 atm, PF = 0.0
- 10 - 20 atm, PF = 0.6
- 20 - 40 atm, PF = 3.0
- 40 - 50 atm, PR = 5.0
- 50 - 100 atm, PF = 10
- 100 - 200 atm, PF = 25

does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects

Carbon Steel MF = 0.0
Stainless Steel MF = 4.0