ChE 455
Fall 2008
Major 1

Ammonia Production

Background

You work for a consulting company that has been hired to evaluate the design of an ammonia synthesis loop designed by an in-house group at your client's small facility. You are only to evaluate the ammonia synthesis portion of a much larger process that takes coal, converts it into a synthesis gas (syngas), adjusts the composition of the syngas, and produces ammonia. Ammonia is one of the five most produced chemicals in the industry. It is a raw material for nitrogen oxides and fertilizers, among others. The process in question is to produce 50,000 tonne/y of ammonia in an 8000-hour year.

Ammonia Production

Unit 600 produces ammonia from syngas, which consists of nitrogen, hydrogen, methane, and trace amounts of carbon dioxide. Figure 1 illustrates the design developed internally by your client. Tables 1 and 2 are the stream tables and utility summary, respectively. Table 3 is a partial equipment summary.

In the design, the syngas feed is assumed to have been pretreated to yield stoichiometric amounts of nitrogen and hydrogen. In the pretreatment, oxygen-containing compounds like CO_2 must be removed, because amounts above 10 ppm in the reactor poison the catalyst. One method for accomplishing this is by methanation, hence the small amounts of methane in the feed syngas. The syngas is compressed, mixed with the recycle stream and the temperature brought to 350°C. The reactor is a shell-and-tube design. Because ammonia production is highly exothermic, heat is removed using a Dowtherm™ A circulation loop. The reaction is equilibrium limited, and it is assumed that the temperature approach to equilibrium is 20°C. The catalyst brings the reaction to this point rapidly. The reaction and equilibrium constant are:

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

$$K = \frac{p_{NH_3}^2}{p_{N_2} p_{H_2}^3} = 3.29 \times 10^{-12} \exp\left[\frac{11806}{T}\right] \tag{2}$$

where the units of K are atm^{-2} and T is in Kelvin. The reactor effluent is cooled and flashed, producing ammonia and light gases. A fraction of the light gases goes to a purge stream, and the remaining light gases are compressed and recycled.

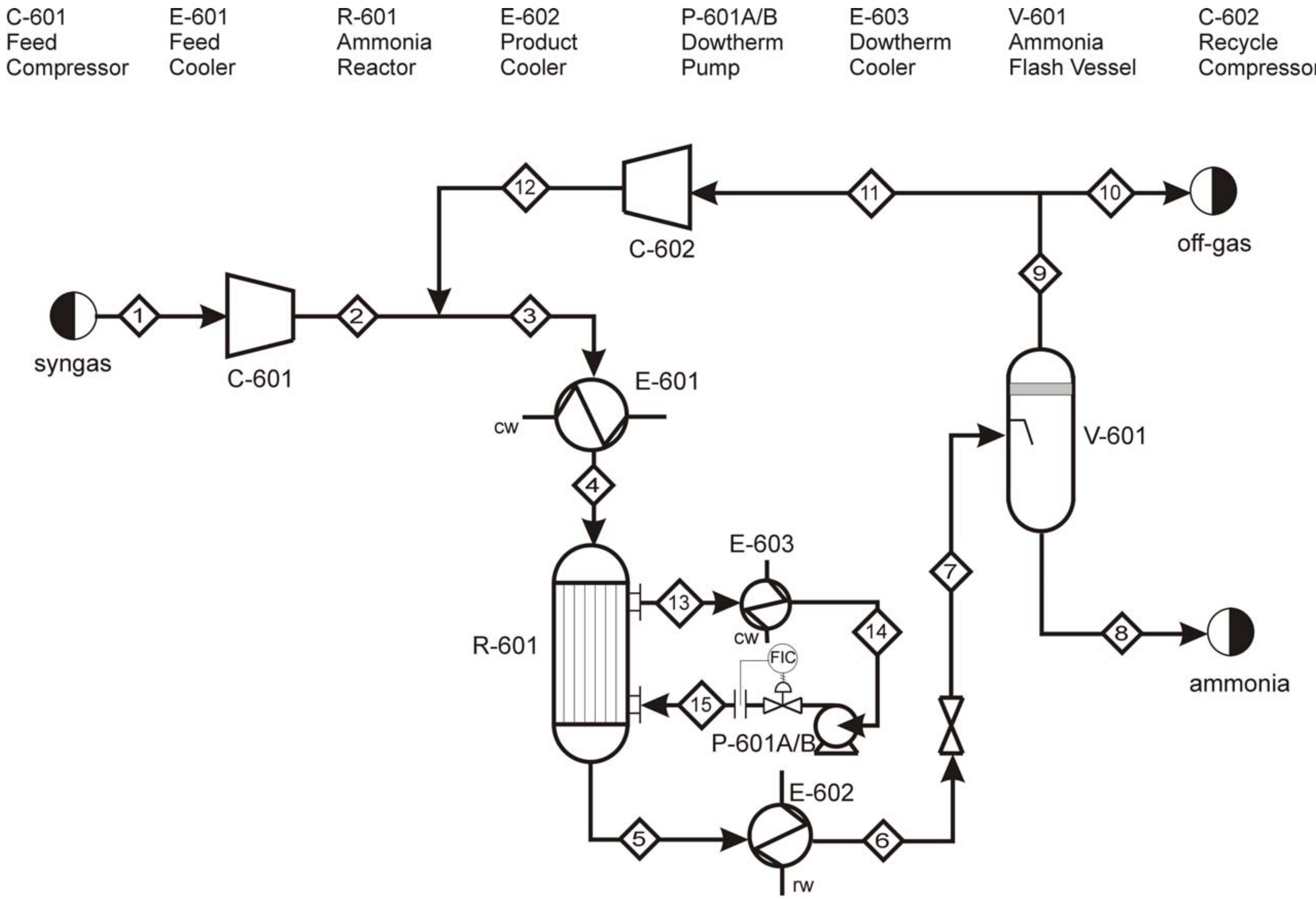


Figure 1: Ammonia Synthesis Loop

Table 1
Stream Table for Unit 600

Stream No	1	2	3	4
Temp °C	200	985.42	574.99	350
Pres kPa	1000	15000	15000	14965
Vapor fraction	1	1	1	1
Total kg/h	13025.36	13025.36	78814.08	78814.08
Total kmol/h	1500.00	1500.00	7973.84	7973.84
Component kmol/h				
nitrogen	366.63	366.63	1663.12	1663.12
hydrogen	1099.88	1099.88	4990.03	4990.03
carbon dioxide	0.0084	0.0084	0.076	0.076
methane	33.48	33.48	334.16	334.16
ammonia	0	0	986.45	986.45

Stream No.	5	6	7	8
Temp °C	350	15	-38.79	-38.79
Pres kPa	14915	14880	500	500
Vapor fraction	1	0.81	0.93	0
Total kg/h	78814.08	78814.08	78814.08	5715.42
Total kmol/h	7528.76	7528.76	7528.76	335.59
Component kmol/h				
nitrogen	1440.58	1440.58	1440.58	0.033
hydrogen	4322.42	4322.42	4322.42	0.023
carbon dioxide	0.076	0.076	0.076	0.0009
methane	334.16	334.16	334.16	0.0697
ammonia	1431.52	1431.52	1431.52	335.47

Stream No.	9	10	11	12
Temp °C	-38.79	-38.79	-38.79	488.54
Pres kPa	500	500	500	15000
Vapor fraction	1	1	1	1
Total kg/h	73098.78	7309.88	65788.90	65788.90
Total kmol/h	7193.17	719.32	6473.85	6473.85
Component kmol/h				
nitrogen	1440.55	144.06	1296.50	1296.50
hydrogen	4322.50	432.24	3890.15	3890.15
carbon dioxide	0.075	0.0075	0.067	0.067
methane	334.09	33.41	300.69	300.69
ammonia	1096.06	109.61	986.45	986.45

Table 1
Stream Table for Unit 600
(continued)

Stream No.	13	14	15
Temp °C	300	250	300
Pres kPa	960	925	1000
Vapor fraction	0	0	0
Total Dowtherm A kg/h	1.893×10^{5}	1.893×10^{5}	1.893×10^{5}

Table 2
Utility Stream Flow Summary for Unit 600

E-601	**E-602**	**E-603**
cw	cw	cw
1.46×10^{6} kg/h	2.43×10^{6} kg/h	5.65×10^{5} kg/h

Table 3
Partial Equipment Summary

Heat Exchangers

E-601 A = 716.0 m^2 1-2 exchanger, floating head, carbon steel process stream in shell Q = 61,030 MJ/h maximum pressure rating of 15,000 kPa	**E-603** A = 45.73 m^2 1-2 exchanger, floating head, carbon steel Dowtherm in tubes Q = 23651 MJ/h maximum pressure rating of 2000 kPa
E-602 A = 758.8 m^2 1-2 exchanger, floating head, carbon steel process stream in shell Q = 101,661 MJ/h maximum pressure rating of 15,000 kPa	

Reactors

R-601 – Heat Exchanger Portion Q = 23651 MJ/h A = 661.9 m^2 counterflow exchanger, floating head, carbon steel process stream in tubes maximum pressure rating of 15,000 kPa	**R-601 – Reactor Portion** catalyst in tubes promoted Ru catalyst on graphite support

Pumps and Compressors

C-601 carbon steel power = 10.33 MW 65% efficient	**P-601 A/B** carbon steel power = 18.96 kW 80% efficient
C-602 carbon steel power = 30.74 MW 65% efficient	

Vessels

V-601 carbon steel height = 4.5 m diameter = 0.9 m maximum pressure rating of 1000 kPa

For additional information on ammonia production, consult the literature. Some possibilities are suggested.[1,2] It is highly recommended that you read about ammonia production before proceeding with this assignment.

Many chemical prices are available at http://www.icis.com/StaticPages/a-e.htm. The value of syngas is $0.10/kg.

Assignment

Your assignment is to evaluate the in-house design, identify problems or errors, if any, that you find, and suggest solutions for these problems. Since the custom-made equipment has already been ordered, solutions to problems that retain as much of this equipment as is possible are desired. You should also recommend any other changes that you feel should be made to improve performance in Unit 600.

Specifically, you are to prepare the following by 9:00 a.m., Monday, November 3, 2008:

1. a written report detailing your evaluation of the present design, recommended modifications (if any), and incremental costs (savings) associated with your recommended modifications. This should include:

    a. an explanation of any errors found in the design of Unit 600.

    b. an explanation and justification for any improvements your recommend to the design of Unit 600.

    c. an incremental economic evaluation (before-tax EAOC at an interest rate of 15%, 10 year lifetime) of the recommended modifications.

    d. a PFD, stream table, utility table, and equipment list for the modified process, if the process is indeed modified. If there are modifications, the report should contain a list of new equipment to be purchased, including size, cost, and materials of construction

Deliverables

Specifically, following is to be completed by 9:00 a.m., Monday, November 3, 2008:

1. Prepare a written report, conforming to the guidelines, detailing the information in items 1, 2, and 3, above.

2. Include a legible, organized set of calculations justifying your recommendations, including any assumptions made.

3. Attach a signed copy of the attached confidentiality statement.

Report Format

This report should be brief and should conform to the guidelines, which are available at the end of the following web page http://www.che.cemr.wvu.edu/publications/projects/index.php. It should be bound in a folder that is not oversized relative to the number of pages in the report. Figures and tables should be included as appropriate. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. The confidentiality statement should be the very last page of the report.

The written report is a very important part of the assignment. Reports that do not conform to the guidelines will receive severe deductions and will have to be rewritten to receive credit. Poorly written and/or organized written reports may also require re-writing. Be sure to follow the format outlined in the guidelines for written reports.

Oral Presentation

You will be expected to present and defend your results some time between November 3, 2008 and November 6, 2008. Your presentation should be 15-20 minutes, followed by about a 30-minute question and answer period. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring at least one hard copy of your slides to the presentation and hand it out before beginning the presentation.

Other Rules

You may not discuss this major with anyone other than the instructor. Discussion, collaboration, or any interaction with anyone other than the instructor is prohibited. This means that any cross talk among students about anything relating to this assignment, no matter how insignificant it may seem to you, is a violation of the rules and is considered academic dishonesty. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (see p. 48 of 2007-09 Undergraduate Catalog or follow the link http://www.arc.wvu.edu/rightsa.html).

Consulting is available from the instructor. Chemcad consulting, *i.e.*, questions on how to use Chemcad, not how to interpret results, is unlimited and free, but only from the instructor. Each individual may receive five free minutes of consulting from the instructor. After five minutes of consulting, the rate is 2.5 points deducted for 15 minutes or any fraction of 15 minutes, on a cumulative basis. The initial 15-minute period includes the 5 minutes of free consulting.

Late Reports

Late reports are unacceptable. The following severe penalties will apply:

- late report on due date before noon: one letter grade (10 points)
- late report after noon on due date: two letter grades (20 points)
- late report one day late: three letter grades (30 points)
- each additional day late: 10 additional points per day

References

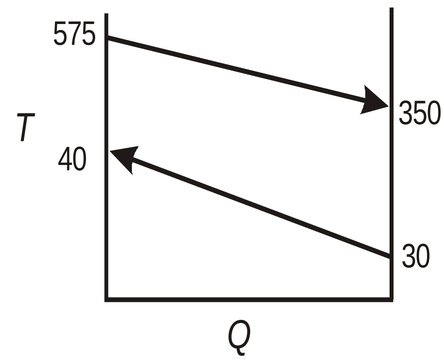
1. Eggeman, T., "Ammonia," *Kirk-Othmer Encyclopedia of Chemical Technology*, on-line version, 10/18/2001. (This encyclopedia is accessible from any University computer at http://www.libraries.wvu.edu/databases. An older print version is available in the Evansdale Library reference section.)

2. Quartulli, Orlando J., William Turner, and Keith W. Padgett, "Ammonia," in *Encyclopedia of Chemical Processing and Design*, (J. J. McKetta, ed.), Marcel Dekker, New York, vol. 3, 256-278 (1977). (This collection is available in the reference section of the Evansdale Library, first floor, back and to the right.)

Appendix
Calculations and Other Pertinent Information

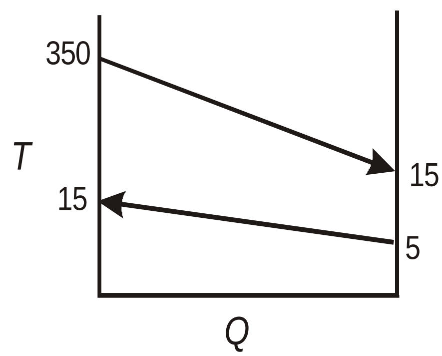
E-601

$Q = 61030 \times 10^6$ J/h
process fluid in shell
cw $h_i = 1000$ W/m^{2}K
process stream $h_o = 60$ W/m^{2}K
$U \approx (1/h_i + 1/h_o)^{-1} = 56.6$ W/m^{2}K
$\Delta T_{lm} = 418.33$°C
$A = 716.0$ m^2
$Q = \dot{m}Cp\Delta T = \dot{m}$ (4.184 kJ/kg°C)(10°C)
$\dot{m} = 1.46 \times 10^6$ kg/h



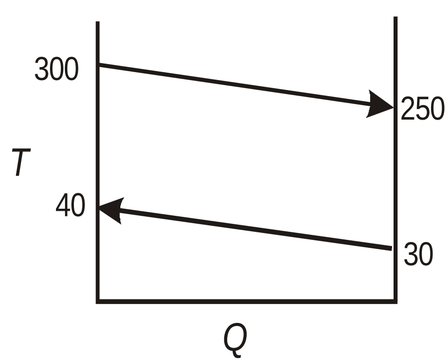
E-602

$Q = 101661 \times 10^6$ J/h
process fluid in shell
cw $h_i = 1000$ W/m^{2}K
process stream partial condensation $h_o = 1000$ W/m^{2}K
$U \approx (1/h_i + 1/h_o)^{-1} = 500$ W/m^{2}K
$\Delta T_{lm} = 87.36$°C
$A = 758.8$ m^2
$F = 0.852$
$Q = \dot{m}Cp\Delta T = \dot{m}$ (4.184 kJ/kg°C)(10°C)
$\dot{m} = 2.43 \times 10^6$ kg/h
assume T-Q diagram at right is approximately true for partial condensation

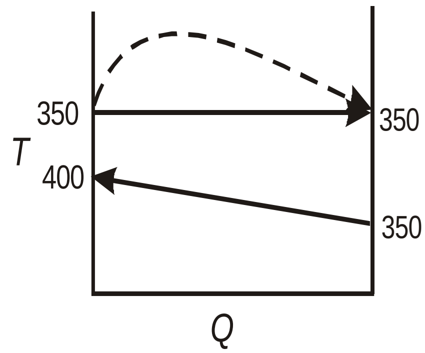


E-603

$Q = 23651 \times 10^6$ J/h
Dowtherm fluid in tubes
Dowtherm $h_i = 1500$ W/m^{2}K
cw $h_o = 1000$ W/m^{2}K
$U \approx (1/h_i + 1/h_o)^{-1} = 600$ W/m^{2}K
$\Delta T_{lm} = 239.44.6$°C
$A = 45.73$ m^2
$Q = \dot{m}Cp\Delta T = \dot{m}$ (4.184 kJ/kg°C)(10°C)
$\dot{m} = 5.65 \times 10^5$ kg/h



R-601 heat exchanger



Q = 23651×10^6 J/h
ΔT_{lm} = 71.135°C
assumes straight line – really get hot spot
this is conservative calculation since ΔT_{lm} is really larger as the T-Q diagram to the right shows
Dowtherm in shell h_o = 2000 W/m^{2}K
reaction stream h_i = 150 W/m^{2}K
$U \approx (1/h_i + 1/h_o)^{-1}$ = 139.53 W/m^{2}K
A = 661.9 m^2
C_p = 2.5 kJ/kg°C for Dowtherm
$\dot{m}_{DT} = Q / C_p \Delta T = Q / [(2.5 \text{ kJ/kg°C})(50°C)]$
$\dot{m}_{DT}$ = 1.893×10^5 kg/h
$\rho \approx$ 1000 kg/m^3 for Dowtherm

V-601

assume 10 min residence time for liquid
assume liquid is half of total volume
from Chemcad:
liquid flowrate in Stream 8 = 8.7427 m^3/h
(8.7427 m^3/h)(h/60 min)(10 min)=1.457 m^3
double volume to 2.915 m^3
2.915 m^3 = $\pi d^2 h/4$
assume $h = 5d$
$d \approx$ 0.9 m
$h \approx$ 4.5 m

P-601 A/B and Loop

all pipe is 3 in schedule 40
d_i = 0.07792 m
A = 0.004769 m^2
10 m equivalent pipe length
4 m elevation change from reactor exit to reactor entrance (Dowtherm out top, in bottom)
choose 75 kPa pressure rise across pump
keep Dowtherm pressurized to reduce volatility and avoid cavitation
pressure out of reactor = 960 kPa
pressure out E-603 = 925 kPa
pressure out of pump 1000 kPa
Dowtherm properties:
C_p = 2.5 kJ/kg°C
ρ = 997 kg/m^3
μ = 0.3 cP

Dowtherm in enters reactor at 250°C, Dowtherm exits reactor at 300°C
for reactor heat exchanger $Q = 2.365\times10^{10}$ J/h = 2.5 J/g°C (50°C) $\dot{m}_{Dowtherm}$

$\dot{m}_{Dowtherm} = 1.893\times10^{5}$ kg/h

$v = \dot{m}_{Dowtherm}/\rho A = 11.0$ m/s

commercial steel pipe $\varepsilon/d = 0.0059$

Re = $dv\rho/\mu = 2.87\times10^{6}$

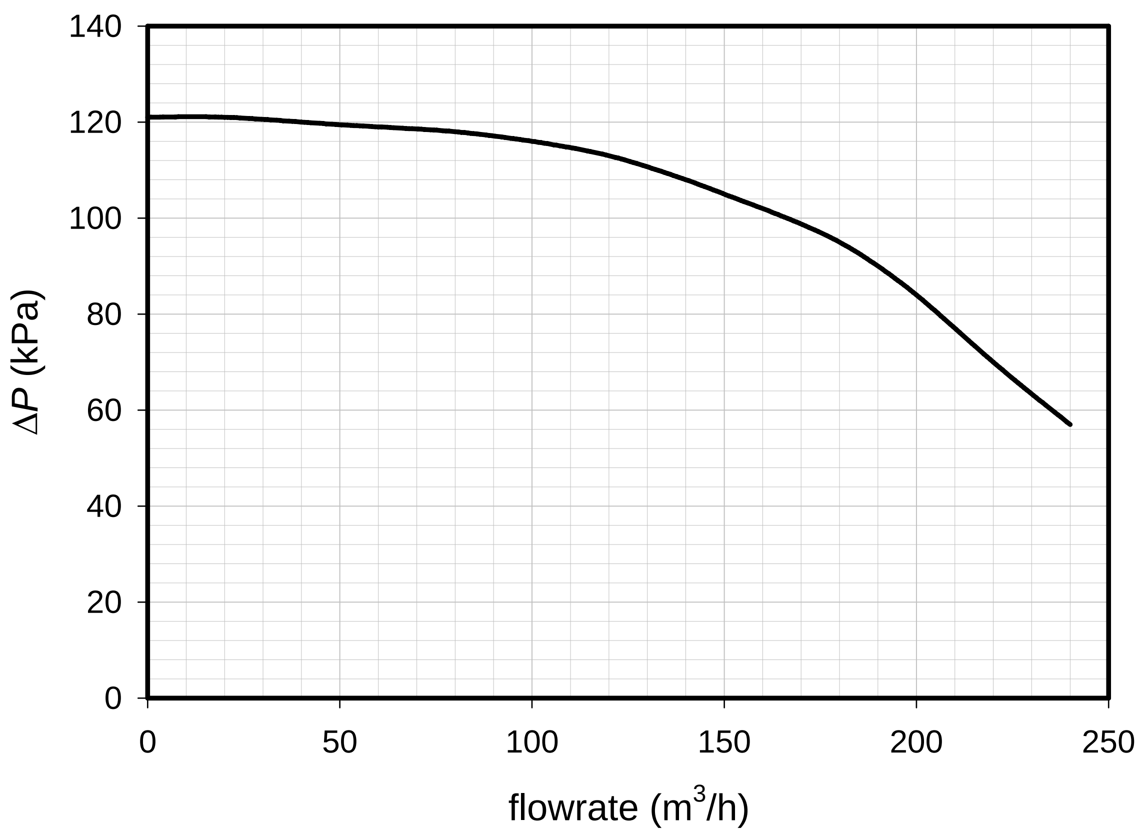
from Pavlov equation: $f = 0.0080$

mechanical energy balance

$$\frac{75000}{997} + 9.81(-4) + \frac{2(10)(0.0080)(11.0)^2}{0.07792} - 0.8W_s = 0$$

$W_s = 356$ J/kg

$\dot{W}_s = 18.96$ kW



Pump Curve for P-601 A/B

Equation for pump curve: $\Delta P(\text{kPa}) = 121.1 - 0.02838\dot{v} + 0.0003209\dot{v}^2 - 0.000005536\dot{v}^3$