Fluid Mechanics, Heat Transfer, Thermodynamics
Design Project

Production of Ethylbenzene

We continue to investigate the feasibility of constructing a new, grass-roots, 80,000 tonne/y, ethylbenzene facility. As part of the feasibility study, we would like you to investigate some of the details of the proposed plant and of the thermodynamics of the components involved in the process.

Chemical Reaction

The production of EB takes place via the direct addition reaction between ethylene and benzene:

$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethyl benzene}}{C_6H_5C_2H_5} \qquad (1)$$

The reaction between ethylbenzene and ethylene to produce di-ethylbenzene may also take place:

$$\underset{\text{ethyl benzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethyl benzene}}{C_6H_4(C_2H_5)_2} \qquad (2)$$

and additional reactions between di-ethylbenzene and ethylene yielding tri- and higher ethyl benzene are also possible. However, for this project, you may assume that the reaction in Equation (1) is the only reaction that occurs as long as the molar ratio of benzene to ethylene is kept high, at approximately 8:1.

Process Description

The PFD for the process is given in Figure 1. It should be used as a starting point for this assignment.

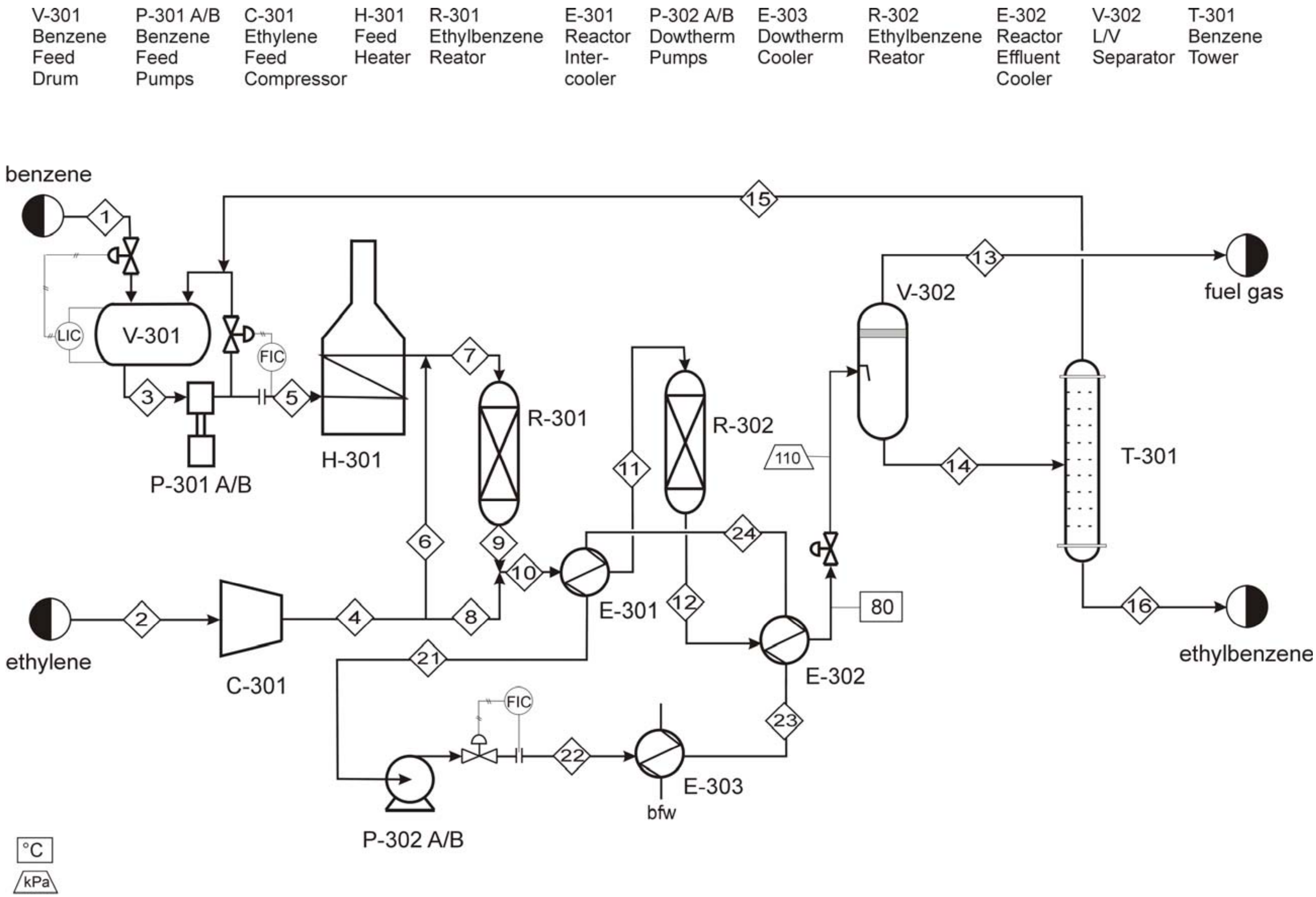

Figure 1: Unit 300 - Ethylbenzene Production Facility

Process Details

Feed Stream and Effluent Streams

Stream 1: benzene feed at 25°C and 110 kPa

Stream 2: ethylene feed at 25°C and 200 kPa, is split so that the benzene to ethylene ratio entering both reactors is fixed at 8/1. The feed contains 5 mol% ethane impurity.

Stream 5: fired heater feed at 2000 kPa

Stream 7: R-301 feed at 380°C, same temperature for R-302 feed, benzene/ethylene ratio at 8/1 for both reactors

Stream 13: fuel gas effluent stream

Stream 16: ethylbenzene product

Equipment

Ethylene Compressor (C-301)

The compressor increases the pressure of the feed ethylene from 200 kPa to 2000 kPa. The compressor may be assumed to be adiabatic with an efficiency of 75%. It may be necessary to use staged compressors with intercooling.

Benzene Feed Mixing Vessel (V-301)

provides reservoir of liquid for feed pump

Pump (P-301 A/B, includes spare pump)

pumps feed benzene to 2025 kPa

Feed Heater – a fired heater (H-301)

effluent at 2000 kPa

Reactors (R-301 and R-302)

adiabatic reactors, conversion in each reactor is 98%, pressure drop of 15 kPa

Heat Exchangers (E301 and E-302)

pressure drop of 25 kPa on the process side

Flash Vessel (V-302)

This flash vessel provides for a one-stage flash separation of the light components from the heavy components. It has a maximum operating pressure of 250 kPa. The base-case conditions are 80°C and 110 kPa.

Distillation Column (T-301)

99.9 % of the benzene enters Stream 15. 99 % of ethylbenzene enters Stream 16, operates at 110 kPa with Stream 15 at the saturation temperature of benzene at 110 kPa and with Stream 16 at the saturation temperature of ethylbenzene at 110 kPa.

Assignment

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

1. Fluid Mechanics and Heat Transfer

The purpose of this design project is to design and evaluate the performance of the cooling loop consisting of E-301, E-302, E-303 and pump, P-302. The purpose of this loop is to circulate a stream of coolant (Dowtherm™ A) through the reactor intercooler and reactor effluent cooler and to use the energy to make steam in the Dowtherm™ cooler. The stream leaving the pump is fed into the Dowtherm™ cooler and then may be fed either through the three exchangers in series, as shown in Figure 1, or split between the two coolers, E-301 and E-302 and then recombined prior to entering the pump. The properties of Dowtherm™ A are available from ChemCAD. In order, to avoid degrading the Dowtherm™ A, its maximum temperature should never exceed 400°C anywhere in the loop. Any steam produced in E-303 may be sold for profit, the values for the different pressure levels of steam are given in Appendix 1.

<u>Process Fluid Mechanics, ChE 310 Assignment</u>

<u>Design Problem</u>

You are to optimize the design of the heating loop in conjunction with the heat transfer assignment. The amount of heat to be removed from the process streams in E-301 and E-302 must be determined from a ChemCAD simulation using the base-case conditions given in this assignment. For exchanger E-301, a detailed design is required and the required details are given in the heat transfer assignment. For the two other exchangers, you may estimate their heat transfer areas (and subsequently their costs) using the following overall heat transfer coefficients:

Liquid-liquid = 300 W/m^2°C
Boiling liquid-liquid = 500 W/m^2°C
Gas-liquid = 80 W/m^2°C
Condensing gas-liquid = 400 W/m^2°C

You should remember that these exchangers may have several zones and that multiple overall coefficients may have to be applied for a given exchanger.

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

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC - R \tag{3}$$

where *CAP* is the capital investment for all the equipment (\$), *AOC* (\$/y) is the annual operating cost, *R* (\$/y) is any revenue produced from the selling of steam, and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{4}$$

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

The cost for the pump, piping components, controls, and exchangers are given in Appendix 1. You are to determine the optimal pipe diameter (and pipe schedule) that minimizes the EAOC. The pressure drops for each exchanger may be estimated as:

2 psi for the shell-side fluid
5 psi for the tube-side fluid

For E-301, which you will design in detail, you may use the above approximate pressure drops in the calculations to determine optimal pipe diameter. However, in the heat exchanger design, you should evaluate the pressure drops in E-301 using the appropriate relationships.

In order to evaluate the amount of piping required for the loop, you should sketch a piping isometric showing the location of all equipment and all the appropriate pipe fittings. You may assume that all the exchangers are located 10 ft above grade (ground level), and that the pump is located at grade with the inlet 1 ft above grade and the outlet 2 ft above grade. The pump will be installed in parallel with a spare and the piping arrangement should be similar to the one shown in the piping isometric given in ChE 310. Assume that the three exchangers are arranged in a horizontal row with approximately 12 ft between each exchanger and that the pump(s) are located within 15 ft of the row of exchangers. A plot plan (looking vertically down on the loop) and an elevation diagram (looking at a side view) are given in Figure 2.

The location and sizes of the equipment in Figure 2 are approximate since the design of the equipment has not yet been performed. However, you may use these diagrams to estimate the length of pipe and the number and types of pipe fittings required for the Dowtherm™ loop. You should assume that for good control, the pressure drop across the control valve should equal 1/3 of the total frictional losses through the loop **<u>or</u>** 5 psi, whichever is the larger value.

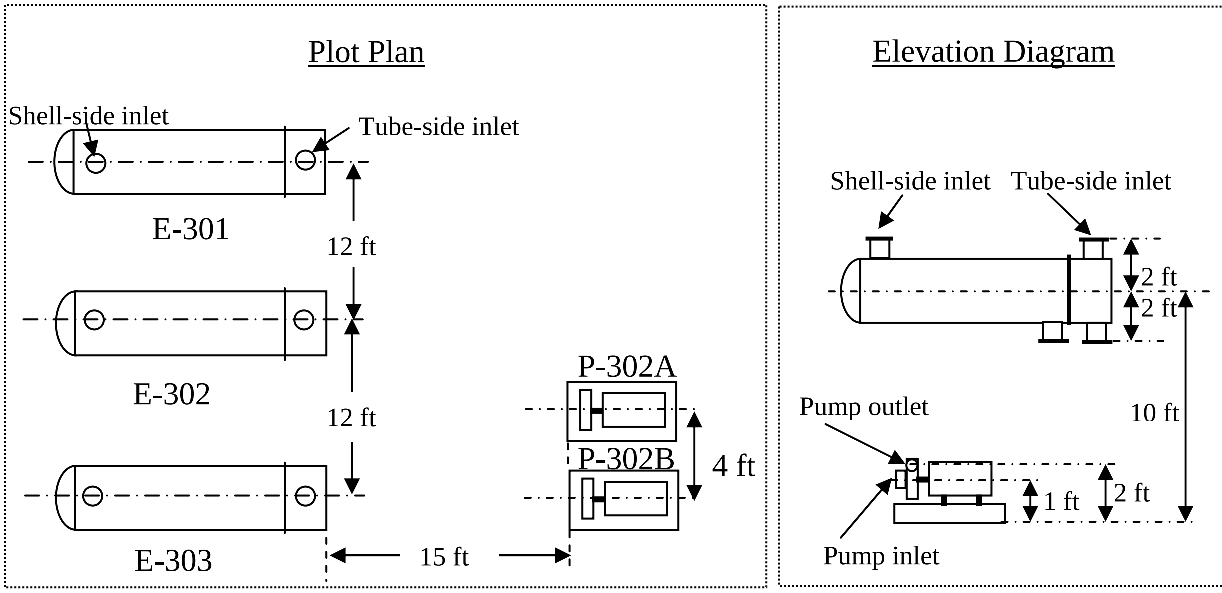

Figure 2: Preliminary plot and elevation diagrams for the equipment in the Dowtherm™ loop.

Performance Problem

Once you have designed and optimized the Dowtherm™ loop, you should determine the maximum heat transfer removal (from E-301 and E-302) possible for the system that you have designed. This will correspond to having the control valve wide open and the pumps running either in parallel or series (the better configuration will depend on your design). The pump characteristics for a typical centrifugal pump are given in Equations (5) and (6)

$$\frac{P}{P_{design}} = 1.1 - 0.1\left[\frac{Q}{Q_{design}}\right]^{7.1265} \tag{5}$$

$$NPSH_R(\text{m of liquid at pump inlet conditions}) = 5 + 2\left(\frac{Q}{Q_{design}}\right)^2 \tag{6}$$

where P_{design} is the pressure increase developed across the pump at the design flowrate, Q_{design}. For this problem, you should calculate the new exit temperatures of the Dowtherm™ as it passes through each heat exchanger and determine the additional heat transfer that occurs in each heat exchanger.

<u>Process Heat Transfer, ChE 311 Assignment</u>

<u>Design of Heat Exchanger, E-301</u>

You should perform a detailed design of E-301. You should assume that utilities are available at the conditions specified in Appendix 1 of this problem statement. For this heat-exchanger design, you should report the following information, as needed for the design:

- 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 and their arrangement (spacing, pitch, type)
- Diameter, 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-project.

2. Thermodynamics – Optimization of the Ethylene Feed Compressor (ChE 320)

You should minimize the equivalent annual operating cost, *EAOC*, for the compressor section of the process with the following in mind:

- The ethylene feed should be taken from the inlet conditions (200 kPa and 25°C) and compressed.

The optimization for this mini-project should include the cost of the compressors, the cost of heat exchangers, the cost of cooling water, and the cost of electricity. Raw material costs should not be included, so *CAP* (the capital investment for equipment used in the equation for *EAOC* given in Equation 3) includes only the installed cost of compressor stages and heat exchangers, and annual operating costs include the electricity to run the compressor stages and the cost of cooling water in the intercoolers, if used. Note that there is no revenue term for this mini-design.

The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC $/y) of the piping system including the compressor. The *EAOC* was defined in Equations 3 and 4.

3. 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. The reactivity and toxicity of the reactants and products will not only affect the design but will also affect the procedures that might be implemented during an unscheduled event such as an emergency shutdown. The purpose of the safety analysis report is to make management aware of risks to personnel due to 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 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.

4. Chemcad/Process Improvements

A Chemcad simulation of one case of the process shown in Figure 1 should be provided. It is your choice whether this is a base case or a final case. You may suggest any process improvements that do not violate the laws of physics. An explanation of the rationale for such process improvements should be provided, including an economic analysis, if possible.

Other Information

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

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 are due by 11:00 a.m. Thursday, November 30, 2006. 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 PFDs from Chemcad are generally unsuitable unless you modify them significantly. 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 and introduction. 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."

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%

A historical account of what each group did is neither required nor wanted. Results and explanations should be what are 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 November 30, 2006, from 11:00 a.m. to 2:00 pm. 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***.

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.

Appendix 1
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, use the minimum attribute value 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, you should use the price for multiple, identical smaller pieces of equipment.

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 70% 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)

Additional Cost Information

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

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

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

Utility Costs

Low-Pressure Steam (618 kPa saturated)	$7.78/GJ
Medium-Pressure Steam (1135 kPa saturated)	$8.22/GJ
High-Pressure Steam (4237 kPa saturated)	$9.83/GJ
Natural Gas (446 kPa, 25°C)	$6.00/GJ
Fuel Gas Credit	$5.00/GJ
Electricity	$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	$2.45/1000 kg
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	$0.354/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	$4.43/GJ
Deionized Water available at 5 bar and 30°C	$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	$7.89/GJ
Wastewater Treatment	$56/1000 m^3

Equipment Cost Factors

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

Pressure	< 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
(absolute)	10 - 20 atm, PF = 0.6	
	20 - 40 atm, PF = 3.0	
	40 - 50 atm, PR = 5.0	
	50 - 100 atm, PF = 10	

Carbon Steel MF = 0.0
Stainless Steel MF = 4.0