Fluid Mechanics, Heat Transfer, Thermodynamics
Design Project

Production of Diethyl Ether

The feasibility of constructing a new, grass-roots, 50,000 tonne/y, diethyl ether plant is being investigated. As part of the feasibility study, some of the details of the proposed plant must be analyzed.

Diethyl Ether Production Reactions

For this analysis, it may be assumed that the only reactions occurring are

$$2C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O \quad (1)$$

ethanol DEE

$$C_2H_5OH \rightarrow C_2H_4 + H_2O \quad (2)$$

ethanol ethylene

For the purposes of this preliminary evaluation, it is assumed that the reaction occurs in an adiabatic packed bed of particles containing high-purity γ-alumina catalyst.

Feed and Reaction Sections

The PFD for the feed and reaction sections is given in Figure 1. The feed to the process is liquid ethanol at 25°C and 1 atm.

The reaction is exothermic, and the reactor is adiabatic. The reactor feed must be 200°C and 1215 kPa. Following the reactor, the reaction products are cooled to 37°C, the three-phase flash conditions. In the three-phase flash, ethylene is separated from the organics, but the liquid forms two, immiscible phases, which are fed to two different locations in the diethyl ether column. Diethyl ether and some remaining ethylene are separated in the first distillation column, which may be assumed to be a perfect separator for this semester's project only. Ethanol and water are separated in the second distillation column. The ethanol is recycled and the wastewater stream must is cooled to 35°C to be sent to waste treatment.

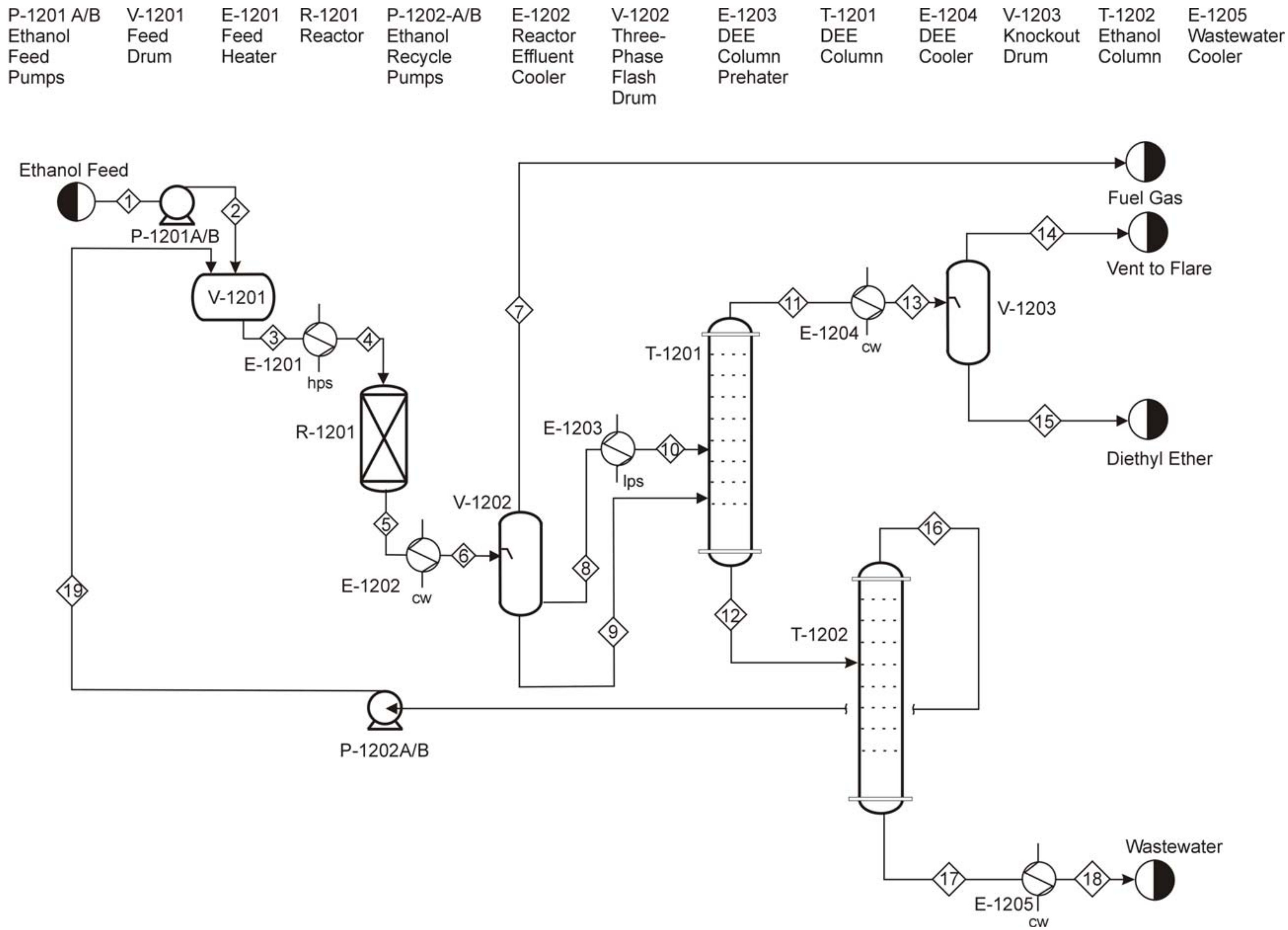

Figure 1: Unit 1200 – Diethyl Ether Production Process

Process Details

Feed Stream

Stream 1: ethanol liquid at 1 atm, 25°C – contains 70 mol% ethanol, 30 mol% water

Effluent Streams

Stream 7: ethylene waste – it can be burned for credit at its LHV

Stream 14: ethylene waste – it can be burned for credit at its LHV

Stream 15: diethyl ether product – must have < 0.1 mol% ethylene

Stream 18: Wastewater stream to treatment – must be at 35°C

Equipment Summary

P-1201 A/B: Ethanol feed pumps – outlet pressure of at least 1260 kPa

V-1201: Feed drum – liquid level may vary but output remains constant – assume 10 kPa pressure drop

E-1201: Feed preheater – reactor feed must be vapor at a minimum of 1215 kPa and 200°C – assume 35 kPa pressure drop

R-1201: Reactor – adiabatic – assume to have a pressure drop of 50 kPa – the fractional conversion of ethanol is 0.8 – the selectivity of the desired reaction to the undesired reaction is 80 moles DEE formed/mole ethylene formed – this must be simulated using a stoichiometric reactor, which only accepts one reaction – a single, overall reaction must be developed based on the stoichiometry, conversion, and selectivity

E-1202: Product cooler – cools reactor outlet stream to 40°C – assume 35 kPa pressure drop

V-1202: Three-phase flash separator with outlet operating at a minimum of 1120 kPa and a minimum of 40°C, as long as multiple phases exists – produces an organic-water-gas three-phase mixture that is assumed to separate easily into three distinct streams – the VLL option must be chosen in the thermodynamics menu screen so the presence of two liquid phases is calculated correctly

E-1203: Heats column feed to 80°C – 35 kPa pressure drop

T-1201: Distillation column – to produce diethyl ether product and ethanol for recycle – the component separator in Chemcad should be used – a perfect separator may be assumed (which is physically impossible) for this semester only, *i.e.*, all diethyl ether and ethylene to the top and all ethanol and water to the bottom – the column operates at 175 kPa, with a top temperature of 46°C and a bottom temperature of 97°C

In a real distillation column, there can be feeds at different locations. This will be discussed next semester. However, the component separator in Chemcad only accepts one feed stream. Therefore, for this semester only, Streams 9 and 10 are to be mixed before entering the component separator. This would never occur in a realistic situation, because it makes no sense to mix streams that are already partially separated only to separate them again. While this is being done for the Chemcad simulation, the PFD should show the more realistic physical situation.

T-1202: Distillation column – to separate ethanol for recycle from wastewater – the component separator in Chemcad should be used – 99.75% of the ethanol and 9.4% of the water entering T-1202 return in the recycle stream – cannot get high-purity ethanol due to the azeotrope – the column operates at 170 kPa with a top temperature of 86°C and a bottom temperature of 115°C

E-1204: Cools and partially condenses the diethyl ether product stream prior to entering V-1203, with an outlet temperature of 37°C

V-1203: Flash vessel allowing separation of volatile ethylene from the diethyl ether product stream

E-1205: Cools wastewater stream to 35°C

P-1202 A/B: Pumps recycle to 1260 kPa

Assignment

The first task is to obtain base-case stream flows for the process using Chemcad.

The remainder of the assignment consists of five “mini-designs.”

1. **Fluid Mechanics (ChE 310) – Optimization of the Feed Pump and the Three-phase Flash Effluents**

   Pump P-1201 A/B should be sized. The optimum pipe size for Streams 6-10 should be determined. The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC in $/y) of the pipe in Streams 7-10 and of P-1201 A/B. The *EAOC* is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{annual operating costs for P-1201 A/B} \tag{3}$$

where *CAP* = the installed cost of P-1201 A/B and the pipe in Streams 6-10, 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).

Raw-material costs or wastewater-treatment costs should not be included, so *CAP* only includes the installed cost of pipes and pumps, and operating costs include the electricity to run the pump. The pump must supply all pressure needed prior to the distillation column. It may be assumed that the pressure drop between the pump and V-1202 outlet is fixed at 1260-1120 = 140 kPa. Stream 7 contains 500 m of equivalent pipe length, and the destination pressure must be at least 1000 kPa. Stream 8 and 10 combined contain 30 m of equivalent pipe length, an elevation increase of 20 m, and there is the pressure drop of 35 kPa in E-1203. Stream 9 contains 20 m of equivalent pipe length and an elevation increase of 10 m.

2. Heat Transfer (ChE 311) – Design of E-1205

The heat exchanger, E-1205, must be designed in detail for the base case. Assume the inlet pressure of the process stream is the same as Stream 17. The outlet pressure must be specified based on the heat-exchanger design. The utility here is cooling water available at 516 kPa and 30°C. The cooling water must be returned at no less than 308 kPa and no hotter than 45°C. Design for no more than 35 kPa pressure drop on the process side. For the heat exchanger design, the following information should be provided:

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

- The EAOC of the heat exchanger. In Equation 3, *CAP* becomes the cost of the heat exchanger, and the annual operating cost is the utility cost.

The maximum heat exchanger length is 6.1 m (20 ft.), and the shell diameter should be the minimum required for the stated duty. 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) – Optimization of V-1203 and thermodynamic package analysis

You are to optimize the product flash, V-1203. The objective function for the optimization should be the Equivalent Annual Operating Cost (*EAOC*, \$/y) for this section only, that is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \tag{5}$$

where *CAP* (\$) is the capital investment for the equipment (includes any equipment that are affected by your optimization), *AOC* (\$/y) is the annual operating cost (includes utility costs for E-1204 as well as the reactant feed cost and product revenue).

Optimization variables can include, but are not limited to the flash pressure and temperature. The equipment and raw material costs, product value, and equipment efficiencies are found in the Appendix.

Additionally, the thermodynamics of the water-ethanol-ethylene-diethyl ether mixture that enters the three-phase flash vessel, V-1202, must be modeled accurately. Inaccuracies in the thermodynamics of the vapor-liquid-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. Your recommendation must be based on more information than simply the Chemcad Wizard.

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. 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 SDS (safety data sheets) for all chemicals in the process should be provided in an appendix, and a brief discussion of the major health and safety 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, an aspect of your process design that addresses one of these safety 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 explored. An explanation of the rationale for such process improvements should be provided, including an economic analysis, if possible. For a process improvement involving additional equipment, use Equation 3, where *CAP*, is the cost of additional equipment and "annual operating costs" are the savings realized (hence a negative number). This is called an "incremental" analysis, and the *EAOC* for a good process modification should be negative, *i.e.*, profitable.

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 fluid mechanics optimization, the heat exchanger design, and the thermodynamics assignment can be completed.

Deliverables

Written Reports

Each team must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor, unless an electronic copy is requested by the instructor after this document is distributed. The written project reports for all teams, regardless of presentation date, are due by 11:00 a.m. Friday, November 30, 2012. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. Guidelines are in 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 (example will be provided). 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 Consolidated Chemcad Report for the base case. The Consolidated Chemcad Report should contain stream compositions, **but not stream properties**. 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-design." These may be hand written if done neatly. Alternatively, Excel spreadsheets may be included, but these must be well documented with comments so that the reader can clearly follow your thought process and interpret the results. In either case, the calculations should be clear and all assumptions made should be explained and justified. 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 main results of the design, emphasizing what was found, not what was done. There should also be an introduction that orients the reader to the all the mini-designs. Then, there should be a results section followed by a discussion section for each "mini-design." A general conclusion and recommendation section 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 team member's writing skills, the results and discussion sections for each mini-design should be written by a different team 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 team member, it is the intent of the instructors that team members should help each other in writing different sections. To this end, it is recommended that input be sought from your team members, including items such as proofreading and critiques.

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 team did is neither required nor desired. 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 team 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 team member must speak. Each team member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Guidelines are in the document entitled *Oral Reports*. The oral presentations will be Monday, December 3, 2012, from 11:00 a.m. to 1:00 p.m.; Tuesday, December 4, 2012, from 11:00 a.m. to 2:00 p.m.; and on Wednesday, December 5, 2012, 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 team 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 7, 2012. Attendance is expected.

Teams

This project will be completed in teams of 3 or 4. More details of team formation will be discussed in class. There will also be peer evaluations of team members, one midway through the project and one after the project is submitted. These will be done on-line, and there will be a window of time when the evaluation must be submitted. **Anyone not completing either the interim or the final peer evaluation will lose one full letter grade in the design grade for all three classes for each evaluation not completed. The results of this evaluation may affect individual team members' grades, so that each team member may not receive the same grade for the project.**

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 1
Other Data

Heat Exchangers

For heat exchangers that do not have to be designed in detail, the following approximations may be used for heat transfer coefficients to calculate the heat transfer area and heat exchanger cost.

situation	***h*** **(W/m²°C)**
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	2000
flowing liquid	600
flowing gas	60

The equations for the log-mean-temperature-difference correction factor, F, for a 1-2, shell-and-tube heat exchanger are:

For $R \neq 1$

$$F = \frac{\sqrt{R^2+1}\ln\left[\frac{1-P}{1-RP}\right]}{(R-1)\ln\left[\frac{2-P\left(R+1-\sqrt{R^2+1}\right)}{2-P\left(R+1+\sqrt{R^2+1}\right)}\right]} \tag{5}$$

and for $R = 1$

$$F = \frac{P\sqrt{2}}{(1-P)\ln\left[\frac{2-2P+P\sqrt{2}}{2-2P-P\sqrt{2}}\right]} \tag{6}$$

where

$$P = \frac{t_{out}-t_{in}}{T_{in}-t_{in}} \tag{7}$$

$$R = \frac{\dot{m}_{tube}C_{p,tube}}{\dot{m}_{shell}C_{p,shell}} = \frac{T_{in}-T_{out}}{t_{out}-t_{in}} \tag{8}$$

the upper-case T is for the tube side and the lower-case t is for the shell side. It is understood that it does not matter which fluid is placed on which side, since the same value for F results for either configuration.

For a 2-4 shell-and-tube heat exchanger, the equations are

For $R \neq 1$

$$F = \frac{\sqrt{R^2+1}\ln\left[\frac{1-P}{1-RP}\right]}{2(R-1)\ln\left[\frac{2-P-PR+2\sqrt{(1-P)(1-PR)}+P\sqrt{R^2+1}}{2-P-PR+2\sqrt{(1-P)(1-PR)}-P\sqrt{R^2+1}}\right]} \tag{9}$$

and for $R = 1$

$$F = \frac{P\sqrt{2}}{2(1-P)\ln\left[\frac{4(1-P)+P\sqrt{2}}{4(1-P)-P\sqrt{2}}\right]} \tag{10}$$

For a 3-6 shell-and-tube heat exchanger, the equations are

For $R \neq 1$

$$F = \frac{\sqrt{R^2+1}\ln\left[\frac{1-P^*}{1-RP^*}\right]}{(R-1)\ln\left[\frac{2-P^*\left(R+1-\sqrt{R^2+1}\right)}{2-P^*\left(R+1+\sqrt{R^2+1}\right)}\right]} \tag{11}$$

and for $R = 1$

$$F = \frac{P^*\sqrt{2}}{(P^*-1)\ln\left[\frac{2-2P^*-P^*\sqrt{2}}{2-2P^*+P^*\sqrt{2}}\right]} \tag{12}$$

where

$$P^* = \frac{1 - \frac{1 - RP}{\sqrt[3]{1 - P}}}{R - \frac{1 - RP}{\sqrt[3]{1 - P}}} \tag{13}$$

Appendix 2
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)
add 25% to the purchased cost for finned tubes

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)
all compressors require a drive in addition to the compressor

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+(sch #)/20)$^{0.25}$
sch = schedule number for pipe
use the same schedule 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)	\$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/Off-gas Credit	at LHV
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

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

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

Raw Material Costs/Product Value

Raw Material or Product	price
ethanol	1.15/kg
diethyl ether	1.70/kg