Fluid Mechanics, Heat Transfer, Thermodynamics
Design Project

Production of Maleic Anhydride

We continue to investigate the feasibility of constructing a new, grass-roots, 40,000 tonne/y, maleic anhydride facility. As part of the feasibility study, we would like you to investigate some of the details of the feed section of the proposed plant and of the thermodynamics of the components involved in the process.

Chemical Reaction

The raw material is benzene. The primary reaction is one in which benzene is partially oxidized to form maleic anhydride (Equation 1). There are three undesired side reactions, the subsequent combustion of maleic anhydride (Equation 2), the complete combustion of benzene (Equation 3), and the formation of the by-product, quinone (Equation 4).

The chemical reactions are as follows:

$$\underset{\text{maleic anhydride}}{C_6H_6 + 4.5O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O} \tag{1}$$

$$C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O \tag{2}$$

$$C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O \tag{3}$$

$$C_6H_6 + 1.5O_2 \rightarrow \underset{\text{quinone}}{C_6H_4O_2} + H_2O \tag{4}$$

Process Description

The PFD for the process is given in Figure 1. Note that this is the same PFD as you were given last spring. It should be used as a starting point for this assignment. You are to focus on the feed section, Streams 1-5.

C-501	E-501	H-501	E-502	R-501	V-501	T-501	T-502	E-503	H-502
Air Feed Compressor	BenzeneFeed Vaporizer	Feed Fired Heater	Reactor Effluent Cooler	Maleic Anhydride Reactor	Dibutyl Phthalate Mixing Vessel	Maleic Anhydride Absorber	Maleic Anhydride Distillation Column	Maleic Tower Condenser	Maleic Tower Reboiler/Fired Heater

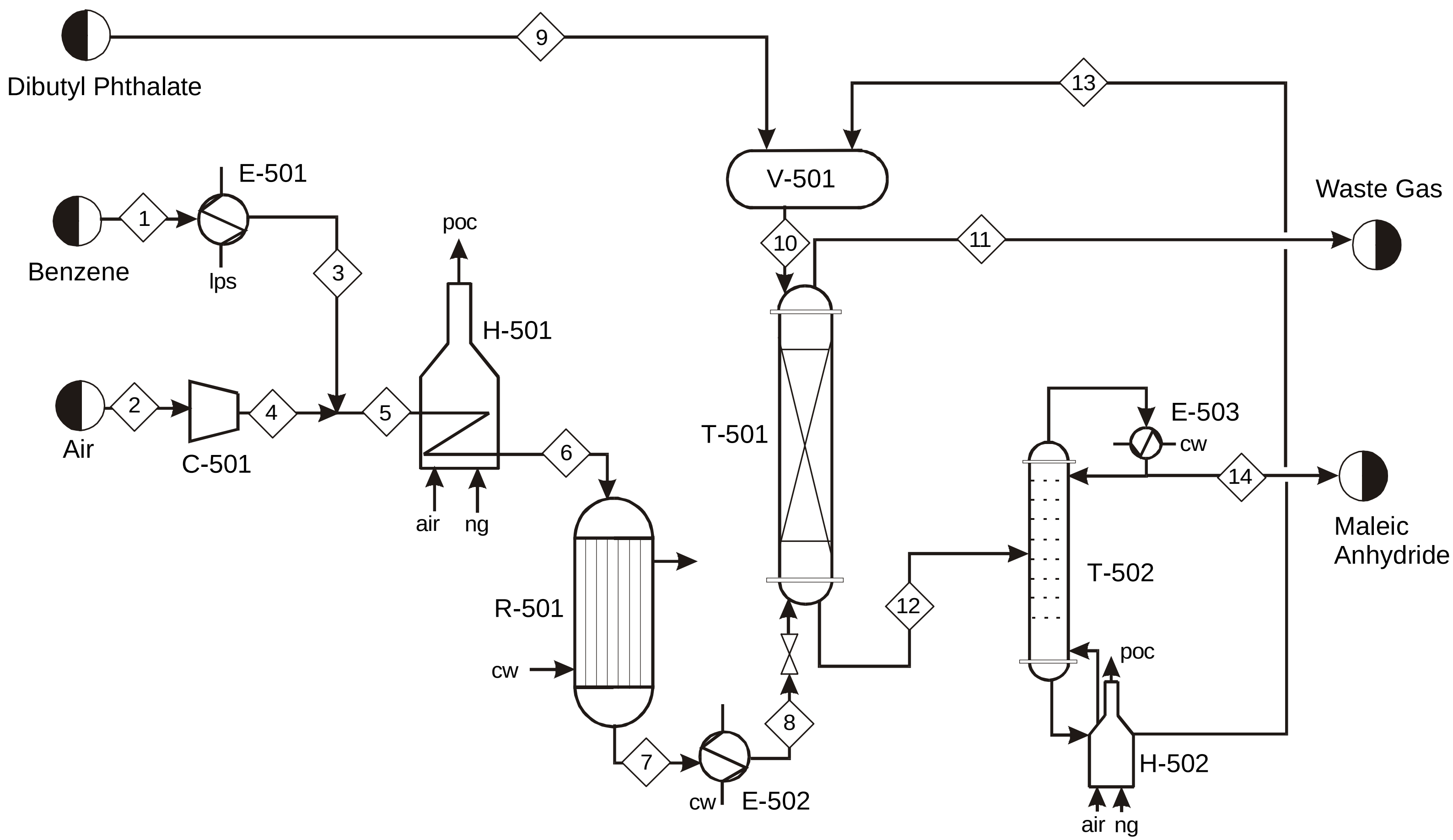


Figure 1: Maleic Anhydride Production Process

Process Details

Feed Stream and Effluent Streams

Stream 1: Benzene – stored as a liquid at atmospheric temperature and pressure (with a blanket of nitrogen gas)

Stream 2: Air – present at 200% excess based on maleic anhydride formation reaction. Consider air to have zero cost and to have 79 mol % N_2, 21 mol % O_2. Assume 100% overall conversion of the limiting reactant in determining the amount of air needed.

Stream 9: Dibutyl phthalate solvent – make-up stream for amount lost in Streams 11 and 14.

Stream 11: Waste gas – contains unreacted benzene and O_2, N_2, CO_2, and H_2O, plus some dibutyl phthalate – sent to treatment process, the cost of which may be considered negligible.

Stream 14: Maleic anhydride product.

Equipment

Compressor (C-501)

The compressor increases the pressure of the feed air to approximately 12 atm. The compressor may be assumed to be adiabatic with an efficiency of 75%. It may be necessary to use staged compressors with intercooling.

Heat Exchanger (E-501)

This heat exchanger vaporizes the benzene feed to saturated vapor at the stream pressure, which you must choose based on the optimization in mini-design #1.

Fired Heater (H-501)

This heats reactor feed vapor to reaction temperature. Natural gas is used as the fuel, and the amount needed is based on the LHV of natural gas and the process heat load. The cost of natural gas is a utility cost, and you should assume that the fired heater is 85% efficient

Reactor (R-501)

This is where the reactions in Equations 1-4 occur.

Process Conditions

In order to complete a material balance for this process, you are to assume that the following process conditions apply.

For the reactions taking place, assume that

88.85 % of benzene of the benzene entering the reactor is converted to maleic anhydride via reaction 1.
30.00% of the maleic anhydride formed by reaction 1 is combusted via reaction 2.
3.35% of the benzene entering the reactor is combusted via reaction 3.
1.66 % of the benzene entering the reactor forms quinone via reaction 4.

The reactor inlet conditions are set at 460°C and 11 bar and the reactor behaves isothermally at the inlet temperature.

The waste gas, Stream 11, contains all the nitrogen, water, oxygen, benzene, and carbon dioxide in Stream 8. In addition, 2% of the maleic anhydride and 70% of the quinine in Stream 8 leave in Stream 11. Finally, Stream 11 also contains 0.1 % of the dibutyl phthalate in Stream 13.

Stream 8 is cooled to 260°C in E-502.

The composition of the solvent recycle, Stream 13, is essentially pure dibutyl phthalate. The mole ratio of Stream 13 to Stream 8 is 0.20.

The composition of Stream 14 is 95 mol% maleic anhydride. The production rate of 40,000 tonne/yr refers to Stream 14.

Stream 11 leaves the process at 84°C and Stream 13 leaves the process at 180°C.

Assignment

The assignment consists of four "mini-designs."

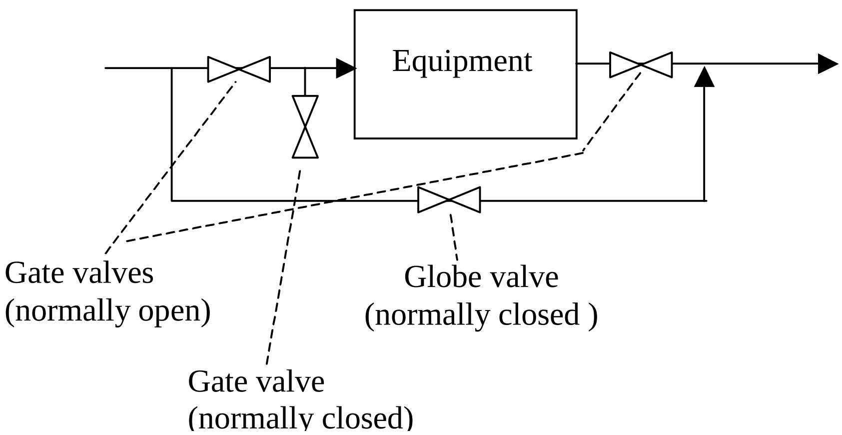
1. Optimization of the Feed Section and Compressor (ChE 310, 320)

You are required to find the optimum pipe sizes and make the pressure drop calculations for the feed section, which includes all piping, pipe fittings, and all heat exchangers between the feeds and the fired heater inlet. Specifically, you should assume the following:

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

- The air feed should be taken from the environment (1 atm and 20°C) and compressed.

- Before compression, the air must flow through a drier/filter to remove any residual moisture and particulates. The drier/filter is standard equipment, and the vendors recommend that at the design flow a pressure drop of 3 psi be used.
- The air should pass through the shell side of any heat exchanger used to heat or cool it.
- For any heat exchanger for which a detailed design is not performed (see the Heat Transfer section), a pressure drop of 3 psi should be used, for the air-side.
- For each piece of equipment in the feed air line (compressors, heat exchangers, drier/filter), isolation gate valves and a bypass line should be provided to allow for use in the event of unscheduled maintenance. The sketch below illustrates this arrangement.



- Each piece of equipment will be separated by at least 10 ft of piping to allow for maintenance.
- The piping between the last piece of equipment before the fired heater should consist of 35 ft of straight pipe, 6 - 90° standard elbows, a gate valve, and an orifice meter with a full scale reading of 100 inches of water pressure drop (the design flow should be 50% of full scale). The orifice meter should have two isolation gate valves with a bypass (similar to the arrangement for equipment shown in the sketch above).
- The benzene storage tank is located 200 m (equivalent length) from the maleic anhydride process unit. The benzene level is 5 m above ground level.

The optimization for this mini-project should include the cost of the compressors, the cost of pumps, the cost of the intercoolers, the cost of all pipe and fittings, 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 below) includes only the installed cost of pipes, valves, compressor stages, pumps, and heat exchangers, and operating costs include the electricity to run the compressor stages and the cost of cooling water in the inter-coolers, if used.

Calculations for the optimum pipe size should be included in an appendix for this mini-project.

You should also do a pressure analysis of the Streams 1 through 5 to make sure all pressures balance. Valves, pumps, or compressors must be added as needed.

The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC) of the piping system including the pump ($/y). The *EAOC* is defined as:

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

where

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{6}$$

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

Using your final design (the one that minimizes *EAOC*), determine the maximum and minimum flowrates that the feed section can supply the process. For this part of the project, you may assume that all pump and compressor curves follow the "standard" curves given below:

$$\frac{P}{P_{design}} = 1.1 - 0.1\left[\frac{\dot{V}}{\dot{V}_{design}}\right]^{7.1265}$$

where P_{design} is the pressure rise across the pump at the design volumetric flowrate of $\dot{V}_{design}$, and $\dot{V}$ is the volumetric flowrate at any pressure rise, P, across the pump.

The compressor curves are shown in Figure 2.

2. Heat Exchanger Design (ChE 311)

You should perform a detailed design of the benzene feed heat exchanger. You should assume that steam is available at the conditions specified in the appendix 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)

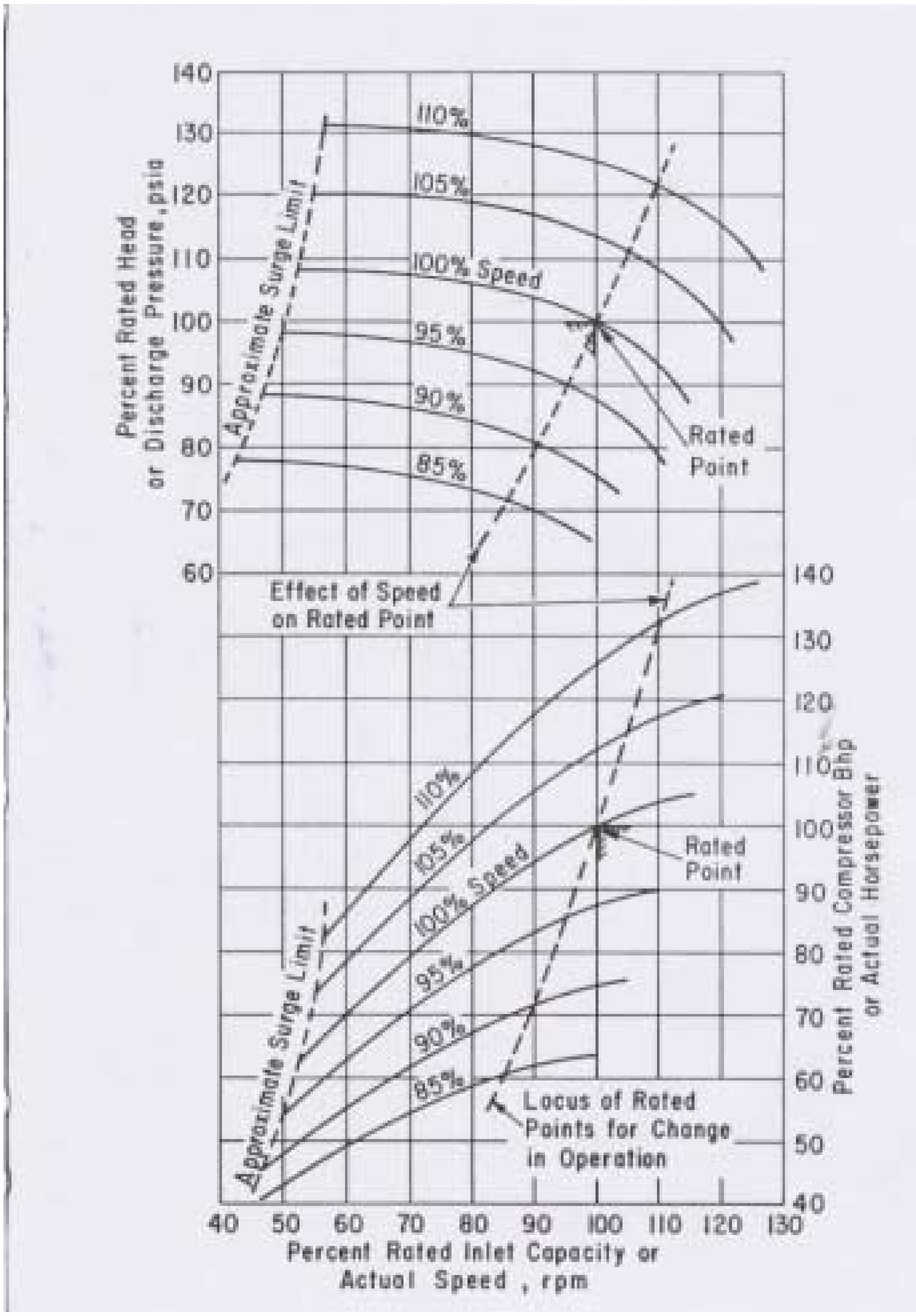


Figure 2: Manufacturer's typical centrifugal compressor curves

- 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
- 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.

3. Thermodynamics of components (ChE 320)

The separations section of this process involves dibutyl phthalate, maleic anhydride, maleic acid, and quinone. It is necessary to understand the vapor-liquid equilibrium between different pairs of these components. Specifically, you are to investigate the vapor-liquid equilibrium between maleic anhydride and quinone, maleic anhydride and maleic acid, and maleic acid and dibutyl phthalate. First of all, check different thermodynamics packages in Chemcad to see if there are differences between the predictions of the packages. The term thermodynamics package means the choice of *K*-value and enthalpy calculation methods. At a minimum, you should investigate ideal, SRK, Peng-Robinson, UNIQAC, UNIFAC, UNIFAC/UNIQAC, plus the recommendation of the expert system if it differs from those listed above. Specifically, examine the *T-xy* diagrams of the pairs of components using the same thermodynamics packages at a variety of possible operating pressures (1-10 atm) for the separation section. The presence of azeotropes strongly affects the ability to do separations. What do you observe? Compare the predictions of the different packages. Explain and discuss reasons for any differences observed.

Additionally, there appears to be a discrepancy in the reported physical properties for some of the components involved in this design. Specifically, the properties in the Chemcad data base do not match those in other published data bases. Please investigate this problem in

depth and determine which information is correct. If the Chemcad data base is in error, discuss how the vapor-liquid equilibrium results would be affected.

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. 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. In addition, briefly discuss possible safety hazards for each piece of equipment in your process. Finally, a feature of your process design that addresses one of these concerns should be explained.

5. **Chemcad**

   A complete Chemcad simulation for the process shown in Figure 1 should be provided for your optimized case. Use the results from all mini designs, including the recommended thermodynamics package.

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 1:00 p.m. Thursday, December 2, 2004. 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 members 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. For groups with four members, the member not authoring a mini-report should author the safety analysis report, which is described below. The remainder of the report, namely the general abstract, general introduction, general results (including Chemcad simulation), general conclusions, and general recommendations sections should be a group effort.

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 you group. The reports will be evaluated as follows:

- section 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 December 2, 2004, 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, 10, 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+(\text{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+(\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}$

Equipment Bypasses

Bypasses around equipment should consist of a minimum of 20 ft of pipe, 2 standard elbows, and 1 gate valve. There will also be a tee at each point where the by-pass connects to the main pipe.

Utility Costs

Low-Pressure Steam (618 kPa saturated)	$7.78/1000 kg
Medium-Pressure Steam (1135 kPa saturated)	$8.22/1000 kg
High-Pressure Steam (4237 kPa saturated)	$9.83/1000 kg
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 (absolute)	< 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
	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

Appendix 2
Other Design Data

Heat Exchangers

For heat exchangers that are not designed in detail, use the following approximations for heat-transfer coefficients to allow you to determine the heat transfer area:

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