Fluid Mechanics, Heat Transfer, Thermodynamics
Design Project

Production of Phthalic Anhydride

Your assignment is to continue evaluating the details of a process to produce 75,000 tonne/y of phthalic anhydride from o-xylene. This is the amount of phthalic anhydride 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.

Process Details

Unit 1700 produces phthalic anhydride (PA) via the partial oxidation of o-xylene using air. The following reactions occur:

$$\underset{\text{o-xylene}}{C_6H_4(CH_3)_2} + 3O_2 \rightarrow \underset{\text{phthalic anhydride}}{C_6H_4(CO)_2O} + 3H_2O \tag{1}$$

$$\underset{\text{phthalic anhydride}}{C_6H_4(CO)_2O} + \frac{15}{2}O_2 \rightarrow 8CO_2 + 2H_2O \tag{2}$$

$$\underset{\text{o-xylene}}{C_6H_4(CH_3)_2} + \frac{21}{2}O_2 \rightarrow 8CO_2 + 5H_2O \tag{3}$$

$$\underset{\text{o-xylene}}{C_6H_4(CH_3)_2} + \frac{15}{2}O_2 \rightarrow \underset{\text{maleic anhydride}}{C_2H_2(CO)_2O} + 4CO_2 + 4H_2O \tag{4}$$

$$\underset{\text{maleic anhydride}}{C_2H_2(CO)_2O} + 3O_2 \rightarrow 4CO_2 + H_2O \tag{5}$$

In order to operate safely, the reaction mixture, Stream 7, must be kept below the lower flammability limit of 1 mol% of o-xylene in air. The oxidation of o-xylene occurs in catalyst-filled tubes to facilitate heat removal. The reactions that take place are highly exothermic, and the temperature everywhere in the reactor must be very carefully controlled. The catalyst, vanadium pentoxide (V_2O_5), sinters above a temperature of 400°C.

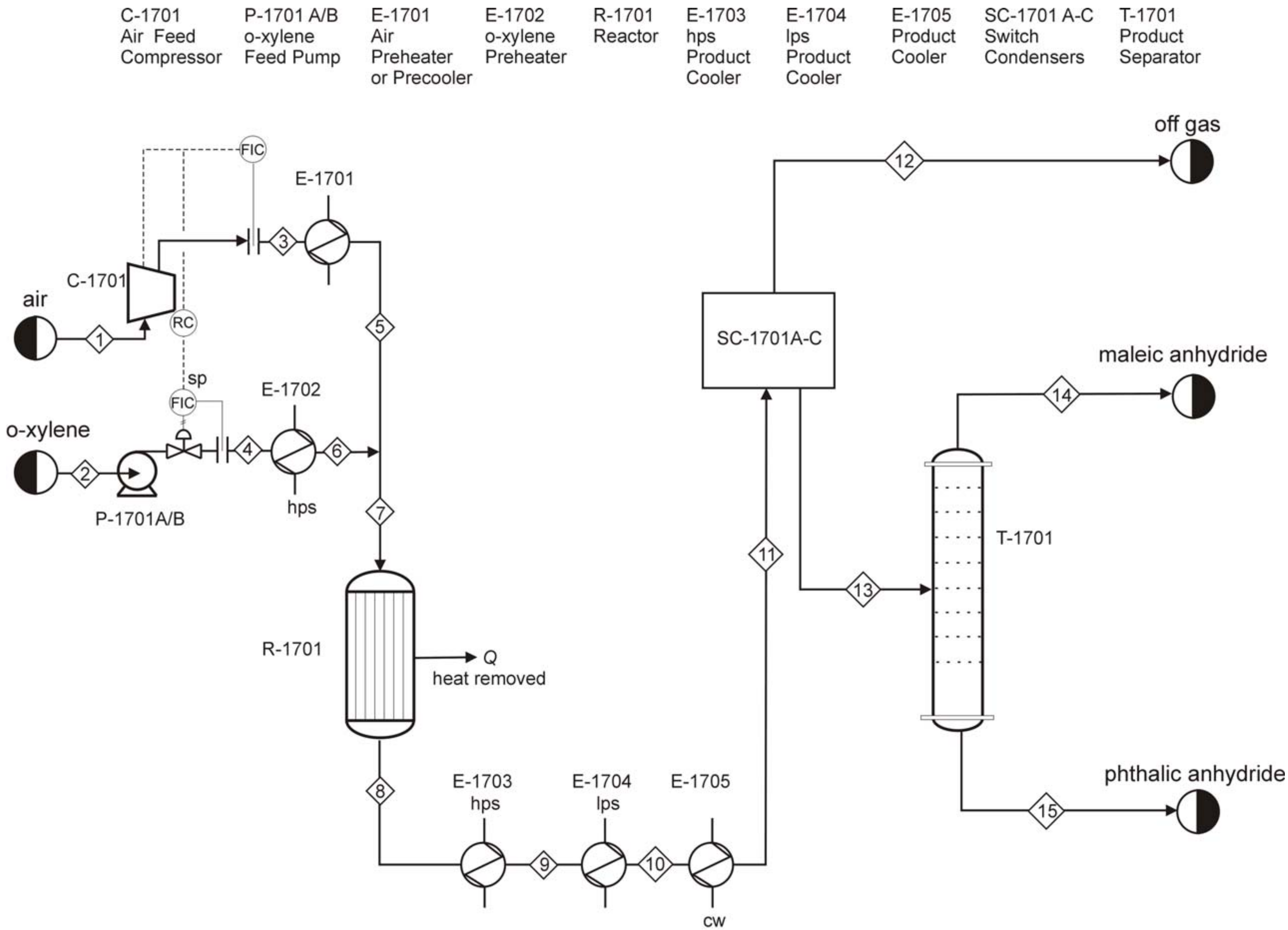

Figure 1: Unit 1700 - Phthalic Anhydride Manufacturing Process

Feed Streams and Effluent Streams

Stream 1: air from the atmosphere that is dried first, so at 25°C and 80 kPa

Stream 2: o-xylene – at 25°C and 101.325 kPa – assumed pure

Stream 12: contains all light gases in Stream 11

Stream 14: maleic anhydride by-product – can be sold

Stream 15: phthalic anhydride product – must contain 75,000 tonne/y of PA

Base-Case Equipment Information

Compressor (C-1701)

This compressor increases the pressure of the air feed to a sufficient value so that the reactor inlet is at 300 kPa. The compressor is adiabatic with a 60% efficiency. In the base case, there is only one stage.

Pump (P-1701 A/B)

This pump increases the pressure of liquid o-xylene feed to a sufficient pressure so that Streams 5 and 6 mix at the same pressure and so the reactor inlet, Stream 7, is at 300 kPa. It is assumed that there is a 10 kPa pressure drop at the mixing point of Streams 5 and 6. The pump is adiabatic with an 80% efficiency.

Heat Exchanger (E-1701)

This heat exchanger preheats the air or precools the air to 240°C, using high-pressure steam or cooling water. The process-side pressure drop is 35 kPa for Chemcad simulations. For the heat transfer design, the pressure drop on the shell side and the tube side should be calculated based on the design details.

Heat Exchanger (E-1702)

This heat exchanger vaporizes the o-xylene to 240°C. The process-side pressure drop is 35 kPa.

Reactor (R-1701)

This is a shell-and-tube reactor, similar to a heat exchanger. The catalyst is in the tubes, and a heat-removal fluid, molten salt, is in the shell. The heat load must be calculated. The reactor exit temperature is to be 360°C, and the pressure drop is 80 kPa, packed bed reactor. At this exit temperature, the selectivity for MA, PA, and CO_2 are 0.1, 0.7, and 0.2, respectively. Of the CO_2 formed, 70% comes from combustion of PA, 20% from combustion of MA, and 10% from combustion of o-xylene. The o-xylene conversion is 100%. The reactor can be simulated on Chemcad by using a “stoichiometric reactor.” A single pseudo-reaction that accounts for both the stoichiometry and the selectivity must be determined and used in the reactor simulation.

Heat Exchanger (E-1703)

This heat exchanger cools the reactor effluent, while recovering some heat by generating high-pressure steam. The effluent temperature is 15°C above the temperature of high-pressure steam. The pressure drop on the process side is 40 kPa.

Heat Exchanger (E-1704)

This heat exchanger further cools the reactor effluent, while recovering some heat by generating low-pressure steam. The effluent temperature is 10°C above the temperature of low-pressure steam. The pressure drop on the process side is 40 kPa.

Heat Exchanger (E-1705)

This heat exchanger cools the reactor effluent using cooling water. The effluent temperature is 45°C. The pressure drop on the process side is 40 kPa.

Switch Condensers (SC-1701)

These are a complex set of three condensers that operate in a semi-continuous mode. The inlet stream is first cooled by cold oil so that the anhydrides are desublimated (condensed as solids). Then hot oil is passed through the same condenser so that the solids are melted. At any given time, one condenser operates to desublimate, one to melt, the third on standby, and the feed is switched between the three. The details of this operation will not be considered here.

The feed to these condensers in Stream 11 must be at 45°C and 100 kPa. All of the light gases and o-xylene go to Stream 12, and 1% of the PA and 2% of the MA go to Stream 12. This unit should be modeled on Chemcad using a “component separator.”

Tower (T-1701)

This tower, which is actually a distillation column, separates the PA and MA. A “component separator” should be used on Chemcad. Distillation columns are not perfect separators. Therefore, 99.8% of the maleic anhydride in Stream 13 enters Stream 14, and 99.8% of the phthalic anhydride in Stream 13 enters Stream 15.

Assignments

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

1. Fluid Mechanics – (ChE 310)

You are to optimize the design of the feed section of the process, which includes Streams 1-7, P-1701 A/B, C-1701, E-1701, and E-1702. The stream conditions should be taken from the base-case simulation performed in Mini Design #5.

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

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \tag{6}$$

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

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{7}$$

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

The costs for the piping components are given in the Appendix. The optimal pipe diameter and schedule number of each stream, the pump duty, and the compressor duty that minimizes the EAOC must be determined.

When doing a Chemcad simulation, pressure drops in pipes are often ignored (unless a pipe is put in as a "unit'). In this optimization only, the pump and the compressor outlet pressures must be sufficient to overcome the pressure drops in the equipment, at the mixing point, and in the pipes. The base-case pressure drops for the heat exchangers should be used.

To evaluate the amount and cost of piping required for the mini-design, it may be assumed that C-1701, P-1701, E-1701, and E-1702 are at grade (ground level). The suction line for the compressor is 0.5 m above grade, and the discharge line for the compressor is 1.5 m above grade. The suction line for the pump is 0.3 m above grade, and the discharge line from the pump is 1 m above grade. The equivalent length of the pipe for Stream 3 is 3 m, the equivalent length of the pipe for Stream 5 is 5 m, the equivalent length of the pipe for Stream 4 is 3 m, the equivalent length of Stream 6 is 2 m, and the equivalent length of Stream 7 is 15 m, including 10 m as an increase in elevation. For this mini-design only, both E-1701 and E-1702 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)

A detailed design of E-1701 is required for base-case conditions. It should be assumed that utilities are 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
- Thickness of shell wall
- 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

The maximum heat exchanger length is 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)

The equivalent annual operating cost, *EAOC*, for the compressor section of the process should be minimized with the following in mind:

- The air feed should be taken from the inlet conditions (80 kPa and 25°C) and compressed to the reactor feed conditions (300 kPa). According to the compressor manufacturer, the maximum compressor operating temperature should be 200°C. Therefore, the compressor section must be optimized within these constraints.

The optimization for this mini-project should include the cost of the compressor(s), 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 6) 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 feed section including the compressor. The *EAOC* was defined in Equations 6 and 7.

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

Deliverables

Written Reports

Each group 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 groups, regardless of presentation date, are due by 11:00 a.m. Thursday, December 2, 2010. 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 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 so that the reader can interpret the results. In either case, your 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 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 2, 2010, from 11:00 a.m. to 2:00 p.m. and on Friday, December 3, 2010, 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 10, 2010. 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 60% 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+(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 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 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 – zero cost
Low-temperature Refrigerant available at -20°C	$7.89/GJ

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
o-xylene	$0.80/kg
maleic anhydride	$1.10/kg
phthalic anhydride	$1.25/kg

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