Fluid Mechanics, Heat Transfer, Thermodynamics Design Project

Production of Phthalic Anhydride from o-Xylene

The subject of this project is a process for manufacturing phthalic anhydride from o-xylene, subject to constraints which will be defined later in this document. A suggested process flow diagram (PFD) is attached. You should use this as a starting point. However, any change that you can justify (and that does not violate the laws of nature) is allowed. Your assignment is to develop an optimum case based upon an objective function defined later. It is your job to define the decision variables, and to choose and implement a method to arrive at an optimum design.

Process Description

The raw materials are air and o-xylene. The o-xylene feed, which may be considered pure and at 0.75 atm, is pumped to a higher pressure and then vaporized in a fired heater, H-701. Air, which may be assumed to contain only O_2 and N_2, is mixed with recycle, if there is any recycle, compressed, and then heated in E-701. The hot air and vaporized o-xylene are mixed and sent to a packed bed reactor. The o-xylene content of Stream 8 must either be below the LFL of o-xylene, which is 1 mole %, or above the UFL of o-xylene, which is 6 mole %. For the purposes of the present design only, assume that essentially 100% of the o-xylene is reacted in this reactor. Most of the o-xylene reacts to form phthalic anhydride, but some complete combustion of o-xylene occurs, and some maleic anhydride is formed. (The yields are given later.) The reactor temperature is controlled by a molten salt loop, Streams 21-24. The reactor effluent is cooled and sent to the separation section. The temperature to the separation section (Stream 10) may be no higher than 180°C, and the pressure may be no lower than 150 kPa. The net result of the separation section is that all light gases and water leave in Stream 11, with small amounts of organics (1% of organic content of Stream 10) . The "dirty air" in Stream 11 or Stream 14 must be treated before it can be vented, and this is an additional expense. It is also possible to recycle some of the "dirty air." Any "dirty air" purged must be sent to a scrubber, not shown on the PFD, and an operating charge is assessed. The effluents from the separation section are Stream 12 containing maleic anhydride, and Stream 13, which must be 99.9 wt % phthalic anhydride and must be 80,000 metric tons/year. Excess organic material may be burned in the fired heater.

Process Details

Feed Streams

Stream 1: air, consisting of 79% N_2 and 21% O_2

Stream 2: o-xylene at 0.75 atm and 150°C

Effluent Streams

Stream 11 or 14: air to treatment plant, appropriate cost charged

Stream 12: waste maleic anhydride, may be burned in fired heater, may not be sold; energy content is equivalent to lower heating value

Stream 13: phthalic anhydride product, 80,000 metric tons/yr, 99.9 wt % pure

Equipment

Compressor (C-701):
The compressor increases pressure of air feed.

Pump (P-701):
The pump increases pressure of the o-xylene feed.

Fired Heater (H-701):
The fired heater vaporizes the o-xylene feed and heats the vapor to any temperature.

Heat Exchanger (E-701):
This heat exchanger heats the air feed

Reactor (R-701):
The reactor feed may be no lower than 300°C. The catalyst is active to produce phthalic anhydride only between 300°C and 420°C.

The following reactions occur:

$$\underset{\text{o-xylene}}{C_8H_{10}} + 3O_2 \rightarrow \underset{\text{phthalic anhydride}}{C_8H_4O_3} + 3H_2O$$

$$C_8H_{10} + 7.5O_2 \rightarrow \underset{\text{maleic anhydride}}{C_4H_2O_3} + 4H_2O + 4CO_2$$

The complete combustion of o-xylene also occurs.

The reactor is a fluidized bed, operating at 5´ minimum fluidization, with a pressure drop of 25 kPa. The reactor installed cost may be assumed to be $2.5 million.

Selectivity data are in Table 1. These data are approximate and are to be used only for this design project this semester, not for next semester.

Table 1
Fractional Conversion of o-Xylene into (Yield of) Indicated Product

T(°C)	maleic anhydride	CO_2	phthalic anhydride
300	1.00	0.00	0.00
320	0.536	0.0339	0.425
340	0.215	0.102	0.683
360	0.100	0.200	0.700
380	0.0463	0.356	0.598
400	0.0215	0.602	0.377
420	0.00	1.00	0.00

Molten Salt Loop: Streams 21-24 contain molten salt. Its properties may be found in Reference [1]. The molten salt removes the heat generated by the exothermic heat of reaction in the reactor.

Power Cycle Section: The energy removed from the molten salt in E-702 is to be used as the energy source in a power cycle. Steam is to be the fluid in the cycle. The turbine generates electricity which can be sold to the power company for 90% of the price of electricity given below, or it can be used internally in the plant. The heat sink in E-704 may be cooling water or refrigerated water. You must evaluate the economics of the power cycle.

Separation Section

This section may be simulated on CHEMCAD with a series of component separators. The installed cost of the separation section, in millions of dollars, may be taken as

$$\$2.25 + 0.5n$$

where n is the number of separation devices needed, not including the one which removes the dirty air. The utility costs associated with the separation section may be assumed to be 50% of the utility costs associated with the process through Stream 10.

Recycle

It is possible to recycle some of the "dirty" air from Stream 11 as long as there is sufficient purge (Stream 14). It is your job to determine the optimal recycle-to-purge ratio. The purge stream must go to the air treatment unit with the appropriate charge taken.

Assignment

1. Optimum pipe sizes should be determined for Streams 1 though 10, subject to the constraints of the pump and compressor curves.

2. Pump and compressor capacities should be specified. There should be flexibility for 25% scale-up and 25% scale-down capacity. Pump and compressor curve equations are in the appendix.

3. Placement of control valves in the feed section should be detailed. Furnish complete designs of orifice plates for flow measurement. There should be flexibility to run either above the UFL or below the LFL.

4. HX-3 must be designed in detail, including tube size and pitch, baffle spacing, shell diameter, detailed pressure drop calculations, etc. All other heat exchange areas may be determined using approximate heat transfer coefficients presented elsewhere in this document.

5. The economics of using the heat transferred from the molten salt in E-702 as a source of energy for a steam power cycle to produce electricity should be evaluated.

Other Data

Equivalent pipe lengths should be taken as follows:

Stream #	Equivalent Length (m)
1	60
2	60
3	20
4	10
5	20
6	30
7	20
8	50
9	20
10	30

Pressure drops for heat exchangers other than E-703 may be estimated as 30 kPa for the tube side and 20 kPa for the shell side.

Individual heat transfer coefficients for all heat exchange devices other than E-703 may be estimated as follows:

situation	h (W/m^2°C)
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	1000
flowing liquid	600
flowing gas	60

Air treatment is accomplished by absorption of the organic matter into water, with the light gases vented to the atmosphere. The water is then sent to a waste-water treatment plant. The annual cost is based upon the volume of vapor sent to the treatment plant and the mole fraction of organic matter (phthalic and maleic anhydrides) in Stream 11 or 15. The cost is:

$$\$/h\ air\ treated = 10^{-4} V_{tot}(0.5 + 1000 x_{or})$$

V_{tot} = total volume of "dirty air" to be treated, m^3

x_{or} = mole fraction of organics (CO_2 is not an organic!) in "dirty air" stream

Utility Costs

Low-Pressure Steam (446 kPa, saturated)	\$3.00/1000 kg
Medium-Pressure Steam (1135 kPa, saturated)	\$6.50/1000 kg
High-Pressure Steam (4237 kPa, saturated)	\$8.00/1000 kg
Natural Gas (446 kPa, 25°C)	\$3.00/10^6 kJ
Electricity	\$0.05/kW hr
Boiler Feed Water (at 549 kPa, 90°C)	\$300.00/1000 m^3

Cooling Water $20.00/1000 m^3
available at 516 kPa and 30°C
return pressure ≥ 308 kPa
return temperature should be no more than 15°C above the inlet temperature, otherwise there is an additional cost of $0.35/10^6 kJ

Refrigerated Water $200.00/1000 m^3
available at 516 kPa and 10°C
return pressure ≥ 308 kPa
return temperature is no higher than 20°C
if return temperature is above 20°C, there is an additional cost of $7.00/10^6 kJ

Equipment Costs (Purchased)

Piping	$/m = 0.7 (dia, in) + 1
Valves	$100 (flow diameter, in)$^{0.8}$ for control valve with orifice plate, double the price
Pumps	$630 (power, kW)$^{0.4}$
Heat Exchangers	$1030 (area, m^2)$^{0.6}$ If extended surfaces are used, area is that for same size tubing without fins. Then add a 25% surcharge for fins.
Compressors	$770 (power, kW)$^{0.96}$ + 400 (power, kW)$^{0.6}$
Steam Turbine	$2.18´ 10^5 (power output, MW)$^{0.67}$ assume 75% efficiency
Fired Heater	$635 (duty, kW)$^{0.8}$ assume 80% thermal efficiency
Storage Tank	$1000V$^{0.6}$ V = volume, m^3

Equipment Cost Factors

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

Pressure (absolute)	< 10 atm, 0.0 10 - 20 atm, 0.6 20 - 40 atm, 3.0 40 - 50 atm, 5.0 50 - 100 atm, 10	does not apply to vessels, packing, trays or catalyst since their cost equations include pressure effects
Carbon Steel	0.0	
Stainless Steel	4.0	

Economic Analysis

When evaluating alternative cases, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = -(product value - feed cost - other operating costs - capital cost annuity)

A negative EAOC means there is a profit. It is desirable to minimize the EAOC; i.e., a large negative EAOC is very desirable.

The costs for phthalic anhydride (the product) and o-xylene (the feed) should be obtained from the *Chemical Marketing Reporter*, which is in the Evansdale Library.

Other Information

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

Unless specifically stated in class, the information in this document is that which is valid for this project. Any information in the sophomore projects not specifically stated in this document is not valid for this project. Information contained in this document will not necessarily be valid for next semester's project.

Deliverables

Each group must deliver a report written using a word processor. The report should be clear and concise. The format is explained in a separate document. Any report not containing a labeled PFD and a stream table will be considered unacceptable. PFDs from CHEMCAD are generally unsuitable unless you modify them significantly. When presenting results for different cases, graphs are superior to tables. The report appendix should contain details of calculations, for the optimal case, that are easy to follow. There should be separate appendices for each class, ChE 110, ChE 111, and ChE 142, each containing calculations appropriate for the respective class. These may be neatly hand-written. Calculations which can not be followed easily will lose credit.

Each group will give an oral report in which the results of this project are presented in a concise manner. The oral report should be no more than 15-20 minutes, and each group member must speak. A 5-10 minute question-and-answer session will follow. Instructions for presentation of oral reports will be provided in a separate document. The oral presentations will be Thursday, November 30, 1995 starting at 11:00 am and running until approximately 3:30 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 in one-letter grade (per occurrence) from your project grade in ChE 110, ChE 111, and ChE 142. Individuals with classes at 2:30 pm will have their group's presentation scheduled first, and are excused from attending presentations after 2:00 pm.

The written project report is due by 11:00 am on Monday, December 4, 1995. Late projects will receive the following automatic deductions:

- after 11:00 am on due date - one letter grade
- before noon, one day late - two letter grades
- after noon, one day late - failure

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 of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

References

1. Perry, R.H. and D. Green, eds., *Perry's Chemical Engineering Handbook (6th ed.)*, McGraw-Hill, New York, 1984, p. 9-74.

Appendix
Equations for Pump Curves

P-701

$$\Delta P\ (\text{kPa}) = 500 - 4.662\times10^{-3}\dot{m} - 1.805\times10^{-6}\dot{m}^2 \qquad \dot{m}\ \text{in kg/h}$$

P-702

for $\dot{m} > 670$ Mg/h

$$\Delta P\ (\text{kPa}) = 196.2 + 0.2972\dot{m} - 2.692\times10^{-4}\dot{m}^2 + 4.899\times10^{-8}\dot{m}^3 \qquad \dot{m}\ \text{in Mg/h}$$

for $\dot{m} < 670$ Mg/h

$$\Delta P\ (\text{kPa}) = 289.0$$

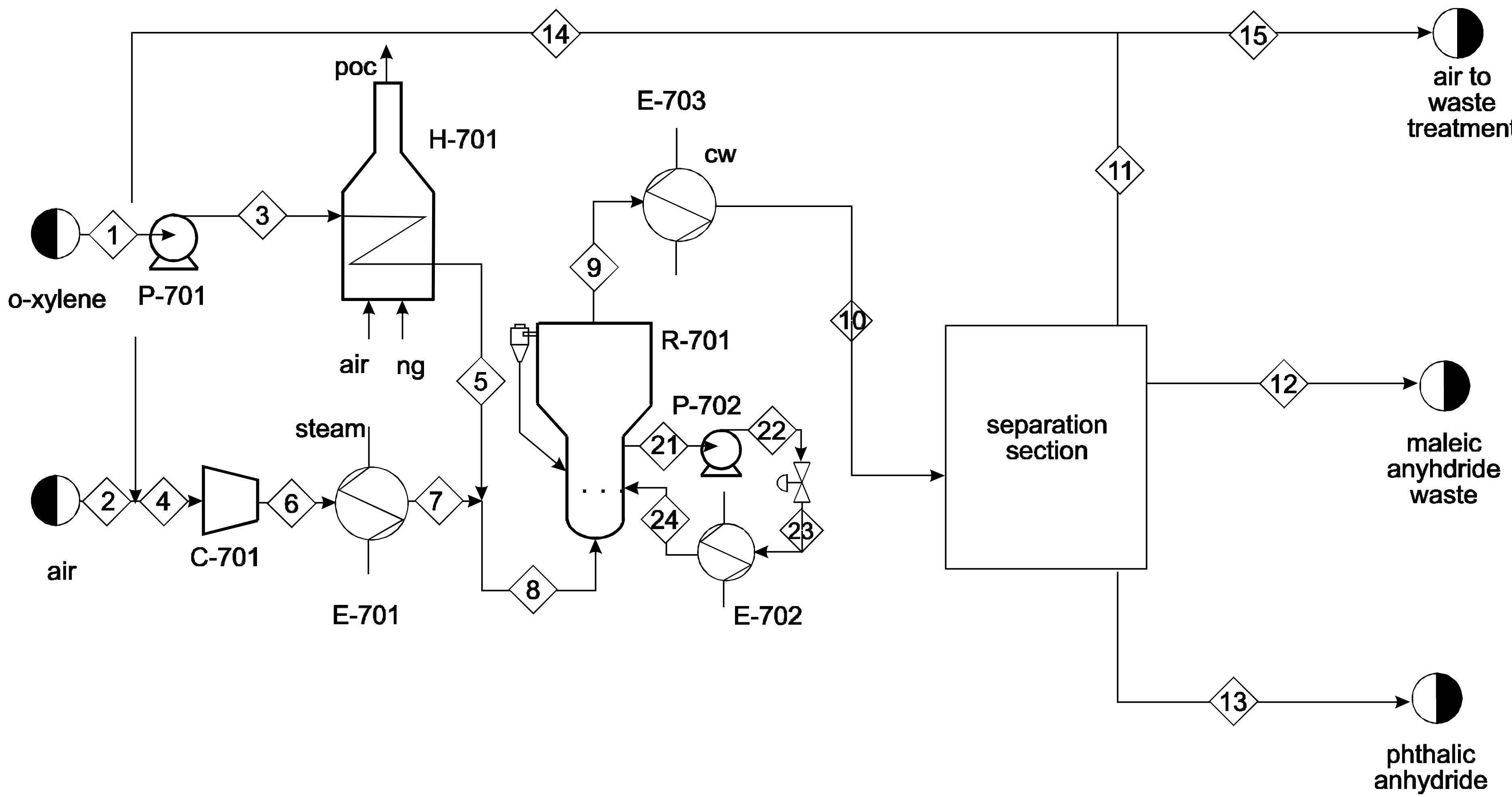
C-701

for 3500 rpm

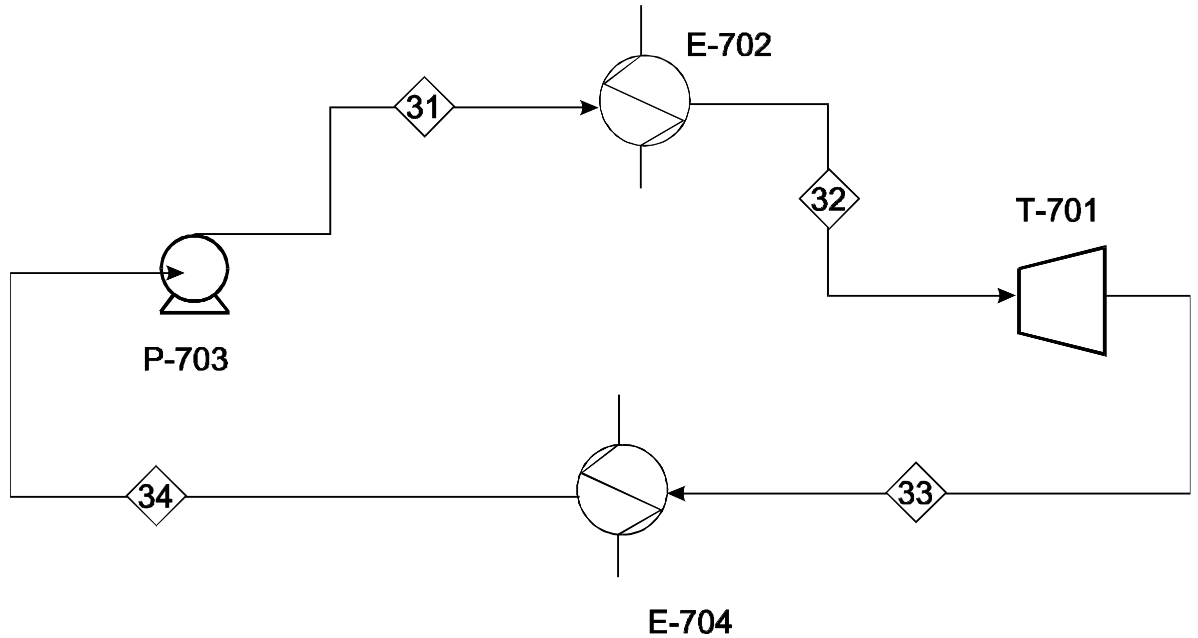
$$P_{out}/\text{P}_{in} = 5.201 + 2.662\dot{m} - 1.358\times10^{-4}\dot{m}^2 + 4.506\times10^{-8}\dot{m}^3 \qquad \dot{m}\ \text{in Mg/h}$$

for 2200 rpm

$$P_{out}/\text{P}_{in} = 4.015 + 5.263\times10^{-3}\dot{m} - 1.838\times10^{-4}\dot{m}^2 \qquad \dot{m}\ \text{in Mg/h}$$



Unit 700 - Phthalic Anhydride from o-Xylene



Power Cycle Section