

# Energy Balances and Numerical Methods 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 3 atm and then vaporized in a fired heater, H-701. Air, which may be assumed to contain only O<sub>2</sub> and N<sub>2</sub>, is mixed with recycle, if there is any recycle, compressed to 3 atm, and heated in E-701. The hot air and vaporized o-xylene are mixed and sent to a packed bed reactor. The contents 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 preliminary 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 21-23. The reactor effluent, which is at 2 atm, enters a complex series of devices known as switch condensers (SC-701). The feed to the switch condensers may be no higher than 180°C; hence, the reactor effluent must be cooled. The net result of the switch condensers is that all light gases and water leave in Stream 11, with small amounts of both anhydrides, and the phthalic anhydride and maleic anhydride leave in Stream 12. The “dirty air” in Stream 11 or Stream 15 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,” as long as there is also a purge stream. Any “dirty air” purged must be sent to a scrubber, not shown on the PFD, and an operating charge is assessed. The contents of Stream 12 are sent to a distillation column which produces liquid waste (Stream 13) which is burned for fuel. The product in Stream 14 must be 99.9 wt % phthalic anhydride. This process must produce 75,000 metric tons/year of phthalic anhydride.

### Process Details

#### Feed Streams

Stream 1: air, consisting of 79% N<sub>2</sub> and 21% O<sub>2</sub>

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

### Effluent Streams

Stream 15: air to treatment plant, appropriate cost charged

Stream 13: waste organic material, may be burned in fired heater  
energy content is lower heating value, energy value identical to natural gas

Stream 14: phthalic anhydride product, 75,000 metric tons/yr, 99.9 wt % pure

### Equipment

Compressor (C-701):

The compressor increases pressure of air feed from 1 atm to 3 atm at the valve outlet.

Pump (P-701):

The pump increases pressure of the o-xylene feed from 0.75 atm to 3 atm at the valve outlet. (For all pumps, the cost of energy may be neglected.)

Fired Heater (H-701):

The fired heater vaporizes the o-xylene feed and heats the vapor to any temperature.

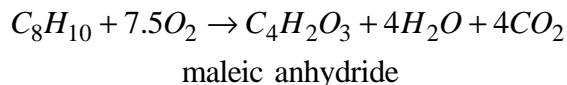
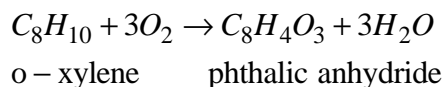
Heat Exchanger (E-701):

This heat exchanger heats the air feed. The air temperature may not exceed 5°C lower than the inlet steam temperature.

Reactor (R-701):

The reactor feed may be no lower than 300°C. The catalyst is only active to produce phthalic anhydride between 300°C and 420°C.

The following reactions occur:



The complete combustion of o-xylene also occurs.

Selectivity data are in Table 1. These data are approximate and are to be used only for this design project this semester, not for more complex versions to be completed in subsequent semesters.

<b>Table 1</b>			
<b>Fractional Conversion of o-Xylene into (Yield of) Indicated Product</b>			
<b>T(°C)</b>	<b>maleic anhydride</b>	<b>CO<sub>2</sub></b>	<b>phthalic anhydride</b>
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 - 23 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. This heat is then used to make high-pressure steam (in E-702) from boiler feed water, with an appropriate credit being taken for the steam made. The pressure of the bfw may be assumed to be the pressure of high-pressure steam. The temperature of Stream 21 may not exceed 5°C lower than Stream 9 (which is also the reactor temperature), and the temperature of Stream 23 may not exceed 5°C lower than the high pressure steam formed in E-702.

Switch Condensers (SC-701): These are a complex set of condensers. The feed may not exceed 180°C, so E-703 removes the necessary heat. The pressure must be less than or equal to 2 atm. The heat load may be assumed to be the equivalent of three times the amount of cooling water that would be needed to condense Stream 10 to Stream 12. This is the heat load necessary to heat and cool the oil. The oil is in a closed loop; the cost of the oil may be considered negligible.

Distillation Column (T-701): Here 99% of the phthalic anhydride goes to Stream 14. All of the maleic anhydride goes to Stream 13. The condenser (E-704) must condense all of the maleic anhydride. The reboiler (E-705) must boil an amount of phthalic anhydride equivalent to that in Stream 14. The distillation column operates at a pressure low enough to make the phthalic anhydride in the reboiler vaporize no higher than 5°C lower than the temperature of the high-pressure steam used in Stream 43.

## Recycle

It is possible to recycle some of the “dirty” air from Stream 11 as long as there is sufficient purge (Stream 15). 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.

## 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 <sup>6</sup> kJ
Electricity	\$0.05/kW hr
Boiler Feed Water (at 549 kPa, 90°C)	\$300.00/1000 m <sup>3</sup>
Cooling Water	\$20.00/1000 m <sup>3</sup>
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 <sup>6</sup> kJ	
Refrigerated Water	\$200.00/1000 m <sup>3</sup>
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 <sup>6</sup> kJ	

## Data

Use data from Reference [2] or from any handbook. The following data are not readily available in these references.

Vapor Heat Capacities (range 150°C - 450°C)

$$\text{form: } C_p(\text{cal/moleK}) = a + bT + cT^2 + dT^3, \quad T \text{ in (K)}$$

	<b>a</b>	<b>10b</b>	<b>10<sup>5</sup>c</b>	<b>10<sup>7</sup>d</b>
<b>o-xylene</b>	-3.786	1.424	-8.224	1.798
<b>phthalic anhydride</b>	-1.064	1.562	-1.023	2.411
<b>maleic anhydride</b>	-3.123	0.8323	-5.217	1.156

Liquid Heat Capacity (range 125°C - 200°C)

$$\text{for any organic: } C_p(\text{cal/mole}^\circ\text{C}) = 41.69 + 7.773 \times 10^{-2} T, \quad T \text{ in } (^\circ\text{C})$$

Vapor Pressures (range 100°C - 300°C)

$$\text{form: } \ln P^*(\text{mmHg}) = A - \frac{B}{T - C}, \quad T \text{ in (K)}$$

	<b>A</b>	<b>B</b>	<b>C</b>
<b>o-xylene</b>	16.1156	3395.57	59.46
<b>phthalic anhydride</b>	15.9984	4467.01	83.15
<b>maleic anhydride</b>	16.2747	3765.65	82.15

Normal heats of vaporization (cal/mole)

<b>o-xylene</b>	8800
<b>phthalic anhydride</b>	11850
<b>maleic anhydride</b>	5850

## 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

$$\text{EAOC} = -(\text{product value} - \text{feed cost} - \text{other operating costs} - \text{capital cost annuity})$$

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.

The capital cost annuity is an annual cost associated with plant construction (like a mortgage payment). A list of capital costs for each piece of equipment will be provided by Spring Break. You have learned to calculate the annuity value in ChE 38.

The other operating costs are for compression and for waste treatment.

Compression costs are:

$$\$/h = 0.007\dot{m} \left[ \left( \frac{P_{out}}{P_{in}} \right)^{0.3} - 1 \right], \quad \dot{m} \text{ in (kg/h)}$$

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:

$$\begin{aligned} \$ / m^3 \text{ air treated} &= 10^{-4} V_{tot} (0.5 + 1000x_{or}) \\ V_{tot} &= \text{total volume of "dirty air" to be treated, } m^3 \\ x_{or} &= \text{mole fraction of organics (CO}^2 \text{ is not an organic!) in "dirty air" stream} \end{aligned}$$

## Other Information

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

You should assume that two streams that mix must be at identical pressures.

## 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. 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. These may be neatly hand-written. Calculations which can not be followed easily will lose credit. Submission of a disk is optional. If a disk is submitted, it should be formatted for a PC (not an Apple). Material on a disk should be in addition to what is in the report; it should not duplicate information already in the report. Under

no circumstances will submission of a disk substitute for the sample calculations required in the appendix.

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 minutes, and each group member must speak. A five-minute question-and-answer session will follow. Instructions for presentation of oral reports will be provided in a separate document. However, the best way to learn how to present an oral report, other than actually presenting one, is to make time to see some of the oral reports presented by the juniors the week before you are to present your report.

The written project report is due upon presentation of the oral report. The oral reports will be Monday, April 24, 1995 (ChE 38 class) and Wednesday, April 26, 1995 (ChE 41 class). There will be a project review on Friday, April 28, 1995 (ChE 41 class). In addition, everyone must attend at least one (and preferably both) of the senior design presentations, either on Tuesday, April 25, 1995, or on Thursday, April 27, 1995 (substitutes for Thursday ChE 38 class). Furthermore, attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the lounge). 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 both ChE 38 and ChE 41.

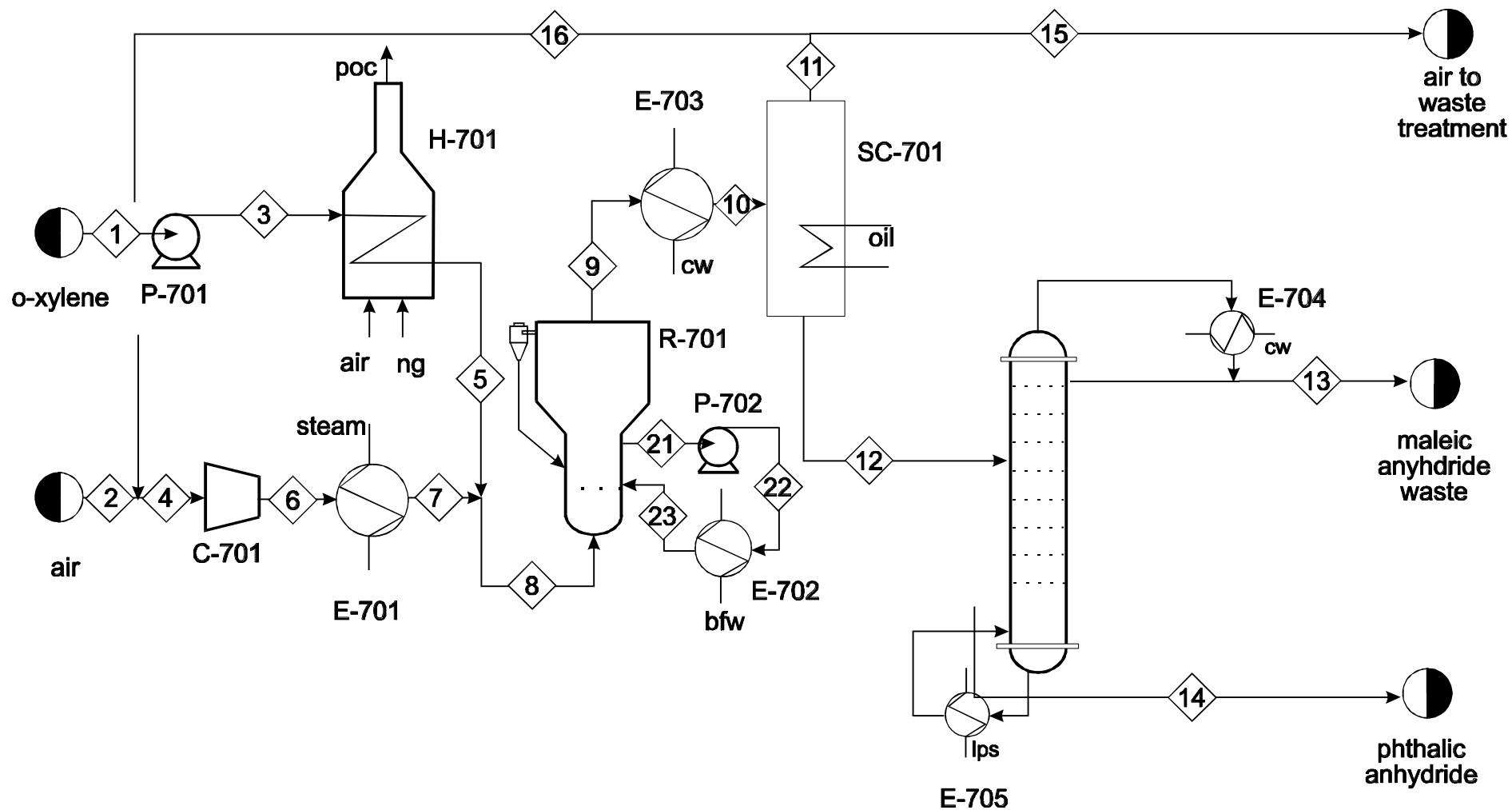
Anyone not participating in this project will automatically receive an F for ChE 38 and ChE 41, regardless of other grades earned in these classes.

## 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.
2. Felder, R.M. and R.W. Rousseau, *Elementary Principles of Chemical Processes (2nd ed.)*, Wiley, New York, 1986.



Unit 700 - Phthalic Anhydride from o-Xylene