Material Balances

Design Project

Production of Phthalic Anhydride from o-Xylene

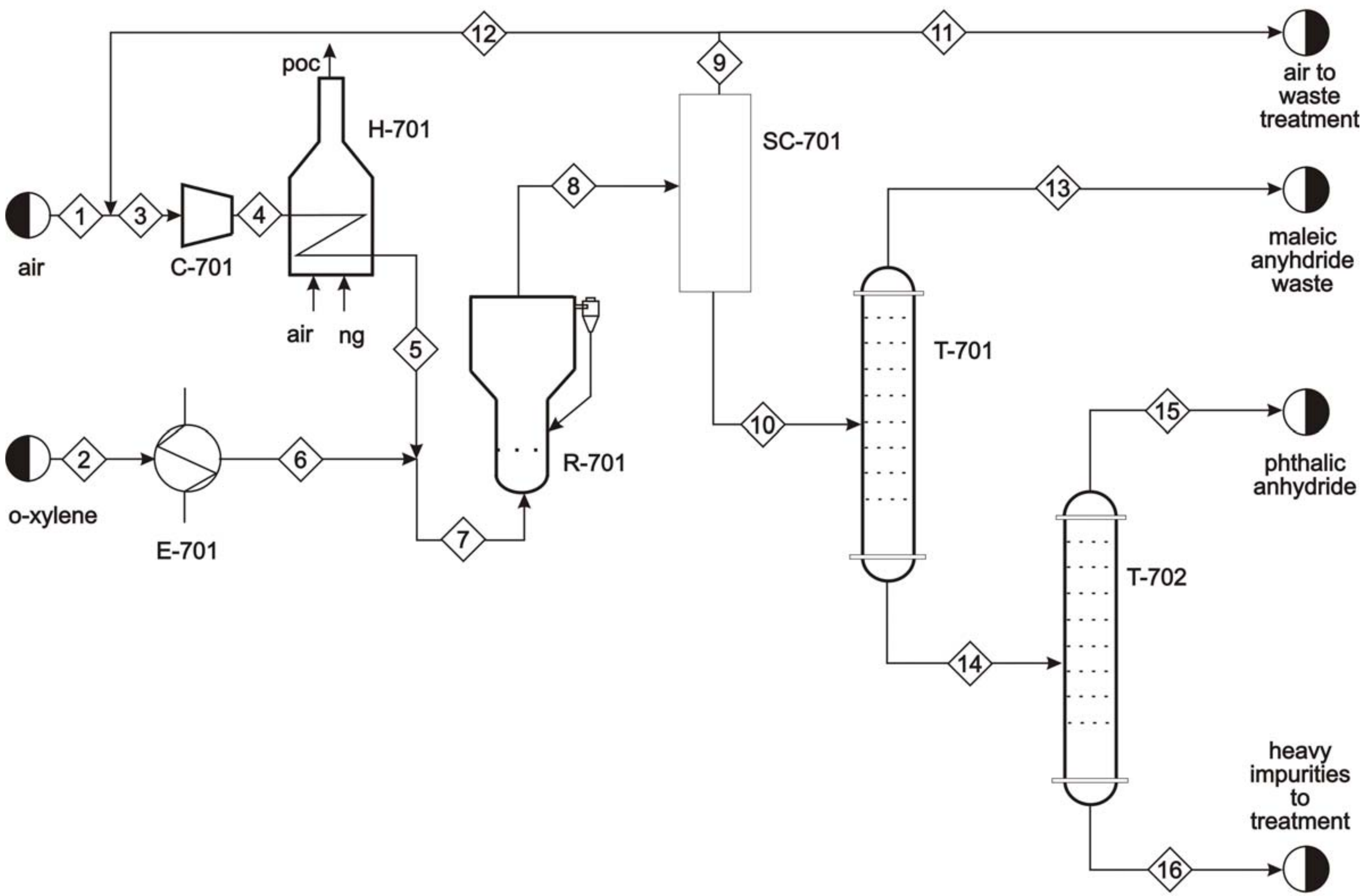
The most common method for production of phthalic anhydride is by oxidation of o-xylene. Phthalic anhydride is used in the manufacture of plasticizers (additives to polymers to give them more flexibility) and polyesters, among other applications. Additional information on phthalic anhydride, it uses, and its manufacture are available.[1] The purpose of this project is to determine the "best" process configuration for a phthalic anhydride from o-xylene process subject to constraints which will be defined later.

A suggested process flow diagram is in Figure 1. You should use this as a starting point. However, any change that you can justify that does not violate the laws of nature is allowed. Your assignment is to develop a "best" case, where "best" is dependent upon economic considerations. The primary issue is how much recycle is necessary/desirable in order to satisfy the flammability limit constraint described below. However, there may be other alternatives which improve process economics which you are left on your own to consider.

Process Description

The raw materials are air and o-xylene. The o-xylene feed, which contains 5 wt% inert impurities is vaporized in unit V-701. Air, which may be assumed to contain only O_2 and N_2, is mixed with recycle, if there is any recycle, and heated. The hot air and vaporized o-xylene are mixed and sent to a fluidized bed reactor. The contents of Stream 7 must be below the LFL of o-xylene, which is 1 mole%. In this reactor, essentially 100% of the o-xylene is reacted. Most goes to form phthalic anhydride, but some complete and incomplete combustion of o-xylene occurs, some maleic anhydride is formed, and a heavy impurity is also formed. The selectivities are given later. The reactor effluent enters a complex series of devices known as switch condensers. The net result is that all light gases and water leave in Stream 9, with small amounts of both anhydrides, and the phthalic anhydride, maleic anhydride, inerts, and heavy impurity leave in Stream 10. The "dirty air" in Stream 9 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" not recycled must be sent to a scrubber, in which the anhydrides are scrubbed into water. The water is then sent to an on-site waste water treatment plant, and an operating charge is assessed. The contents of Stream 10 are sent to a series of two distillation columns which produce liquid waste (Streams 13 and 16) which is burned for fuel. No economic credit is allowed. The product in Stream 15 must be 99.9 mass % phthalic anhydride. This process must produce 75,000 metric tons/year of phthalic anhydride.

C-701	E-701	H-701	R-701	SC-701	T-701	T-702
Feed Air Compressor	Feed o-Xylene Heat Exchanger	Fired Heater	Phthalic Anhydride Reactor	Switch Condensers	Maleic Anhydrice Tower	Phthalic Anhydride Tower



Unit 700 - Phthalic Anhydride from o-Xylene

Process Details

Feed Streams

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

Stream 2: o-xylene with 5 wt % inert impurity

Equipment

Compressor (C-701): increases pressure of air feed from 1 atm to 3 atm

Vaporizer (E-701): vaporizes o-xylene feed which is already above 3 atm

Fired Heater (H-701): heats air to rection temperature

Reactor (R-701): the following reactions occur:

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

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

The selectivity for the phthalic anhydride reaction is 70%, for the complete combustion of o-xylene is 15%, for the incomplete combustion of o-xylene is 5%, for maleic anhydride is 9%, and for the heavy impurity is 1%. The heavy impurity consumes a negligible amount of oxygen and produces a negligible amount of light gases.

Switch Condensers (SC-701): These are a complex set of condensers. Phthalic anhydride is first condensed as a solid (desublimated) and then melted. There are three condensers, one in the desublimation mode, one in the melting mode, and one in stand-by mode.

The recovery of phthalic anhydride is done using a set of switch condensers that desublimate the phthalic anhydride using cooled oil. This unit operation has been modeled as a component separator with the following fractions leaving in the off gas.

o-Xylene	1.00
Oxygen	1.00
Nitrogen	1.00
Water	1.00
Carbon Dioxide	1.00
Carbon Monoxide	1.00
Phthalic Anhydride	0.010
Maleic Anhydride	0.89
Heavy Impurity	0.00

Distillation Column (T-701): Here, 99% of the phthalic anhydride and all of the heavy impurity goes to Stream 14. All of the inert and enough of the maleic anhydride to allow Stream 15 to satisfy its purity requirement go to Stream 13.

Distillation Column (T-702): Here, 99.9% of the phthalic anhydride, and any remaining maleic anhydride go to Stream 15, and all of the heavy impurity goes to Stream 16.

Economic Analysis

When evaluating alternative cases, the following relationship should be used:

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

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

Phthalic anhydride is valued at \$1.54/kg, and o-xylene costs \$0.80/kg. The capital cost annuity is an annual cost associated with plant construction (kind of like mortgage payments), and may be assumed to be $\$2.4\times10^6$/yr. 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 cost is based upon the amount of organic matter (phthalic and maleic anhydrides) in Stream 11. The cost is:

$$\$500/1000\ \text{kg organic matter}$$

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 word processed report. It should be clear and concise. The format is explained in a separate document. When presenting results for different cases, graphs are superior to tables. The body of the report should be short, emphasizing only the results and briefly summarizing computational strategies. The report appendix should contain details of calculations that are easy to follow. Calculations which can not be followed easily will lose credit.

The project is due December 9, 2009, at the beginning of class.

Computational Methods

You may not use CAD software, but should use Excel spreadsheet calculations. Before developing a spreadsheet, you must solve the material balance by hand for at least one case to demonstrate that the spreadsheet is set-up correctly.

Groups

A student design group will consist of 4 group members. You are encouraged to choose a partner for this project to form a pair. When you have formed a pair, please write your names on the chart posted on Dr. Kugler's door. Dr. Kugler will combine pairs to form groups of four. Group assignments will be made on November 12.

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.

References

1. "Phthalic Acids and other Benzenepolycarboxylic Acids," *Kirk-Othmer Encyclopedia of Chemical Technology*, on-line version, 10/18/2001. (This encyclopedia is accessible from any University computer at http://www.libraries.wvu.edu/databases. An older print version is available in the Evansdale Library reference section.)