

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.

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. As part of the integrated chemical engineering curriculum at WVU, you will work on more complex versions of this problem through the end of your junior year, when you will have completed the design and evaluation of this process, including design of the equipment and more sophisticated energy and economic analyses than are possible in this semester.

A suggested process flow diagram is attached. 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 O₂ and N₂, is mixed with recycle, if there is any recycle, and heated. The hot air and vaporized o-xylene are mixed and sent to a packed 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% phthalic anhydride. This process must produce 75,000 metric tons/year of phthalic anhydride.

Process Details

Feed Streams

Stream 1: air, consisting of 79% N₂ and 21% O₂ - free

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

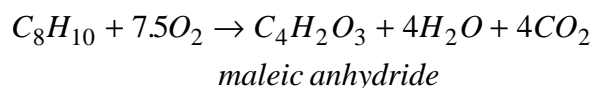
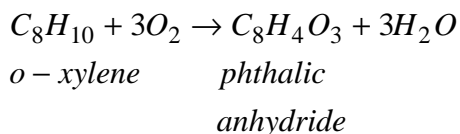
Equipment

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 reaction temperature

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



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 desublimated and then melted. There are three condensers, one in the desublimation mode, one in the melting mode, and one in stand-by mode.

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:

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

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 \$0.77/kg, and o-xylene costs \$0.30/kg. The capital cost annuity is an annual cost associated with plant construction (kind of like mortgage payments), and may be assumed to be $\$1.2 \cdot 10^6/\text{yr}$. 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:

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

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 November 30, 1994, at the beginning of class.

Anyone not participating in this project will automatically receive an F for ChE 40, regardless of other grades earned in this class.

Computational Methods

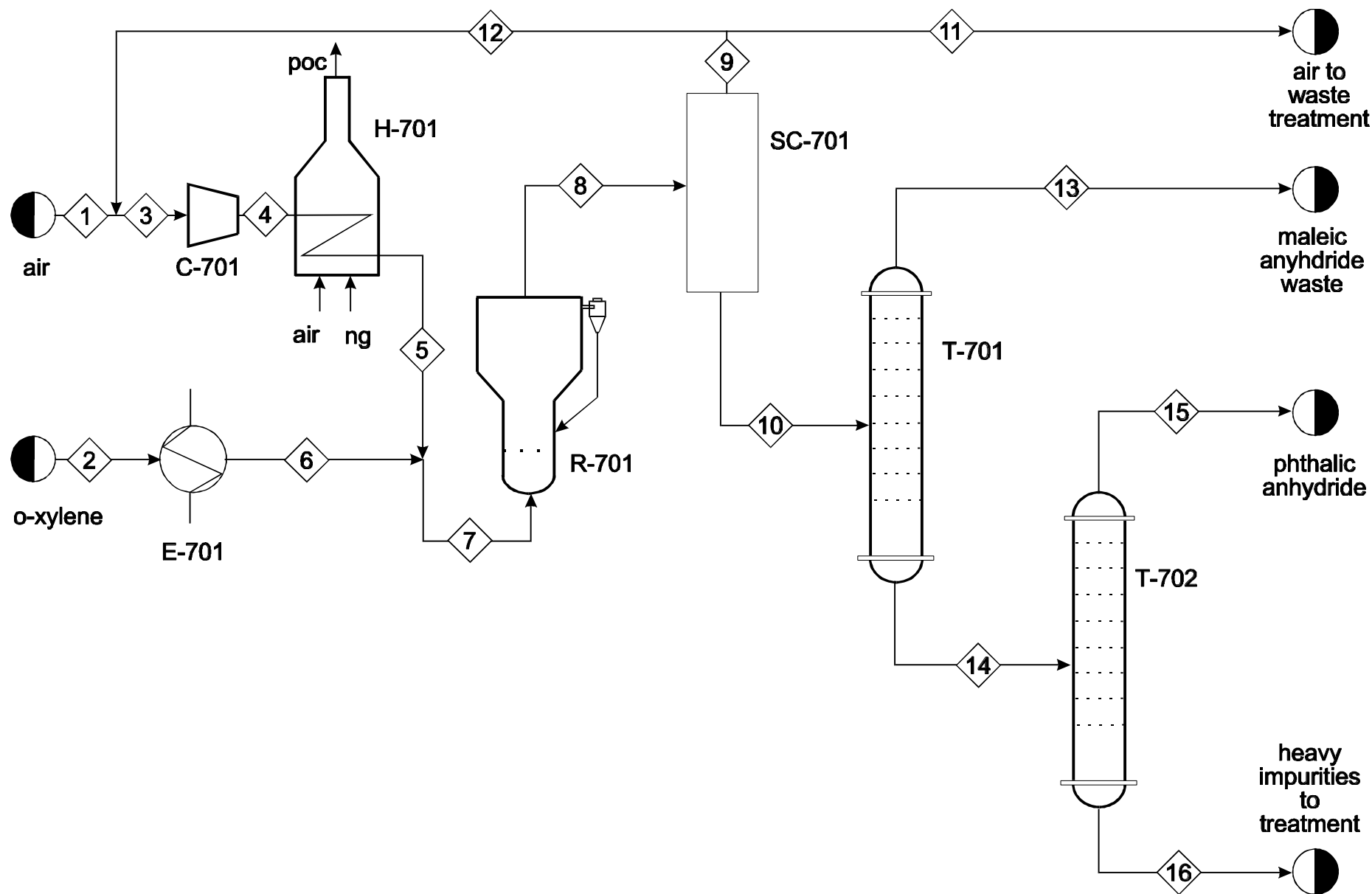
You may choose among several methods to do the necessary calculations. If you use Fortran or Basic programming, a clearly documented source code is required, along with a logic flow diagram. If you use a spreadsheet, a disk must be submitted which contains the spreadsheet in either .wk1 or .xls format (lotus or excel). If you use Quattro, the file you submit should be saved as a lotus (.wk1) file. It is also permissible to use MathCad, and a hard copy of the program should be submitted.

Groups

Groups of 3 or 4 are permissible. These must be selected so as to minimize the number of reports submitted. More details of group formation 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.



Unit 700 - Phthalic Anhydride from o-Xylene