The Design of a New, 100,000 Metric Tons Per Year, Phthalic Anhydride Production Facility

Background

The operation of Unit 700, phthalic anhydride facility, has been successfully scaled down by 50%. Over the long term, we are still considering changing to o-xylene as the raw material. The catalysis and reaction engineering group has finished preliminary research and is very optimistic about their new catalyst. They promise that it will be superior to other versions of o-xylene to phthalic anhydride catalysts in that most side products are minimized. At this point we are uncertain as to whether Unit 700 will be retrofitted to accommodate the new catalyst or whether we will build a new, grass-roots facility at another site, nearer to an o-xylene producer.

In order for us to have enough information to make an informed decision, we need a preliminary process design for a grass-roots facility to produce phthalic anhydride from what may be assumed to be pure o-xylene. Your job is to prepare a preliminary design for the new 100,000 metric tons/yr phthalic anhydride from o-xylene plant, and it must be completed within the next month. You may assume that the o-xylene feed is available at 100°C and 1.1 bar and that the required purity for phthalic and maleic anhydride products are 99.9 wt% and 95.0 wt% respectively.

Other Information

Concentrated organic waste streams may be burned instead of natural gas only if a fired heater is included in the design. Dilute organic waste streams must be sent to a treatment facility, with the appropriate operating cost charged. The capital cost of this facility may be assumed to be included in the grass roots cost of the new facility. Other pertinent information is given below and in Tables 1, 2 and 3.

Assignment

Your assignment is to provide:

1. an optimized preliminary design of a plant to make phthalic anhydride from o-xylene using the new catalyst

2. an economic evaluation giving the *NPV* (net present value), after-tax, of the new project. For your evaluation you should use the following economic information:

   After tax internal hurdle rate = 9%

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Depreciation = MACRS (6 year schedule given in Prob. 4.18)
Marginal taxation rate of 35%
Construction period of 2 years
Project plant life = 10 years after start-up

Specifically, you are to prepare the following by ...... (4 weeks from now):

1. a written report detailing your design and profitability evaluation of the new process

2. a clear, complete, labeled process flow diagram of your optimized process

3. a clear stream flow table giving the T, P, total flowrate in kg/hr and kmol/hr, component flowrate in kmol/hr, and phase for each important process stream.

4. a list of new equipment to be purchased, including size, cost, and materials of construction

5. an evaluation of the after-tax NPV, and the discounted cash flow rate of return on investment ($DCFROR$) for your recommended (optimized) process

6. a legible, organized set of calculations justifying your recommendations, including any assumptions made
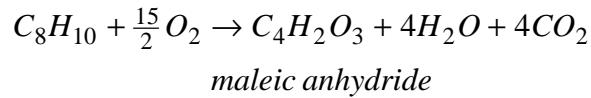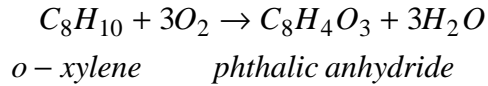
Report Format

This report should be in the "standard" design report format. It should include an abstract, results, discussion, conclusions, recommendations, and an appendix with calculations. The report format rules given in Chapter 22 of your textbook [1].

References

1. Turton, R., Bailie, R.C., Whiting, W.B., and J.A. Shaeiwitz, Analysis, Synthesis, and Design of Chemical Processes, Prentice-Hall, Upper Saddle River, NJ, 1998.

Table 1: Information on Reaction Kinetics (Unit 700)

The catalysis and reaction engineering group has obtained the following kinetic information regarding the o-xylene to phthalic anhydride reaction. The reactions are

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

$$C_8H_{10} + \tfrac{15}{2}O_2 \rightarrow C_4H_2O_3 + 4H_2O + 4CO_2$$
$$maleic\ anhydride$$

In addition, the complete combustion reaction for each organic component occurs. The reaction network is given below. As you can see, a major advantage of our catalyst is that CO formation is essentially eliminated and no heavy impurity is made.
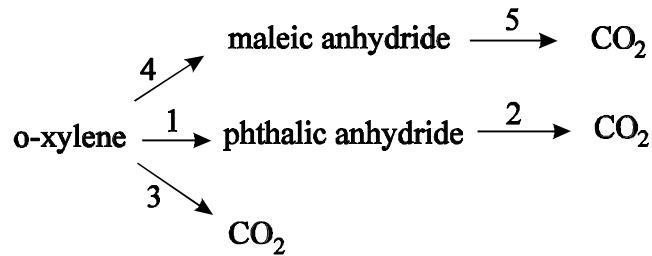
The catalyst must operate between 300°C and 400°C, and at pressures between 1 atm and 3 atm. In this range, the kinetics are as follows: (partial pressures in atmospheres, r_i in kmol hr^{-1} (kg catalyst)$^{-1}$, $k_0 = 1$ kmol hr^{-1}(kg catalyst)$^{-1}$atm^{-2}, $R = 1.987$ cal/K mole, and T is in K)

$$r_1 = k_1 p_{xy} p_{o_2} \qquad \ln \frac{k_1}{k_0} = -\frac{27{,}000}{RT} + 19.837$$

$$r_2 = k_2 p_{pa} p_{o_2} \qquad \ln \frac{k_2}{k_0} = -\frac{31{,}000}{RT} + 20.86$$

$$r_3 = k_3 p_{xy} p_{o_2} \qquad \ln \frac{k_3}{k_0} = -\frac{28{,}600}{RT} + 18.97$$

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$$r_4 = k_4 p_{xy} p_{o_2} \qquad \ln \frac{k_4}{k_0} = -\frac{27{,}900}{RT} + 19.23$$

$$r_5 = k_5 p_{ma} p_{o_2} \qquad \ln \frac{k_5}{k_0} = -\frac{30{,}400}{RT} + 20.47$$

The lower flammability limit of o-xylene in air is 1 mol%, and the upper flammability limit is 6 mole%. For safety reasons, it is necessary that process conditions not be within these limits. It is also necessary that the o-xylene content of the reactor never exceed 10 mole%, because, if that limit is exceeded, the catalyst no longer operates at the desired selectivity, the reaction could become oxygen starved, forming significant amounts of CO and other undesired byproducts.

At this time, we are unsure as to whether a packed bed reactor (shell and tube type - modeled as plug flow reactor) or a fluidized bed reactor (modeled as an isothermal plug flow reactor with 10 % feed gas bypass) is the better choice. Please address this in your preliminary design. For the shell and tube packed bed, the catalyst would be in the tubes. We do believe, however, that tube diameters exceeding one inch in a shell and tube configuration would not allow for rapid enough heat removal, causing significant hot spots, and subsequent catalyst damage.

For a fluidized bed, the following data may be assumed:

spherical catalyst particle, diameter range d_p = 300 - 600µm
catalyst particle density r_{cat} = 1600 kg/m^3
void fraction at minimum fluidization e_{mf} = 0.50
heat transfer coefficient from fluidized bed to tube wall h = 300 W/m^2°C
reactor should operate between $2u_{mf}$ (bubbling) and $50u_{mf}$ (turbulent)
the reactor has a rectangular cross section (width of sides = w & v)
range of acceptable side ratios $0.2 < v/w < 5$
maximum value of v or w = 8 m
maximum volume of bed displaced by tube banks is 40%

for u_{mf}, use the correlation of Wen & Yu:

$$\mathrm{Re}_{mf} = \frac{d_p u_{mf} \rho_g}{\mu} = \left[(33.7)^2 + \frac{0.0408 d_p^3 \rho_g (\rho_s - \rho_g) g}{\mu^2} \right]^{0.5} - 33.7$$

where r_g is the density of the gas in the fluidized bed (at average conditions) and r_s is the solid catalyst particle density (called r_{cat} above).

For a shell and tube packed bed, the following data may be assumed:

catalyst particle diameter d_p = 3 mm
catalyst particle density r_{cat} = 1600 kg/m^3
void fraction e = 0.50
heat transfer coefficient from packed bed to tube wall h = 60 W/m^2°C
use standard tube sheet layouts as for a heat exchanger
shell diameter is a function of heat transfer characteristics and frictional losses

It is anticipated that a heat transfer fluid will be used in a closed loop to remove the highly exothermic heat of reaction from either type of reactor. We anticipate that all surplus high pressure steam made can be sold elsewhere in the plant. Since we have had many years of successful operation using the HiTec™ molten salt, we anticipate using it again for the new process. However, you should feel free to recommend an alternative if you can justify superior performance at the same cost, or equal performance at a lower cost.

Table 2: Design of the Switch Condensers and Air Treatment Costs (Unit 700)

These are a complex set of condensers. There are three. Because of the low partial pressure of phthalic anhydride in the stream, it desublimates rather than condenses. Therefore, the process stream is cooled using a low temperature oil in tubes to promote desublimation. Then, after solid is loaded on the heat transfer surface, gas flow to this condenser is stopped, and higher temperature oil is circulated in the tubes to melt the solid. There are three such devices, one operating in desublimation mode, one operating in melting mode, and one on standby. The net result is a liquid stream containing the condensables and a vapor stream containing some maleic anhydride, some phthalic anhydride, and all of the non-condensables.

These condensers will once again be designed and maintained under contract by Condensex. They indicate that operation at any scale is possible as long as the pressure of the feed to the condensers is between 1.70 and 2.00 bar. You may assume that all light gases are neither condensed nor dissolved, and that 99 % of the organics are desublimated and melted. Based on past experience, Condensex suggests that we may estimate the capital cost of these condensers as 15% of all the other capital costs for the new process. In addition, the annual operating cost is 3 times the cost of an equivalent amount cooling water needed to satisfy the cooling duty from the energy balance on the condenser unit modeled as a component separator.

The following cost of treating the waste (dirty) air stream leaving the switch condensers should be used in your cost estimates.

Air Treatment Cost = $10^{-4}V_{tot}(0.5+1000x_{or})$

where V_{tot} = the total volume of "dirty air" to be treated, m^3 and x_{or} = mole fraction of organics in "dirty air" stream

Table 3: Simulator Hints (Unit 700)

The following hints were developed for students using the CHEMCAD ™ simulator. These should also provide help to people using other simulator packages.

Use SRK (Soave Redlich Kwong) for the VLE and enthalpy options in the thermodynamic package for all the units in this process.

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger.. For the switch condensers, use a component separator, and then calculate the heat duty from the inlet and outlet streams

When simulating a process using "fake" streams and equipment, it is imperative that the process flow diagram that you present not included any "fake" streams and equipment. It must represent the actual process.