

Your assignment is to provide recommendations as to how much immediate scale-down is possible and what, if any, modifications would be needed to scale down by 50%. For now, you are to consider only the portion of the process prior to the switch condensers. You should also recommend any other changes that you feel should be made to improve performance in Unit 700. Because our plant is due for annual shutdown in a few months, we want specific recommendations as to what should be done at that time and the cost of these alterations and/or modifications.

Specifically, you are to prepare the following by two weeks from now:

1. A written report detailing the maximum scale-down possible, how to achieve 50% scale-down, recommendations, and costs associated with scaling down production in Unit 700.
2. A list of new equipment to be purchased, including size, cost, and materials of construction.
3. An analysis of any change in the annual operating cost created by your recommended modifications.
4. A legible, organized set of calculations justifying your recommendations, including any assumptions made.

### **C.3.5. Report Format**

This report should be brief. Most of the report should be an executive summary, not to exceed five double-spaced, typed pages, that summarizes your diagnosis, recommendations, and rationale. Figures and tables may be included (and do not count against the page limit) in the executive summary. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. In general, the written report should follow the guidelines given in [Chapter 29](#) (in this CD).

## **PROJECT 4. The Design of a New 100,000-Metric-Tons-per-Year Phthalic Anhydride Production Facility**

### **C.4.1. Background**

The operation of Unit 700, our 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 its 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, grassroots 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 grassroots 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/y 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 is 99.9 wt% and 95.0 wt%, respectively.

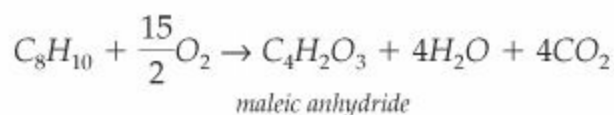
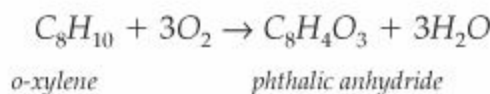
### **C.4.2. Other Information**

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

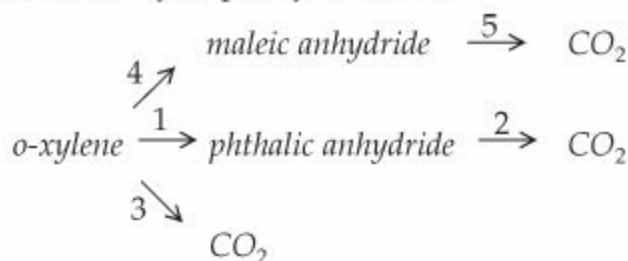
appropriate operating cost charged. The capital cost of this facility may be assumed to be included in the grassroots cost of the new facility. Other pertinent information is given below and in [Tables C.10](#), [C.11](#), and [C.12](#).

**Table C.10. 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



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  $\text{kmol h}^{-1} (\text{kg catalyst})^{-1}$ ,  $k_0 = 1 \text{ kmol h}^{-1} (\text{kg catalyst})^{-1} \text{ atm}^{-2}$ ,  $R = 1.987 \text{ cal/K mole}$ , and  $T$  is in K.)

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

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

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

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

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

The lower flammability limit of o-xylene in air is 1 mol%, and the upper flammability limit is 6 mol%. 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 mol%, because if that

limit is exceeded, the catalyst no longer operates at the desired selectivity, and the reaction could become oxygen starved, forming significant amounts of CO and other undesired by-products.

At this time, we are unsure as to whether a packed-bed reactor (shell-and-tube type, modeled as a 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 1 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  $d_p = 300\text{--}600\mu\text{m}$

Catalyst particle density  $\rho_{cat} = 1600\text{ kg/m}^3$

Void fraction at minimum fluidization  $\varepsilon_{mf} = 0.50$

Heat transfer coefficient from fluidized bed to tube wall  $h = 300\text{ W/m}^2\text{C}$

Reactor should operate between  $2u_{mf}$  (bubbling) and  $50u_{mf}$  (turbulent)

The reactor has a rectangular cross section (width of sides =  $w$  and  $v$ )

Range of acceptable side ratios  $0.2 < v/w < 5$

Maximum value of  $v$  or  $w = 8\text{ m}$

Maximum volume of bed displaced by tube banks is 40%

The cost of the fluidized bed should be estimated as 5 times the cost of a vessel of the same volume

For  $u_{mf}$ , use the correlation of Wen and Yu:

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

where  $\rho_g$  is the density of the gas in the fluidized bed (at average conditions) and  $\rho_s$  is the solid catalyst particle density (called  $\rho_{cat}$  above).

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

Catalyst particle diameter  $d_p = 3\text{ mm}$

Catalyst particle density  $\rho_{cat} = 1600\text{ kg/m}^3$

Void fraction  $\varepsilon = 0.50$

Heat transfer coefficient from packed bed to tube wall  $h = 60\text{ W/m}^2\text{C}$

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. Because 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 C.11. Design of the Switch Condensers and Air Treatment Costs (Unit 700)**

These are a complex set of three condensers. 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 noncondensables.

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 other capital costs for the new process, and that the annual operating cost is 3 times the cost of an equivalent amount of 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:

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

where  $V_{tot}$  = the total volume of “dirty air” to be treated,  $\text{m}^3$ , and  $x_{or}$  = mole fraction of organics in “dirty air” stream.

### Table C.12. 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 include any fake streams and equipment. It must represent the actual process.

### C.4.3. Assignment

Your assignment is to provide the following:

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%
  - Depreciation = MACRS (6-year schedule given in [Chapter 9](#))
  - 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 . . . (four 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/h and kmol/h, component flowrate in kmol/h, 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

#### C.4.4. 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 29](#) (in this CD) should be followed.

### PROJECT 5. Problems at the Cumene Production Facility, Unit 800

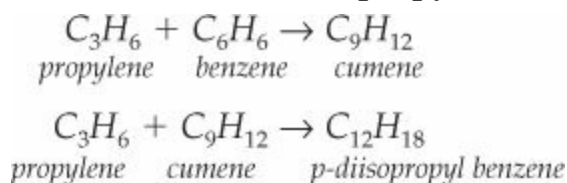
#### C.5.1. Background

Cumene (isopropyl benzene) is produced by reacting propylene with benzene. During World War II, cumene was used as an octane enhancer for piston engine aircraft fuel. Presently, most of the worldwide supply of cumene is used as a raw material for phenol production. Typically, cumene is produced at the same facility that manufactures phenol.

The plant at which you are employed currently manufactures cumene in Unit 800 by a vapor-phase alkylation process that uses a phosphoric acid catalyst supported on kieselguhr. Plant capacity is on the order of 90,000 metric tons per year of 99 wt% purity cumene. Benzene and propylene feeds are brought in by tanker trucks and stored in tanks as a liquid.

#### C.5.2. Cumene Production Reactions

The reactions for cumene production from benzene and propylene are as follows:



#### C.5.3. Process Description

The PFD for the cumene production process, Unit 800, is given in [Figure C.8](#). The reactants are fed from their respective storage tanks. After being pumped up to the required pressure (dictated by catalyst operating conditions), the reactants are mixed, vaporized, and heated in the fired heater to the temperature required by the catalyst. The shell-and-tube reactor converts the reactants to desired and undesired products as per the above reactions. The exothermic heat of reaction is removed by producing high-pressure steam from boiler feed water in the reactor. The stream leaving the reactor enters the flash unit, which consists of a heat exchanger and a flash drum. The flash unit is used to