ChE 321: Kinetics and Reactor Design
(Due: 2/9/2011, Wednesday)

1. In the class, I have explained how to derive the following Equation 1 by doing the mole balance on the PFR,

$$\frac{dF_i}{dz} = A\, r_i \qquad \text{(Equation 1)}$$

Derive Equation 2 from Equation 1.

$$\frac{dV}{F_{io}} = \frac{dx_i}{-r_i} \qquad \text{(Equation 2)}$$

[F_i=molar flow rate of species "i," z = direction of flow, A = cross sectional area of the reactor, r_i=reaction rate of species "i."]

2. There were 820 million pounds of phthalic anhydride produced in the United States in 1995. One of the end uses of phthalic anhydride is in the fiberglass of sailboat hulls. Phthalic anhydride can be produced by the partial oxidation of naphthalene in either a fixed or a fluidized catalytic bed. A flowsheet for the commercial process is shown in Figure P3-11. Here the reaction is carried out in a fixed-bed reactor with a vanadium pentoxide catalyst packed in 25-mm-diameter tubes. A production rate of 31,000 tons per year would require 15,000 tubes.

Set up a stoichiometric table for this reaction for an initial mixture of 3.5% naphthalene and 96.5% air (mol %), and use this table to develop the relations listed below. P_0 = 10 atm and T_0 = 500 K.

(a) For an isothermal flow reactor in which there is no pressure drop, determine each of the following as a function of the conversion of naphthalene, X_N.

(1) The partial pressures of O_2 and CO_2 (*Ans.*: $P_{CO_2} = 0.345\ [5.8 - 9/2\ X]/(1 - 0.0175\ X)$)

(2) The concentrations of O_2 and naphthalene (*Ans.*: $C_N = 0.084\ (1 - X)/(1 - 0.0175\ X)$)

(3) The volumetric flow rate v

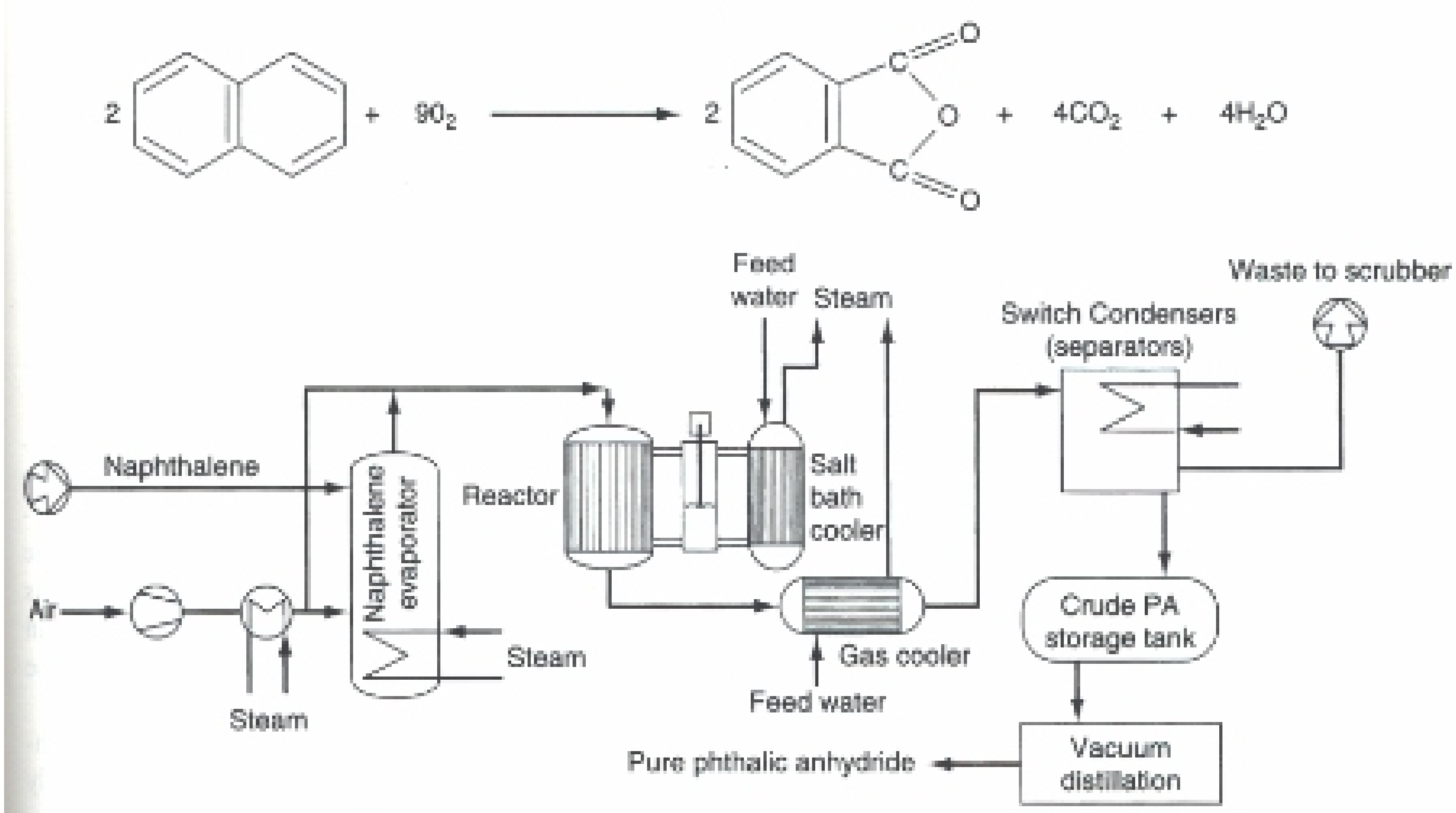

Figure P3-11 [Adapted from *Chemical Engineering, Process Technology and Flowsheet*, Vol. IIK pp. 111 and 125.]

(c) If the reaction just happened to be first order in oxygen and second order in naphthalene with a value of k_N of 0.01 $dm^6/mol^2 \cdot s$, write an equation for $-r_N$ solely as a function of conversion for parts (a) and (b).

3. The reaction

$$A \longrightarrow B$$

is to be carried out isothermally in a continuous-flow reactor. Calculate both the CSTR and PFR reactor volumes necessary to consume 99% of A (i.e., $C_A = 0.01C_{A0}$) when the entering molar flow rate is 5 mol/h, assuming the reaction rate $-r_A$ is:

(a) $-r_A = k$ with $k = 0.05 \dfrac{\text{mol}}{\text{h} \cdot \text{dm}^3}$ (*Ans.*: $V = 99$ dm³)

(b) $-r_A = kC_A$ with $k = 0.0001\ \text{s}^{-1}$

(c) $-r_A = kC_A^2$ with $k = 3 \dfrac{\text{dm}^3}{\text{mol} \cdot \text{h}}$ (*Ans.*: $V_{CSTR} = 66{,}000$ dm³)

The entering volumetric flow rate is 10 dm³/h. [*Note*: $F_A = C_A v$. For a constant volumetric flow rate $v = v_0$, then $F_A = C_A v_0$. Also, $C_{A0} = F_{A0}/v_0 =$ (5 mol/h)/(10 dm³/h) = 0.5 mol/dm³.]

4. Radial reactors are sometimes used in catalytic processes where pressure drop through the reactor is an important economic parameter. For example, radial reactors are frequently used in ammonia synthesis and in naphtha reforming to produce high-octane gasoline. Top and cross-sectional views of a typical radial catalytic reactor are shown below.