CE 329 Fall 2015

Class 22 Worksheet

1. The rate of liquid-phase reaction (1) is adequately described by the rate expression given in equation (2). Reactant A is fed to a CSTR at a rate of 0.01 lbmol min^{-1}, and reactant B is fed at a rate of 0.25 lbmol min^{-1}. This corresponds to an inlet volumetric flow rate of 0.08 ft^3 min^{-1}. The CSTR has a fluid volume of 18 ft^3, and it operates adiabatically. The heat of reaction may be taken to be constant and equal to -1.7 x 10^4 BTU lbmol^{-1}. The heat capacities of A, B and Z are equal to 1000, 180 and 1200 BTU lbmol^{-1} °R^{-1}, respectively, and they may be considered to be independent of temperature. What will the conversion and outlet temperatures equal if the combined feed enters at 600, 650 or 700 °R.

$$A + B \rightleftarrows Z \tag{1}$$

$$r_1 = \left(1.2 \times 10^{14}\ \text{ft}^3\ \text{lbmol}^{-1}\ \text{min}^{-1}\right)\exp\left\{\frac{-23000\ °\text{R}}{T}\right\}C_AC_B \times\left[1-\frac{C_Z}{\left(6.5 \times 10^{-13}\ \text{ft}^3\ \text{lbmol}^{-1}\right)\exp\left\{\frac{20000\ °\text{R}}{T}\right\}C_AC_B}\right] \tag{2}$$

2. A certain kind of living cell grows according to the Monod equation as given in equation (1). The concentrations in equation (1) are mass concentrations. Under the conditions to be studied (for which equation (1) is accurate), 2.2 grams of substrate are consumed for every one gram of cells that is produced. An isothermal, steady-state chemostat that performs like an ideal CSTR is being to be used to grow the cells. The reactor volume is 4000 cm^3, and the feed stream contains 0.04 g cm^{-3} of substrate and 8.0 x 10^{-5} g cm^{-3} of cells. If the feed rate is 60 cm^3 min^{-1}, determine what would happen if the cells were suddenly removed from the feed and comment upon what you find. Then repeat the analysis for the case where the inlet volumetric flow rate is 50 cm^3 min^{-1}.

$$r = \frac{\left(0.014\ \text{min}^{-1}\right)[S][X]}{\left(0.001\ \text{g cm}^{-3}\right)+[S]} \tag{1}$$

3. A 500 cm^3 CSTR will operate adiabatically with a feed of 1.0 cm^3 s^{-1} containing equal amounts of A and B (0.015 mol cm^{-3}) at 50 °C. The heat capacity of the fluid is essentially equal to that of the solvent, 0.35 cal g^{-1} K^{-1} and can be considered to be constant. The (constant) density of the fluid is 0.93 gm cm^{-3}. The reaction of interest is given in equation (1). The standard heat of this reaction is constant and equal to -20 kJ mol^{-1}. The rate expression is given in equation (2). The reactor will first be filled with pure solvent at 190 °C, and then a valve will be opened, admitting the feed. How long will it take for the reactor to reach 260 °C, and what will the conversion of A equal?

$$A + B \rightarrow Y + Z \tag{1}$$

$$r_1 = 3.24\times10^{12}\left(\frac{\text{cm}^3}{\text{mol s}}\right)\exp\left\{\frac{-25\text{ kcal mol}^{-1}}{RT}\right\}C_AC_B \qquad (2)$$

4. Reactants A and B can react irreversibly to produce either a desired product, D, or an undesired product, U, as shown in equations (1) and (2). The corresponding rate expressions are given in equations (3) and (4). A feed stream containing 10 mol A per gal and 12 mol B per gal at 350 K is fed to a 25 gal adiabatic CSTR at a rate of 12.5 gal min^{-1}. If the standard heats at 298 K of reactions (1) and (2) are -12.0 and -21.3 kJ mol^{-1}, respectively, and if the temperature-independent heat capacities of A, B, D and U are 85, 125, 200 and 170 J mol^{-1} K^{-1}, what are the conversion of the limiting reagent, the outlet selectivity (in mol D per mol U) and the outlet temperature, and how will they vary with time?

$$\text{A + B} \rightarrow \text{D} \qquad (1)$$

$$\text{A + B} \rightarrow \text{U} \qquad (2)$$

$$r_1 = \left(1.12\times10^2\text{ min}^{-1}\right)\exp\left\{\frac{-15300\text{ J mol}^{-1}}{RT}\right\}C_A \qquad (3)$$

$$r_2 = \left(1.87\times10^2\text{ min}^{-1}\right)\exp\left\{\frac{-23700\text{ J mol}^{-1}}{RT}\right\}C_B \qquad (4)$$

5. A certain kind of living cell grows according to the Monod equation as given in equation (1). The concentrations in equation (1) are mass concentrations. Under the conditions to be studied (for which equation (1) is accurate), 2.2 grams of substrate are consumed for every one gram of cells that is produced. An isothermal, steady-state chemostat that performs like an ideal CSTR is going to be used to grow the cells. The reactor volume is 4000 cm^3, and the feed stream contains 0.04 g cm^{-3} of substrate and 8.0 x 10^{-5} g cm^{-3} of cells. If the feed rate is 60 cm^3 min^{-1}, calculate the inlet and outlet mass flow rates of substrate and cell mass, along with the percentage increase in the cell mass.

$$r = \frac{\left(0.014\text{ min}^{-1}\right)[S][X]}{\left(0.001\text{ g cm}^{-3}\right)+[S]} \qquad (1)$$

6. Reaction (1) takes place in an adiabatic CSTR with a volume of 1.5 L. The feed to the reactor consists of 5 mol% ethane in air at 2 atm and 350 °C. The kinetics are given by equation (2) with k_0 = 1.4 x 10^8 min^{-1} and E = 30 kcal mol^{-1}. The heat of reaction at 298 K is -211 kJ mol^{-1}. The heat capacities of the gases may be taken as constant (in J mol^{-1} K^{-1}); C_2H_6 – 99, O_2 – 33.5, N_2 – 31, C_2H_4 – 77.7, H_2O – 37.5. The reactor is going to be started up at a space time of 10 min by one of two procedures. Calculate and plot the ratio of inlet ethane flow to outlet ethane flow and the outlet temperature as a function of time for each of the following initial conditions: (a) the reactor is initially filled with unreacted feed at an initial temperature of 425 °C and (b) the reactor is initially filled with completely reacted feed at 425 °C. You may neglect the change in volumetric flow rate caused by the change in moles, but you should still account for

the change caused by thermal expansion. Put differently, you may assume that the outlet and inlet volumetric flow rates are related according to equation (3)

$$2\ C_2H_6 + O_2 \rightarrow 2\ C_2H_4 + 2\ H_2O \tag{1}$$

$$r = k_0 e^{\frac{-E}{RT}} C_{C_2H_6} \tag{2}$$

$$\dot{V} = \dot{V}^{in}\left(\frac{T}{T^{in}}\right) \tag{3}$$

7. Consider an adiabatic CSTR with a fluid volume of 0.4 L. Suppose the liquid phase reaction A → Z takes place in the reactor. The feed to the reactor is at 330 K; it flows at 1 L min^{-1} and it contains 5 mol A L^{-1}. The heat capacity of the solution is 1000 cal L^{-1} K^{-1}, and it is independent of both temperature and composition. The reaction is exothermic with a heat of -30,000 cal mol^{-1}. The rate is first order in the concentration of A. The pre-exponential factor equals 4.8 x 10^{13} min^{-1} and the activation energy is 24,000 cal mol^{-1}. Determine the outlet concentration of Z as a function of time.

8. The irreversible, homogeneous, liquid-phase reaction A → R + S takes place in an adiabatic CSTR. Pure A is fed to the reactor at a rate of 50 L min^{-1}, 4 mol/L, and at a temperature of 350 K. The reactor operates at a constant pressure of 10 atm. The reaction is first order in A with a rate coefficient given by equation (5).

$$k = (4.4 \times 10^{-1}\ s^{-1}) \exp\{-(17{,}300 cal/mol)/(RT)\} \tag{5}$$

Heat capacities of the species, in cal mol^{-1} K^{-1}, are as follows: A = 11.3, R = 10.1, and S = 13.0; and the heat of reaction is constant and equal to -22 kcal/mol. What must the space velocity equal for the conversion to be 50%, and what will be the outlet temperature at this space velocity?

9. The irreversible aqueous reaction A → B is to be run in an adiabatic CSTR using a feed at 300 K with a concentration of A of 2 mol/L (there is no B in the feed). The reactor volume is 1000 L, and the space time is to be 1.5 min. The thermal properties of the fluid may be taken to equal those of the solvent, water (1 cal g^{-1} K^{-1} = 18 cal mol^{-1} K^{-1}). The reaction is first order in A with a rate coefficient of 0.02 min^{-1} at 300K and an activation energy of 30 kcal/mol. The heat of reaction is −25,000 cal/mol and may be taken to be constant. In order to start up the reactor, it will be filled initially with only water at 335 K. Show how to calculate the conversion versus time until the reactor reaches steady state.

10. A jacketed CSTR with a fluid volume of 0.4 L is cooled using water flowing at 2.0 L min^{-1}. The coolant is supplied at 20 ºC. The jacket heat transfer area is 0.7 m^2 and the heat transfer coefficient is 100 BTU h^{-1} ft^{-2} $ºR^{-1}$. The liquid phase reaction A → Z takes place in the reactor. The feed to the reactor is at 330 K; it flows at 1 L min^{-1} and it contains 5 mol A L^{-1}. The heat capacity of the solution is 1000 cal L^{-1} K^{-1}, and it is independent of both temperature and composition. The reaction is exothermic with a heat of -30,000 cal mol^{-1}. The rate is first order in the concentration of A. The pre-exponential factor equals 4.8 x 10^{13} min^{-1} and the activation energy is 24,000 cal mol^{-1}. Determine the outlet concentration of Z as a function of time if the cooling water temperature is changes to 35 ºC.