CE 329 Fall 2015

Class 19 Worksheet

Suppose the catalytic reaction (1) below is reactant inhibited with a rate expression of the form shown in equation (2). The reaction is irreversible, and K is very, very small in magnitude. Predict, qualitatively, how the rate and the conversion will vary as a function of isothermal batch reaction time (a) if $P_A^0 = P_B^0$ and (b) if $P_A^0 > P_B^0$.

$$A + B \rightarrow Y + Z \quad (1)$$

$$r = \frac{kP_B}{K + P_A} \quad (2)$$

1. Read through the problem statement and identify (a) the type(s) of reactor(s) being used, (b) the reactor operating procedure being used (isothermal vs. adiabatic, steady state vs. transient, etc.), (c) the type of reaction(s) taking place (reversible/irreversible, typical, auto-catalytic, product inhibited, etc.) and (d) the quantities whose variation you are asked to describe

2. Sketch a plot of reactant concentration(s), product concentrations, temperature, reaction rate and other quantities of interest versus time (for a batch reactor) or space time (for a flow reactor)
   a. Draw sets of axes for the plots

b. Determine the initial values of each of these quantities (at the start of the reaction or inlet to the reactor) and add to the corresponding plots

c. Determine the initial slope of the plots of these quantities by considering the first small increment in time (or space time) and add to the plots
    i. Do the reactant concentrations, product concentrations and temperature increase or decrease during this interval?

    ii. Will those changes cause the reaction rate to increase or decrease during this interval?

    iii. Do the quantities of interest increase or decrease during this interval?

    iv. Will those changes cause the equilibrium conversion to increase or decrease during this interval?
    v. if comparing two or more systems, for each plot, determine the which system will have the largest slope, the second largest slope, etc.
d. Determine the curvature of the plots by considering the next small increment in time (or space time) and add to the plots
    i. Do the reactant concentrations, product concentrations, temperature and rate change by a greater or lesser amount than during the preceding interval?

    ii. Do the quantities of interest change by a greater or lesser amount than during the preceding interval?

e. Determine whether continuing the initial trends will result in the rate asymptotically approaching equilibrium
    i. If not, infer what must happen so that the system approaches equilibrium properly (i. e. so the rate progressively decreases to zero)

f. If comparing two or more systems, determine the relative magnitudes of the equilibrium concentrations and temperatures in order to ascertain whether or not the curves for the systems being compared cross each other

3. Use the plot(s) to answer the questions posed in the problem