EEC 503 Spring 2013

REVIEW 2: IDEAL REACTOR CONCEPTS

SINGLE PHASE, ISOTHERMAL SYSTEMS

1. What are the basic assumptions in describing an ideal batch reactor of constant volume for processing either a liquid phase or gas phase system? Apply the conservation equation to species j and define the pertinent symbols used. If you have a single reaction how many species balances are needed? How many balances are needed for R multiple reactions.

2. A single liquid phase reaction of known stoichiometry occurs in an isothermal ideal batch reactor of constant volume. You know the initial composition of this mixture and monitor the change of concentration of reactant A in the system in time. From this information you need to obtain the dependence of the rate of reaction on reactant concentration and the value of the rate constant. Describe how you would do that using: a) differential analysis, b) integral analysis method!

3. A single gas phase reaction of known stoichiometry occurs in an isothermal ideal batch reactor of constant volume. You know the initial composition of this mixture and monitor the change of total pressure in the system in time. Describe how the pressure change is related to the stoichiometric coefficients, initial composition and molar extent of reaction, or some other measure of reaction progress. From this information you need to obtain the dependence of the rate of reaction on reactant concentration and the value of the rate constant. Describe how you would do that using: a) differential analysis, b) integral analysis!

4. Two ideal reactor concepts for steady state operation of continuous flow reactors are: a) ideally mixed continuous flow stirred tank reactor (IMFR or CSTR or CFSTR), and b) plug flow reactor (PFR) or piston flow reactor (PF). State the basic assumptions for each, and write a species mass balance for reactant A that is involved in a single reaction of stoichiometry A +bB = pP. Assume that the reaction rate of disappearance of A is given as a function of pertinent concentrations and relate the reactor volume V needed to reach a specified conversion of A, x_A , in processing a feed at volumetric flow rate Q with fixed feed concentrations of A and B. a) What is the space time for each reactor? b) Find the volumetric productivity for each reactor and compare for reaction of first and second order.

5. Sketch the reciprocal of the reaction rate versus conversion for an n-th order reaction and discuss using the graph what space time in a CSTR and PFR is at a given conversion and how they compare.

6. Describe how you would evaluate the reaction rate as a function of reactant concentration from a series of steady state runs in a constant volume CSTR when you varied the flow rate and measured steady state exit concentration at each flow rate used while keeping the feed composition constant.

7. In multiple reactions conducted in a PFR or a CSTR you need to solve as many species balances as there are independent reactions. To gain insight it is useful, whenever possible to monitor the behavior of the point yield (ratio of the rate of desired product formation over the consumption rate of key reactant involved in several reactions) as a multi-dimensional surface over the permissible composition field in order to determine what optimal contacting patterns might be. Assume that such a point yield (R_R/-R_A) can be expressed as a function of concentration of A, C_A , only. To maximize the yield of R would you use a) CSTR or b) PFR if the point yield is: i) a monotonically rising function of $C_{A,}$ b) a monotonically decreasing function of C_A. What is the best choice if the point yield exhibits a maximum at some concentration C_{Am} between the feed value and zero?

NONISOTHERMAL, SINGLE PHASE SYSTEMS

1. List the assumptions needed to represent the energy balance for a single reaction as shown below:

$$\underset{(I)}{\rho Q \underline{C}_{pm}(T - T_o)} + \underset{(II)}{\dot{X}\Delta H_R} = \underset{(III)}{\dot{q}}$$

a) Define all the symbols used in the above equation with appropriate consistent units.

b) Explain what each of the terms I, II, III represents.

c) Is the above equation valid for any reactor type?

2. Consider a single reaction A+bB = pP in a system of constant density conducted in a CSTR. a)Present the energy and species balances that need to be solved to calculate rate of heat removal or addition needed to keep the system isothermal. b) Show equations that need to be solved for an adiabatic system. c) what is the adiabatic temperature rise as a function of conversion?

3. For a single exothermic reaction, of stoichiometry discussed above, in cooled CSTR of given size and at fixed flow rate and feed composition and temperature, sketch graphically how to obtain the steady state conversion and temperature. You can assume that the heat removal rate is proportional to the product of the overall heat transfer coefficient, total heat exchange area and the difference between the reactor temperature and constant coolant temperature. Under what conditions based on the graph are multiple steady states possible?

4. Consider a single reaction A+bB = pP in a system of constant density conducted in a PFR . Present the energy and species balance that need to be solved to calculate the conversion change along the reactor (i.e. change with increased space time) in an adiabatic reactor . What is the criterion used to ensure safe adiabatic operation?

5. Consider a single reaction A+bB = pP in a system of constant density conducted in a PFR . Present the energy and species balance that need to be solved to calculate the conversion and temperature change along the reactor (i.e. change with increased space time) if the cooling rate is every proportional to the product of the overall heat transfer coefficient, total heat exchange area per unit reactor volume and the difference between the local reactor temperature and constant coolant temperature. What is the criterion used to ensure safe operation and avoid hot-spots?