Study Guide Final Exam

In order to do well on the next test, you should be able to do the following:

1. Explain in your own words that the terms *elementary reactions*, *non-elementary reactions*, *rate equation*, *rate constant, reaction order, reaction dependence on temperature (Arrhenius' Law)*, *collision theory vs. transition theory.*

2. Be able to derive the relationship between rates of reaction of all reaction species and their stoichiometry coefficients.

3. Be able to derive relationship between time and concentration or conversion (C vs. t, X vs. t) for different types of reaction rate models (ie. zero order, 1^{st} order, 2^{nd} order, n^{th} order).

4. Be able to develop reaction rate models from reaction mechanisms and apply necessary assumption (ie. regarding transition species behavior dx/dt = 0, [x]=constant, etc) to see if rate equations fit observed behavior (see examples 2.1 and 2.2 in text).

5. Be able to derive M-M rate equation for an enzymatic reaction as well as its integration form for obtaining the relationship between concentration and time.

6. Be able to derive the terms *Km, Vm* for different inhibition enzymatic kinetics (ie. competitive inhibition, uncompetitive inhibition, non-competitive inhibition) and understand how concentrations of inhibitor [I] affect Km and Vm using the Lineweaver-Burke plot.

7. Explain in your own words that the terms *space-time* and *space-velocity.*

8. Be able to apply the mass balance for any reactant (or product) in reactor.

9. Be able to derive performance equations for ideal batch and steady-flow reactors and their integrated expressions for various types of reactions (ie. enzymatic reactions, zero order, 1^{st} order, 2^{nd} order).

10. Be able to solve for the sizes, flow rates, and production rates (qC_0X) of mixed and plug flow reactors, and compare the performance of MFR and PFR for a given duty.

11. Be able to derive performance equations for single reactors in series (PFR, MFR) or combinations in terms of C_n and overall conversion, X, i.e. X = f(tau, k).

12. Be able to determine the performance differences for both single reactors (MFR and PFR) and mixed reactors in series (MFR/PFR) in terms of C_n and overall conversion, X.

13. Explain in your own words for the terms *RTD*, *E(t)*, *F(t)*, and convolution integral.

14. Be able to determine E(t) and F(t) using pulse input and step input.

15. Be able to plot the E(t) curve given an F(t) curve or F(t) curve given an E(t) curve.

16. Be able to determine the conversion (X) for a reaction (ie. zero order, 1st order, 2nd order) in a non-ideal reactor as a function of C_0, k, and E(t).

17. Explain in your own words for the Shrinking Core Model *Film Diffusion Controls*, *Ash Diffusion Controls*, and *Reaction Controls* as well as Shrinking spheres.

18. Be able to determine τ, t/τ, and conversion of the solid reactant X(t) for various shapes of particles in the shrinking core models.

19. Be able to develop/derive the models for different reaction mechanisms (i.e. 1st, 2nd order reactions and M-M kinetics) for each limiting situation (film layer, reacted layer, reaction) and each geometrical shape (plate, cylinder, sphere).

20. Be able to determine the significant resistance in fluid solid reactions and calculate the reaction time for a given conversion (i.e. Problem 3 in exam 4).

21. Explain in your own words for difference between the units/dimensions of the reaction rate, r, for homogeneous vs. heterogeneous reactions, thiele modulus and the effectiveness factor (i.e. what does it measure/quantify and how is it used).

22. Be able to calculate thiele modulus and the effectiveness factor and determine actual reaction rates for catalysts of various shapes (i.e. Equations 13, 20, 22 in pp 386-387)

23. Be able to determine conversion for mixed flow and plug flow reactors containing catalysts.

Practice problems:

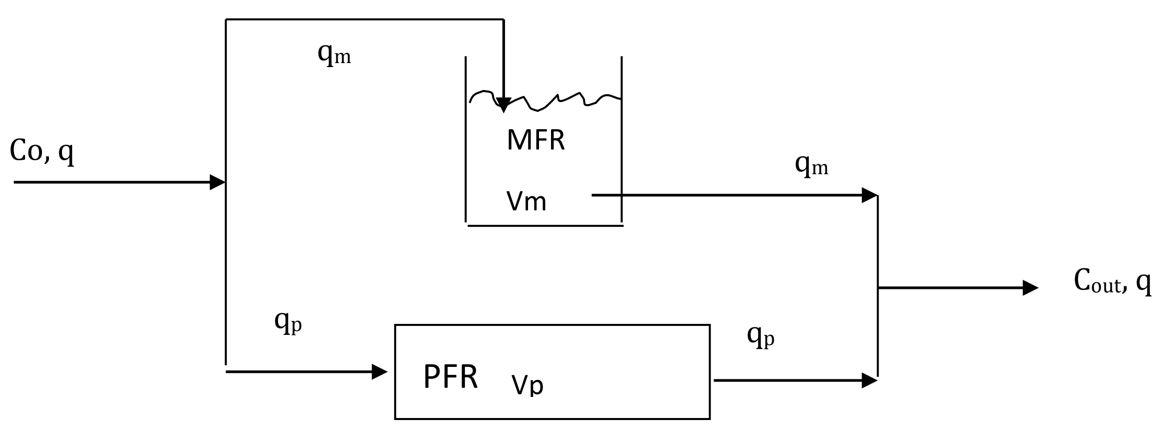
Problem 1:

A process is used to make product Z by a 1st order reaction ($k=0.186\ min^{-1}$) in 2 ideal mixed flow reactors in series. The required overall conversion is 96.0% using an inlet reactant concentration = 5.7 mol/L (both fixed values)

Process operating conditions: Flowrate = 500 L/hr.

A. Calculate the size (L) of an individual reactor.
B. If you were to shift production (same flow rate) over to using only one PFR, what would be the size (L) of the reactor?

Problem 2: Derive the equation giving C_{out} as a function of Co, q_p, q, V_m, V_p, and k, assuming an zero order reaction occurs in the ideal reactors of this steady state system.



Assume outlet concentrations of each reactor are C_m and C_p, respectively.

Problem 3:

For a chemical reaction in which 'ash' layer diffusion controls the overall reaction, a flat plate (total thickness 2L) requires 10 minutes to be completely reacted. Under the same reaction conditions, calculate how long it would take (in min) for a cylinder and a sphere made of the same material to be completely reacted, assuming R = L in both cases.

How can we improve effectiveness (i.e. increase reaction rate) of the systems of different geometries?