ASSIGNMENT-6, CHE331A, 2020-21 1st Semester

1. The elementary reversible liquid-phase reaction $A \leftrightarrow B$ takes place in a CSTR with a heat exchanger. Pure A enters the reactor. Derive an expression (or set of expressions) to calculate heat of generation, G(T), as a function of heat of reaction, equilibrium constant, temperature. Show a sample calculation for G(T) at T = 450 K.
Given: Ua = 3600 cal/min K, V = 20 dm^3, ΔH_{RXN} = – 60,000 cal/ mol A, volumetric flowrate = 1 dm^3/min, K_e= 200 at 450 K, Molar flow rate of A = 10 mol/min, k = 2 min^{-1} at 450 K

2. The elementary irreversible gas-phase reaction $A \rightarrow B+C$ is carried out adiabatically in a PFR packed with a catalyst. Pure A enters the reactor at a volumetric flow rate of 20 dm^3/s at a pressure of 10 atm and a temperature of 550 K. What catalyst weight is necessary to achieve 75% conversion in a CSTR?
Given: Initial concentration of A = 2 mol/dm^3, ΔH_{RXN} = – 15000 J/mol, Activation energy = 25000 J/mol, k = 0.133 dm^3/kgcat.s at 550 k, $C_{P,A}$ = 40 J/(mol.K), C_{PB} = 25 J/(mol.K), $C_{P,C}$ =15 J/mol.K)

3. For an adiabatic reaction with W_s and ΔC_P = 0, sketch the conversion, X_{EB}, as a function of temperature for: a) an exothermic reaction. b) an endothermic reaction and c) give X_{MB} = f(T) using the combined mole balance, rate law, and stoichiometry for a first order irreversible reaction $A \longrightarrow B$ carried out in a CSTR. Show how to locate the steady state conversion and temperature. Sketch necessary graphs. X_{MB} and X_{EB} are conversions based on mol balance and energy balance equations, respectively.

4. The acid catalyzed irreversible liquid phase reaction $A \longrightarrow B$ is carried out adiabatically in a CSTR. The reaction is second order in A. The feed, which is equimolar in water (which contains the catalyst) and A, enters the reactor at a temperature of 62˚C and a total volumetric flow rate of 20 dm^3/min. The concentration of A entering the reactor is 8 mol/dm^3.

   a) What is the reactor volume to achieve 90% conversion?
   b) How to calculate exit conversion and temperature when volume of reactor is given? Sketch necessary graphs and justify your answer.

Given: ΔH_{RXN} = – 4000 cal/mol, C_{PA} = 20 cal/mol.K= C_{PB}, C_{PW} = 25 cal/mol.K, E = 10000 cal/mol, and k = 0.0005 dm^3/(mol.s) @ 25°C