Midterm Examination #2
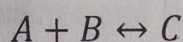
(200) 1. The following reversible gas-phase reaction is carried out in a cylindrical plug flow reactor (PFR) of radius R:

$$A + B \leftrightarrow C$$

The reactor is isothermal with temperature T_1, at which temperature the reaction equilibrium constant is K_1. The reaction exhibits elementary kinetics with forward rate constant k_1 and reverse rate constant k_{-1}. Species A is fed to the reactor with molar flowrate F_{A0} along with an equimolar flow of species B. You may assume ideal gas behavior.

(20) a) Suppose that the reaction goes to equilibrium. Write the expression for the equilibrium constant in terms of the mole fractions of A, B, and C, and the pressure at the reactor outlet, P. What are the units of K_1? Should the reactor be run at low or high pressure and why?

(25) b) Using species mole balances and the equilibrium constant derived in part a), derive an expression for the equilibrium conversion of A (X_A) in terms of K_1, F_{A0}, and the pressure at the reactor outlet, P

(35) c) Explain qualitatively how long the reactor must be for equilibrium to be reached. The reverse rate constant has units of inverse time. Using this fact, find an expression to estimate quantitatively the necessary length of the reactor, L, to reach equilibrium in terms of k_{-1}, F_{A0}, the inlet concentration of A (C_{A0}), and R.

(35) d) Suppose that the reactor temperature is increased to a higher temperature T_2. Assuming that the enthalpy of reaction (ΔH_{rxn}) is negative, qualitatively explain how the equilibrium conversion will change. Write an expression that can be solved algebraically to determine K_2 from T_1, T_2, ΔH_{rxn}, and K_1. What assumption(s) must be made in order to use this expression?

(40) e) Write (but do not solve) the PFR design equations (which are equivalent to the PFR mole balances) for species A, B, and C, and each boundary condition required to solve the equations. Is the volumetric flow rate through the reactor constant? Why or why not?

(45) f) Let the plug-flow reactor be cylindrical with radius R. Suppose now that the reactor wall is a cylindrical membrane that allows species C to permeate through it but not species A or B. The rate at which species C permeates through the membrane per unit surface area is directly proportional to the concentration of species C. Derive (but do not solve) a new PFR design equation for species C for this membrane reactor and list its boundary condition. How are the mole balance equations for species A and B affected by the membrane-wall modification? Why would a membrane reactor be used?