Chemical Reaction Engineering—Homework #5

Due: Online submission on Canvas, **Wednesday, February 26, 2020 at 11:59pm.**

No late submissions will be accepted.

Problems that require a numeric answer should have 3 significant figures.
Units, where required, are shown in blue. Please use these units.

Problem 1: Unsteady-state CSTR operation

MN Chemicals has a CSTR that is close to overflowing. Inside of the CSTR the following reaction is occurring:

$$A \rightarrow 2P$$

The reaction is run in the liquid phase in isothermal operation. To stop the overflow from occurring, the operator changes the outlet volumetric flow rate to be 1.5 times the inlet volumetric flow rate. Assume that the volume of the CSTR is large enough that it does not run dry under these conditions. The rate law for this reaction is:

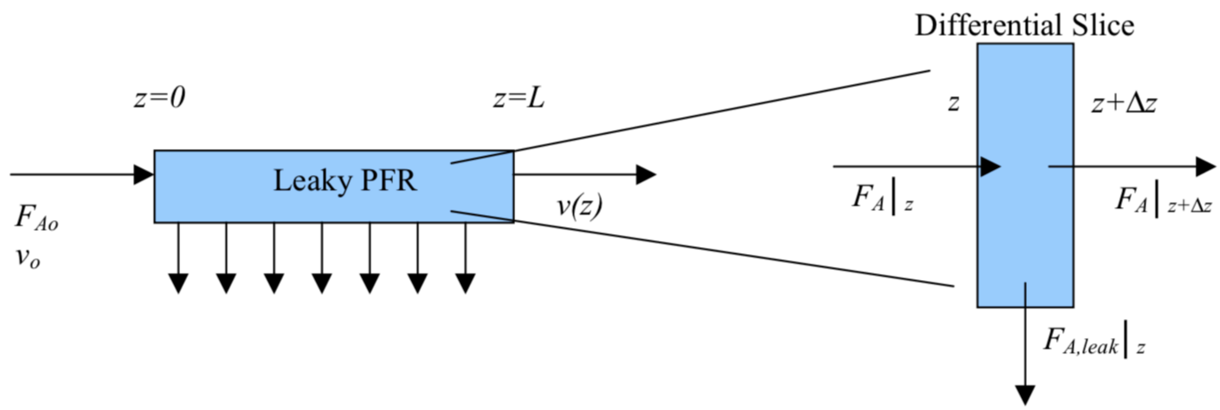
$$-r_A = k_1 c_A^2$$

a. Write the differential equations showing how c_A and c_P change with time.

b. The inlet volumetric flow rate is 10 L/hr. If the reaction is run for 2 hours with a 1000 L reactor charged initially with 200 mol of A and $k_1 = 0.02$ $M^{-1}s^{-1}$, how much product leaves the reactor? [10 mol]

Problem 2: Leaky PFR

You found that the PFR in your chemical plant has loose screws and has a continuous leak along its axial direction.
The volumetric flow rate along the axial direction decreases as a result of the leak and is



a function of axial position, z, as follows:

$$v(z) = v_0\left(1 - \frac{z}{L}\right)$$

The first order gas phase reaction A → B is to be carried out isothermally and isobarically.

a. Determine an expression for $F_{A,leak}|_z$ in terms of dv/dz, c_A, Δz.

b. Write a mole balance on a differential slice of the reactor. Assume the PFR has a constant cross-sectional area A_c. Obtain an equation in terms of Δz, dv/dz, F_A, c_A, A_c, k, and z. Be sure to include the term for the amount of A lost through the leak in a differential volume element—denoted by $F_{A,leak}|_z$.

c. Allow Δz to approach 0 and obtain a differential equation for conversion X in terms of dv/dz, dX/dz, A_c, F_{A0}, C_A, k, and z. Your dependent variables should be v and X while the independent variable should be z.

d. Write an expression for dX/dz. Use $v(z) = v_0\left(1 - \frac{z}{L}\right)$ to simplify further the equation.

e. Integrate to find X as a function of z.

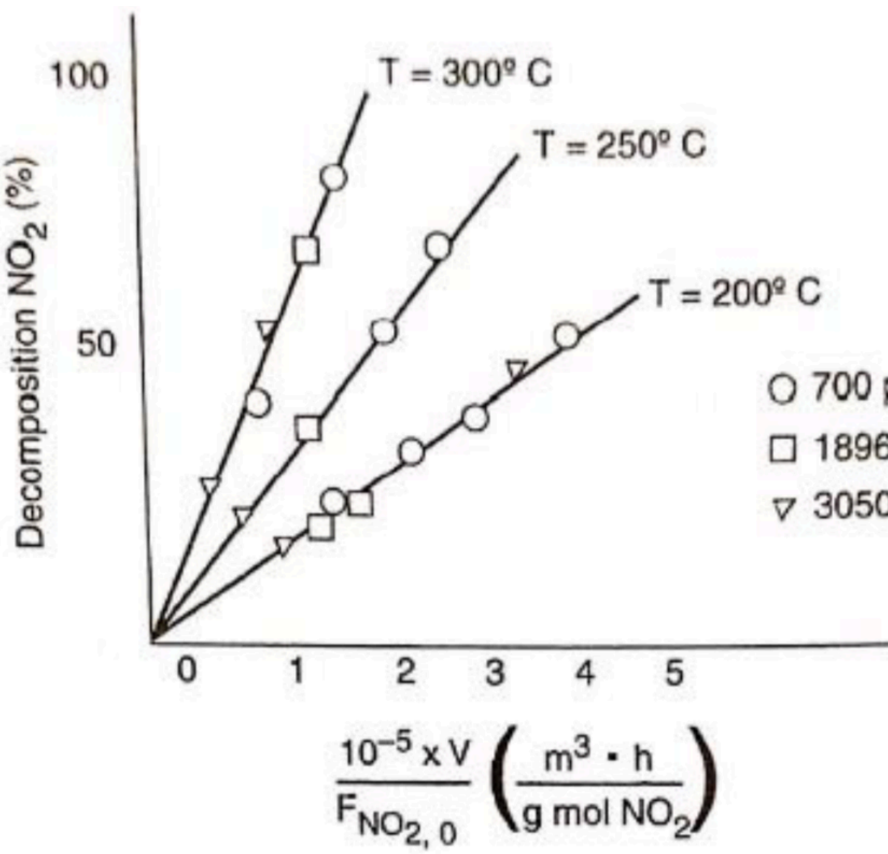
Problem 3: Membrane reactor

The elementary, gas-phase reversible reaction A $\leftrightarrow$ B + 2C occurs in an isothermal, isobaric, steady-state membrane PFR with a forward rate constant of k_1 and an overall equilibrium constant of K_C. The reactor is tubular with a constant cross-sectional area. Pure A enters the reactor, and B diffuses out through the membrane. Unfortunately, a small amount of reactant A also diffuses through the membrane. The rate of diffusion of species i through the membrane at any given point along the reactor is equal to the constant, β_i, multiplied by the local concentration of species i.

Plot the flow rate of A, B, and C along the length of the reactor, from z = 0 to z = $L_{reactor}$.

Additional information:
$k_1 = 10\ \text{min}^{-1}$
$K_C = 0.01\ M^2$
$\beta_A = 1\ \text{min}^{-1}$
$\beta_B = 40\ \text{min}^{-1}$
$F_{A0} = 100$ mol/min
$v_0 = 100$ L/min
Cross sectional area: 2 dm^2
$L_{reactor} = 10$ dm

Problem 4: Differential reactor



A steady-state differential reactor was used to study the decomposition of nitrogen oxides in automobile exhaust. In one series of experiments, a stream containing various concentrations of NO_2 was fed to a reactor, and the kinetic data is shown below. The plot gives the fractional decomposition of NO_2 versus the ratio of the reactor volume V in cm^3 to the NO_2 feed rate, $F_{NO2,0}$ in mol/hr at different feed concentrations of NO_2 in ppm (by weight).

a. Derive the mole balance for a differential flow reactor that relates the rate of NO_2 consumption, $-r_{NO2}$, to the conversion of NO_2, X_{NO2}. Why is the equation an algebraic one rather than a differential one?

b. Estimate the order of reaction in NO_2. Justify your estimation.

c. Estimate the activation energy.