Chemical Reaction Engineering—Homework #9
Due: Online submission on Canvas as PDF, **Wednesday, April 8, 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: Non-ideal reactors

Experiments are being performed using a reactor with non-ideal flow. The exit concentration in response to a pulse input with an inlet volumetric flow rate of 0.1 L/s is given below.

$C = 0$	for $t < 3$ s
$C = 0.5t - 1.5$	for $3s < t < 5s$
$C = -t + 6$	for $5s < t < 6s$
$C = 0$	for $t > 6s$

C has units of mol/L.

a. What is the total amount of tracer fed at t = 0? [0.15 mol]

b. Find an algebraic expression for the residence time distribution function E(t) and graph this as a function of time.

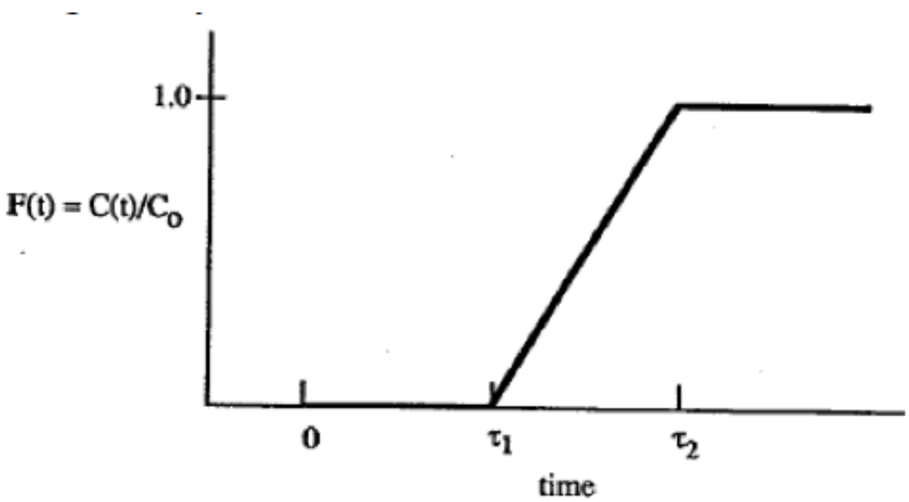
c. Plot F(t) of this reactor to a step change in inlet concentration from 0 to 1 mol/L at t = 0.

d. What is the mean residence time in this reactor? [4.5 s] What is the volume of this reactor? [0.45 L]

e. Using the segregation model of mixing, what is the mean conversion for the second order reaction $A \rightarrow B$ with k = 0.5 L/(mol*s), and C_{A0} = 1 mol/L? [0.7] How does this compare to the conversions achieved in a CSTR and a PFR operating at the same residence time?

Problem 2: Writing E(t) from F(t)

The response of an isothermal tubular reactor to a step change in concentration at t = 0 is given by the following graph.



a. Write an expression for E(t) and sketch the predicted response of this reactor to a pulse input.

b. Calculate the conversion of A in this reactor using a segregated model for this non-ideal tubular reactor for the liquid phase reaction. The experimental conversion is 35%. [0.35]

Reaction: $A + B \rightarrow C$

Rate law: $-r_A = kC_AC_B$

$C_{A0} = 2C_{B0}$ $kC_{A0} = 0.05\ s^{-1}$

$\tau_1 = 30s$ $\tau_2 = 50\ s$

Problem 3: Mass transfer limited or kinetically limited systems

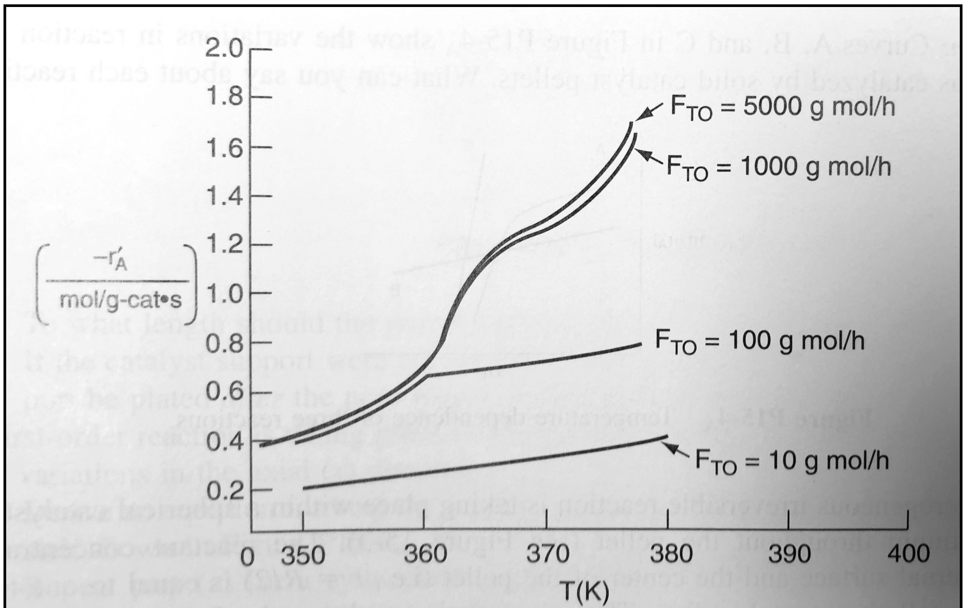


Figure P15-2$_B$ Reaction rates in a catalyst bed.

Answer the following questions using the figure above from Fogler.

a. Is the reaction limited by external diffusion?
b. If your answer from part a was Yes, under what conditions (flow rate and temperature) is the reaction limited by external diffusion?
c. Is the reaction "kinetically limited?"
d. If your answer from part c was Yes, under what conditions (flow rate and temperature) is the reaction limited by the rate of chemical reaction?
e. Is the reaction limited by internal diffusion?
f. If your answer from part e was Yes, under what conditions (flow rate and temperature) is the reaction limited by internal diffusion?

Problem 4: Concentration gradients and internal effectiveness factor

Consider an irreversible first-order heterogeneous reaction inside a porous spherical pellet that is coated on the inside with platinum. Let the reactant concentration halfway between the external surface and the center of the pellet ($r = R/2$) be equal to one-tenth of the concentration of the pellet's external surface. At the external surface, the concentration is 0.001 mol/L, the effective diffusion coefficient is 0.1 cm^2/s, and the diameter is 0.002 cm. Assume that the pellet is isothermal.

a. At a radial distance of 0.0003 cm inside from the external pellet surface, what is the concentration of the reactant? [2×10^{-4} M]

b. What diameter of particle must be used to have an effectiveness factor of 0.8? [7×10^{-4} cm]

Problem 5: Sizing a reactor with internal mass transfer limitations

The second order, ideal gas phase decomposition reaction of $A \rightarrow B$ is carried out isothermally and isobarically in a tubular reactor packed with catalyst pellets 0.4 cm in diameter. These large pellets are used to make pressure drop negligible, but as a consequence, the reaction becomes internal mass transfer limited. Pure A enters the reactor at a superficial velocity of 3 m/s, temperature of 250 degrees C and a pressure of 5 kPa. The reaction rate constant is $k'' = 0.0005$ $m^4/(mol*s)$. Assume that the forced axial convection term in the mole balance is much larger than axial diffusion.

Calculate the length of the bed necessary to achieve 80% conversion with the 0.4 cm diameter pellets. [0.04 m]

<u>Additional information:</u>
Effective diffusivity: $2.66(10^{-8})$ m^2/s
Bed void fraction: 0.4
Pellet density $2(10^6)$ g/m^3
Internal surface area: 400 m^2/g