

CRE Homework #9

$$1a. \quad N_0 = \int_0^{\infty} v C(t) dt$$

$$N_0 = v \left[\int_3^5 0.5t - 1.5 dt + \int_5^6 -t + 6 dt \right]$$

$$N_0 = 0.15 \text{ MOL}$$

$$1b. \quad E(t) = \frac{v C(t)}{\int_0^{\infty} v C(t) dt} = \frac{C(t)}{\int_0^{\infty} C(t) dt}$$

$$3s < t < 5s$$

$$E(t) = \frac{0.5t - 1.5}{\int_0^{\infty} C(t) dt} = \frac{0.5t - 1.5}{1.5}$$

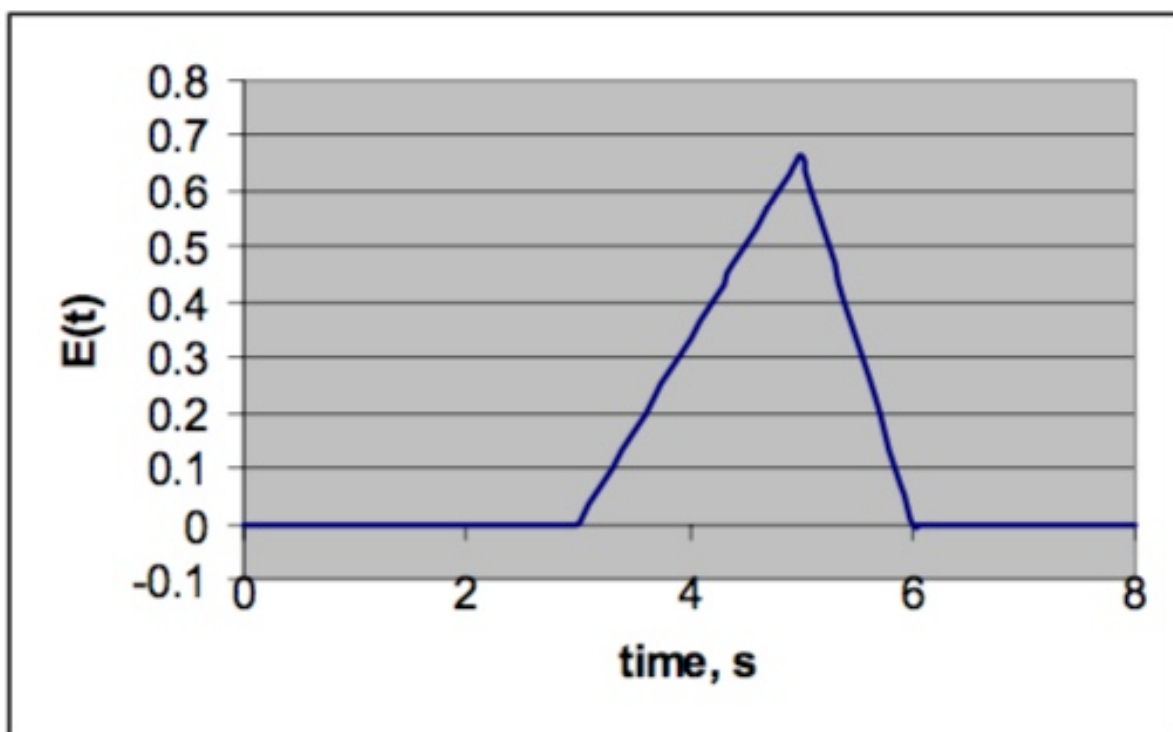
$$E(t) = \frac{1}{3}t - 1$$

$$5s < t < 6s$$

$$E(t) = \frac{-t + 6}{\int_0^{\infty} C(t) dt} = -\frac{2}{3}t + 4$$

$$E(t) = \begin{cases} 0 & t < 3 \\ \frac{1}{3}t - 1 & 3 < t < 5 \\ -\frac{2}{3}t + 4 & 5 < t < 6 \\ 0 & t > 6 \end{cases}$$

GRAPH ON NEXT PAGE



1c. $F(t) = \int_0^t E(t) dt$

$t < 3$ $F(t) = \int_0^t 0 dt = 0$

$3 < t < 5$ $F(t) = 0 + \int_3^t \frac{1}{3}t - 1 dt = \frac{3}{2} - t + \frac{1}{6}t^2$

$5 < t < 6$

$F(t) = \frac{3}{2} - 5 + \frac{1}{6}(5)^2 + \int_5^t -\frac{2}{3}t + 4 dt = -11 + 4t - \frac{1}{3}t^2$

$t > 6$ $F(t) = 1$

$$F(t) = \begin{cases} 0 & t < 3 \\ \frac{3}{2} - t + \frac{1}{6}t^2 & 3 < t < 5 \\ -11 + 4t - \frac{1}{3}t^2 & 5 < t < 6 \\ 1 & t > 6 \end{cases}$$

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1d. $\tau = \int_0^\infty t \cdot E(t) dt$

$\tau = \int_3^5 t \left(\frac{1}{3}t - 1 \right) dt + \int_5^6 t \left(-\frac{2}{3}t + 4 \right) dt$

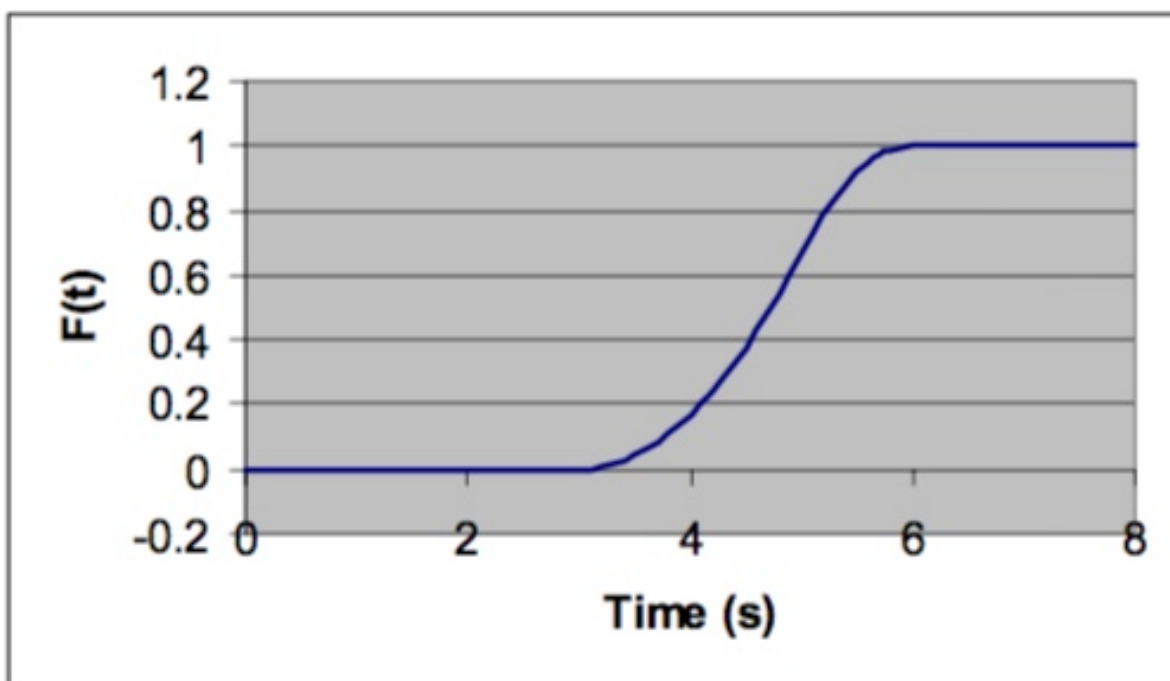
$\tau = 4.67 \text{ s}$

$V = \tau v = (0.1 \text{ L/s})(4.67 \text{ s}) = 0.467 \text{ L}$

1e. THINK OF THE SYSTEM AS SMALL BATCH REACTORS.

$$\bar{X} = \int_0^\infty X(t) E(t) dt$$

$X(t)$ IS SAME AS BATCH REACTOR



BATCH REACTOR MOLE BALANCE

$$\frac{dN_A}{dt} = r_A V \quad \longrightarrow \quad C_{A0} \frac{dX_A}{dt} = k C_{A0}^2 (1-X_A)^2$$

$$\int_0^X \frac{dX_A}{(1-X_A)^2} = \int_0^t k C_{A0} dt$$

$$\frac{1}{1-X_A} = k C_{A0} t$$

$$X_A(t) = 1 - \frac{1}{k C_{A0} t}$$

$$\bar{X} = \int_{0.3}^5 \left(1 - \frac{1}{k C_{A0} t}\right) \left(\frac{1}{3} - 1\right) dt + \int_5^6 \left(1 - \frac{1}{k C_{A0} t}\right) \left(4 - \frac{2}{3}t\right) dt$$

$$\bar{X} = 0.563 \text{ VIA COMPUTER}$$

IN A CSTR W/ SAME MEAN RESIDENCE TIME

$$F_{A0} X = V k [C_{A0} (1-X)]^2$$

$$X = 2k\tau C_{A0} + 1 - \sqrt{4k\tau C_{A0} + 1} / 2k\tau C_{A0}$$

$$X = 0.525$$

PFR: SAME EXPRESSION AS BATCH REACTOR

$$X = 0.563$$

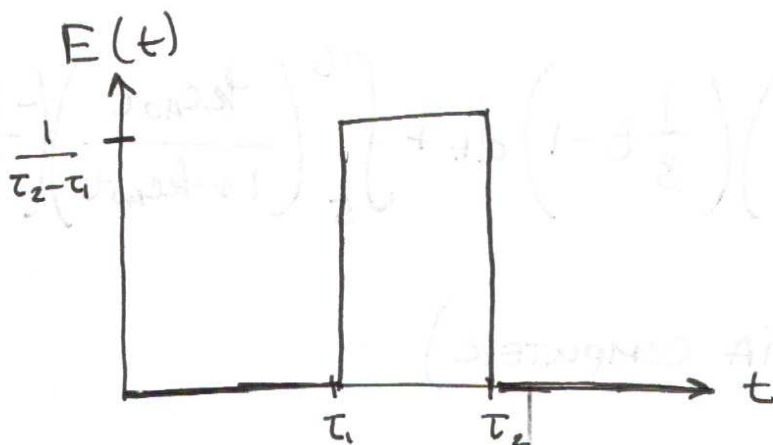
SIMILAR CONVERSIONS FOR NON-IDEAL & PFR,
CSTR IS A BIT LESS.

2a.

$$E(t) = \frac{dF(t)}{dt}$$

SLOPE OF $F(t)$ CURVE

$$E(t) = \begin{cases} 0 & \text{for } t < \tau_1 \\ \frac{1}{\tau_2 - \tau_1} & \text{for } \tau_1 < t < \tau_2 \\ 0 & \text{for } t > \tau_2 \end{cases}$$



2b.

$$\overline{C_A} = \int_{\tau_1}^{\tau_2} \frac{C_A(t)}{\tau_2 - \tau_1} dt$$

$$\frac{dN_A}{dt} = r_A V \longrightarrow \frac{dC_A}{dt} = -k C_A C_B$$

$$C_A = C_{A0}(1 - X_A) \quad C_B = C_{B0}\left(\frac{1}{2} - X_A\right)$$

$$-C_{A0} \frac{dX_A}{dt} = -k C_{A0}^2 (1 - X_A) \left(\frac{1}{2} - X_A\right)$$

System of 2 ODEs

$$\frac{dX}{dt} = 0.05(1-X)\left(\frac{1}{2}-X\right)$$

$$\frac{d\bar{X}}{dt} = \frac{X}{20}$$

$$\bar{X} = 0.385 \text{ (via computer soln)}$$

Problem #3

Problem Statement

Look at Figure P15-2B in the 5th Edition of Fogler and answer the following questions using that figure.

- 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?

Solutions

- a) Yes
- b) $F_{T0} = \frac{10 \text{ g mol}}{h}$ at all Temperatures
- c) Yes
- d) $F_{T0} = 100 \frac{\text{mol}}{h}$ ($T < 362\text{K}$)
 $F_{T0} = 1000 \frac{\text{mol}}{h}, 5000 \frac{\text{mol}}{h}$ ($T < 367\text{K}$)
- e) Yes
- f) $F_{T0} = 100 \frac{\text{mol}}{h}$ ($T > 362\text{K}$)
 $F_{T0} = 1000 \frac{\text{mol}}{h}, 5000 \frac{\text{mol}}{h}$ ($T > 367\text{K}$)

Problem #4

Problem Statement

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 $0.1 \text{ cm}^2/\text{s}$, and the diameter is 0.002 cm. Assume that the pellet is isothermal.

Given variables:

$$\begin{aligned} D_e &= 0.1 \frac{\text{cm}^2}{\text{s}} \\ D &= 2R = 0.002 \text{ cm} \\ c_{AS} &= 0.001 \frac{\text{mol}}{\text{L}} \\ c_A(r = \frac{R}{2}) &= 0.1 c_{AS} \end{aligned}$$

Required:

- At a radial distance of 0.003 cm inside from the external pellet surface, what is the concentration of the reactant?
- What diameter of particle must be used to have an effectiveness factor of 0.8?

Solutions

a)

$$\Psi = \frac{c_A}{c_{AS}} = \frac{1}{\lambda} \left(\frac{\sinh(\phi_1 \lambda)}{\sinh(\phi_1)} \right)$$

$$\lambda = \frac{r}{R}$$

$$\text{At } r = 0.0007, \lambda = 0.7$$

$$\text{At } r = \frac{R}{2}, c_A = 0.1 c_{AS}$$

Solve for ϕ_1 using that information:

$$\frac{c_A}{c_{AS}} = \frac{1}{\lambda} \left(\frac{\sinh(\phi_1 \lambda)}{\sinh(\phi_1)} \right)$$

$$0.1 = \frac{1}{0.5} \left(\frac{\sinh(\phi_1/2)}{\sinh(\phi_1)} \right)$$

$$\boxed{\phi_1 = 6}$$

$$\Psi = \frac{1}{\lambda} \left(\frac{\sinh(\phi_1 \lambda)}{\sinh(\phi_1)} \right) = \frac{1}{0.7} \frac{\sinh(6 \cdot 0.7)}{\sinh(6)}$$

$$\boxed{\Psi = 0.236}$$

$$c_A = c_{AS}\Psi$$

$$\boxed{\mathbf{c_A} = \mathbf{2.36} \times \mathbf{10^{-4}} \frac{\mathbf{mol}}{\mathbf{L}}}$$

b)

$\eta = 0.8$, find d_p

$$\phi_n^2 = \frac{k_N R^2 c_{AS}^{n-1}}{D_e}$$

$$\eta = \frac{3}{\phi_1^2} (\phi_1 \coth \phi_1 - 1)$$

solve for ϕ_1

$$\boxed{\phi_1 = 2.04}$$

$$\phi_1^2 = \frac{k_N R^2 S_a \rho_B}{D_e}$$

We know $\phi_1 = 6$ at $R = 0.001 \text{ cm}$

$$6^2 = k_N S_a \rho_B \cdot \frac{(0.001 \text{ cm})^2}{0.1 \text{ cm}^2/\text{s}}$$

$$k_N S_a \rho_B = 3.6 \times 10^6 \frac{1}{\text{s}}$$

Now solve for the actual R:

$$2.04^2 = (3.6 \times 10^6 \frac{1}{\text{s}}) \cdot \frac{R^2}{0.1 \text{ cm}^2/\text{s}}$$

$$R = 3.4 \times 10^{-4} \text{ cm}$$

$$\boxed{\mathbf{D} = \mathbf{6.8} \times \mathbf{10^{-4}} \mathbf{cm}}$$

Problem #5

Problem Statement

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 $k'' = 0.0005 \text{ m}^4/(\text{mol}\cdot\text{s})$. Assume that the forced axial convection term in the mole balance is much larger than axial diffusion.

Given variables:

$$d_p = 0.4 \text{ cm}$$

$$v = 3 \text{ m/s}$$

$$T = 250^\circ \text{C}$$

$$P = 5 \text{ kPa}$$

$$k'' = 0.0005 \frac{\text{m}^4}{\text{mol}\cdot\text{s}}$$

$$\text{Effective diffusivity: } 2.66 \times 10^{-8} \frac{\text{m}^2}{\text{s}}$$

$$\text{Bed void fraction: } 0.4$$

$$\text{Pellet density: } 2 \times 10^6 \frac{\text{g}}{\text{m}^3}$$

$$\text{Internal surface area: } 400 \frac{\text{m}^2}{\text{g}}$$

Required:

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

Solutions



$$r_A'' = k'' c_A^2$$

$$c_{A0} = \frac{P_A}{RT} = \frac{5 \times 10^3 \text{ Pa}}{8.31 \frac{\text{J}}{\text{mol}\cdot\text{K}} (250 + 273) \text{ K}} = 1.15 \frac{\text{mol}}{\text{m}^3}$$

Thiele Modulus for 2nd Order Rxn:

$$\phi_2^2 = \frac{k_n R^2 c_{AS}}{De}$$

$$c_{AB} = c_{AS} \text{ (No external diffusion limitations)}$$

$$\phi_2 = R \cdot \sqrt{\frac{k'' \rho_c S_a c_{AB}}{De}}$$

Check to see if ϕ_2 is large:

$$\phi_2 = 0.02m \cdot \sqrt{\frac{(0.05 \frac{m^4}{mol \cdot s}) \cdot (2 \times 10^6 \frac{g}{m^3}) \cdot (400 \frac{m^2}{g})(1.15 \frac{mol}{m^3})}{2.66 \times 10^{-8} \frac{m^2}{s}}}$$

$$\phi_2 = 8400$$

ϕ_2 is large, therefore:

$$\eta = \sqrt{\frac{2}{n+1}} \frac{3}{\phi_2}$$

$$\eta = \sqrt{\frac{2}{3}} \frac{3}{\phi_2}$$

$$-r_A = \eta r_{AS}$$

$$-r''_{AS} = k'' c_{AS}$$

$$-r_A = \eta k'' \rho_B S_a c_{AB}^2$$

Mole Balance:

$$D_{AB} \frac{d^2 c_{AB}}{dz^2} - v \frac{dc_{AB}}{dz} + r_A = 0$$

$$\frac{dc_{AB}}{dz} = \frac{r_A}{v}$$

$$\frac{dc_{AB}}{dz} = \frac{-\eta k'' \rho_B S_a c_{AB}^2}{v}$$

$$\frac{dc_{AB}}{dz} = - \left(\sqrt{\frac{2}{3}} \frac{3}{R \cdot \sqrt{\frac{k'' \rho_c S_a c_{AB}}{De}}} \right) \left(\frac{k'' \rho_B S_a c_{AB}^2}{v} \right)$$

$$c_A = 0.2 c_{A0} (80\% \text{ conversion})$$

Solving the ODE for $0 \rightarrow L$ for the bounds on dz :

$$\boxed{\mathbf{L = 0.04m}}$$