

ChE 344
Chemical Reaction Engineering
Winter 2000
Exam I
Solutions

Part 1, Closed Book

Name _____

Honor Code _____

Signed _____

[Don't sign until the end of the exam]

1) ____/10 pts

2) ____/10 pts

3) ____/30 pts

4) ____/10 pts

5) ____/15 pts

6) ____/ 5 pts

Total 80 pts

Exam I

1. Simpson's Three-eighths rule (4 points)

$$\int_{x_0}^{x_3} f(x) dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

2. $\frac{dy}{dW} = -\frac{a(1+eX) \frac{dT}{T_0}}{2y \frac{dT}{T_0}}$ where $a = \frac{2b_0}{A_c r_c (1-f) R_0}$, and $b_0 = \frac{G(1-f) \dot{E} 1.5(1-f) m}{g_c r_0 D_p f^3} + 1.75 \frac{m}{D_p}$, $G = \frac{\dot{m}}{A_c}$

$$\frac{dy}{dW} = -\frac{a \frac{dT}{T_0}}{2y \frac{dT}{T_0}}$$

3. Integrals

$$\int \frac{dx}{1-x} = \ln \frac{1}{1-x}$$

$$\int \frac{1+e^x}{(1-x)^2} dx = \frac{1+e^x}{1-x} - e \ln \frac{1}{1-x}$$

$$\int \frac{dx}{(1-x)^2} = \frac{x}{1-x}$$

$$\int \frac{(1+e^x)^2}{(1-x)^2} dx = 2e(1+e) \ln(1-x) + e^2 x + \frac{(1+e)^2 x}{1-x}$$

$$\int \frac{dx}{1+e^x} = \frac{1}{e} \ln(1+e^x)$$

$$\int \frac{1+e^x}{1-x} dx = (1+e) \ln \frac{1}{1-x} - e^x$$

$$\int \frac{dx}{(1-x)(q_b - x)} = \frac{1}{q_b - 1} \ln \frac{q_b - x}{q_b(1-x)} \quad q_b \neq 1$$

$$\int \frac{dx}{ax^2 + bx + c} = \frac{-2}{2ax + b} + \frac{2}{b}$$

for $b^2 = 4ac$ where p and q are the roots of the equation.

$$\int (1-aw)^{1/2} dw = \frac{2}{3a} [1 - (1-aw)^{3/2}]$$

$$ax^2 + bx + c = 0 \text{ i.e., } p, q = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\int \frac{dx}{ax^2 + bx + c} = \frac{1}{a(p-q)} \ln \left| \frac{q - x - p}{p - x - q} \right|$$

$$\text{for } b^2 > 4ac \quad \int \frac{a + bx}{c + gx} dx = \frac{bx}{g} + \frac{ag - bc}{g^2} \ln \left| \frac{c + gx}{c} \right|$$

4. Finite Difference

First Point: $-\frac{dC_A}{dt} \Big|_0 = -\frac{\dot{E} - 3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$

Middle Points: $-\frac{dC_A}{dt} \Big|_1 = -\frac{\dot{E} C_{A(1+1)} - C_{A(1-1)}}{2\Delta t}$

e.g., $-\frac{dC_A}{dt} \Big|_3 = -\frac{\dot{E} C_{A4} - C_{A2}}{2\Delta t} = \frac{C_{A2} - C_{A4}}{2\Delta t}$

Last Point: $-\frac{dC_A}{dt} \Big|_5 = -\frac{\dot{E} C_{A3} - 4C_{A4} + 3C_{A5}}{2\Delta t}$

5. Ideal Gas Constant

$$R = \frac{8309 \text{ kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}}$$

$$R = \frac{1.987 \text{ BTU}}{\text{lbmol} \cdot \text{R}}$$

$$R = \frac{0.73 \text{ ft}^3 \cdot \text{atm}}{\text{lbmol} \cdot \text{R}}$$

$$R = \frac{8.314 \text{ J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082 \frac{\text{liter} \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082 \text{ m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}}$$

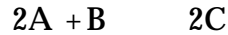
$$R = \frac{1.987 \text{ cal}}{\text{mol} \cdot \text{K}}$$

Volume of Ideal Gas

1 lbmol of an ideal gas at 32°F and 1 atm occupies 359 ft³.

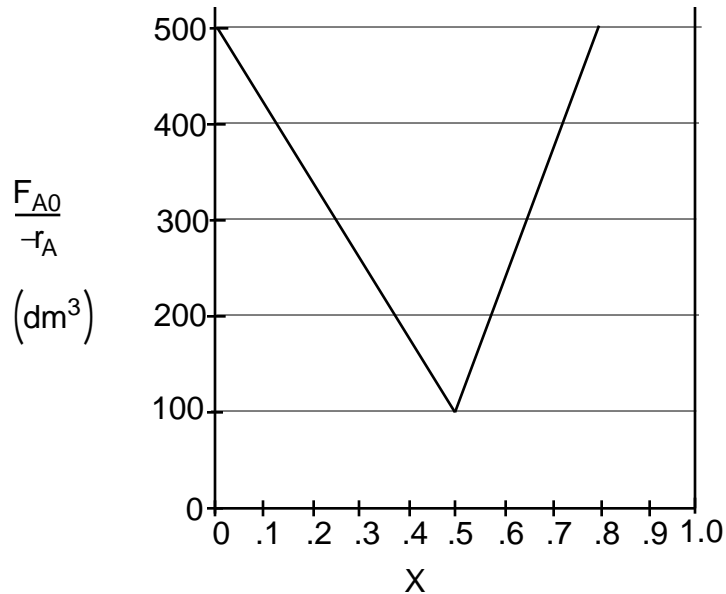
1 g mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm³.

(10%) 1) The adiabatic exothermic irreversible gas phase reaction



is to be carried out in a flow reactor for an equimolar feed of A and B.

Additional Information



a) What is ϵ , the volume change parameter?

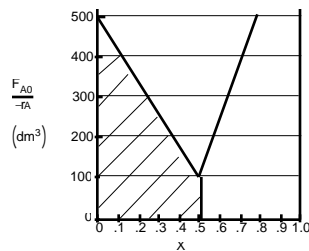
Equimolar feed of A and B. Base all calculations on limiting reactant, A.

$$\epsilon = y_{A0} \delta, y_{A0} = 0.5, \delta = 1 - 1 - .05 = -0.5$$

$$\epsilon = (0.5)(-0.5) = -0.25$$

$$= \underline{-0.25}$$

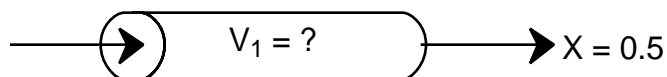
b) What PFR volume is necessary to achieve 50% conversion?



$$V_{PFR} = F_{A0} \int_0^{0.5} \frac{dx}{-r_A} = \text{area under curve}$$

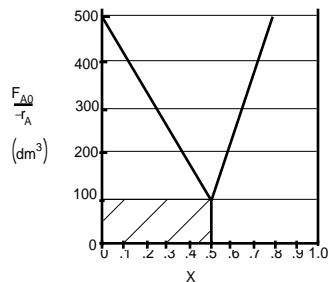
$$V_{PFR} = (100 \cdot 0.5) + 0.5 \cdot (400 \cdot 0.5) = 150$$

$$V_1 = \underline{150 \text{ dm}^3}$$



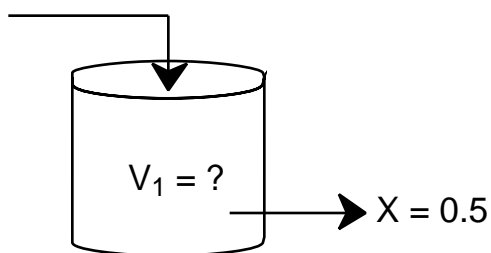
c) What CSTR volume is necessary to achieve 50% conversion?

CSTR, therefore volume calculated using conditions at the exit (i.e. $X=0.5$)



$$V_{CSTR} = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A0,exit}} 0.5 * 100 = 50$$

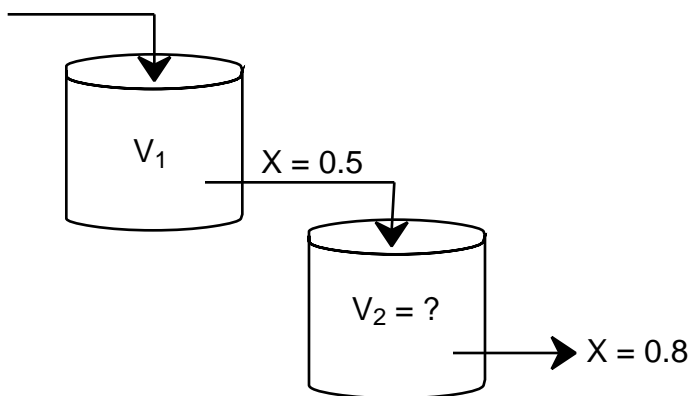
$$V_1 = \underline{50 \text{ dm}^3}$$

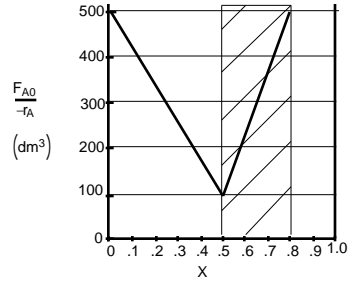


continued

- d) What CSTR volume must be added to raise the conversion in Part (c) to 80%?

$$V_2 = \underline{150 \text{ dm}^3}$$

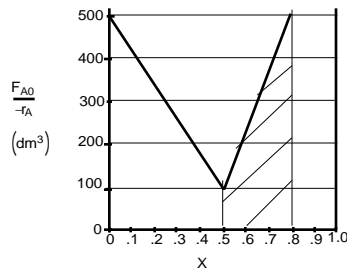
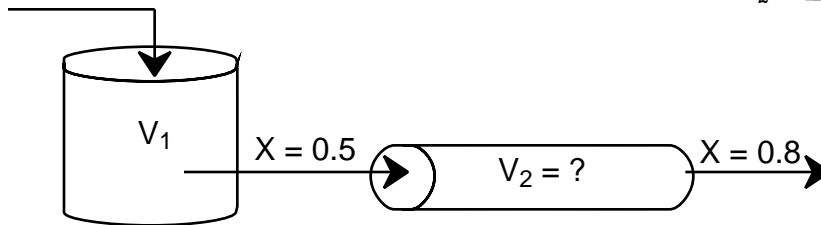




$$V_2 = (X_2 - X_1) * \frac{F_{A0}}{-r_A} = (0.8 - 0.5) * (500) = 150$$

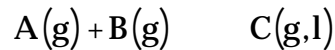
e) What PFR volume must be added to raise the conversion in Part (c) to 80%?

$$V_2 = \underline{90 \text{ dm}^3}$$



$$V_2 = \int_{0.5}^{0.8} \frac{F_{A0}}{-r_A} dX = (0.8 - 0.5) * (100) + 0.5 * (0.8 - 0.5) * (400) = 90$$

(10%) 2) The elementary irreversible gas reaction



is carried out isothermally in a PFR in which there is no pressure drop. As the reaction proceeds the partial pressure of C builds up and a point is reached at which C begins to condense. The vapor pressure of C is 0.4 atm. What is the rate of reaction at the point at which C first starts to condense. The feed is equal molar in A and B, there are no inerts or other species entering the reactor and the total pressure at the entrance is 2 atm.

Additional Information

$$C_{A0} = 0.02 \text{ mol/dm}^3$$

$$k_A = 100 \text{ dm}^3 \text{ mol}^{-1} \text{ min}^{-1}$$

Ans

$$-r_A = \underline{2.56 \text{ mol/dm}^3 \text{ min}}$$

Find X where C begins to condense (X_{cond})

$$F_A = F_{A0}(1 - X)$$

$$F_B = F_{A0}(1 - X)$$

$$F_C = F_{A0}(X)$$

$$F_T = F_A + F_B + F_C = F_{A0}(2 - X)$$

$$y_{C,cond} = \frac{P_{C,cond}}{P_T} = \frac{0.4}{2} = 0.2 = \frac{F_{C,cond}}{F_{T,cond}} = \frac{F_{A0}X_{cond}}{F_{A0}(2 - X_{cond})}$$

$$\frac{X_{cond}}{2 - X_{cond}} = 0.2 \quad X_{cond} = \frac{0.4}{1.2} = \frac{1}{3}$$

Now proceed to the rate law

$$-r_A = k_A C_A C_B$$

$$C_A = \frac{C_{A0}(1 - X)}{(1 + \epsilon X)} = C_B$$

$$\epsilon = y_{A0} \delta = 0.5 * (1 - 1 - 1) = -0.5$$

$$-r_A = k_A \frac{C_{A0}^2 (1 - X)^2}{(1 + \epsilon X)^2} = 100 \frac{\text{dm}^3}{\text{mol min}} \frac{(0.02 \frac{\text{mol}}{\text{dm}^3})^2 (1 - 1/3)^2}{(1 + (-1/2)(1/3))^2} = 2.56 \frac{\text{mol}}{\text{dm}^3 \text{ min}}$$



(30%)

3) It is desired to carry out the gaseous reaction

A + B in an existing *tubular reactor* consisting of 50 parallel tubes 40 ft long with a 0.75-in. inside diameter. Bench-scale experiments have given the reaction rate constant for this first-order reaction as 0.00152 s^{-1} at 200°F and 0.0740 s^{-1} at 300°F . At what temperature should the reactor be operated to give a conversion of A of 80% with a feed rate of 500 lb/h of pure A and an operating pressure of 100 psig? A has a molecular weight of 73. Departures from perfect gas behavior may be neglected, and the reverse reaction is insignificant at these conditions.

Ans

$$T = 278^\circ\text{F or } 738^\circ\text{R}$$

$$V_{total} = N_{tubes} [\pi r^2 L] = 50 \pi \frac{0.75 \text{ in}^2}{2} \frac{40 \text{ ft}}{1 \text{ ft}/12 \text{ in}} = 10603 \text{ in}^3 = 6.14 \text{ ft}^3$$

$$F_{A_o} = \frac{500 \text{ lb/hr}}{73 \text{ lb/lbmol}} = 6.85 \text{ lbmol/hr}$$

Mole Balance, Rate Law, Stoichiometry, Combine

$$V = F_{A_o} \frac{dX_A}{-r_A}, \quad -r_A = kC_A, \quad C_A = C_{A_o}(1-X), \quad V = F_{A_o} \frac{dX_A}{kC_{A_o}(1-X)}$$

$$V = \frac{F_{A_o}}{kC_{A_o}} \ln \frac{1}{1-X} \quad k = \frac{F_{A_o}}{VC_{A_o}} \ln \frac{1}{1-X}$$

$$C_{A_o} = \frac{y_{A_o} P_o}{RT_o}, \quad P_o = 100 \text{ psig} + 14.7 = 114.7 \text{ psia} = 7.8 \text{ atm}, \quad y_{A_o} = 1$$

$$k = \frac{F_{A_o} RT_o}{VP_o} \ln \frac{1}{1-X} = \frac{6.85 * 0.73 * T_o}{6.14 * 7.8} \ln \frac{1}{0.2} = 0.168 * T_o$$

$$k = k(T) = A e^{\frac{-E}{RT}} \quad \text{use given k values to find E and A}$$

$$\ln \frac{k_1}{k_2} = \frac{E}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \quad \ln \frac{0.00152}{0.074} = \frac{E}{R} \left(\frac{1}{760^\circ\text{R}} - \frac{1}{660^\circ\text{R}} \right) \quad \frac{E}{R} = 19498^\circ\text{R}$$

$$A = k e^{\frac{E}{RT}} = \frac{0.00152}{\text{s}} * \frac{3600 \text{ s}}{\text{hr}} \exp \frac{19489}{660} = 3.65 E^{13} \text{ hr}^{-1}$$

$$k = 3.65 E^{13} \text{ hr}^{-1} \exp \frac{19489}{T_o}$$

Now set the two expressions for k equal to each other and solve for T_o

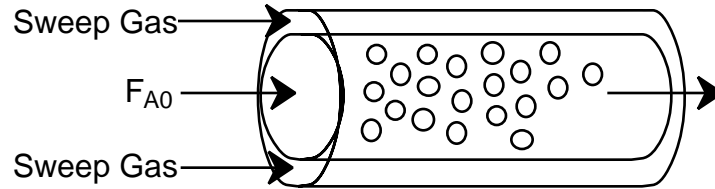
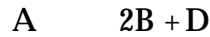
$$0.168 T_o = 3.65 E^{13} \text{ hr}^{-1} \exp \frac{19489}{T_o}$$

Iterate to solve for T_o (or use solver)

$$T_o = 738^\circ\text{R} = 278^\circ\text{F}$$

(10%)

4) The following reaction is carried out in a membrane reactor packed with 100 kg of catalyst. The reaction is carried out isothermally and there is no pressure drop.



The following is a sketch of the concentration profile in a conventional PBR

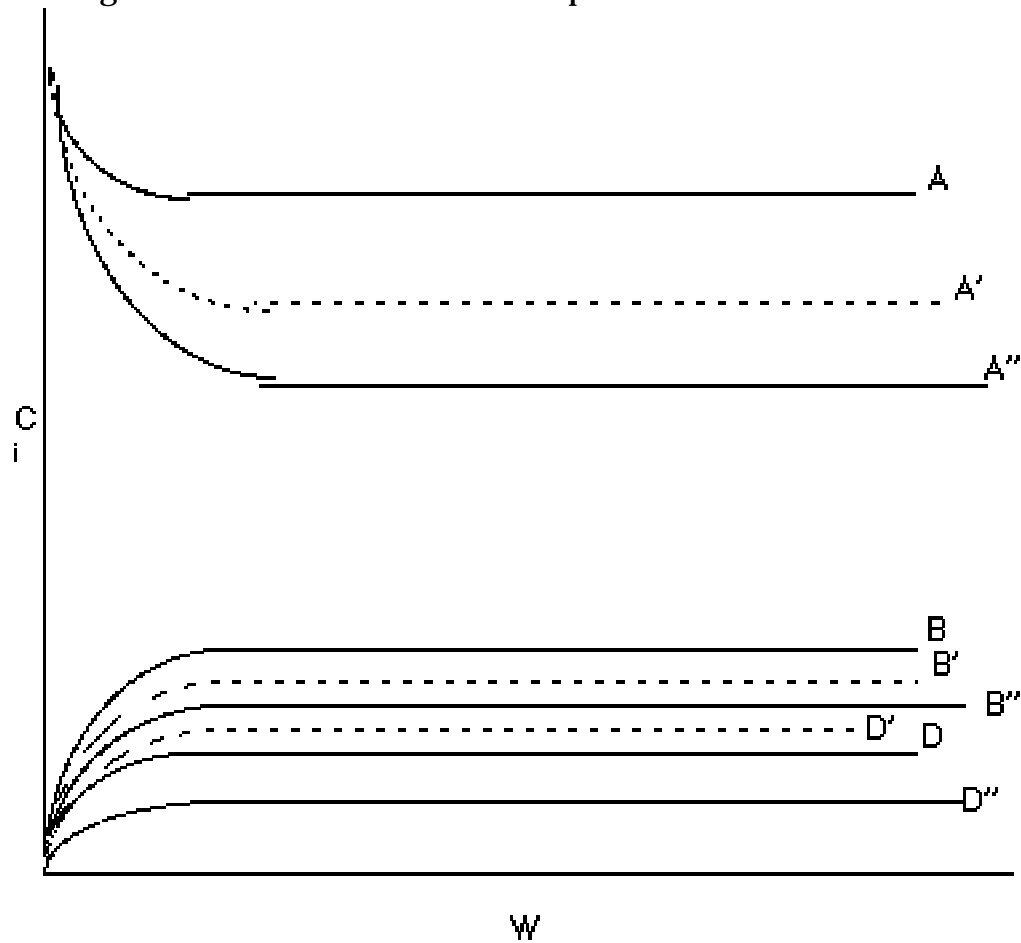


Figure 1

- a) Suppose B diffuses out through the membrane. Using a dashed line (-----) sketch the concentration profiles in a membrane reactor for a moderate value of the mass transfer coefficient for B, k_{CB} , sketch the profiles of A, B and D on Figure 1.

The traces are shown in Figure 1, represented by the dotted lines and A', B', and D'. Final concentrations A', and B' will be lower than PBR, while D' will be greater

- b) Now suppose that both B and D can diffuse out of the reactor, use a solid line (____) to sketch the profiles of A, B, and D on Figure 1. Assume the mass transfer coefficients of B and D are the same, $k_{CB} = k_{CD}$.

The traces are shown in Figure 1, represented by the solid lines and A'', B'', and D'' Final concentrations A'', B'', and C'' will all be lower than in a PBR. Final concentrations A'' and B'' are lower than final concentrations A' and B'

- c) Suppose you could choose from two types of membranes, one in which only B would diffuse out, and one in which only D would diffuse out. In both cases the mass transfer coefficient would be very very very large. Which membrane would give the greatest conversion of A?

Why?

According to Le Chatelier's Principle, you want to remove products to push reaction forward. If you remove B, you are removing 2 moles. If you remove D, you are only removing one mole. Therefore, you would want to remove B. Analytically:

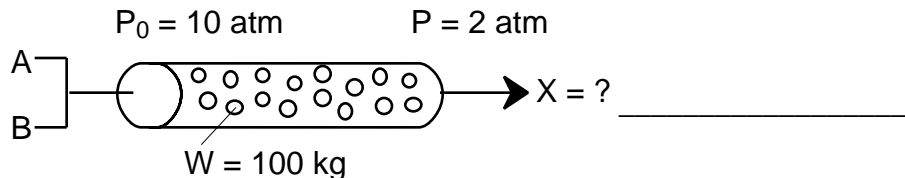
$$C_A = C_{T0} \frac{F_A}{F_T} = C_{T0} \frac{F_A}{F_A + F_B + F_C}$$

$$-r_A = k C_A - \frac{C_B^2 C_C}{K_C}, \text{ keep } C_A \text{ high}$$

(15%) 5) The irreversible gas phase reaction



is carried out in a PBR. The reaction is non-elementary in that it is first order in A and zero order in B. The feed is equal molar in A and B, and the pressure at the entrance is 10 atm and the pressure at the exit is 2 atm.



Additional Information

$$F_{A0} = 100 \text{ mol/s}$$

$$k = 1 \frac{\text{dm}^3}{\text{kg s}}$$

$$C_{A0} = 1 \text{ mol/dm}^3$$

a) What is the conversion exiting the reactor? X=0.5

b) If the flow were turbulent, what would be the pressure drop if the cross sectional area was increased by a factor of 2 and the particle size decreased by a factor of 10? All other conditions remain the same.

Pressure drop too great, no flow under these conditions

Find X

Mole Balance, Rate Law, Stoichiometry, Combine

$$\frac{dX}{dW} = \frac{-r'_A}{F_{A0}}, \quad -r'_A = k' C_A, \quad C_A = C_{A0}(1-X) \frac{P}{P_0}, \quad \frac{dX}{dW} = \frac{k' C_{A0}(1-X) P}{F_{A0} P_0}$$

$$\epsilon = 0 \quad \frac{P}{P_0} = (1 - \alpha W)^{\frac{1}{2}} \quad \frac{2}{10} = (1 - \alpha * 100 \text{ kg})^{\frac{1}{2}} \quad \alpha = 0.0096 \text{ kg}^{-1}$$

$$\frac{dX}{dW} = \frac{k' C_{A0}(1-X)}{F_{A0}} (1 - \alpha W)^{\frac{1}{2}} \quad \frac{dX}{1-X} = \frac{k' C_{A0}}{F_{A0}} (1 - \alpha W)^{\frac{1}{2}} dW \quad \int_0^X \frac{dX}{1-X} = \frac{k' C_{A0}}{F_{A0}} \int_0^{100 \text{ kg}} (1 - \alpha W)^{\frac{1}{2}} dW$$

$$\ln \frac{1}{1-X} = \frac{k' C_{A0}}{F_{A0}} \frac{2}{3\alpha} [1 - (1 - \alpha W)^{\frac{3}{2}}]_0^{100 \text{ kg}} \quad \ln \frac{1}{1-X} = \frac{1 * 1}{100} \frac{2}{3 * 0.0096} [1 - (1 - 0.0096 * 100)^{\frac{3}{2}}] = 0.6938$$

$$\frac{1}{1-X} = 2.00 \quad X = 0.5$$

Find the new α

$$\alpha \sim \frac{\beta_o}{A_c}, \beta_o \sim \frac{G^2}{D_p} \text{ (for turbulent flow)}, G \sim \frac{1}{A_c}$$

$$\text{Combining yields } \alpha \sim \frac{1}{A_c^3 D_p}$$

$$A_{c,2} = 2A_{c,1}, D_{p,2} = \frac{1}{10} D_{p,1}$$

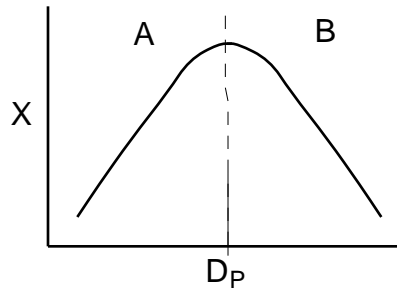
$$\frac{\alpha_1}{\alpha_2} = \frac{A_{c,2}^3 D_{p,2}}{A_{c,1}^3 D_{p,1}} = \frac{8A_{c,1}^3 \frac{1}{10} D_{p,1}}{A_{c,1}^3 D_{p,1}} = \frac{8}{10} \quad \alpha_2 = \frac{10}{8} \alpha_1$$

Calculate new pressure drop

$$\frac{P}{P_o} = (1 - \alpha_2 W)^{\frac{1}{2}} = 1 - \frac{10}{8} \alpha_1 W^{\frac{1}{2}} = 1 - \frac{10}{8} 0.0096 * 100^{\frac{1}{2}} = (-0.2)^{\frac{1}{2}} = \text{imaginary numbers}$$

Pressure drop will be too great, no flow under these conditions

- (5%) 6) Below is a sketch showing the exit conversion as a function of catalyst particle size in a packed bed reactor.



Why does the conversion increase with increasing particle size in region A?

Decreasing pressure drop with increasing particle size. Increasing pressure, therefore increases concentration, increasing rate of reaction, thus increasing conversion

Why does the conversion decrease with increasing particle size in region B?

Larger particles the smaller the effective rate of reaction; therefore, the smaller the conversion.

