

(0905421) Chemical Reaction Engineering I

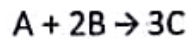
In-Class Assessment # 1 (Chapter 1)

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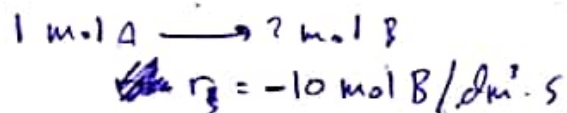
Q1: Consider the reaction



In which the rate of disappearance of A is 5 moles of A per  $\text{dm}^3$  per second at the start of the reaction. At the start of the reaction:

(a) What is  $-r_A$ ?  $r_A = 5 \text{ mol A} / (\text{dm}^3 \cdot \text{s})$

(b) What is the rate of formation of B?



(c) What is the rate of formation of C?

$$r_C = 15 \text{ mol C} / (\text{dm}^3 \cdot \text{s})$$

(d) What is the rate of disappearance of C?

$$r_C = -15 \text{ mol C} / (\text{dm}^3 \cdot \text{s})$$

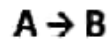
(e) What is the rate of formation of A,  $r_A$ ?

$$r_A = -5 \text{ mol A} / (\text{dm}^3 \cdot \text{s})$$

(f) What is  $-r_B$ ?

rate of disappearance of B

Q2: For the reaction



Calculate the time to reduce the number of moles by a factor of 10 ( $N_A = \frac{N_{A0}}{10}$ ) in a batch reactor for the above reaction with  $-r_A = kC_A$ , when  $k = 0.046 \text{ min}^{-1}$ .

$$\begin{aligned} t &= \int_{N_{A0}}^{N_A} \frac{dN_A}{-r_A V} \\ &= \int_{N_{A0}}^{N_A} \frac{dN_A}{k C_A V} \\ &= \int_{N_{A0}}^{N_A} \frac{dN_A}{k \frac{N_A}{V} V} \\ &= \frac{-1}{k} \int_{N_{A0}}^{N_A} \frac{dN_A}{N_A} \\ &= \frac{1}{k} \ln \left| \frac{N_{A0}}{N_A} \right| \\ &= \frac{1}{k} \ln \left| \frac{N_{A0}}{N_{A0}/10} \right| \\ &= \frac{1}{k} \ln(10) \\ &= 50.056 \text{ min} \end{aligned}$$

$$N_{A0} = 10 N_A$$

The reaction  $A \rightarrow B$  is to be carried out isothermally in a continuous-flow reactor.

- (a) Calculate the PFR volume to consume 99% of A ( $C_A = 0.01 C_{A0}$ ) when the entering molar flow rate is 5 mol A/h, the volumetric flow rate is constant at  $10 \text{ dm}^3/\text{h}$  and the rate is  $-r_A = (3 \text{ dm}^3/\text{mol} \cdot \text{h}) C_A^2$ .
- (b) Calculate the CSTR volume to consume 99% of A ( $C_A = 0.01 C_{A0}$ ) when the entering molar flow rate is 5 mol A/h, the volumetric flow rate is constant at  $10 \text{ dm}^3/\text{h}$  and the rate is  $-r_A = (3 \text{ dm}^3/\text{mol} \cdot \text{h}) C_A^2$ .
- (c) Compare the CSTR and PFR volumes!

a)  $V = \int_{F_{A0}}^{F_A} \frac{dF_A}{-r_A}$

$= \int_{F_{A0}}^{F_A} \frac{dF_A}{3 C_A^2}$

$= \frac{1}{-3} \int_{F_{A0}}^{F_A} \frac{dF_A}{C_A^2}$

$= \frac{1}{-3} \left[ \frac{1}{C_A} \right]_{F_{A0}}^{F_A}$

$= \frac{1}{-3} \left( \frac{1}{0.05} - \frac{1}{5} \right)$

$= 66000$

$C_A = 0.01 C_{A0}$

$C_{A0} = \frac{5 \text{ mol/h}}{10 \text{ dm}^3/\text{h}}$

$= 0.5 \text{ mol/dm}^3$

$C_A = 5 \times 10^{-3}$

$F_{A0} = 0.05 \text{ mol/h}$

b)  $V = \frac{F_{A0} C_{A0} - V C_A}{-r_A}$

$= \frac{F_{A0} C_{A0} - V C_A}{3 C_A^2}$

$= \frac{10 (0.5 - 5 \times 10^{-3})}{-3 (5 \times 10^{-3})^2}$

$C_{A0} = \frac{5 \text{ mol/h}}{10 \text{ dm}^3/\text{h}}$

$= 0.5 \text{ mol/dm}^3$

$C_A = 5 \times 10^{-3} \text{ mol/dm}^3$



$$\textcircled{A} \quad V = \int_{F_A}^{F_A} \frac{dF_A}{r_A}$$

$$= \int_{F_A}^{F_A} \frac{dF_A}{-3C_A^2}$$

$$= \int_{F_A}^{F_A} \frac{dF_A}{3C_A^2}$$

$$= \int_{C_{A0}}^{C_A} \frac{V dC_A}{3C_A^2}$$

$$= \frac{V}{3} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2}$$

$$= \frac{10}{3} \int_{0.5}^{0.005} \frac{dC_A}{C_A^2}$$

$$= 660 \text{ dm}^3$$

$$F_A = C_A V$$

$$dF_A = V dC_A$$

$$C_{A0} = 0.5 \text{ mol/dm}^3$$

$$C_A = 0.005 \text{ mol/dm}^3$$

$$\textcircled{b} \quad V = \frac{F_{A0} - F_A}{-r_A} = \frac{5 - 0.05}{3(0.005)^2} = 66000 \text{ dm}^3$$

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In-Class Assessment # 2 (Chapter 2)

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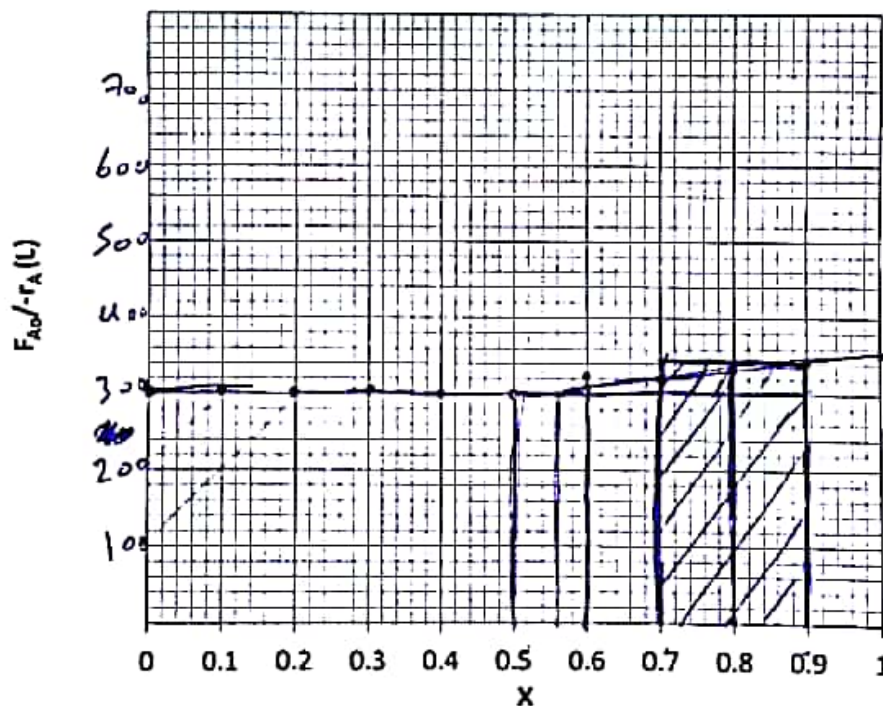
For the irreversible gas-phase reaction:  $A \rightarrow 2B$  the following correlation was determined from laboratory data (the initial concentration of A is 2 mol/L):

$$\text{For } X \leq 0.5: \frac{1}{-r_A} = 30 \frac{\text{L.s}}{\text{mol}}$$

$$\text{For } X > 0.5: \frac{1}{-r_A} = 30 + 10(X - 0.5) \frac{\text{L.s}}{\text{mol}}$$

The volumetric flow rate is 5 L/s.

$$F_{A0} = \frac{2 \text{ mol/L} \times 5 \text{ L/s}}{1} = 10 \text{ mol/s}$$



a. Graph Levenspiel plot ( $F_{A0}/-r_A$  vs. X)

$$\frac{1}{2} \times 0.1 \times 10$$

b. Over what range of conversions are the plug-flow reactor and CSTR volumes identical?

$$0 \leq X \leq 0.5$$

c. What conversion will be achieved in a CSTR that has a volume of 90 L?

$$V = \frac{F_{A0} X}{-r_A} = \frac{V - r_A}{F_{A0}} = X = \frac{90}{10 \times 30} = 0.3$$

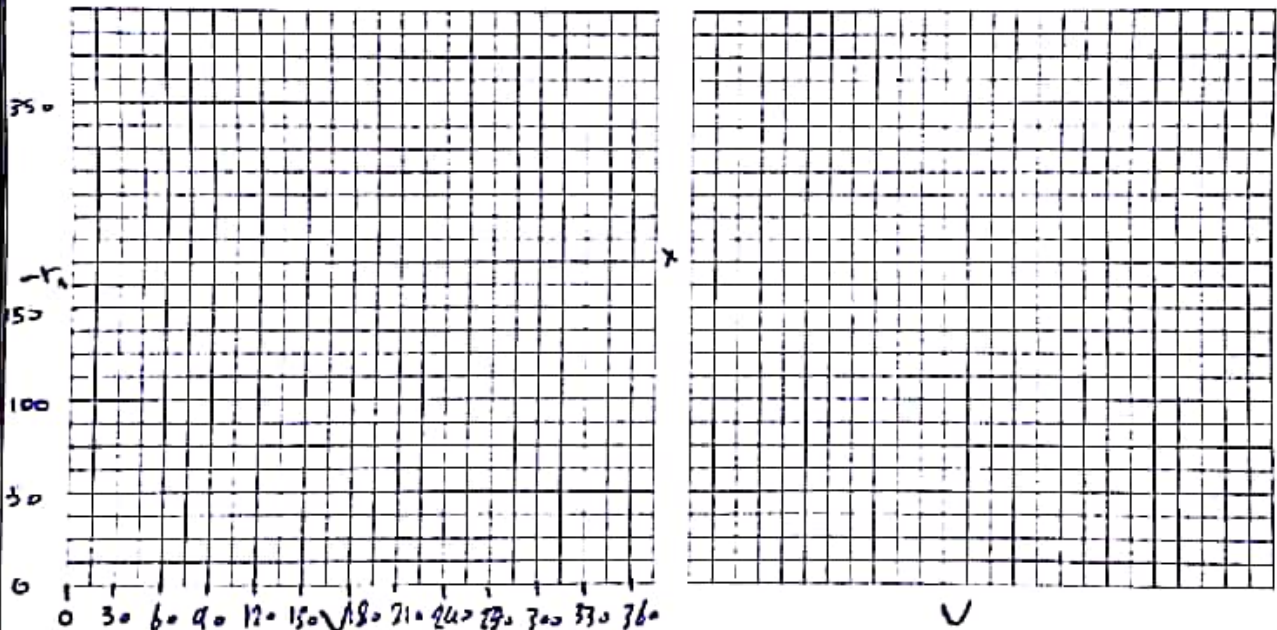
d. What plug-flow reactor volume is necessary to achieve 70% conversion?

$$V = F_{A0} \int_0^{0.7} \frac{dX}{-r_A} = 0.7 \int_0^{0.7} \frac{F_{A0}}{-r_A} dX = \frac{0.75}{3} [300 + 4 \times 300 + 320] = 212.33 \text{ L}$$

e. What CSTR reactor volume is required if effluent from the plug-flow reactor in part (d) is fed to a CSTR to raise the conversion to 90%?

$$A = 0.2 \times 340 = 68 \text{ L}$$

f. Plot the rate of reaction and conversion as a function of PFR volume.



g. If the reaction is carried out in a constant-pressure batch reactor in which pure A is fed to the reactor, what length of time is necessary to achieve 40 % conversion?

|      |      |     |      |     |      |       |      |       |      |     |       |
|------|------|-----|------|-----|------|-------|------|-------|------|-----|-------|
| X    | 0    | 0.1 | 0.2  | 0.3 | 0.4  | 0.5   | 0.6  | 0.7   | 0.8  | 0.9 | 1.0   |
| -r_A | 1/30 |     | 1/70 |     | 1/50 |       | 1/35 |       | 1/25 |     | 1/10  |
| V    | 0    | 60  |      | 120 |      | 180.5 |      | 244.5 |      |     | 312.5 |



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In-Class Assessment # 10 (Chapter 5)

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The reaction  $A \rightarrow B$  is carried out in a constant volume batch reactor. Determine the reaction order and specific reaction rate from the following data.

|                              |   |     |     |     |
|------------------------------|---|-----|-----|-----|
| t (min)                      | 0 | 10  | 20  | 30  |
| $C_A$ (mol/dm <sup>3</sup> ) | 1 | 0.6 | 0.4 | 0.3 |

$$-\Delta C_A / \Delta t \quad 0.04 \quad 0.02 \quad 0.01$$

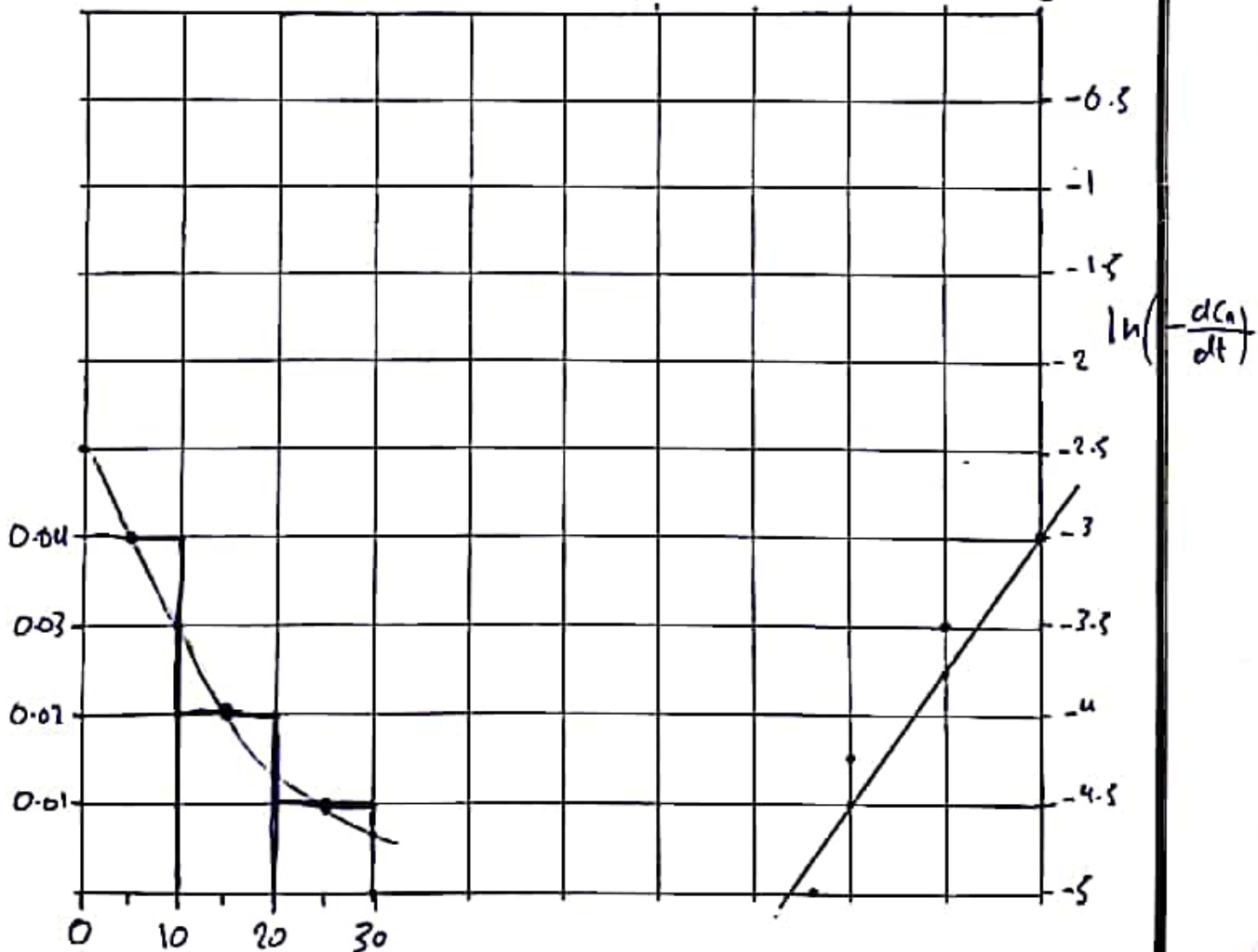
$$-dC_A/dt = 0.05 \quad 0.03 \quad 0.013 \quad 0.007$$

$$\ln C_A \quad -1.5 \quad -1 \quad -0.5 \quad 0$$

$$\ln\left(-\frac{dC_A}{dt}\right) = \ln k_p + \alpha \ln C_A$$

$$\ln\left(-\frac{dC_A}{dt}\right) \quad 3 \quad -3.5 \quad -4.3 \quad -5$$

$$\ln(C_A) \quad 0 \quad -0.5 \quad -1 \quad -1.2$$



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$$\alpha = \frac{\Delta y}{\Delta x} = \frac{-4.8 + 3.75}{-1 + 0.5} = 1.5$$

$$\ln k_p = -3$$

$$k_p = 0.05$$

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In-Class Assessment # 12 (Chapter 6)

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P6-12 The following liquid-phase reactions were carried out in a CSTR at 325 K.



$$-r_{1A} = k_{1A}C_A$$

$$k_{1A} = 7.0 \text{ min}^{-1}$$



$$r_{2D} = k_{2D}C_C^2C_A$$

$$k_{2D} = 3.0 \text{ L}^2/\text{mol}^2\cdot\text{min}$$



$$r_{3E} = k_{3E}C_D C_C$$

$$k_{3E} = 2.0 \text{ L/mol}\cdot\text{min}$$

The concentrations measured *inside* the reactor were  $C_A = 0.10$ ,  $C_B = 0.93$ ,  $C_C = 0.51$ , and  $C_D = 0.049$  all in mol/L.

(a) What are  $r_{1A}$ ,  $r_{2A}$ , and  $r_{3A}$ ?

$$\frac{-r_{1A}}{1} = \frac{r_{2D}}{3}$$

$$-r_{2A} = \frac{1}{3} r_{2D}$$

$$r_{3A} = 0$$

$$r_A = -k_{1A}C_A - \frac{k_{2D}C_C^2C_A}{3}$$

(b) What are  $r_{1B}$ ,  $r_{2B}$ , and  $r_{3B}$ ?

$$\frac{+r_{1B}}{1} = \frac{1}{3} (-r_{1A})$$

$$r_{2B} = 0$$

$$r_{3B} = 0$$

$$r_B = \frac{+k_{1A}C_A}{3}$$

(c) What are  $r_{1C}$ ,  $r_{2C}$ , and  $r_{3C}$ ?

$$r_{1C} = +\frac{1}{3} r_{1A}$$

$$r_C = \frac{+k_{1A}C_A}{3} - \frac{2}{3} k_{2D}C_C^2C_A - k_{3E}C_D C_C$$

$$\frac{+r_{1C}}{2} = \frac{r_{2D}}{3} \Rightarrow -r_{2C} = \frac{2}{3} r_{2D}$$

$$r_{3C} = r_{3E}$$

(d) What are  $r_{1D}$ ,  $r_{2D}$ , and  $r_{3D}$ ?

$$r_{1D} = 0$$

$$r_{2D} = k_{2D}C_C^2C_A$$

$$r_{3D} = \frac{4}{3} r_{3E}$$

$$r_D = k_{2D}C_C^2C_A - \frac{4}{3} k_{3E}C_D C_C$$



(c) What are  $r_{1E}$ ,  $r_{2E}$ , and  $r_{3E}$ ?

$$r_{1E} = 0$$

$$r_{2E} = 0$$

$$r_{3E} = k_{3E} C_D C_C$$

$$r_E = k_{7E} C_D C_C$$

(f) What are the net rates of formation of A, B, C, D, and E?

(g) The entering volumetric flow rate is 100 L/min and, the entering concentration of A is 3 M. What is the CSTR reactor volume?

Parts (h), (i), (j) are HOMEWORK! (Solve them using POLYMATH or MATLAB)

$$V_0 = 100 \text{ L/min}$$

$$C_{A0} = 3 \text{ mol/L}$$

$$V = \frac{F_{A0} - F_A}{-r_A} = \frac{(C_{A0} - C_A)V_0}{-r_A}$$

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(0905421) Chemical Reaction Engineering I

First Semester – 2016/2017

In-Class Assessment # 14 (Chapter 8)

Partner (1) Name: \_\_\_\_\_ Partner (2) Name: \_\_\_\_\_

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**P8-6 (Continued)**

The elementary irreversible organic liquid-phase reaction  $A + B \rightarrow C$  is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C, and the volumetric flow rate is  $2 \text{ dm}^3/\text{s}$  and  $C_{A0} = 0.1 \text{ kmol/m}^3$ .

(d) Calculate the conversion that can be achieved in one  $500\text{-dm}^3$  CSTR and in two  $250\text{-dm}^3$  CSTRs in series.

**Additional Information**

$$H_A^0(273 \text{ K}) = -20 \text{ kcal/mol}$$

$$H_B^0(273 \text{ K}) = -15 \text{ kcal/mol}$$

$$H_C^0(273 \text{ K}) = -41 \text{ kcal/mol}$$

$$C_{pA} = C_{pB} = 15 \text{ cal/(mol} \cdot \text{K)}$$

$$C_{pC} = 30 \text{ cal/(mol} \cdot \text{K)}$$

$$k = 0.01 \text{ L/(mol} \cdot \text{s)} \text{ at } 300 \text{ K}$$

$$E = 10,000 \text{ cal/mol}$$

$$T = 300 + 200X$$

$$V = \frac{F_{A0} X}{-r_A}$$

$$-r_A = k C_A C_B$$

$$C_A = C_{A0} (1-X)$$

$$C_B = C_{A0} (1-X)$$

$$-r_A = k C_{A0}^2 (1-X)^2$$

$$V = \frac{V_0 C_{A0} X}{k C_{A0}^2 (1-X)^2}$$

$$V = \frac{V_0}{k C_{A0}} \frac{X}{(1-X)^2}$$

$$\frac{X}{(1-X)^2} = \frac{0.01 \text{ L/(mol} \cdot \text{s)} \times 0.1 \times 10^3 \text{ L/mol}}{2 \text{ dm}^3/\text{s}} \times \frac{500 \text{ dm}^3}{10^3 \text{ dm}^3}$$

$$\frac{X}{(1-X)^2} = \frac{1}{u}$$

$$X^2 - 6X + 1 = 0$$

$$(1-X)^2 = 4X \quad Y = 0.17$$

$$1 - 2X + X^2 = 4X$$

(0905421) Chemical Reaction Engineering I

First Semester – 2016/2017

In-Class Assessment # 13 (Chapter 8)

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**P8-5 CSTR with Heat Effect**

The endothermic liquid-phase elementary reaction  $A + B \rightarrow 2C$  proceeds, substantially, to completion in a single steam-jacketed, continuous-stirred reactor. From the following data, calculate the steady-state reactor temperature:

Reactor volume: 125 gal      Steam jacket area: 10 ft<sup>2</sup>      Agitator shaft horsepower: 25 hp

Jacket steam: 150 psig (365.9 °F saturation temperature)

Overall heat-transfer coefficient of jacket,  $U$ : 150 Btu/h.ft<sup>2</sup>.°F

Heat of reaction,  $\Delta H_{Rx}^\circ = +20,000$  Btu/lb mol of A (independent of temperature)

| Component                      | A    | B    | C    |
|--------------------------------|------|------|------|
| Feed (lbmol/hr)                | 10.0 | 10.0 | 0    |
| Feed temperature (°F)          | 80   | 80   | -    |
| Specific heat (Btu/lb mol. °F) | 51.0 | 44.0 | 47.5 |
| Molecular weight (lb/lbmol)    | 128  | 94   | 222  |
| Density (lb/ft <sup>3</sup> )  | 63.0 | 67.2 | 65.0 |

$$V = \frac{F_{A0} X}{-r_A}$$

$$-r_A = k C_A C_B$$

$$C_A = C_{A0}(1-X)$$

$$C_B = C_{A0}(\theta_0 - X)$$

$$V = 125 \text{ gal} \rightarrow = 16.7 \text{ ft}^3$$

$$\frac{\text{lb}}{\text{lbmol}} \quad \frac{\text{lb}}{\text{ft}^3}$$

$$\frac{\text{lb}}{\text{ft}^3} \rightarrow \frac{\text{lbmol}}{\text{ft}^3}$$

$$V_0 = V_{A0} + V_{B0} \\ = 34.3 \text{ ft}^3/\text{h}$$

$$C_{A0} = \frac{10}{34.3} = 0.29 \text{ lbmol/ft}^3$$

$$Q - W - F_{A0} X$$



P8-13<sub>A</sub> The reaction

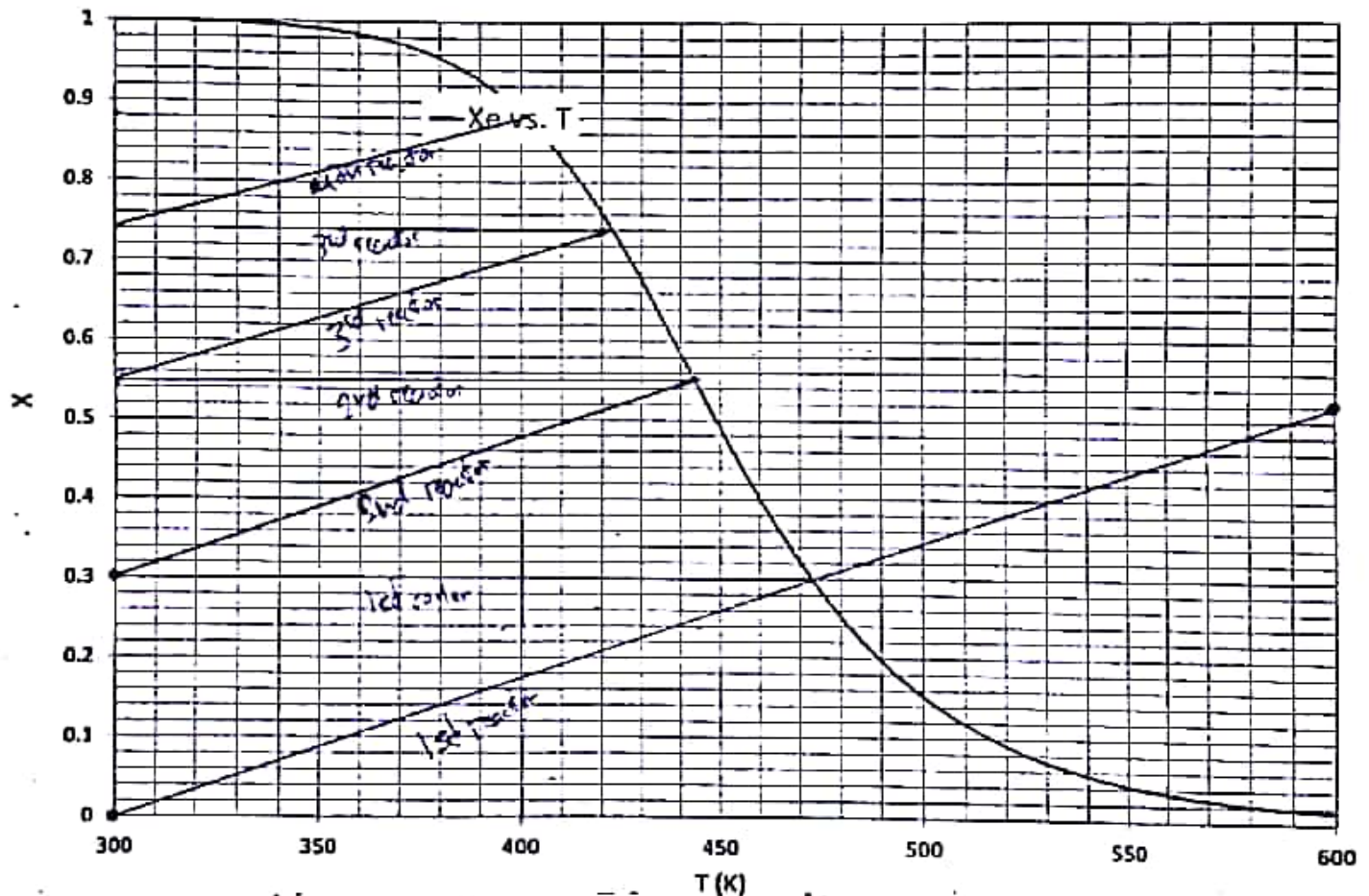


is carried out adiabatically in a series of staged packed-bed reactors with inter-stage cooling. The lowest temperature to which the reactant stream may be cooled is  $27^\circ\text{C}$ . The feed is equimolar in A and B and the catalyst weight in each reactor is sufficient to achieve 99.9% of the equilibrium conversion. The feed enters at  $27^\circ\text{C}$  and the reaction is carried out adiabatically. If four reactors and three coolers are available, what conversion may be achieved?

Additional information:

$$\Delta H_{Rx}^\circ = -30,000 \text{ cal/mol A} \quad C_{pA} = C_{pB} = C_{pC} = C_{pD} = 25 \text{ cal/g mol} \cdot \text{K}$$

$$K_e(50^\circ\text{C}) = 500,000 \quad F_{A0} = 10 \text{ mol A/min}$$



$$T = 300 + \frac{30000X}{100}$$

$$T = 300 + 300X$$

$$T = 300 + 600(X - X_1)$$

$$\sum \Theta_i C_{pi}$$

$$X = 0.88$$