– MASS BALANCES FOR REACTORS OF VARIOUS CONFIGURATIONS

1. **CSTR vs. Batch reactor *A—> M*, exothermic reaction** (60 points)

Consider a simple first order reaction of *A—>M*. A batch reactor will be compared to a CSTR with the required conversion, $f_A = .9$ (that is, the exit C_A concentration/molar flow will be 10% of the feed, C_{A0}.)

Consider first the batch reactor. Suppose that its volume of $V = 100$ l is filled with reactant *A* that has a concentration, $C_{A0} = 1$ mole/l. The heat capacity of the *A* and *M* are the same: $C_{pA} = C_{pM} = 100$ J/(mole K). The initial temperature is $T_{feed} = 300$ K. The reaction rate constant is $k = 10^{15}$ Exp[-12000/*T*] (1/s) and the heat of reaction is $\Delta H_r = -4{,}000$ J/mol.

a. What batch time will be needed for the requisite conversation of 90% of the *A* into *M* if the temperature is kept at 300K?
b. What quantity of heat must be removed to keep the reactor at 300K?
c. If the reactor were operated adiabatically, what would the final temperature be?
d. For an adiabatic reactor, the maximum reaction **rate** does not always occur at $f_A = 0$. Explain why this is so.
e. Sketch the reactor temperature as a function of time for the adiabatic case.
f. Under what conditions could the reactor temperature rise and then decrease during the course of a reaction?

A ISOTHERMAL BATCH REACTOR

$$\frac{d(VC_A)}{dt} = \underset{\text{NO FLOW}}{\sim} - kC_A V$$

V = CONST

$k = .0042/s$

$$\frac{dC_A}{dt} = -kC_A$$

$$\int \frac{dC_A}{C_A} = -k\int dt$$

$$\ln\left(\frac{C_A}{C_A^0}\right) = -kt$$

$$C_A = C_A^0 \exp(-kt)$$

$$t = \frac{-\ln\left(\frac{.1}{1}\right)}{k}$$

$$\boxed{t = 542\,s}$$

HEAT REMOVED TO KEEP T=300 $= \Delta H_r \, m \, f$

$= -4000 \frac{J}{MOLE} \times 100 \text{ MOLES} \times .9$

$Q = -360{,}000 \, J$

SUPPOSE ADIABATIC — ALL HEAT GOES TO RAISING T OF FLUID

(HEAT REMOVED) $0 = \Delta H \, m \, f + m \, C_p (T - T^{INITIAL})$

$\Delta T = \frac{\Delta H f}{C_p} = \frac{(4000 \, J/MOLE)(.9)}{100 \, J/MOLE \cdot K}$

$\Delta T = 36 \, K$

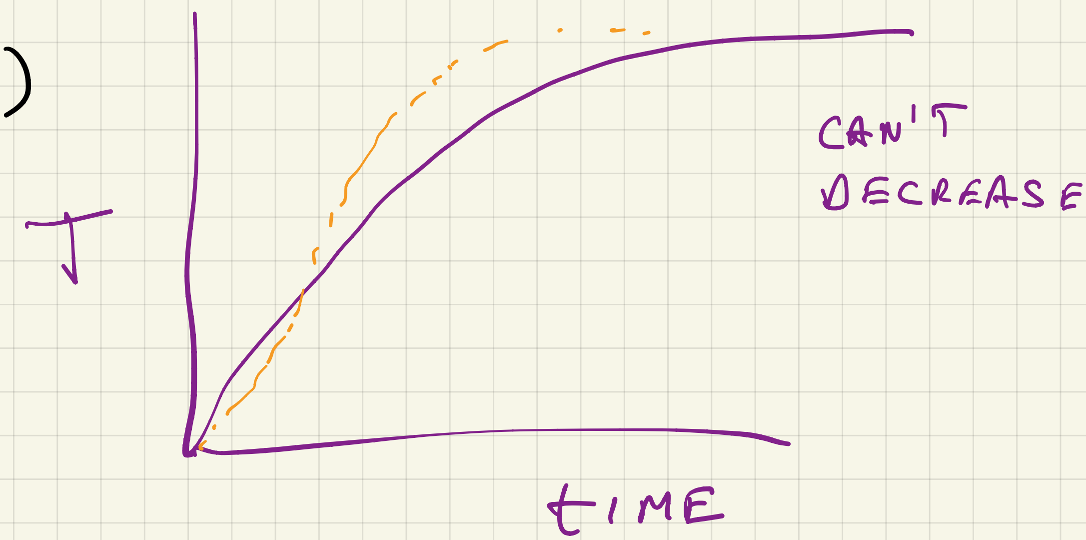
ADIABATIC TEMP RISE!

d) $r = k C_A$

IF T ↑ k ↑ FASTER THAN

C_A ↓.

e)



f) WOULD REQUIRE COOLING

Now, independently consider a CSRT with a feed stream of 1 l/s at 300K, where C_{A0} = 1 mol/l. The heat capacity of the *A* and *M* are the same: $C_{pA} = C_{pM}$ = 100 J/(mole K). The reaction rate constant is $k = 10^{15}$ Exp[-12000/*T*] (1/s) and the heat of reaction is ΔH_r = - 4,000 J/mol.

g. What reactor volume is needed to accomplish the requisite conversion of 90% of the *A* into *M* if the temperature is kept at 300K?
h. If the reactor is operating at 300K, what is the heat removal rate?
i. If the reactor is operated adiabatically, what is the steady state temperature?
j. For this case, what is the necessary residence time?

ISOTHERMAL CSTR

$$\frac{d\, VC_A}{dt} = q\, C_{Af} - q\, C_A - k C_A V \quad (\to 0)$$

$$\frac{C_A}{C_{Af}} = \frac{1}{1 + k\tau} \qquad \tau = \frac{V}{q}$$

$$\tau = \frac{C_{Af} - C_A}{C_A k}$$

$$\tau = 2120 \text{ s} \qquad q = 1\ \text{l/s}$$

$$\boxed{V = 2120 \text{ L}}$$

HEAT REMOVAL THROUGH WALL/COILS = RATE OF GENERATION

$$\left(\frac{J}{TIME}\right) \quad \dot{Q} = (\Delta H_r)\left(\begin{array}{c}\text{RATE OF}\\ \text{REACTION}\end{array}\right)$$

$$\left(\frac{J}{MOLE}\right)\left(\frac{MOLES}{TIME}\right)$$

$$= \Delta H_r \, k C_A V \quad (= \Delta H F_A f)$$

$$= -4000 \, J/_{MOL} \left(\frac{.0042}{s}\right)\left(0.1 \frac{M}{L}\right)(21202)$$

$$\dot{Q} = -3600 \, J/s$$

ADIABATIC, BUT SOMEHOW STILL GET SAME f.

$$0 = \Delta H_r F_A f + F_A\left[(1-f) C_{p_A} + f C_{p_M}\right] \Delta T$$

$$-\Delta T = \frac{-3600 \, J/s}{\left(1 \, MOLE/s\right)\left(.1 \; \frac{100 J}{MOLE K} + .9 \; \frac{100 J}{MOLE K}\right)}$$

$$\Delta T = 36 \, K$$

I AGAIN PICKED THE CONCEPT

OF 90% CONVERSION + T_{FINAL}

= 336

$k_2(336) = .31/s$

$\tau = 30s$

COMPARE BATCH + CSTR

FOR BOTH

$$\Delta T = \frac{\Delta H f}{C_{p\,FINAL\,MIX}}$$

AS LONG AS NO DILUENTS

OR AT LEAST IF

$$\frac{\text{MOLES A}}{\text{MOLES INERT}} = \text{SAME FOR BOTH}$$

NO MATTER WHAT...

IF A MOLE OF M IS PRODUCED

$\Delta H = -4000$ J

IF FLUIDS ARE TO STAY ISOTHERMAL

THIS MUCH HEAT HAS TO BE REMOVED

#2 a. $U = 0$ SO

$$\frac{df}{dt} = g(T, f_A)$$

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$$\frac{dT}{dt} = \frac{-\Delta H_r m_A^0 g(T, f_A)}{m_A^0 \left((1-f_A)c_{pA} + (1.2-f_A)c_{pB} + f_A c_{pC}\right)}$$

$$\Longrightarrow \frac{dT}{df_A} = \frac{\Delta H_r}{\left((1-f_A)c_{pA} + (1.2-f_A)c_{pB} + f_A c_{pC}\right)}$$

b. THE PROBLEM IS THAT THE NUMBER OF MOLES IS CHANGING.

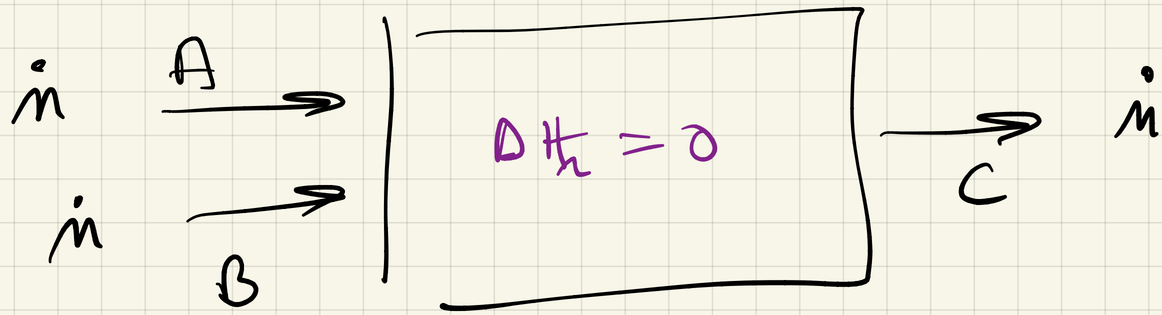
REFERENCE T

IF WE DEFINE: $\underline{H}_A = \underline{c}_{pA}(T - T_0)$

$\underline{H}_B = \underline{c}_{pB}(T - T_0)$

$\underline{H}_C = \underline{c}_{pC}(T - T_0)$

CONSIDER



FOR THIS CASE $\Delta H = 0$

$$0 = \dot{m}(\underline{H}_A + \underline{H}_B) - \dot{m}\,\underline{H}_C$$

$$0 = (C_{pA} + C_{pB})(T - T_0) - C_{pC}(T - T^0)$$

→ THIS IS ONLY CORRECT IF $C_{pA} + C_{pB} = C_{pC}$

(10)

3)

a) MOST LIKELY THE PACKING HAS SETTLED

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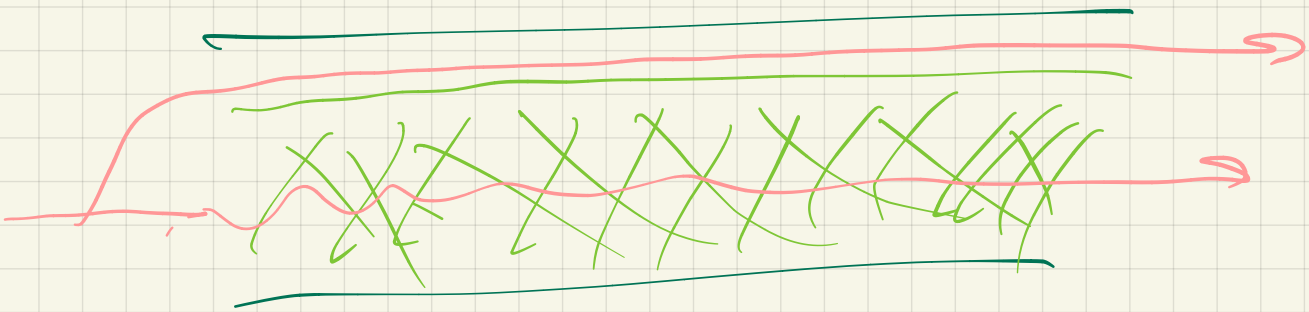

b) ΔP (FLOW RATE)

RESULT WILL NOT MATCH ERGUN EQ.

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