

Name: \_\_\_\_\_

ADA SLAW

**Problem 3 (25 points)***const assume elementary rxn.*

Consider synthesizing R via the liquid-phase reaction,  $A + B \leftrightarrow R$ . However, over-accumulation of B leads to undesired side reactions. Therefore, a semi-batch reactor is proposed to be used in the following manner: initially charge with A ( $N_{A0}$ ,  $V_0$ ), and feed a stream of B ( $v_0$ ,  $C_{B0}$ ) until the desired  $X_A$  is achieved.

- While the reactor is being filled, the volume  $V$  varies with time. Perform an overall mass balance to determine  $V(t)$ .
- What is  $N_A$ ,  $N_B$  and  $N_R$  in terms of conversion  $X_A$ ? *so they want me to write 3 eqns.*
- Write the mole balance on species A and obtain a differential equation for  $X_A$  as a function of time. DO NOT SOLVE FOR  $X_A$  - leave as a differential equation.
- If the reaction reached equilibrium after feeding species B for a time  $t$ , write an expression for  $K_c$ , in terms of time  $t$ , and  $X_{Ae}$  - the equilibrium conversion of A.

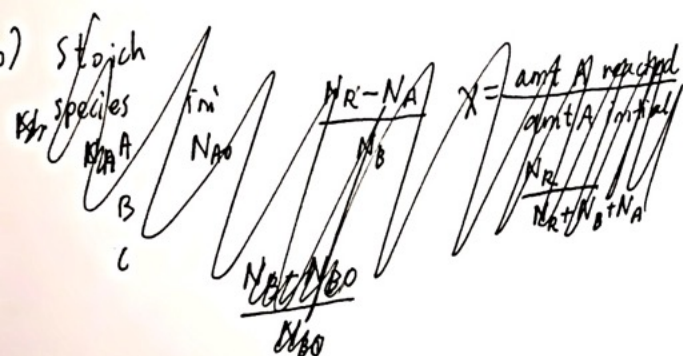
a)  $acc = in - out + gen$

$$\frac{dm}{dt} = v_0 \rho$$

$$\rho \frac{dV}{dt} = v_0 \rho$$

$$\int_{V_0}^{V(t)} dV = v_0 \int_0^t dt$$

$$V(t) = v_0 t + V_0$$



$$N_A = N_{A0} - N_{A0} X_A$$

$$N_B = -N_{A0} X_A + C_{B0} v_0 t$$

$$N_R = N_{A0} X_A$$

Part D:

$$K_c = \frac{C_R}{C_A C_B} = \frac{N_{A0} X_A (v_0 t + V_0)}{N_{A0} (1 - X_A) (N_{A0} X_A + C_{B0} v_0 t)}$$

c)  $\frac{dN_A}{dt} = F_{A0} - F_A + r_A$

$$-N_{A0} \frac{dX_A}{dt} = -F_{A0}(1 - X_A) + (k_1 C_A C_B - k_{-1} C_R) V$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1 - X_A)}{v_0 t + V_0}$$

$$C_B = \frac{N_B}{V} = \frac{-N_{A0} X_A + C_{B0} v_0 t}{v_0 t + V_0}$$

$$C_R = \frac{N_R}{V} = \frac{N_{A0} X_A}{v_0 t + V_0}$$

$$\frac{dX_A}{dt} = \left( -k_1 \left( \frac{N_{A0}(1 - X_A)}{v_0 t + V_0} \right) \left( \frac{-N_{A0} X_A + C_{B0} v_0 t}{v_0 t + V_0} \right) + k_{-1} \left( \frac{N_{A0} X_A}{v_0 t + V_0} \right) \right) \frac{v_0 t + V_0}{N_{A0}}$$

$$= \left( -k_1 N_{A0} (1 - X_A) (-N_{A0} X_A + C_{B0} v_0 t) + k_{-1} N_{A0} X_A \right) / N_{A0}$$

$$= -k_1 (1 - X_A) (X_A + C_{B0} v_0 t / N_{A0}) + k_{-1} X_A$$

$$+ k_{-1} X_A$$