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Problem 3 (25 points)

Consider synthesizing R via the liquid-phase reaction, A + B ↔ 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.

a) While the reactor is being filled, the volume V varies with time. Perform an overall mass balance to determine V(t).
b) What is N_A, N_B and N_R in terms of conversion X_A?
c) 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.
d) If the reaction reached equilibrium after feeding species B for a time t, write an expression for Kc, in terms of time t, and X_{Ae} – the equilibrium conversion of A.

const ρ assume elementary rxn.

so they want me to write 3 eqns.

a) acc = in − out + gen

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

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

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

$V(t) = v_0 t + V_0$

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

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

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

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

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

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

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

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

b) Stoich

Species	N_i	$\frac{N_R - N_A}{N_B}$	$X = \frac{\text{amt A reacted}}{\text{amt A initial}}$
A	N_{A0}		$\frac{N_R}{N_R + N_B + N_A}$
B	$C_{B0} v_0 t$		
C			

$\frac{N_{A0} X_A}{N_{B0}}$

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

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

$N_R = N_{A0} X_A$

Part D:

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