Josh Whitehead 09 Feb 2022

HW 3

1) $P_1 = P_2 = 101\ kPa$ $\quad A + 2B \rightarrow C + D$

$T_1 = T_2 = 25°C$

$y_C^{sat} = 0.25$

1° order in A, B

$F_{A0} = 1\ \frac{mol}{sec}$

$F_{B0} = 2\ \frac{mol}{sec} = 2F_{A0}$

$\dot{V} = 1.5\ \frac{L}{min}$

$k = 0.035\ \frac{L}{mol \cdot sec}$

a) first order in A, B $\therefore$ $-r_A = k\, C_A^1 C_B^1$

If elementary then $-r_A = k\, C_A C_B^2$

$\therefore$ $\boxed{\text{this is not an elementary rxn/step}}$

b)

Species	I	Δ	F (before condense)
A	F_{A0}	$-x_A F_{A0}$	$F_{A0}(1-x_A)$
B	$2F_{A0}$	$-2x_A F_{A0}$	$2F_{A0}(1-x_A)$
C	0	$+x_A F_{A0}$	$x_A F_{A0}$
D	0	$+x_A F_{A0}$	$x_A F_{A0}$
Total	$3F_{A0}$	$-x_A F_{A0}$	$3F_{A0}(1-x_A) + 2x_A F_{A0}$ $= F_{A0}(3-x_A)$

c) $P_{vap} = y_C \cdot P_{tot} = 0.25 \cdot 101\ kPa$ $\boxed{= 25.3\ kPa}$

$y_C = \frac{F_C}{F_{tot}} = \frac{x_A \cancel{F_{A0}}}{\cancel{F_{A0}}(3-x_A)} \rightarrow x_A = \frac{3y}{1+y}$ $\boxed{= 0.6}$ mol

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1) d) Finish table:

	F (after condens.)
A	$F_{A0}(1-X_A)$
B	$2F_{A0}(1-X_A)$
C	$y_C F_{tot}$
D	$X_A F_{A0}$
tot	$3F_{A0}(1-X_A)+X_A F_{A0}+y_C F_{tot} = y_C F_T + 3F_{A0} - 2F_{A0}X_A$

– C is only one that condenses

$-r_A = C_A C_B$

$$C_i = \frac{C_{A0}\left(\Theta_j - \frac{\nu_j}{\nu_A} X_A\right)}{1+\varepsilon X_A} \quad \therefore \; C_A = \frac{C_{A0}(1-X_A)}{1-\frac{1}{3}X_A}$$

$$\varepsilon = y_{A0}\delta = \frac{1}{3}(1+1-2-1) = -\frac{1}{3}$$

$$C_B = \frac{C_{A0}(2-2X_A)}{1-\frac{1}{3}X_A}$$

$$\therefore \boxed{-r_{A\,before} = 2kC_{A0}^2\left(\frac{(1-X_A)^2}{(1-\frac{1}{3}X_A)^2}\right)}$$

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1) d)

$$C_A = \frac{F_A}{\dot{v}} \qquad C_B = \frac{F_B}{\dot{v}} \qquad \text{where } \dot{v} = \dot{v}_0 \left(\frac{F_T}{F_{T_0}}\right)$$

$$F_T = y_C F_T + 3F_{A_0} - 2F_{A_0} X_A$$

$$\rightarrow F_T = \frac{2F_{A_0}(1.5 - X_A)}{1 - y_C}$$

$$\dot{v} = \dot{v}_0 \left(\frac{2\cancel{F_{A_0}}(1.5 - X_A)}{3\cancel{F_{A_0}}(1 - y_C)} \right) = \frac{\dot{v}_0 2 \cdot \left(\frac{3}{2} - X_A\right)}{3(1 - y_C)}$$

$$\therefore C_A = \frac{F_{A_0}(1 - X_A) \cdot 3(1 - y_C)}{2\dot{v}_0(1.5 - X_A)}$$

$$C_B = \frac{\cancel{2} F_{A_0}(1 - X_A) \cdot 3(1 - y_C)}{\cancel{2}\dot{v}_0\left(\frac{3}{2} - X_A\right)}$$

$$\boxed{\therefore -r_A = \frac{k\, 4.5\, C_{A_0}^2 (1 - y_C)^2 (1 - X_A)^2}{(1.5 - X_A)^2}}$$

↑

after condense

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HW #3

1)e) $V = \frac{F_{A0} X_A}{-r_A}$

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2) a) Given $\bar{K}_{eq}$, k_f, and T, find

E_A, A, H_{rxn}

for E_A

$$k_f(T) = k_f(T_0) \exp\left(\frac{+E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right)$$

$$\rightarrow E_A = \frac{R \ln\left(\frac{k(T)}{k(T_0)}\right)}{\frac{1}{T_0} - \frac{1}{T}}$$

using $T_0 = 30^\circ$
- Solve for each set of data and average!

$$\boxed{E_A = 111. \frac{kJ}{mol}}$$

for A $k_f(T) = A \exp\left(\frac{-E}{RT}\right)$

$$\rightarrow A = \frac{k_f(T)}{\exp\left(\frac{-E}{RT}\right)} \Rightarrow \boxed{2.42 \times 10^{12}}$$

for ΔH^{rxn}

$$\bar{K}(T) = \bar{K}(T_0) \exp\left(\frac{\Delta H}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right)$$

$$\rightarrow \Delta H^{rxn} = \frac{R \ln\left(\frac{\bar{K}(T)}{\bar{K}(T_0)}\right)}{\frac{1}{T_0} - \frac{1}{T}} \Rightarrow \boxed{-63.0 \frac{kJ}{mol}}$$