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HW 10

a.)

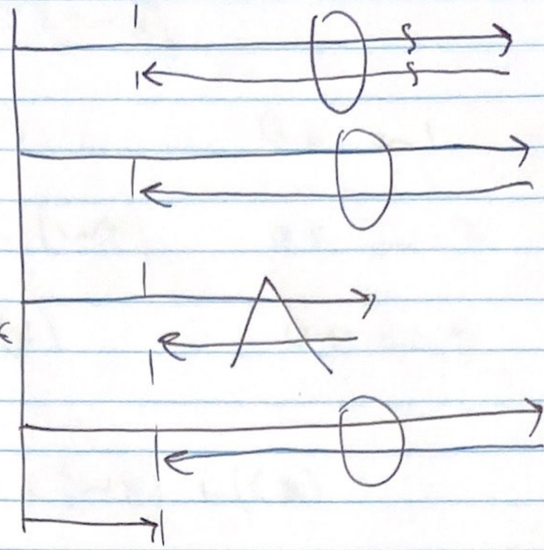
$D + * \rightleftarrows D*$

$W + * \rightleftarrows W*$

$D* + W* \rightarrow C* + *$

$C* \rightleftarrows C + *$

Net



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b) $r = r_3 = k_R (D*)(W*)$

$\underline{K}_D (D)(*) = (D*)$ QE on 1

$\underline{K}_W (W)(*) = (W*)$ QE on 2

$\underline{K}_C (C*) = (C)(*)$ QE on 4

$C_T = (*) + (D*) + (W*) + (C*)$

$C_T = (*) + \underline{K}_D (D)(*) + \underline{K}_W (W)(*) + \frac{(C)(*)}{\underline{K}_C}$

$C_T = * \left(1 + \underline{K}_D (D) + \underline{K}_W (W) + \frac{(C)}{\underline{K}_C}\right)$

$r = k_R (*)^2 \underline{K}_D (D) \underline{K}_W (W)$

$$\boxed{\therefore r = k_R \underline{K}_D \underline{K}_W (D)(W) \cdot \left(\frac{C_T}{1 + \underline{K}_D (D) + \underline{K}_W (W) + \frac{(C)}{\underline{K}_C}}\right)^2}$$

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c) $C_T = (*)$

$$\therefore \boxed{r = k_R \bar{k}_D(D)\, \bar{k}_w(w)\, C_T^2}$$

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d) $\frac{C_A}{C_{AS}} = \frac{1}{10}$

$\lambda = 0.8$

$\frac{C_A}{C_{AS}} = \frac{1}{\lambda} \frac{\sinh(\phi_1 \lambda)}{\sinh(\phi_1)} \rightarrow \phi_1 = 12.63 > 2$

$\therefore \eta = \frac{3}{\phi_1^2}(\phi_1 - 1) \boxed{= 0.219}$

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e) $$V_{PFR} = F_{A0} \int_0^{x_A} \frac{dx_A}{-r_A} = \dot{v} C_{A0} \int_0^{x_A} \frac{dx_A}{k C_A}$$

$$C_A = \frac{C_{A0}\left(\Theta - \frac{\nu_i}{\nu_A} x_A\right)}{1 + \epsilon x_A} = \frac{C_{A0}(1 - x_A)}{1 + x_A\left(1(0.2 + 1 - 1)\right)}$$

$$\rightarrow C_A = \frac{C_{A0}(1 - x_A)}{1 + 0.2 x_A}$$

$$\rightarrow V = \frac{\dot{v} \cancel{C_{A0}}}{k \cancel{C_{A0}}} \int_0^{x_A} dx_A \frac{(1 + 0.2 x_A)}{1 - x_A}$$

$$= \frac{\dot{v}}{k}\left[-0.2(x_A - 1) - (1.2)\ln(|x_A - 1|)\right]_{x_A = 0.6}$$

$$= 58.98 \; \boxed{= 59.0 \text{ L}}$$

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f.) The conversion estimated in (e) should be the same as the conversion calculated by the segregation model.

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9) $A \leftrightarrows B + 0.2C$

$$r = -r_A = \frac{k_1 (A)}{k_1} - \frac{k_{-1} (B)(C)^{0.2}}{k_1}$$

$$\rightarrow = \left((A) - \frac{(B)(C)^{0.2}}{\underline{K}} \right) k_1$$

$$(A) = \frac{C_{A0}(1 - X_A)}{1 + 0.2 X_A}$$

$$(B) = \frac{C_{A0} X_A}{1 + 0.2 X_A} \qquad (C) = \frac{0.2 C_{A0} X_A}{1 + 0.2 X_A}$$

$$-r_A = 0 = \cancel{k_1} \left[\frac{C_{A0}(1 - X_A)}{1 + 0.2 X_A} - \frac{\frac{C_{A0} X_A}{1 + 0.2 X_A} \left(\frac{0.2 C_{A0} X_A}{1 + 0.2 X_A} \right)^{0.2}}{1 + 0.2 X_A} \right]$$

$$C_{A0} = \frac{P_0}{T_0 R} = \frac{10}{700 \cdot 0.0821} = 0.174$$

$$\boxed{\rightarrow X_A = 0.939}$$

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h) $Q = F_{A0} X_A (-\Delta H_R)$

$\Delta H_R = -5000 \frac{J}{mol}$

$X_A = 0.60$

$F_{A0} = C_{A0} \dot{V} = \frac{P_0}{T_0 R} \cdot 5 \frac{L}{sec} = \frac{10}{700(0.0821)} \cdot 5 = 0.870 \frac{mol}{sec}$

$\therefore \; Q = 0.870 (0.6)(5000) = 2610.1 \frac{J}{\cancel{mol}\; sec}$

$\cancel{= 2.61 \frac{KJ}{mol}}$

$\boxed{= 2.61 \text{ KW}}$

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i) $A \to B + 0.2C$

$\Delta H_R = -5000 \frac{J}{mol}$

$$T = T_0 + \frac{(-\Delta H_R)\chi_A}{\Sigma\Theta_i C_{p_i}}$$

$\Theta_A = 1$

$\Theta_B = \Theta_C = 0$

$\Sigma\Theta_i = 1$

$C_p = 35 \frac{J}{mol\,K}$

$$\frac{dF_A}{dV} = kC_A = -r$$

$T_0 = 700K$

$\dot{V} = 5 \frac{L}{sec}$

$$\rightarrow \frac{d\chi_A}{dV} = \frac{kC_A}{F_{A_0}} = \frac{kC_A}{\dot{V}C_{A_0}}$$

$k = 0.1 \frac{1}{sec}$

$$C_A = \frac{C_{A_0}(1-\chi_A)}{1+0.2\chi_A}\left(\frac{T_0}{T}\right)$$

$$\therefore \frac{d\chi_A}{dV} = \frac{k(1-\chi_A)}{\dot{V}(1+0.2\chi_A)}\left(\frac{T_0}{T}\right)$$

$\rightarrow$ odeint in python

$$\rightarrow \boxed{\begin{array}{l}\chi_A = 0.639 \\ T = 791\,K\end{array}}$$

HW10_i

April 26, 2022

[ ]:
```
import numpy as np
from scipy.integrate import odeint

T0 = 700
dHR = -5000
thet = 1
cp = 35
k = .1
v = 5

def ode(x,V):
    T = T0 + -dHR*x/thet/cp
    dxdv = k/v*(1-x)/(1+.2*x)*T0/T

    return dxdv

V = np.linspace(0,59)
init = 0

x = odeint(ode,init,V)
print(x[-1][-1])
T = T0 + -dHR*x/thet/cp
print(T[-1][-1])
```

```
0.6391271620690431
791.3038802955775
```

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i)

Species	Enter	Change	Before	After
A	F_{A0}	$-X_A F_{A0}$	$F_{A0}(1-X_A)$	$F_{A0}(1-X_A)$
B	0	$X_A F_{A0}$	$X_A F_{A0}$	$Y F_T$
C	0	$0.2 X_A F_{A0}$	$0.2 X_A F_{A0}$	$0.2 F_{A0} X_A$
tot	F_{A0}	$0.2 X_A F_{A0}$	$F_{A0}(1+0.2X_A)$	$F_{A0}(1-X_A) + Y F_T + 0.2 F_{A0} X_A$

for $A \rightarrow B + 0.2C$

$$Y = \frac{F_B}{F_T} = \frac{X_A \cancel{F_{A0}}}{\cancel{F_{A0}}(1+0.2X_A)} = \frac{X_A}{1+0.2X_A}$$

$Y = 0.2$

$\therefore \boxed{X_A = 0.208}$