Josh Whitehead 15 Mar 2022

HW 6

1)

a)

$A + 2B \rightarrow C$

$-r_A = k C_B^2$

$R = 8.314 \frac{J}{mol K}$

assume: adiabatic, steady state, isobaric

$k = A e^{-E_a/RT} \rightarrow A = \frac{k}{\exp\left(\frac{-E_a}{RT}\right)} = \frac{0.0055}{\exp\left(\frac{-500}{R(300)}\right)} = 0.00672$

$$C_B = \frac{C_{A_0}\left(\Theta_B - \frac{\nu_B}{\nu_A} x_A\right) T_0}{(1 + \varepsilon x_A) T}$$

where $C_{A_0} = \frac{F_0 y_{A_0}}{V_0}$, $\Theta_B = \frac{y_{B_0}}{y_{A_0}}$, $\frac{\nu_B}{\nu_A} = 2$

$\varepsilon = -2 y_{A_0}$

E-bal:

$$\underbrace{\frac{dE}{dt}}_{SS} = \underbrace{\cancel{\dot{Q}}}_{adiabatic} - \underbrace{\cancel{\dot{W}_s}}_{no\ shaft} - F_{A_0} \sum \Theta_i \tilde{C}_{p_i} (T - T_0) - F_{A_0} x_A \left(\Delta H_R^\circ + \underbrace{\cancel{\Delta C_p (T - T_R)}}_{\Delta C_p = 0}\right)$$

$$\therefore T = T_0 - \frac{x_A \, \Delta H_R^\circ}{\sum \Theta_i C_p}$$

Design Eq

$$\frac{dx_A}{dV} = \frac{r_A}{F_{A_0}} = \frac{k C_B^2}{F_{A_0}}$$

→ use "ODEINT" with $\phi = x$ as ~~initial~~ on [0, 150]

→ ~~x @ ...~~ $\boxed{@ \ 150 L \quad x = 3.22 \times 10^{-3} \quad T = 500.03 K = 500. K}$

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1) b) $T = 600\,K$

$$T_0 = T + \frac{x_A\, \Delta H_R^{\circ}}{\sum \theta_i C_P}$$

C_B = same as ~~…~~ problem 1.a.

since ~~$\frac{dV}{dx}$~~ $\frac{dx}{dV} = \frac{k C_B^2}{F_{A0}}$

$$\rightarrow \frac{dV}{dx} = \frac{F_{A0}}{k C_B^2}$$

→ use "ODEInt" with $V=0$ as initial ~~and~~ on $x = [0, 0.95]$

@ $x = 0.95$: $\boxed{\begin{array}{l} T_0 = 591.\,K \\ V = 6.88 \times 10^4\ L \end{array}}$

```python
import numpy as np
import scipy.integrate as inte
import matplotlib.pyplot as plt

Ea = 500                                        #j/mol
k_arr = .0055                                   #L/mol/sec
T_arr = 300                                     #k
R = 8.314                                       #j/mol/k
V = 150                                         #L
cp = 150                                        #j/mol/k
dHR = -7000                                     #j/mol
dcp = 0
F0 = 5                                          #mol/s
v0 = 50                                         #L/sec
yA0 = .2
yB0 = .6
yC0 = .2
T0 = 500                                        #k
eps = yA0*(1-2-1)
thetA = 1
thetB = yB0/yA0
thetC = yC0/yA0
FA0 = F0*yA0
thet = np.array([thetA,thetB,thetC])
cA0 = FA0/v0


A = k_arr/np.exp(-Ea/T_arr/R)

def k(temp):
    return A*np.exp(-Ea/R/temp)

def mass(x,V):
    T = T0-x*dHR/sum(thet)/cp


    cB = cA0*(thetB-2*x)*T0/T/(1+eps*x)

    dxdv = k(T)*cB**2/FA0
    return dxdv

sol = inte.odeint(mass,0,np.linspace(0,V))

print(sol[-1][0])
print(T0-sol[-1][0]*dHR/sum(thet)/cp)

# plt.plot(sol)
# plt.show()
```

```
print(A)

def prob(V,x):
    T = 600
    T0 = T+x*dHR/sum(thet)/cp
    cb = cA0*(thetB-2*x)*T0/(1+eps*x)/T

    dvdx = FA0/k(T)/cb**2
    return dvdx

sol = inte.odeint(prob,0,np.linspace(0,.95))
plt.plot(np.linspace(0,.96),sol)
plt.show()
print(np.linspace(0,.95)[-1],sol[-1][0])
T0 = 600+.95*dHR/sum(thet)/cp
print(T0)
```

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2) a) $A + B \longrightarrow C$

Assume: elementary
isobaric

$$\left.\begin{aligned} C_{P,A} &= 25 \\ C_{P,B} &= 35 \\ C_{P,C} &= 60 \end{aligned}\right\} \frac{kJ}{mol\,K}$$

$V = 1\ m^3$
$\dot{V}_0 = 0.5\ \frac{m^3}{min}$
$C_{A_0} = 1\ \frac{mol}{L} = 1000\ \frac{mol}{m^3}$

$T_0 = 300\ K$
$T_{adiab} = 350\ K$

$$\dot{Q} = F_{A_0} X_A (-\Delta HR)$$

$F_{A_0} = C_{A_0} \cdot \dot{V}_0 = 500\ \frac{mol}{m^3}$, $X_A = 0.4$

$$\Delta H_R = H_A + \frac{\nu_B}{\nu_A} H_B + \frac{\nu_C}{\nu_A} H_C = H_A + H_B - H_C$$
$$= (C_{P,A} + C_{P,B} - C_{P,C})T$$

~~$\Delta HR = CP_A \Delta T$~~ $\Delta H_R = \dfrac{(C_{PA} + C_{PB})(T_0 - T)}{2 X_A}$

$$= 3750\ \frac{kJ}{mol}$$

$\therefore \dot{Q} = F_{A_0} X_A (-\Delta H_R) = 500 \cdot 0.4 (-3750) = -750{,}000$

$$\boxed{= -7.50 \times 10^5\ \frac{kJ}{min}}$$

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3) $V_{CSTR} = \frac{F_{A0} X_A}{-r_A}$ $-r_A = k C_A C_B$

$C_A = C_{A0}(1-X_A)\frac{T_0}{T} = C_B$ $\therefore$ $\underline{-r_A = k C_A^2}$

E-Bal: $\Delta C_p = -\sum \frac{\nu_i}{\nu_A} C_{pi} = 0$

$0 = F_{A0}\sum \Theta \tilde{C}_{pi}(T-T_0) + F_{A0}X_A(\Delta H_R^\circ + \cancel{\Delta C_p(T-T_R)})$

$\rightarrow \underline{T = T_0 - \frac{X \cdot \Delta H_R^\circ}{C_{PA} + C_{PB}}}$

$V = \frac{F_{A0} X_A}{k\left(C_{A0}(1-X_A)\frac{T_0}{T}\right)^2}$

$\rightarrow$ Solve in python: $\boxed{\begin{array}{l} T = 505\ K \\ X_A = 0.860 \end{array}}$

$k = A\exp\left(\frac{-E}{RT}\right)$ $\rightarrow A = \frac{k_{300}}{\exp\left(\frac{-E}{R \cdot 300}\right)}$

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.optimize as opt


T0 = 300                                            #k
V = 10                                              #L
v0 = 2                                              #L/s
c = 6                                               #mol/L
Ha0 = -10                                           #kcal/mol @273k
Hb0 = -5
Hc0 = -20
Cpa = 10/1000                                       #kcal/mol/k
Cpb = 12/1000
Cpc = 22/1000
k300 = .02                                             #L/mol/s @300k
E = 8                                               #kcal/mol
cA0 = 6
FA0 = cA0*v0
R = 1.986e-3
A = k300/np.exp(-E/R/300)
def k(temp):
    return A*np.exp(-E/R/temp)

dCp = -(Cpa+Cpb-Cpc)
TR = 273
dHR = Hc0-Hb0-Ha0

def prob(x):
    T = T0-x*dHR/(Cpa+Cpb)
    ca = cA0*(1-x)*T0/T
    cb = ca
    # cc = cA0*(x)*T0/T
    r = k(T)*ca*cb
    vol = FA0*x/r
    # eb = FA0*(Cpa+Cpb-Cpc)+FA0*x*(dHR+dCp*(T-TR))
    return vol
plt.plot(np.linspace(0,1),prob(np.linspace(0,1)))
plt.ylim(0,20)
plt.grid()
plt.show()
# sol = opt.fsolve(prob,[.9,500])
# print(sol)

ca = cA0*(1-.9)*T0/500

v = FA0*.9/k(500)/ca**2

# print(dCp)
T = T0-.9*dHR/(Cpa+Cpb)
```

```
print(T)
```

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4) $-r_A = k \quad \therefore V_{CSTR} = \frac{C_{A0} \dot{V}_0 X_A}{k}$

$$\rightarrow \frac{V}{\dot{V}} = \frac{C_{A0} X_A}{k} = \tau \qquad k = A\exp\left(\frac{-E}{RT}\right)$$

$$X_A = \frac{\sum \Theta_i C_{p,i}(T-T_0)}{-\Delta H_R^\circ - \Delta C_p(T-T_R)} = \frac{C_{p,A}(T-T_0)}{-\Delta H_R^\circ - \Delta C_p(T-T_{ref})}$$

$$\Delta C_p = -\sum \frac{\nu_i}{\nu_A} C_{p_i} = -(C_{pA} - C_{pB} - C_{pC}) = -(C_{pA} - 0.5C_{pA} - 0.5C_{pA}) = 0$$

$$\therefore \Delta C_p = 0, \quad X_A = \frac{C_{pA}(T-T_0)}{-\Delta H_R^\circ}$$

$$\therefore \boxed{\tau = \frac{C_{A0}}{k} \cdot \frac{C_{pA}(T-T_0)}{-\Delta H_R^\circ}}$$