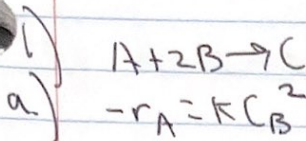


Josh Whitehead

15 Mar 2022

HW 6



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

assume
adiabatic steady state
isobaric

$k = A e^{-E_a/RT} \rightarrow A = \frac{k}{\exp(-E_a/RT)} = \frac{0.0055}{\exp(-500/(8.314(300)))} = 0.00672$

~~XXXX~~ $C_B = \frac{C_{A0}(\Theta_B - \frac{\nu_B}{\nu_A} X_A) T_0}{(1 + \epsilon X_A) T}$

where $C_{A0} = \frac{F_0 Y_{A0}}{V_0}$, $\Theta_B = \frac{T_{B0}}{T_{A0}}$, $\frac{\nu_B}{\nu_A} = 2$

$\epsilon = -2 Y_{A0}$

E-bal: $\frac{dE}{dt} = \dot{Q} - W_s + F_{A0} \sum \Theta_i (C_{pi}(T - T_0)) - F_{A0} X_A (\Delta H_R^\circ + DCP(T - T_0))$
SS, no shaft, adiabatic, DCP=0

$\therefore T = T_0 - \frac{X_A \Delta H_R^\circ}{\sum \Theta_i C_{pi}}$

Design Eq

$\frac{dX_A}{dV} = \frac{-r_A}{F_{A0}} = \frac{kC_B^2}{F_{A0}}$

→ use 'ODEINT' with $\phi = X$ as initial on $[0, 150]$

→ ~~XXXX~~ @ 150 L

$X = 3.22 \times 10^{-3}$
 $T = 500.03 K \approx 500 K$

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Hw 6

1) b) $T = 600 \text{ K}$

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

C_B = Same as ~~Problem~~ Problem 1.a.

Since ~~$\frac{dV}{dx}$~~ $\frac{dx}{dV} = \frac{KC_B^2}{F_{A0}}$

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

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

@ $x = 0.95$:

$$\begin{aligned} T_0 &= 591. \text{ K} \\ V &= 6.88 \times 10^4 \text{ L} \end{aligned}$$

```

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

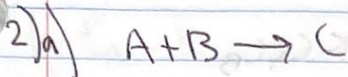
sol = inte.odeint(prob,0,np.linspace(0,.95))
plt.plot(np.linspace(0,.96),sol)
plt.show()
print(np.linspace(0,.95)[-1],sol[-1][0])
T0 = 600+.95*dHR/sum(thet)/cp
print(T0)

```


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HW 6



Assume: elementary
isobaric

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

$$V = 1 m^3$$

$$\dot{V}_0 = 0.5 \frac{m^3}{min}$$

$$C_{A0} = 1 \frac{mol}{L} = 1000 \frac{mol}{m^3}$$

$$T_0 = 300 K$$

$$T_{ad,iso} = 350 K$$

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

$$F_{A0} = C_{A0} \cdot \dot{V}_0 = 500 \frac{mol}{min}$$

$$X_A = 0.4$$

$$\Delta H_R = H_A + \frac{V_B}{V_A} H_B + \frac{V_C}{V_A} H_C = H_A + H_B - H_C$$

$$= (C_{P,A} + C_{P,B} - C_{P,C}) T$$

$$\Delta H_R = \frac{(C_{P,A} + C_{P,B})(T_0 - T)}{2 X_A}$$

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

$$\therefore \dot{Q} = F_{A0} X_A (-\Delta H_R) = 500 \cdot 0.4 (-3750) = -750,000$$

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

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16 Mar 2022

HW6

$$3) V_{\text{CSTR}} = \frac{F_{A0} X_A}{-r_A}$$

$$-r_A = K C_A C_B$$

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

E-Bal:

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

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

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

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

→ Solve in python:

$$T = 505 \text{ K}$$
$$X_A = 0.860$$

$$K = A \exp\left(\frac{-E}{RT}\right)$$

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

```

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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Hw 6

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

$$\rightarrow \frac{V}{\dot{V}} = \frac{C_{A0} X_A}{k} = \tau$$

$$k = A \exp\left(\frac{-E}{RT}\right)$$

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

$$D_{CP} = -\sum \frac{V_i}{V_A} C_{p,i} = -(C_{p,A} - C_{p,B} - C_{p,C}) = -(C_{p,A} - 0.5 C_{p,A} - 0.5 C_{p,B}) = 0$$

$$\therefore D_{CP} = 0, \quad X_A = \frac{C_{p,A} (T - T_0)}{-\Delta H_R^\circ}$$

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