CRE HOMEWORK #6

PROBLEM #1

a. **NON-ISOTHERMAL PFR**

$$A + 2B \longrightarrow C$$

$$-r_A = k C_B^2$$

$$T = T_0 + \frac{(-\Delta H_R) X}{\sum \Theta_i \, c_{p,i}}$$

$y_{A0} = 0.2$ A is LIMITING

$y_{B0} = 0.6$

PFR DESIGN EQN.

$$\frac{dF_A}{dV} = \frac{-F_{A0}\, dX}{dV} = -k C_B^2$$

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

$\Theta_A = 1$ $\Theta_B = 3$

$\Theta_i = 1$

$\sum \Theta = 5$

GAS PHASE REACTION

$P = P_0$

$$C_A = C_{A0}\left(\frac{1 - X}{1 + \epsilon X}\right)\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right)$$

$$C_B = C_{A0}\left(\frac{\Theta_B - \frac{\nu_B}{\nu_A} X}{1 + \epsilon X}\right)\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right)$$

$$= C_{A0}\left(\frac{\Theta_B - 2X}{1 + \epsilon X}\right)\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right)$$

$$\epsilon = \delta y_{A0} = (-2)(0.2) = -0.4 \qquad \Theta_B = 3$$

BACK TO DESIGN EQN.

$$\frac{dX}{dV} = \frac{k C_{A0}^2}{F_{A0}} \left(\frac{\Theta_B - 2X}{1-0.4X} \right)^2 \left(\frac{T_0}{T} \right)^2$$

V from 0 to 150 L

Arrehinus EQN

$$k(T_2) = k_1(T_1) \exp\left[\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right]$$

$T_1 = 500K$

$$T = T_0 + \frac{7000 \frac{J}{Mol} (X)}{150 \frac{J}{Mol \cdot K} (5)}$$

$T = 500.05 K$

$X = 0.0032$

b. $T_{MAX} = 600K$

$X_{Af} = 0.95$

$$600K = T_0 + \frac{7000X}{(150)(5)} \leftarrow 0.95$$

~~$T_0 = 592.6K$~~

$T_0 = 591.1K$

$$\frac{dV}{dX} = \frac{F_{A0}}{k}\left(\frac{1-0.4X}{3-2X}\right)^2\left(\frac{T}{T_0}\right)^2\frac{1}{C_{A0}^2}$$

Integrate from $X = 0$ to 0.95

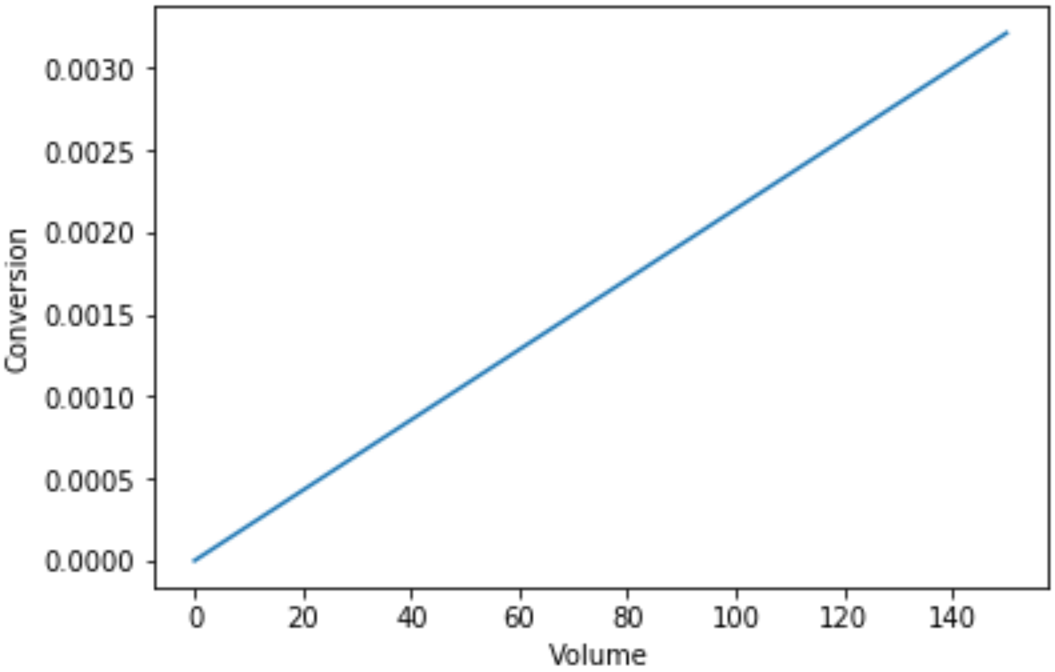
$$\boxed{V_R = 7\times10^4 \text{ L}}$$

Solution HW6.1A

In [26]:

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt


def ode(X,V):
    yA0 = 0.2
    ThetaB = 3
    DeltaHR = -7000
    EA = 500
    Tref = 300
    kref = 0.0055
    T0 = 500
    F0 = 5
    FA0 = yA0*F0
    v0 = 50
    cA0 = FA0/v0

    T = T0 + (-DeltaHR*X/(150*5))
    k = kref*np.exp((EA/8.314)*((1/Tref)-(1/T)))
    dXdV = (k*cA0**2/FA0)* ((T0/T)**2) *((ThetaB-2*X)/(1-0.4*X))**2

    return dXdV

Vspan = np.linspace(0,150)
init = 0

X = odeint(ode,init,Vspan)

plt.plot(Vspan,X)
plt.xlabel('Volume')
plt.ylabel('Conversion')

from scipy.interpolate import interp1d
Xint = interp1d(Vspan,X[:,0])
print('Conversion is {0}'.format(Xint(150)))
```

```
Conversion is 0.0032150185314418836
```



Soln HW6.1B

In [25]:

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt


def ode(V,X):
    yA0 = 0.2
    EA = 500
    DeltaHR = -7000
    Tref = 300
    kref = 0.0055
    T0 = 591.1
    F0 = 5
    FA0 = yA0*F0
    v0 = 50
    cA0 = FA0/v0

    T = T0 + (-DeltaHR*X/(150*5))
    k = kref*np.exp((EA/8.314)*((1/Tref)-(1/T)))
    dVdX = (FA0/k)*(1/cA0**2)*((T/T0)**2)*((1-0.4*X)/(3-2*X))**2

    return dVdX

Xspan = np.linspace(0,0.95)
init = 0

V = odeint(ode,init,Xspan)

from scipy.interpolate import interp1d
Vint = interp1d(Xspan,V[:,0])
print('Volume = {0}'.format(Vint(0.95)))
```

```
Volume = 68805.53925386531
```

Problem # 2

$A + B \longrightarrow C$

Liquid phase rxn

$V = 1\,m^3 \qquad v_0 = 0.5\,\frac{m^3}{min}$

$C_{A0} = \frac{1\,mol}{L} \qquad C_{B0} = \frac{1\,mol}{L}$

When $T = T_0 = 300K$

$X = 0.20$

CSTR Design Eqn.

$$V = \frac{F_{A0}X}{(-r_A)} \qquad -r_A = k C_A C_B$$

$$C_A = C_{A0}(1-X)$$

$$C_B = C_{A0}(1-X)$$

a. Energy Balance

$$\dot{Q} - \cancel{F_{A0}\sum_i \Theta_i C_{p,i}}(T-T_0) - F_{A0}X\Delta H_R(T) = 0$$

isothermal

$$\dot{Q} = F_{A0}X\Delta H_R(300K)$$

ADIABATIC CSTR

$$\cancel{\dot{Q}}_{0} - F_{A0}\sum \Theta_i c_{p,i}(T-T_0) - F_{A0} X \Delta H_R(T) = 0$$

$$F_{A0}\sum \Theta_i c_{p,i}(T-T_0) = -F_{A0} X \Delta H_R(350K)$$

$$\Delta H_R(350K) = -\frac{(T-T_0)\sum \Theta_i c_{p,i}}{X}$$

$$\sum \Theta_i c_{p_i} = \Theta_A c_{pA} + \Theta_B c_{pB}$$

$$= (1)\left(25 \frac{kJ}{mol\,K}\right) + (1)\left(35 \frac{kJ}{mol\,K}\right)$$

$$= 60 \frac{kJ}{mol\,K}$$

$$\Delta H_R(350K) = -\frac{(350K - 300K)\left(60 \frac{kJ}{mol\,K}\right)}{0.40}$$

$$\Delta H_R(350K) = -7500 \frac{kJ}{mol}$$

$$\Delta H_R(300K) = \Delta H_R(350K) + \Delta c_p(T - 350K)$$

$$\Delta c_p = \frac{c}{a} c_{pC} - \frac{b}{a} c_{pB} - \frac{a}{a} c_{pA}$$

$$\Delta c_p = (60 - 25 - 30) \frac{kJ}{mol \cdot K} = 0$$

$$\Delta H_R(300K) = \Delta H_R(350K)$$

$$= -7500 \frac{kJ}{mol}$$

$$\dot{Q} = \left(1\ \frac{mol}{L}\right)\left(500\ \frac{L}{MIN}\right)(0.2)\left(-7500\ \frac{kJ}{MOL}\right)$$

$$\dot{Q} = -750{,}000\ \frac{kJ}{MIN}$$

b. WHEN COOLANT TEMP IS CONSTANT:

$$\frac{UA(T_a - T)}{F_{A0}} - \sum \Theta_i c_{p,i}(T - T_0) - \Delta H_R(T) X = 0$$

$T_a = 350$ $\quad T_0 = 300K$ $\quad UA = 4\ \frac{KJ}{MOL}$

$F_{A0} = 400\ \frac{MOL}{MIN}$

$$\begin{aligned}\sum \Theta_i c_{p,i} &= \Theta_A c_{pA} + \Theta_B c_{pB} + \Theta_C c_{pC} \\ &= (1)\left(25\ \frac{kJ}{MOL \cdot K}\right) + (1)\left(35\ \frac{kJ}{MOL \cdot K}\right) \\ &\quad + \left(\frac{1}{4}\right)\left(60\ \frac{kJ}{MOL \cdot K}\right) \\ &= 75\ \frac{kJ}{MOL \cdot K}\end{aligned}$$

$$V = \frac{F_{A0} X}{k(T) C_{A0}^2 (1-X)^2}$$

Solve $X_{MB} = X_{EB}$

Isothermal CSTR

$$1000\,L = \frac{500\,\frac{mol}{min}(0.2)}{k(300K)\left(1\,\frac{mol}{L}\right)^2(0.8)^2}$$

$$k(300K) = 0.156\,\frac{L}{mol \cdot min}$$

Adiabatic CSTR

$$1000\,L = \frac{500\,\frac{mol}{min}(0.4)}{k(350K)\left(1\,\frac{mol}{L}\right)^2(0.6)^2}$$

$$k(350K) = 0.556\,\frac{L}{mol \cdot min}$$

$$\ln\left(\frac{k_2}{k_1}\right) = -\frac{E_A}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\ln\left(\frac{0.156}{0.556}\right) = -\frac{E_A}{R}\left(\frac{1}{300K} - \frac{1}{350K}\right)$$

$$\frac{E_A}{R} = 2668\,K$$

$$k(T) = 0.556\exp\left(2668K\left(\frac{1}{350K} - \frac{1}{T}\right)\right)$$

$X_2 = 0.277$ (from Polymath)

$$X_{Af} = \frac{F_{A0} - F_{A2}}{F_{A0}} = \frac{F_{A0} - F_{A1}(1 - X_2)}{F_{A0}}$$

$$X_{Af} = \frac{500 - 500(0.8)(1-0.277)}{500}$$

$$\boxed{X_{Af} = 0.421}$$

c. $$\frac{dX}{dV} = \frac{k(T)\, C_{A0}^2 (1-X)^2}{F_{A0}}$$ PFR M.B.

$$\frac{dT}{dV} = \frac{r_A\, \Delta H_R(T) + Ua(T_a - T)}{F_{A0}\left(\sum \theta_i C_{p,i} + \cancel{\Delta C_p}_0 X\right)}$$ PFR E.B.

$\sum \Theta_i c_{p,i} = 75 \frac{kJ}{MOL \cdot K}$ $\quad Ua = 0.01 \frac{kJ}{L \cdot min \cdot K}$

$T_a = 300 K$ $\quad F_{A0} = 400 \frac{mol}{min}$

Solve M.B. & E.B. simultaneously

$X_2 = 0.270$

$$X_{Af} = \frac{F_{A0} - F_{A1}(1 - X_2)}{F_{A0}} = 0.416$$

d. DESIGN EQN.

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

$$-r_A = k\left(C_A C_B - \frac{C_C}{K}\right)$$

$$C_A = C_{A0}(1-X) \quad C_B = C_{A0}(1-X)$$

$$C_C = C_{A0}(\Theta_C + X) \quad \Theta_C = 1/4$$

$$k(T) = 0.556 \exp\left[2668\left(\frac{1}{350K} - \frac{1}{T}\right)\right]$$

$$K(T) = \frac{2L}{mol} \exp\left[-\frac{7500}{R}\left(\frac{1}{310K} - \frac{1}{T}\right)\right]$$

E.B. SAME AS IN PART c.

Solve for X_2 $\quad X_2 = 0.1014$

$$X_{Af} = \frac{F_{A0} - F_{A1}(1-X_2)}{F_{A0}} = 0.281$$

HWK 6.2B

In [14]:

```
    import scipy.optimize as opt
    from numpy import exp


    def f(variables) :
        (X,T) = variables

        UA = 4
        T0 = 300
        Ta = 350
        Cpo = 75
        DeltaHR = -7500
        V = 1000
        v0 = 500
        cA0 = 0.8
        FA0 = cA0*v0
        cA = cA0*(1-X)
        cB = cA0*(1-X)

        k = 0.556*exp(-2668*((1/T)-(1/350)))
        rA = -k*cA*cB

        first_eq = UA * (Ta-T)/FA0-(T-T0)*Cpo-DeltaHR*X
        second_eq = V-FA0*X/(-rA)
        return [first_eq, second_eq]

    solution = opt.fsolve(f, (0.2,300) )
    print('Conversion is {0}'.format(solution[0]))
    print('Temperature is {0} K'.format(solution[1]))
```

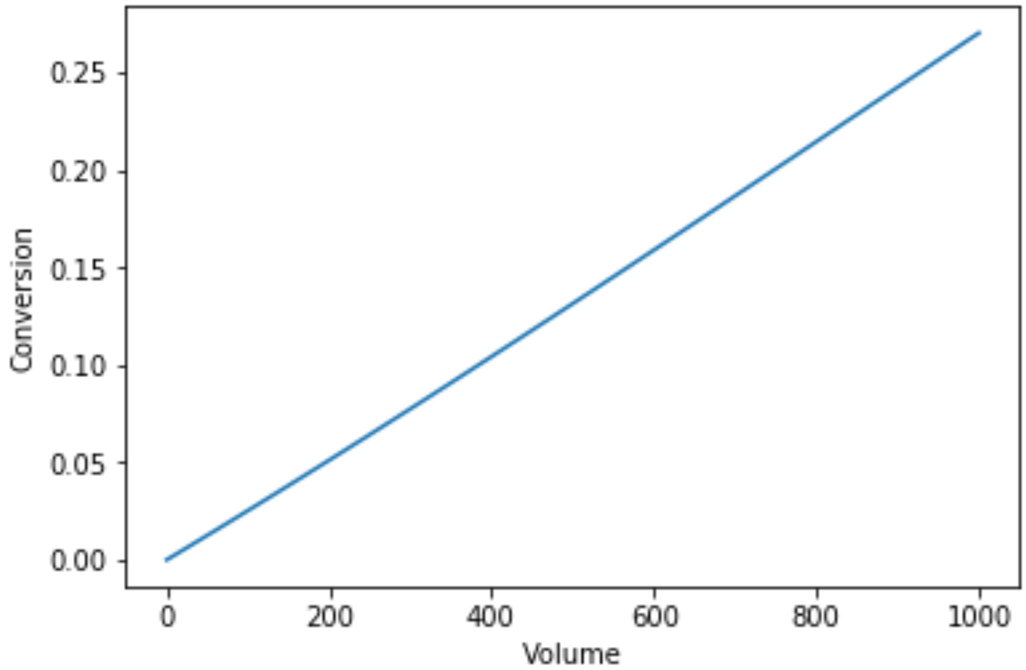
```
Conversion is 0.27684597125346194
Temperature is 327.68757211573075 K
```

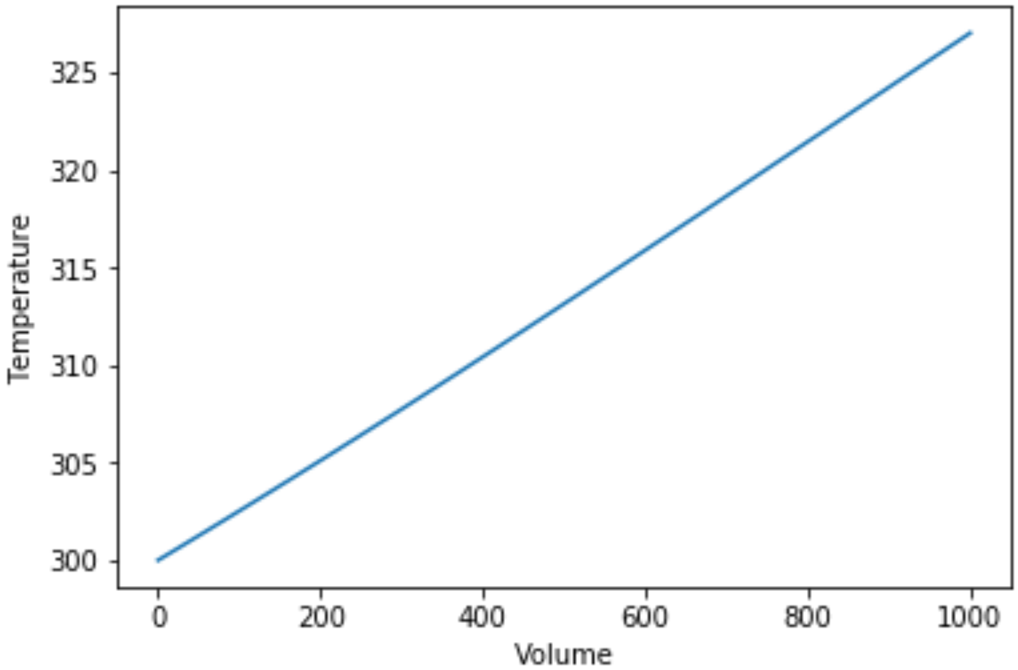
HWK 6.2C

In [37]:

```
from scipy.integrate import odeint
import numpy as np
import matplotlib.pyplot as plt

def myode (F,V):

    X = F[0]
    T = F[1]

    cA0 = 0.8
```

```
    cA0 = 0.8
    v0 = 500
    FA0 = cA0 * v0
    DeltaHR = -7500
    UA = 0.01
    Ta = 300
    Cpo = 75
    cA = cA0*(1-X)
    cB = cA0*(1-X)
    rA = -0.556*np.exp(-2668*((1/T)-(1/350))) * cA * cB

    dXdV = -rA/FA0
    dTdV = (rA*DeltaHR+UA*(Ta-T))/(FA0*Cpo)

    dFdV = [dXdV,dTdV]

    return dFdV

Vspan = np.linspace(0,1000)

init = [0,300]

F = odeint(myode,init,Vspan)

X = F[:,0]
T = F[:,1]
plt.figure()
plt.plot(Vspan, X)
plt.xlabel('Volume')
plt.ylabel('Conversion')
plt.show()
plt.figure()
plt.plot(Vspan, T)
plt.xlabel('Volume')
plt.ylabel('Temperature')
plt.show()

from scipy.interpolate import interp1d
Xint = interp1d(Vspan, F[:,0])
Tint = interp1d(Vspan, F[:,1])

print('Conversion is {0}'.format(Xint(1000)))
print('Temperature is {0} K'.format(Tint(1000)))
```





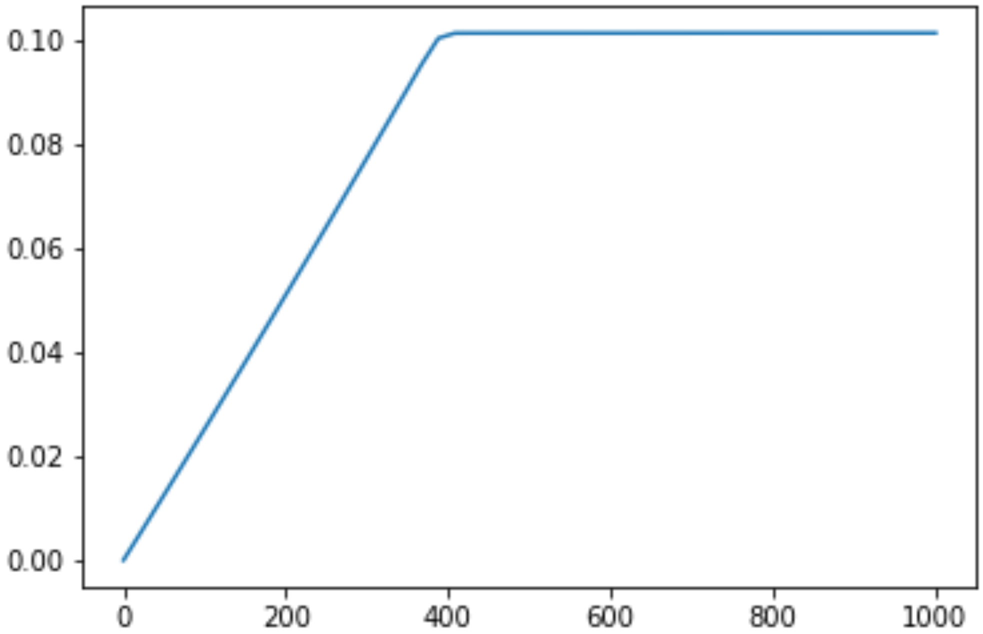

```
Conversion is 0.27020953379625523
Temperature is 327.01653097191905 K
```

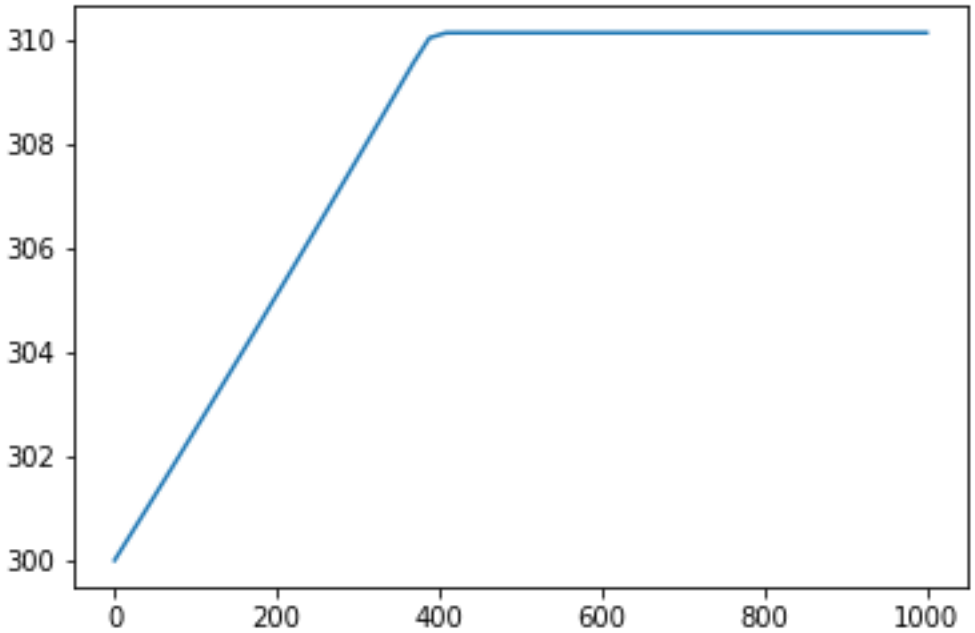
HWK 6.2D

In [36]:

```
from scipy.integrate import odeint
import numpy as np
import matplotlib.pyplot as plt

def myode (F,V):

    X = F[0]
    T = F[1]

    cA0 = 0.8
    cC0 = 0.2
    v0 = 500
    FA0 = cA0 * v0
```

```
    FC0 = cC0 * v0

    DeltaHR = -7500
    UA = 0.01
    Ta = 300
    Cpo = 75
    R = 8.314/1000
    cA = cA0*(1-X)
    cB = cA0*(1-X)
    cC = cA0*(FC0/FA0 + X)
    k = 0.556*np.exp(-2668*((1/T)-(1/350)))
    Kc = 2*np.exp(DeltaHR/R*(1/310-1/T))
    rA = -k * (cA*cB-cC/Kc)

    dXdV = -rA/FA0
    dTdV = (rA*DeltaHR+UA*(Ta-T))/(FA0*Cpo)

    dFdV = [dXdV,dTdV]

    return dFdV

Vspan = np.linspace(0,1000)

init = [0,300]

F = odeint(myode,init,Vspan)

X = F[:,0]
T = F[:,1]
plt.figure()
plt.plot(Vspan, X)
plt.show()
plt.figure()
plt.plot(Vspan, T)
plt.show()

from scipy.interpolate import interp1d
Xint = interp1d(Vspan, F[:,0])
Tint = interp1d(Vspan, F[:,1])

print('Conversion is {0}'.format(Xint(1000)))
print('Temperature is {0} K'.format(Tint(1000)))
```






```
Conversion is 0.10141455779186818
Temperature is 310.13874296348797 K
```

PROBLEM #3

$$A + B \longrightarrow P$$

$$-r_A = k C_A C_B$$

$$C_A = C_{A0}(1 - X_A)$$
$$C_B = C_{A0}(1 - X_A)$$

$$X_A = \frac{r_A V}{F_{A0}} = \frac{k C_A C_B V}{F_{A0}} = \frac{k C_{A0}^2 (1-X_A)^2 V}{F_{A0}} \quad \boxed{1}$$

MASS BALANCE

ENERGY BALANCE CALC.

$$\Delta H_R^\circ = H_P^\circ - H_B^\circ - H_A^\circ = (-20 + 10 + 5)\frac{kcal}{mol}$$
$$= -5 \frac{kcal}{mol}$$

$$\Delta H_R = \Delta H_R^\circ + (C_{p,P} - C_{p,A} - C_{p,B})(T - T_0)$$

$$\Delta H_R = \Delta H_R^\circ + \underbrace{(22 - 10 - 12)}_{0}(T - T_0)$$

$$\Delta H_R = \Delta H_R^\circ$$

$$\underbrace{\frac{dE}{dt}}_{0} = \underbrace{\dot{Q}}_{0} - \underbrace{\dot{W}_s}_{0} - F_{A0}\sum \Theta_i c_{pi}(T - T_0) - F_{A0} X_A \Delta H_R$$

$$0 = F_{A0}(C_{PA} + C_{PB})(T - T_0) - F_{A0} X_A \Delta H_R \quad \boxed{2}$$

SOLVE $\boxed{1}$ AND $\boxed{2}$ SIMULTANEOUSLY WITH COMPUTATIONAL METHODS. SEE PYTHON CODE ATTACHED

$$\boxed{X = 0.88,\ T = 501 K}$$

HWK 6.3

In [3]:

```
import scipy.optimize as opt
import numpy as np

def f(var):
        (X,T)= var
        HA = -10000
        HB = -5000
        HP = -20000
        CPA = 10
        CPB = 12
        #CPP = 22
        kref = 0.02
        EA = 8000
        cA0 = 3
        #cB0 = 3
        v0 = 2
        T0 = 300
        Vtotal = 10
        R = 1.986
        FA0 = cA0 * v0
        DeltaHR = HP - HA - HB
        k = kref * np.exp((EA/R)*((1/T0)-(1/T)))

        massBal = ((k* cA0**2 * (1-X)**2 * Vtotal)/FA0)-X
        eBal = FA0 * (CPA+CPB) * (T0-T)-(FA0 * X * DeltaHR)

        return[massBal, eBal]

solution = opt.fsolve(f, (0.83,460) )
print ('Conversion is {0}'.format(solution[0]))
print ('Temperature is {0} K'.format(solution[1]))
```

```
Conversion is 0.8837651662895825
Temperature is 500.85571961126874 K
```

PROBLEM #4

CSTR DESIGN EQN.

$$\tau = \frac{C_{A0} X_A}{-r_A}$$

$$-r_A = k$$

$$\tau = \frac{C_{A0} X_A}{k}$$

$$k = k_{ref} \exp\left[\frac{-E}{R}\left(\frac{1}{T_R} - \frac{1}{T}\right)\right]$$

ADIABATIC ENERGY BALANCE

$$T = \frac{X_A\left[-\Delta H_R(T_R)\right] + \sum \Theta_i c_{p,i} T_0 + X_A \Delta c_p T_R}{\sum \Theta_i c_{p,i} + X_A \Delta c_p}$$

$$\Delta c_p = c_{p,C} + c_{p,B} - c_{p,A}$$

$$= \tfrac{1}{2} c_{p,A} + \tfrac{1}{2} c_{p,A} - c_{p,A} = 0$$

$$\sum \Theta_i c_{p,i} = 1\,(c_{pA}) = c_{p,A}$$

$$T = \frac{X_A(-\Delta H_R) + c_{pA} T_0}{c_{pA}}$$

$$X_A = \frac{c_{pA}(T - T_0)}{-\Delta H_R} = \frac{c_{pA}(T_0 - T)}{\Delta H_R}$$

$$\tau = \frac{C_{A0}\left(c_{p,A}(T_0 - T)\right)}{\Delta H_R\, k_{ref} \exp\left[-E/R\left(\frac{1}{T_R} - \frac{1}{T}\right)\right]}$$