CRE HOMEWORK #5

PROBLEM #1

MOLE BALANCE ON A

$$\frac{dN_A}{dt} = F_{A0} - F_A + r_A V$$

$$\frac{d(c_A \cdot V)}{dt} = c_{A0} v_0 - c_A v_0 (1.5) + r_A V$$

$$-r_A = k_1 c_A^2$$

$$V \frac{dc_A}{dt} + c_A \frac{dV}{dt} = c_{A0} v_0 - 1.5\, c_{A0} v_0 + r_A V$$

$$\frac{dV}{dt} = v_0 - 1.5 v_0 = -0.5 v_0$$

$$V \frac{dc_A}{dt} - 0.5 v_0 c_A = c_{A0} v_0 - 1.5 c_A v_0 - k_1 c_A^2 V$$

$$\frac{dc_A}{dt} = \frac{c_{A0} v_0}{V_i - 0.5 v_0 t} - \frac{v_0 c_A}{V_i - 0.5 v_0 t} - k_1 c_A^2$$

MOLE BALANCE ON P

$$\frac{dc_P V}{dt} = 0 - c_P (1.5 v_0) + r_P V$$

$$2 r_P = -r_A$$

$$\frac{V\,dc_p}{dt} + c_p(-0.5v_0) = -c_p(1.5v_0) + 2k_1 c_A^2 V$$

$$\frac{dc_p}{dt} = \frac{-c_p v_0}{V_i + v_0(-0.5)t} + 2k_1 c_A^2$$

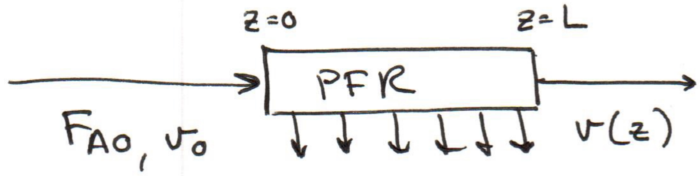
$$\frac{dc_p}{dt} = 2k_1 c_A^2 - \frac{v_0 c_p}{V_i - 0.5v_0 t}$$

INTEGRATE USING AN ODE SOLVER.

$$N_p = \int c_p(t)\,dt \cdot v_{out}$$

$$\boxed{N_p = 10.55 \text{ mol}}$$

PROBLEM #2



a. $$F_{A,LEAK}\big|_z = C_A\big|_z \left(-v\big|_{z,LEAK}\right)$$

$$v\big|_{z,LEAK} = \frac{dv}{dz}\Delta z$$

$$F_{A,LEAK}\big|_z = -C_A\big|_z \left(\frac{dv}{dz}\Delta z\right)$$

b. IN − OUT + GEN = ACCUM. = 0

$$F_A\big|_z - \left(F_A\big|_{z+\Delta z} + F_{A,LEAK}\big|_z\right) + (-kC_A)A_c\Delta z = 0$$

$$F_A\big|_z - F_A\big|_{z+\Delta z} + C_A\big|_z\left(\frac{dv}{dz}\right) = kC_A A_c \Delta z$$

c. DIVIDE BY Δz

$$\frac{-\left(F_A\big|_{z+\Delta z} - F_A\big|_z\right)}{\Delta z} + C_A\frac{dv}{dz} = kC_A A_c$$

TAKE LIMIT AS $\Delta z \rightarrow 0$

$$\frac{-dF_A}{dz} + C_A\frac{dv}{dz} = kC_A A_c$$

$$F_A = F_{A0}(1-X)$$

$$\frac{-d(F_{A0}(1-X))}{dz} + C_A\frac{dv}{dz} = kC_A A_c$$

$$F_{A0}\frac{dX}{dz} + C_A\frac{dv}{dz} = k\,C_A A_c$$

d. $$\frac{dv}{dz} = \frac{-v_0}{L}$$

$$\frac{-dF_A}{dz} - C_A\frac{v_0}{L} = k\,C_A A_c$$

PUT FLOWRATES & CONCENTRATIONS IN TERMS OF CONVERSIONS

$$F_A = F_{A0}(1-X) \qquad C_A = \frac{F_{A0}(1-X)}{v(z)}$$

$$\cancel{F_{A0}}\frac{dX}{dz} - \frac{\cancel{F_{A0}}(1-X)}{v(z)}\frac{v_0}{L} = \frac{k\,\cancel{F_{A0}}(1-X)}{v(z)}A_c$$

$$\frac{dX}{dz} = \frac{(1-X)\,v_0}{v_0(1-z/L)}\frac{1}{L} = \frac{k(1-X)}{v_0\left(1-\frac{z}{L}\right)}A_c$$

$$\frac{dX}{dz} = \frac{(1-X)}{1-\frac{z}{L}}\left[\frac{k A_c}{v_0} + \frac{1}{L}\right]$$

e. $$\int_0^X \frac{dX}{1-X} = \left[\frac{kA_c}{v_0} + \frac{1}{L}\right] \int_0^z \frac{dz}{1-z/L}$$

$$-\ln(1-X)\Big|_0^X = \left[\frac{kA_c}{v_0} + \frac{1}{L}\right]\left[-L\ln\left(1-\frac{z}{L}\right)\Big|_0^z\right]$$

$$\ln(1-X) = \left(\frac{LkA_c}{v_0} + 1\right)\ln\left(1-\frac{z}{L}\right)$$

$$\boxed{X = 1 - \left(1-\frac{z}{L}\right)^{\frac{LkA_c}{v_0}+1}}$$

PROBLEM #3

$$A \rightleftharpoons B + 2C$$

$$\frac{dF_A}{dV} = r_A - R_A = \frac{dF_A}{dz}\left(\frac{1}{A}\right)$$

$$\frac{dF_B}{dV} = r_B - R_B = \frac{dF_B}{dz}\left(\frac{1}{A}\right)$$

$$\frac{dF_C}{dV} = r_C = \frac{dF_C}{dz}\left(\frac{1}{A}\right)$$

IF SYSTEM IS ISOTHERMAL + ISOBARIC, THEN $C_{TO} = C_T$

$$-r_A = k_1\left(C_A - \frac{C_B C_C^2}{K_C}\right) = k_1\left(\frac{C_{TO} F_A}{F_T} - \left(\frac{C_{TO}}{F_T}\right)^3\left(\frac{F_B F_C^2}{K_C}\right)\right)$$

$$= r_B = \frac{1}{2} r_C$$

$$R_A = \frac{\beta_A F_A C_{TO}}{F_T} \qquad R_B = \beta_B C_B = \frac{\beta_B F_B C_{TO}}{F_T}$$

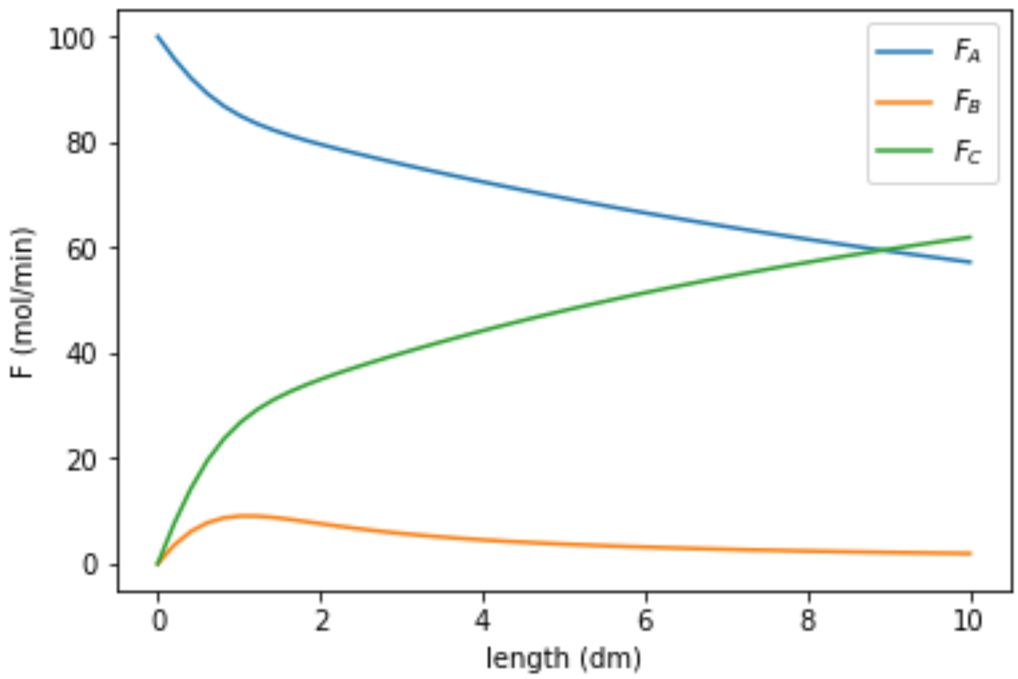
$$\frac{dF_A}{dz} = A(r_A - R_A) = -A\left[k_1\left(\frac{C_{TO} F_A}{F_T} - \left(\frac{C_{TO}}{F_T}\right)^3\left(\frac{F_B F_C^2}{K_C}\right)\right) + \frac{\beta_A F_A C_{TO}}{F_T}\right]$$

$$\frac{dF_B}{dz} = A\left[k_1\left(\frac{C_{T0}F_A}{F_T} - \left(\frac{C_{T0}}{F_T}\right)^3\left(\frac{F_B F_C^2}{K_C}\right)\right) - \frac{\beta_B F_B C_{T0}}{F_T}\right]$$

$$\frac{dF_C}{dz} = 2Ak_1\left(\frac{C_{T0}F_A}{F_T} - \left(\frac{C_{T0}}{F_T}\right)^3\left(\frac{F_B F_C^2}{K_C}\right)\right)$$

In [3]:

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

def myode(F,z):
    A = 2
    k1 = 10
    C_T0 = 1
    Kc = 0.01
    BetaA = 1
    BetaB = 40

    FA = F[0]
    FB = F[1]
    FC = F[2]

    rA = k1*(((C_T0*FA)/(FA+FB+FC))-(C_T0**3/((FA+FB+FC)**3))*(FB*FC**2/Kc))
    RA = BetaA * FA * C_T0/(FA+FB+FC)
    RB = BetaB * FB * C_T0/(FA+FB+FC)

    dFAdz = -A * (rA+RA)
    dFBdz = A *(rA-RB)
    dFCdz = 2*A*rA

    dFdz= [dFAdz,dFBdz,dFCdz]
    return dFdz

zspan = np.linspace(0,10)

init = [100,0,0]
F = odeint(myode,init,zspan)

FA = F[:,0]
FB = F[:,1]
FC = F[:,2]

plt.plot(zspan, FA, zspan, FB, zspan, FC)
plt.xlabel('length (dm)')
plt.ylabel('F (mol/min)')
plt.legend(['$F_A$', '$F_B$', '$F_C$'])
plt.savefig('membrane.png')
```



100
80
60
40
20
0
F (mol/min)
0
2
4
6
8
10
length (dm)
F_A
F_B
F_C

PROBLEM #4

a. · MOLE BALANCE ON "A" (NO_2)

IN − out + gen = acc.

$$F_{A0} - F_A + r_A V = 0$$

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

b. ASSUME POWER LAW FORM OF RATE LAW

$$-r_A = k C_A^{\alpha}$$

$$k C_A^{\alpha} = \frac{F_{A0} X_A}{V} \qquad X_A = \frac{\text{fractional decomp. of } NO_2}{100\ \%}$$

$$X_A = k C_A^{\alpha} \left(\frac{V}{F_{A0}} \right)$$

WHEN PLOTTING X_A VS. $\frac{V}{F_{A0}}$, $k C_A^{\alpha}$ IS THE SLOPE. AT 200°C, THE SLOPE IS THE SAME FOR ALL CONCENTRATIONS TESTED. THE REACTION ORDER IS EQUAL TO 0.

c. $$k = A \exp\left(\frac{-E_A}{RT}\right) \Rightarrow \ln k = \ln A + \left(\frac{-E_A}{RT}\right)\left(\frac{1}{T}\right)$$

At 200°C $$k = \frac{X_A}{\frac{V}{F_{A0}}} \approx \frac{0.5}{4 \frac{m^3\, h}{mol\ NO_2}} = 0.125 \frac{mol\ NO_2}{m^3\, h}$$

At 250°C $k \approx \dfrac{0.5}{2 \frac{m^3 h}{mol\ NO_2}} = 0.25 \dfrac{mol\ NO_2}{m^3 h}$

At 300°C $k \approx \dfrac{0.6}{1 \frac{m^3 h}{mol\ NO_2}} = 0.6 \dfrac{mol\ NO_2}{m^3 h}$

Plot $\ln(k)$ vs. $\dfrac{1}{T}$

Slope $= -4223$

$E_A = -4223\left(8.314 \frac{J}{mol\ K}\right) = 35 \frac{kJ}{mol\ K}$