Chemical Reaction Engineering—Spring 2020—Homework 0

PROBLEM #1

$$2\,Sb(s) + 3\,I_2(s) \longrightarrow 2\,SbI_3(s)$$

A. MOL OF SbI_3 PRODUCED

a) FROM 1.20 mol Sb:

$$1.20 \text{ mol Sb} \left(\frac{2 \text{ mol } SbI_3}{2 \text{ mol Sb}} \right) = 1.20 \text{ mol } SbI_3$$

b) FROM 2.40 mol I_2:

$$2.40 \text{ mol } I_2 \left(\frac{2 \text{ mol } SbI_3}{3 \text{ mol } I_2} \right) = 1.60 \text{ mol } SbI_3$$

Sb is LIMITING REAGENT

THEORETICAL YIELD: 1.20 mol SbI_3

B. FROM 1.20 g Sb:

$$1.20 \text{ g Sb} \left(\frac{1 \text{ mol Sb}}{121.8 \text{ g Sb}} \right) \left(\frac{2 \text{ mol } SbI_3}{2 \text{ mol Sb}} \right) \left(\frac{502.5 \text{ g } SbI_3}{\text{mol } SbI_3} \right)$$

$$= 4.95 \text{ g } SbI_3$$

FROM 2.40g I_2

$$2.40 \text{ g } I_2 \left(\frac{\text{mol } I_2}{253.8 \text{ g } I_2} \right) \left(\frac{2 \text{ mol } SbI_3}{3 \text{ mol } I_2} \right) \left(\frac{502.5 \text{ g } SbI_3}{\text{mol } SbI_3} \right)$$

$$= 3.17 \text{ g } SbI_3$$

I_2 is LIMITING

MASS OF Sb REQUIRED

$$3.17\,g\ SbI_3 \left(\frac{121.8\ g\ Sb}{502.5\,g\ SbI_3} \right) = 0.768\ g\ Sb$$

MASS OF Sb REMAINING

$$1.20\,g - 0.768\,g = \boxed{0.43\,g\ Sb}$$

PROBLEM #2

NET IONIC EQUATION

$$Fe^{3+} + 3OH^- \longrightarrow Fe(OH)_3 \downarrow$$

MOLES OF Fe^{3+}

$$0.03000\ L\ Fe(NO_3)_3 \left(\frac{0.125\ mol\ Fe(NO_3)_3}{1\ L\ Fe(NO_3)_3}\right) \times \left(\frac{1\ mol\ Fe^{3+}}{1\ mol\ Fe}\right) = 3.75E\text{-}3\ mol\ Fe^{3+}$$

MOLES OF OH^-

$$0.05000\ L\ NaOH \left(\frac{0.200\ mol\ NaOH}{1L\ NaOH}\right)\left(\frac{1\ mol\ OH^-}{1\ mol\ NaOH}\right)$$

$$= 1.00E\text{-}2\ mol\ OH^-$$

IF Fe^{3+} IS LIMITING:

$$3.75E\text{-}3\ mol\ Fe^{3+} \left(\frac{mol\ Fe(OH)_3}{mol\ Fe^{3+}}\right) = 3.75E\text{-}3\ mol\ Fe(OH)_3$$

IF OH^- IS LIMITING:

$$1.00E\text{-}2\ mol\ OH^- \left(\frac{1\ mol\ Fe(OH)_3}{3\ mol\ OH^-}\right) = 3.33E\text{-}3\ mol\ Fe(OH)_3$$

OH^- IS LIMITING

MASS OF $Fe(OH)_3$

$$3.33E\text{-}3\ mol\ Fe(OH)_3 \left(\frac{106.87g\ Fe(OH)_3}{mol\ Fe(OH)_3}\right) = 0.356\ g\ Fe(OH)_3$$

PROBLEM # 3

ASSUME A VOLUME OF 1 L

$$\frac{PV}{RT} = n = \frac{(0.950\ \text{ATM})(1\ \text{L})}{\left(0.0821\ \frac{\text{L}\cdot\text{ATM}}{\text{MOL}\cdot\text{K}}\right)(298\ \text{K})}$$

$$n = 0.0388\ \text{mol}$$

$$n_{H_2} = 0.0259\ \text{mol}\ H_2 \qquad n_{O_2} = 0.0129\ \text{mol}\ O_2$$

AFTER REACTION :

$$n_{H_2} = (1-0.88)\,0.0259\ \text{mol}\ H_2 = 0.00311\ \text{mol}\ H_2$$

$$n_{O_2} = (1-0.88)\,0.0129\ \text{mol}\ H_2 = 0.00155\ \text{mol}\ O_2$$

$$n_{H_2O} = (0.88)\big((0.0259)\ \text{mol}\ H_2\big)\left(\frac{2\ \text{mol}\ H_2O}{2\ \text{mol}\ H_2}\right) = 0.228\ \text{mol}\ H_2O$$

$$\Sigma n = (0.00311 + 0.00155 + 0.228)\ \text{mol} = 0.02746\ \text{mol}$$

$$\frac{nRT}{V} = P = \frac{(0.02746\ \text{mol})(398\ \text{K})\left(0.0821\ \frac{\text{L}\cdot\text{ATM}}{\text{mol}\cdot\text{K}}\right)}{1\ \text{L}}$$

$$\boxed{P = 0.897\ \text{ATM}}$$

PROBLEM #4

OVERALL REACTION

$$2N_2 + 5O_2 \longrightarrow 2N_2O_5$$

MULTIPLY SECOND EQN BY -2

$$4HNO_3 \longrightarrow 2N_2O_5 + 2H_2O$$

$$\Delta H = -2(-73.7\,kJ)$$

MULTIPLY ~~first~~ THIRD EQN BY 4

$$2N_2 + 6O_2 + 2H_2 \rightarrow 4HNO_3$$

$$\Delta H = 4(-174.1\,kJ)$$

ADD EQNS 2 + 3

$$2N_2 + 6O_2 + 2H_2 \rightarrow 2N_2O_5 + 2H_2O$$

Substract Eqn 1:

$$2N_2 + 6O_2 + \cancel{2H_2} \rightarrow 2N_2O_5 + \cancel{2H_2O}$$

$$\cancel{2H_2O} \rightarrow \cancel{2H_2} + O_2$$

$$2N_2 + 5O_2 \longrightarrow 2N_2O_5$$

$$\Delta H = -2(-73.7\,kJ) + 4(174.1\,kJ) + 571.6\,kJ$$

$$\Delta H = 22.6\,kJ / 2\,mol\,N_2O_5$$

$$\Delta H = 11.3\,kJ / mol\,N_2O_5$$

PROBLEM #5

$$K = \frac{(P_{NO_2})^2}{P_{N_2O_4}}$$

	I	Δ	F
N_2O_4	1.00 ATM	$-x$	$(1.00 - x)$
NO_2	0	$2x$	$2x$

$$11 = \frac{(2x)^2}{(1.00 - x)}$$

$x = 0.78$

$P_{NO_2} = 2(0.78) = \boxed{1.56 \text{ ATM}}$

$P_{N_2O_4} = ((1 - 0.78)\text{ATM}) = \boxed{0.22 \text{ ATM}}$

14.21 Plug flow reactor with a pressure drop

If there is a pressure drop in a plug flow reactor, [2] there are two equations needed to determine the exit conversion: one for the conversion, and one from the pressure drop.

$$\frac{dX}{dW} = \frac{k'}{F_A0}\left(\frac{1-X}{1+\epsilon X}\right) y \tag{49}$$

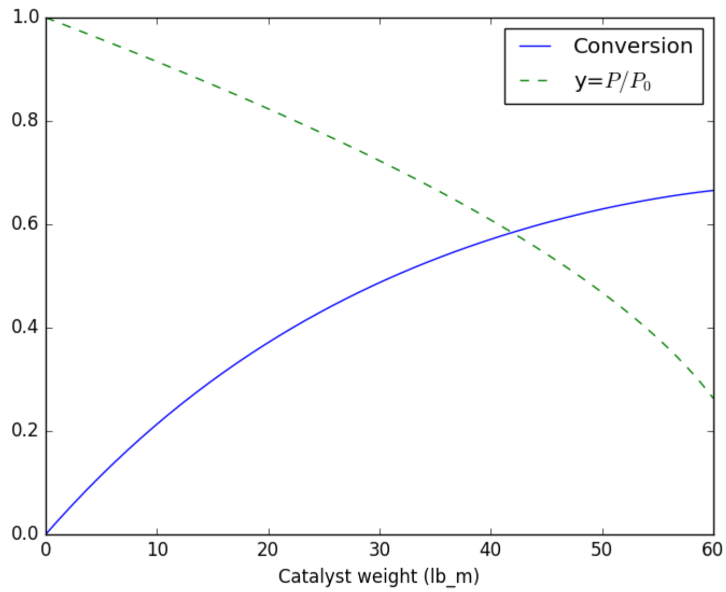
$$\frac{dX}{dy} = -\frac{\alpha(1+\epsilon X)}{2y} \tag{50}$$

Here is how to integrate these equations numerically in python.

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

kprime = 0.0266
Fa0 = 1.08
alpha = 0.0166
epsilon = -0.15

def dFdW(F, W):
    'set of ODEs to integrate'
    X = F[0]
    y = F[1]
    dXdW = kprime / Fa0 * (1-X) / (1 + epsilon*X) * y
    dydW = -alpha * (1 + epsilon * X) / (2 * y)
    return [dXdW, dydW]

Wspan = np.linspace(0,60)
X0 = 0.0
y0 = 1.0
F0 = [X0, y0]
sol = odeint(dFdW, F0, Wspan)

# now plot the results
plt.plot(Wspan, sol[:,0], label='Conversion')
plt.plot(Wspan, sol[:,1], 'g--', label='y=$P/P_0$')
plt.legend(loc='best')
plt.xlabel('Catalyst weight (lb_m)')
plt.savefig('images/2013-01-08-pdrop.png')
```

Here is the resulting figure.

[2] Fogler, 4th edition. page 193.



14.22 Solving CSTR design equations

Given a continuously stirred tank reactor with a volume of 66,000 dmˆ3 where the reaction $A \rightarrow B$ occurs, at a rate of $-r_A = kC_A^2$ ($k = 3$ L/mol/h), with an entering molar flow of F_{A0} = 5 mol/h and a volumetric flowrate of 10 L/h, what is the exit concentration of A?

From a mole balance we know that at steady state $0 = F_{A0} - F_A + V r_A$. That equation simply states the sum of the molar flow of A in in minus the molar flow of A out plus the molar rate A is generated is equal to zero at steady state. This is directly the equation we need to solve. We need the following relationship:

1. $F_A = v0 C_A$

```python
from scipy.optimize import fsolve

Fa0 = 5.0
v0 = 10.

V = 66000.0  # reactor volume L^3
k = 3.0      # rate constant L/mol/h

def func(Ca):
    "Mole balance for a CSTR. Solve this equation for func(Ca)=0"
```