Chemical Reaction Engineering—Homework #0

Due: Online submission on Canvas, <u>Friday</u>, <u>January 10</u>, <u>2020 at 11:59pm</u>. No late submissions will be accepted.

Problems that require a numeric answer should have 3 significant figures.

Units, where required, are shown in blue. Please use these units. Approximate answers are indicated in blue.

This homework is a basic review of chemistry and solving systems of ODE's computationally. These are some of the essentials of this course.

Problem 1: Stoichiometry, Limiting Reagent

Consider the reaction:

$$2 \text{ Sb (s)} + 3 \text{ I}_2 (s) \rightarrow 2 \text{ SbI}_3 (s)$$

Determine the limiting reagent and the theoretical yield when:

- a. $1.20 \text{ mol of Sb and } 2.40 \text{ mol of } I_2 \text{ are mixed.}$
- b. 1.20 g of Sb and 2.40 g of I_2 are mixed. What mass of excess reactant is left when the reaction is complete?

Problem 2: Precipitation reactions

An aqueous solution of sodium hydroxide and iron(III) nitrate are mixed and a red precipitate forms in the bottom of the flask. Calculate the mass of the precipitate that is formed when 50.00 mL of 0.200 M NaOH and 30.00 mL of 0.125 M Fe(NO₃)₃ are mixed.



Precipitation of Fe(OH)₃

Problem 3: Gas phase reactions

A mixture in which the mole ratio of hydrogen to oxygen is 2:1 initially is used to prepare water using the reaction below.

$$2 H_2(g) + O_2(g) \rightarrow 2 H_2O(g)$$

The total pressure in the container is 0.950 atm at 25°C before the reaction. What is the final pressure in the container at 125°C after the reaction, assuming an 88.0% yield and no volume change?

Problem 4: Thermochemistry

Given the following system, calculate ΔH for the formation of one mole of dinitrogen pentoxide from its elements in their stable state at 25°C and 1 atm.

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l); \ \Delta H = -571.6 \text{ kJ}$$

 $N_2O_5(g) + H_2O(l) \rightarrow 2HNO_3(l); \ \Delta H = -73.7 \text{ kJ}$
 $0.5 \ N_2(g) + 1.5 \ O_2(g) + 0.5 \ H_2(g) \rightarrow HNO_3(l); \ \Delta H = -174.1 \text{ kJ}$

Problem 5: Chemical Reaction Equilibrium

For the reaction,

$$N_2O_4(g) \rightleftharpoons 2 NO_2(g)$$

The equilibrium constant is known to be 11 atm at 373K. Starting with pure N_2O_4 at a pressure of 1.00 atm, what are the equilibrium partial pressures of NO_2 and N_2O_4 ?

Problem 6: Systems of ordinary differential equations, Plug flow reaction with a pressure drop

Using the system of ODEs below graph X and y on a plot of X vs. W for $0 \le W \le 60$.

$$\frac{dX}{dW} = \frac{k'}{F_{A0}} \left(\frac{1 - X}{1 + \epsilon X} \right) y$$

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

The following values are known: k' = 0.0266, $F_{A0} = 1.08$, $\alpha = 0.0166$, $\epsilon = -0.15$. Initially, X(0) = 0 and y(0) = 1.