Introduction to Chemical Engineering

Problem Sheet 2 – Week 4 – October 4 2024

Goals:
Introduction to reactive systems

Problem 1: Reactive Systems (Fraction Conversion Specified)

The chlorination of methane occurs by the following reaction:

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

Determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH_4, 50% Cl_2, and 10% N_2.

Suggested Steps:

1. Draw diagram process with known data inserted
2. Select a basis
3. Determine limiting reactant:
   Compare maximum extent of reaction for each reactant
4. Degree-of-freedom analysis (good practice)
5. Obtain composition

Problem 2: Reactive Systems (Fraction Conversion to be calculated)

Mercaptans, hydrogen sulfide, and other sulfur compounds are removed from natural gas by various so-called "sweetening processes" that make available otherwise useless "sour" gas. H_2S is known to be toxic in very small quantities and is quite corrosive to process equipment.

A proposed process to remove H2S is by reaction with SO2:

$$H_2S\ (g) + SO_2\ (g) \rightarrow S\ (s) + H_2O$$

In a test of the process, a gas stream containing 20% H2S and 80% CH4 was combined with a stream of pure SO2. The process produced 5000 kg of S (s), and in the product gas the ratio of SO2 to H2S was equal to 3, and the ratio of H2O to H2S was 10. **Determine the fractional conversion of the limiting reactant**.

(Hint: ξ will have to be calculated from the material balance equations before calculating the fractional conversion)

Suggested Steps:

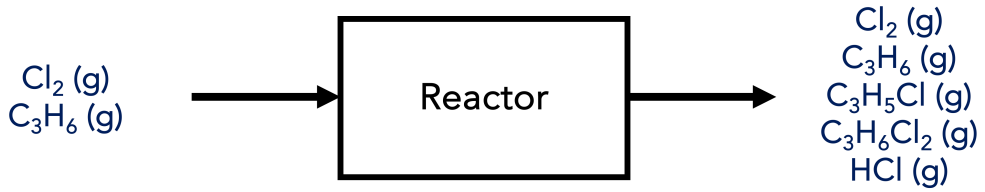
1. Draw diagram process with known data inserted
2. Determine Basis
3. Degree-of-freedom analysis (good practice)
4. Balance Species, form equations, and solve ☺

Problem 3: Reactive Systems 101 (Reactive system)

Let's take a quick look at the chemistry of allyl chlorides. The two reactions of interest for this example are:

$$\text{(a)}\ \ Cl_2\ (g) + C_3H_6\ (g) \rightarrow C_3H_5Cl\ (g) + HCl\ (g)$$

$$\text{(b)}\ \ Cl_2\ (g) + C_3H_6(g) \rightarrow C_3H_6Cl_2\ (g)$$



Species involved:

- C_3H_6 is propylene (propene) (MW = 42.08)
- C_3H_5Cl is allyl chloride (3-chloropropene) (MW = 76.53)
- $C_3H_6Cl_2$ is propylene chloride (1,2-dichloropropane) (MW = 112.99)

The species recovered after the reaction takes place for some time are listed in the table below:

Species	mol
Cl_2	141.0
C_3H_6	651.0
C_3H_5Cl	4.6
$C_3H_6Cl_2$	24.5
HCl	4.6

Based on the product distribution, assuming that no allyl chlorides were present in the feed, calculate the following:

a. How much Cl_2 and C_3H_6 were fed to the reactor in mol?
b. What was the limiting reactant?
c. What was the excess reactant?
d. What was the fraction conversion of C_3H_6 to C_3H_5Cl?
e. What was the selectivity of C_3H_5Cl relative to $C_3H_6Cl_2$?
f. What was the yield of C_3H_5Cl expressed in grams of C_3H_5Cl to the grams of C_3H_6 fed to the reactor?
g. What was the extent of reaction of the first and second reactions?
h. In the application of green chemistry, you would like to identify classes of chemical reactions that have the potential for process improvement, particularly waste reduction. In this example, the waste is HCl(g). The Cl_2 is not considered to be a waste because it is recycled. What is the mole efficiency, i.e., the fraction of an element in the entering reactants that emerges in the exiting products, for chlorine?

Problem 4: Reactive Systems (Simultaneous Reactions)

Formaldehyde (CH_2O) is produced industrially by the catalytic oxidation of methanol according to the following reaction:

$$CH_3OH + O_2 \rightarrow CH_2O + H_2O \quad \cdots (1)$$

Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is:

$$CH_2O + O_2 \rightarrow CO + H_2O \quad \cdots (2)$$

Assume that methanol is twice the stoichiometric amount of air neededd for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) are fed to the reactor. Also, assume that 90% conversion of the methanol results, and that a 75% yield of the formaldehyde occurs based on the theoretical production of CH_2O by Reaction 1. Determine the composition of the product gas leaving the reactor.