Leture 15

Example 5

The two reactions of interest for this example are**:**

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

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

C_3H_6 is propylene (propene) (MW = 42.08)

C_3H_5C1 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 Table**:**

species	**Cl_2**	**C_3H_6**	**C_3H_5Cl**	**$C_3H_6Cl_2$**	**HCl**
mol	141	651	4.6	24.5	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?

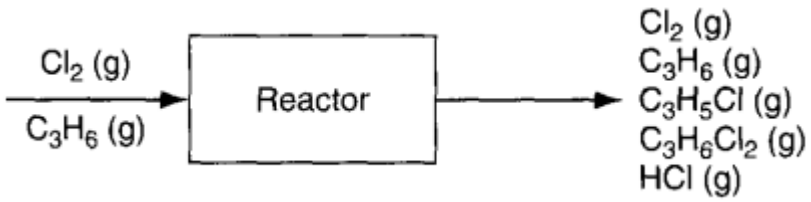
d. What was the fraction conversion of C_3H_6 to C_3H_5C1?

e. What was the selectivity of C_3H_5C1 relative to $C_3H_6Cl_2$?

f. What was the yield of C_3H_5C1 expressed in g of C_3H_5C1 to the g of C_3H_6 fed to the reactor?

g. What was the extent of reaction of the first and second reactions?

Solution



A convenient basis is what is given in the product list in Table**.**

Reaction (a): 1 mol of Cl_2 equivalent to 1 mole of C_3H_7Cl

moles of Cl_2 reacts = $4.6\ mol\ C_3H_7Cl * \frac{1\ mol\ Cl2}{1\ mol\ C_3H_7Cl} = 4.6\ mol\ Cl_2$

Reaction (b): 1 mol of Cl_2 equivalent to 1 mole of $C_3H_6Cl_2$

moles of Cl_2 reacts = $24.5\ mol\ C_3H_6Cl_2 * \frac{1\ mol\ Cl2}{1\ mol\ C_3H_6Cl_2} = 24.5\ mol\ Cl_2$

Total = 4.6 + 24.5 = 29.l mol Cl_2 reacts

Cl_2 in product = 141.0 mol from Table

(a) Total Cl_2 fed = 141.0 + 29.1 = 170.1 mol Cl_2

Total C_3H_6 fed = 651.0 + 29.1 = 680.1 mol of C_3H_6

(b) and (c) Since both reactions involve the same value of the respective reaction stoichiometric coefficients, both reactions will have the same limiting and excess reactants**:**

$$\xi^{max}(\text{based on } C_3H_6) = \frac{-680.1\ \text{mol}\ C_3H_6}{-1} = 680.1\ \text{mol reacting}$$

$$\xi^{max}(\text{based on } Cl_2) = \frac{-170.1\ \text{mol}\ Cl_2}{-1} = 170.1\ \text{mol reacting}$$

Thus, C_3H_6 was the excess reactantand Cl_2 the limiting reactant.

(d) The fraction conversion of C_3H_6 to C_3H_5C1 was

$$f = \frac{4.6 \text{ mol } C_3H_6 \text{ reacted}}{680.1 \text{ mol } C_3H_6 \text{ fed}} = 0.0067$$

(e) The selectivity was**:**

$$\text{selectivity} = \frac{4.6 \text{ mol } C_3H_5Cl}{24.5 \text{ mol } C_3H_6Cl_2} = 0.19 \frac{\text{mol } C_3H_5Cl}{\text{mol } C_3H_6Cl_2}$$

(f) The yield was:

$$\text{Yield} = \frac{(76.53)(4.6) \text{ g } C_3H_5Cl}{(42.08)(680.1) \text{ g } C_3H_6} = 0.012 \frac{\text{g } C_3H_5Cl}{\text{g } C_3H_6}$$

(g) Because $C_3H_5C1$is produced only by the first reaction, the extent of reactionof the first reaction is:

$$\xi_1 = \frac{n_i - n_{io}}{\nu_i} = \frac{4.6-0}{1} = 4.6 \text{ mol reacting}$$

Because $C_3H_6C1_2$ is produced only by the second reaction, the extent of reaction of the second reaction is

$$\xi_2 = \frac{n_i - n_{io}}{\nu_i} = \frac{24.5-0}{1} = 24.5 \text{ mol reacting}$$

Problems

1. If 1 kg of benzene (C_6H_6) is oxidized with oxygen, how many kilograms of O_2 are needed to convert all the benzene to $CO_2$and H_2O?

2. Two well-known gas phase reactions take place in the dehydration of ethane:

$$C_2H_6 \rightarrow C_2H_4 + H_2 \quad (a)$$

$$C_2H_6 + H_2 \rightarrow 2\,CH_4 \quad (b)$$

Given the product distribution measured in the gas phase reaction of C_2H_6 as follows: C_2H_6 27%, C_2H_4 33%, H_2 13%, and CH_4 27%.

a. What species was the limiting reactant?

b. What species was the excess reactant?

c. What was the conversion of C_2H_6 to CH_4?

d. What was the degree of completion of the reaction?

e. What was the selectivity of C_2H_4 relative to CH_4?

f. What was the yield of C_2H_4 expressed in kg mol of C_2H_4 produced per kg mol of C_2H_6?

g. What was the extent of reaction of C_2H_6?