Lecture 14

Limiting and Excess Reactants

The reactant that would run out if a reaction proceeded to completion is called the limiting reactant, and the other reactants are termed excess reactants.

A reactant is limiting if it is present in less than its stoichiometric proportion relative to every other reactant.

If all reactants are present in stoichiometric proportion, then no reactant is limiting.

Suppose $n_{(A)feed}$ is the number of moles of an excess reactant, A, and $n_{(A)stoich}$ is the stoichiometric requirement of A, or the amount needed to react completely with the limiting reactant. Then:

$$\text{fractional excess of A} = \frac{n_{(A)feed} - n_{(A)stoich}}{n_{(A)stoich}}$$

As a straightforward way of determining the limiting reactant, you can determine the maximum extent of reaction, ξ^{max} , for each reactant based on the complete reaction of the reactant.

The reactant with the smallest maximum extent of reaction is the limiting reactant.

For example, for the chemical reaction equation:

$$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8H_2O$$

If 1 mol of C_7H_{16} and 12 mol of O_2 are mixed, then:

$$\xi^{max}(based\ on\ O_2) = \frac{0\ mol\ O_2 - 12\ mol\ O_2}{-11} = 1.09\ mol\ reacting$$

$$\xi^{max}(based\ on\ C_7H_{16}) = \frac{0\ mol\ C_7H_{16} - 1mol\ C_7H_{16}}{-1} = 1\ mol\ reacting$$

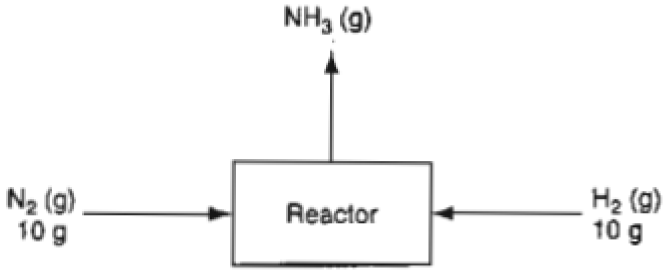
Therefore, heptane is the limiting reactant and oxygen is the excess reactant.

Example 3

If you feed 10 grams of N_2 gas and 10 grams of H_2 gas into a reactor:

a. What is the maximum number of grams of NH_3 that can be produced?
b. What is the limiting reactant?
c. What is the excess reactant?

Solution



	$N_2(g)$	+	$3H_2(g)$	→	$2NH_3(g)$
Given g:	10		10		0
MW:	28		2.016		17.02
Calcd. g mol:	0.357		4.960		0

$$\xi^{max}\ (\text{based on } N_2) = \frac{-0.357\ \text{g mol } N_2}{-1\ \text{g mol } N_2/\text{moles reacting}} = 0.357\ \text{moles reacting}$$

$$\xi^{max}\ (\text{based on } H_2) = \frac{-4.960\ \text{g mol } H_2}{-3\ \text{g mol } H_2/\text{moles reacting}} = 1.65\ \text{moles reacting}$$

You can conclude that (b) N_2 is the limiting reactant, and that (c) H_2 is the excess reactant. The excess H_2 is 4.960 – 3(0.357) = 3.89 g mol. To answer question (a), the maximum amount of NH_3 that can be produced is based on assuming complete conversion of the limiting reactant

$$\frac{0.357 \text{ g mol } N_2}{} \left| \frac{2 \text{ g mol } NH_3}{1 \text{ g mol } N_2} \right| \frac{17.02 \text{ g } NH_3}{1 \text{ g mol } NH_3} = 12.2 \text{ g } NH_3$$

Conversion and degree of completion

The fractional conversion of a reactant is the ratio:

$$f = \frac{\text{moles reacted}}{\text{moles fed}}$$

Example 4

for the chemical reaction equation:

$$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8H_2O$$

If 14.4 kg of CO_2 are formed in the reaction of 10 kg of C_7H_{16}, what is the fractional conversion of heptan?

Solution

1. moles of C_7H_{16} in the feed:

moles of C_7H_{16} fed = $\frac{10\ kg\ C7H16}{101.1\ \frac{kg\ C7H16}{k\ mol\ C7H16}} = 0.099\ kmol\ C_7H_{16}$

2. moles of C_7H_{16} reacted:

moles of CO_2 = $\frac{14.4\ kg\ CO2}{44\ \frac{kg\ CO2}{k\ mol\ CO2}} = 0.327\ kmol\ CO_2$

then from reaction equation: 1 mol of C_7H_{16} equivalent to 7 moles of CO_2:

moles of C_7H_{16} reacted $= 0.327\ \text{k mol}\ CO_2 * \frac{1\ \text{kmol}\ C_7H_{16}}{7\ \text{kmol CO2}} =$ $0.0467\ \text{k mol}\ C_7H_{16}$

$$f = \frac{0.0468\ \text{kmol reacted}}{0.0999\ \text{kmol fed}} = 0.468$$

$$\text{conversion} = \frac{\text{extent of reaction that actually occurs}}{\text{extent of reaction that would occur if complete reaction took place}}$$

$$= \frac{\xi}{\xi^{max}}$$

Selectivity

Selectivity is the ratio of the moles of the desired product produced to the moles of undesired product produced in a set of reactions.

$$\text{selectivity} = \frac{\text{moles of desired product}}{\text{moles of undesired product}}$$

For example, methanol (CH_3OH) can be converted into ethylene (C_2H_4) or propylene (C_3H_6) by the reactions**:**

$$2CH_3OH \rightarrow C_2H_4 + 2H_2O$$

$$3CH_3OH \rightarrow C_3H_6 + 3H_2O$$

What is the selectivity of C_2H_4 relative to the C_3H_6 at 80% conversion of the CH_3OH? Given that At 80% conversion: C_2H_4 19 mole % and for C_3H_6 8 mole %.

Because the basis for both values is the same,

$$\text{selectivity} = \frac{19\ \text{moles}}{8\ \text{moles}} = 2.4\ \text{mol}C_2H_4/\text{mol}C_3H_6$$

Yield

Yield (based on feed)—the amount (mass or moles) of desired product obtained divided by the amount of the key (frequently the limiting) reactant fed.