**Answers:**

1. 33.3 kg
2. 178 kg/hr
3. (a) 28% $Na_2SO_4$ ; (b) 33.3
4. Salt: 0.00617; Oil: 0.99393.

### 2.4 The Chemical Reaction Equation and Stoichiometry

**Stoichiometry**

- The stoichiometric coefficients in the chemical reaction equation
  $C_7H_{16}(\ell) + 11\ O_2(g) \rightarrow 7\ CO_2(g) + 8\ H_2O(g)$ $C_7H_{16}$, 11 for $O_2$ and so on).
- Another way to use the chemical reaction equation is to indicate that **1 mole of $CO_2$** is formed from each **(1/7) mole of $C_7H_{16}$**, and **1 mole of $H_2O$** is formed with each **(7/8) mole of $CO_2$**. The latter ratios indicate the use of **stoichiometric ratios** in determining the relative proportions of products and reactants.

**For example** how many kg of $CO_2$ will be produced as the product if 10 kg of $C_7H_{16}$ react completely with the **stoichiometric quantity** of $O_2$? On the basis of 10 kg of $C_7H_6$

$$\frac{10\text{ kg } C_7H_{16}}{} \left| \frac{1\text{ kg mol } C_7H_{16}}{100.1\text{ kg } C_7H_{16}} \right| \frac{7\text{ kg mol } CO_2}{1\text{ kg mol } C_7H_{16}} \left| \frac{44.0\text{ kg } CO_2}{1\text{ kg mol } CO_2} \right. = 30.8\text{ kg } CO_2$$

**Example 15**

The primary energy source for cells is the aerobic catabolism (oxidation) of glucose ($C_6H_{12}O_6$, a sugar). The overall oxidation of glucose produces $CO_2$ and $H_2O$ by the following reaction

$$C_6H_{12}O_6 + aO_2 \rightarrow b\ CO_2 + c\ H_2O$$

Determine the values of a, b, and c that balance this chemical reaction equation.

**Solution**

**Basis: The given reaction**

By inspection, the carbon balance gives b = 6, the hydrogen balance gives c = 6, and an oxygen balance

$6 + 2a = 6 * 2 + 6$

Gives a = 6. Therefore, the balanced equation is $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

**Example 16**

In the combustion of heptane, $CO_2$ is produced. Assume that you want to produce 500 kg of dry ice per hour, and that 50% of the $CO_2$ can be converted into dry ice, as shown in Figure E9.2. How many kilograms of heptane must be burned per hour? (MW: $CO_2$ = 44 and $C_7H_{16}$ = 100.1)

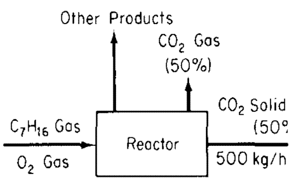



**Figure E9.2**

**Solution**

The chemical equation is $C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

**Basis: 500 kg of dry ice (equivalent to 1 hr)**

The calculation of the amount of $C_7H_{16}$ can be made in one sequence:

$$\frac{500 \text{ kg dry ice}}{} \left| \frac{1 \text{ kg } CO_2}{0.5 \text{ kg dry ice}} \right| \frac{1 \text{ kg mol } CO_2}{44.0 \text{ kg } CO_2} \left| \frac{1 \text{ kg mol } C_7H_{16}}{7 \text{ kg mol } CO_2} \right| \frac{100.1 \text{ kg } C_7H_{16}}{1 \text{ kg mol } C_7H_{16}} = 325 \text{ kg } C_7H_{16}$$

**Example 17**

A limestone analyses (weight %): $CaCO_3$ 92.89%, $MgCO_3$ 5.41% and Inert 1.70%

By heating the limestone you recover oxides known as lime.

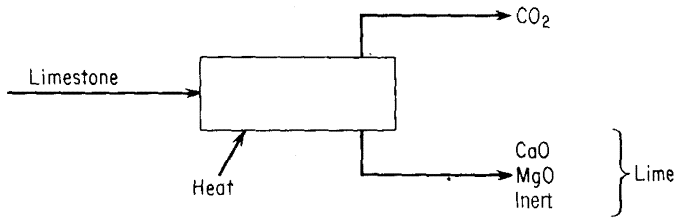
(a) How many pounds of calcium oxide can be made from 1 ton of this limestone?

(b) How many pounds of $CO_2$ can be recovered per pound of limestone?

(c) How many pounds of limestone are needed to make 1 ton of lime?

Mol. Wt.: $CaCO_3$ (100.1) $MgCO_3$ (84.32) CaO (56.08) MgO (40.32) $CO_2$ (44.0)

**Solution**




Chemical Equation:

$$CaCO_3 \rightarrow CaO + CO_2$$

$$MgCO_3 \rightarrow MgO + CO_2$$

**Basis: 100 lb of limestone**

| Limestone | | | Solid Products | | |
|---|---|---|---|---|---|
| Component | lb = percent | lb mol | Compound | lb mol | lb |
| $CaCO_3$ | 92.89 | 0.9280 | CaO | 0.9280 | 52.04 |
| $MgCO_3$ | 5.41 | 0.0642 | MgO | 0.0642 | 2.59 |
| Inert | 1.70 | | Inert | | 1.70 |
| Total | 100.00 | 0.9920 | Total | 0.9920 | 56.33 |

The quantities listed under Products are calculated from the chemical equations. For example, for the last column:

$$\frac{92.89 \text{ lb } CaCO_3}{} \left| \frac{1 \text{ lb mol } CaCO_3}{100.1 \text{ lb } CaCO_3} \right| \frac{1 \text{ lb mol CaO}}{1 \text{ lb mol } CaCO_3} \left| \frac{56.08 \text{ lb CaO}}{1 \text{ lb mol CaO}} \right. = 52.04 \text{ lb CaO}$$

$$\frac{5.41 \text{ lb } MgCO_3}{} \left| \frac{1 \text{ lb mol } MgCO_3}{84.32 \text{ lb } MgCO_3} \right| \frac{1 \text{ lb mol MgO}}{1 \text{ lb mol } MgCO_3} \left| \frac{40.32 \text{ lb MgO}}{1 \text{ lb mol MgO}} \right. = 2.59 \text{ lb MgO}$$

The production of $\mathbf{CO_2}$ is:

**0.9280 lb mol CaO** is equivalent to **0.9280 lb mol $CO_2$**

**0.0642 lb mol MgO** is equivalent to **0.0642 lb mol $CO_2$**

Total lb mol $CO_2$ = 0.9280 + 0.0642 = **0.992 lb mol $CO_2$**

$$\frac{0.992 \text{ lb mol } CO_2}{} \left| \frac{44.0 \text{ lb } CO_2}{1 \text{ lb mol } CO_2} \right. = 44.65 \text{ lb } CO_2$$

Alternately, you could have calculated the **lb $CO_2$** from a total balance: **100 - 56.33 = 44.67**.

Now, to calculate the quantities originally asked for:

(a) CaO produced = $\frac{52.04 \text{ lb CaO}}{100 \text{ lb limestone}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right. = 1041 \text{ lb CaO/ton}$

(b) $CO_2$ recovered = $\frac{43.65 \text{ lb } CO_2}{100 \text{ lb limestone}} = 0.437 \text{ lb } CO_2\text{/lb limestone}$

(c) Limestone required = $\frac{100 \text{ lb limestone}}{56.33 \text{ lb lime}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right. = \frac{3550 \text{ lb limestone/}}{\text{ton lime}}$

**Terminology for Applications of Stoichiometry**

**Extent of Reaction**

The **extent of reaction**, ξ, is based on a particular stoichiometric equation, and denotes how much reaction occurs.

The extent of reaction is defined as follows: ... 9.1

$$\xi = \frac{n_i - n_{io}}{v_i}$$

Where:

$n_i$ = moles of species *i* present in the system after the reaction occurs

$n_{io}$ = moles of species *i* present in the system when the reaction starts

$v_i$ = coefficient for species *i* in the particular chemical reaction equation (moles of species *i* produced or consumed per moles reacting)

ξ = extent of reaction (moles reacting)

- The **coefficients** of the **products** in a chemical reaction are assigned **positive** values and the **reactants** assigned **negative** values. Note that ($n_i$ - $n_{io}$) is equal to the **generation** or **consumption** of component *i* by reaction.

Equation (9.1) can be rearranged to calculate the number of moles of component *i* from the value of the extent of reaction

$$n_i = n_{i0} + \xi v_i \qquad \text{... 9.2}$$

**<u>Example 18</u>**

Determine the extent of reaction for the following chemical reaction $N_2 + 3H_2 \rightarrow 2NH_3$ given the following analysis of feed and product:

| | $N_2$ | $H_2$ | $NH_3$ |
|---|---|---|---|
| Feed | 100 g | 50 g | 5 g |
| Product | | | 90 g |

Also, determine the g and g mol of $N_2$ and $H_2$ in the product.

**Solution**

The extent of reaction can be calculated by applying Equation 9.1 based on $NH_3$:

$$n_i = \frac{90 \text{ g } NH_3}{} \left| \frac{1 \text{ g mol } NH_3}{17 \text{ g } NH_3} \right. = 5.294 \text{ g mol } NH_3$$

$$n_{i0} = \frac{5 \text{ g } NH_3}{} \left| \frac{1 \text{ g mole } NH_3}{17 \text{ g } NH_3} \right. = 0.294 \text{ g mol } NH_3$$

$$\xi = \frac{n_i - n_{i0}}{v_i} = \frac{(5.294 - 0.204)\text{g mol } NH_3}{2 \text{ g mol } NH_3\text{/moles reacting}} = 2.50 \text{ moles reacting}$$

Equation 9.2 can be used to determine the g mol of $N_2$ and $H_2$ in the products of the reaction

$$N_2: \quad n_{i0} = \frac{100 \text{ g } N_2}{} \left| \frac{1 \text{ g mol } N_2}{28 \text{ g } N_2} \right. = 3.57 \text{ g mol } N_2$$

$$n_{N_2} = 3.57 + (-1)(2.5) = 1.07 \text{ g mol } N_2$$

$$m_{N_2} = \frac{1.07 \text{ g mol } N_2}{} \left| \frac{28 \text{ g } N_2}{1 \text{ g mol } N_2} \right. = 30 \text{ g } N_2$$

$$H_2: \quad n_{i0} = \frac{50 \text{ g } H_2}{} \left| \frac{1 \text{ g mol } H_2}{2 \text{ g } H_2} \right. = 25 \text{ g mol } H_2$$

$$n_{H2} = 25 + (-3)(2.5) = 17.5 \text{ g mol } H_2$$

$$m_{H2} = \frac{17.5 \text{ g mol } H_2}{} \left| \frac{2\text{g } H_2}{1 \text{ g mol } H_2} \right. = 35 \text{ g } H_2$$

**Note**: If several independent reactions occur in the reactor, say $k$ of them, ξ can be defined for each reaction, with $v_{ki}$ being the stoichiometric coefficient of species $i$ in the $k$th reaction, the total number of moles of species $i$ is

$$n_i = n_{i0} + \sum_{k=1}^{R} v_{ki}\,\xi_k \qquad \ldots 9.3$$

Where $R$ is the total number of independent reactions.

---

**Limiting and Excess Reactants**

- The **excess material** comes out together with, or perhaps separately from, the product, and sometimes can be used again.
- The **limiting reactant** is the species in a chemical reaction that would theoretically run out first (**would be completely consumed**) if the reaction were to proceed to completion according to the chemical equation—**even if the reaction does not proceed to completion!** All the other reactants are called **excess reactants**.

$$\%\,\text{excess reactant} = \frac{\left\{\begin{array}{c}\text{amount of the excess reactant fed - amount of the excess reactant required to} \\ \text{react with the limiting reactant}\end{array}\right\}}{\{\text{amount of the excess reactant required to react with the limiting reactant}\}} \times 100$$

- **For example**, using the chemical reaction equation in **Example 9.2**,

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

If **1 g mol of $C_7H_{16}$** and **12 g mol of $O_2$** are mixed.

As a straightforward way of determining the **limiting reactant**, you can determine the **maximum extent of reaction**, $\xi^{max}$, 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 the example, for **1 g mol** of $C_7H_{16}$ plus **12 g mole** of $O_2$, you calculate

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

$$\xi^{max}\text{ (based on } C_7H_{16}) = \frac{0 \text{ g mol } C_7H_{16} - 1 \text{ g mol } C_7H_{16}}{-1 \text{ g mol } C_7H_{16}/\text{moles reacting}} = 1.00 \text{ moles reacting}$$

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

As an **alternate** to determining the **limiting reactant**,

| | *Ratio in feed* | | *Ratio in chemical equation* |
|---|---|---|---|
| $\frac{O_2}{C_7H_{16}}$: | $\frac{12}{1} = 12$ | > | $\frac{11}{1} = 11$ |

❖ Consider the following reaction $A + 3B + 2C \rightarrow \text{Products}$

If the feed to the reactor contains **1.1 moles of A**, **3.2 moles of B**, and **2.4 moles of C**. The extents of reaction based on complete reaction of **A, B,** and **C** are

$$\xi^{max}\text{ (based on A)} = \frac{-1.1 \text{ mol A}}{-1} = 1.1$$

$$\xi^{max}\text{ (based on B)} = \frac{-3.2 \text{ mol B}}{-3} = 1.07$$

$$\xi^{max}\text{ (based on C)} = \frac{-2.4 \text{ mol C}}{-2} = 1.2$$

As a result, **B** is identified as the **limiting reactant** in this example while **A** and **C** are the **excess reactants**.

As an **alternate** to determining the **limiting reactant** for same example: اذا كانت النسبة في ال feed اكبر فالمقام هو Limiting

We **choose A** as the **reference substance** and calculate اذا كانت النسبة في ال معادلة الكيميائية اكبر فالبسط هو Limiting

| | *Ratio in feed* | | *Ratio in chemical equation* |
|---|---|---|---|
| $\frac{B}{A}$: | $\frac{3.2}{1.1} = 2.91$ | < | $\frac{3}{1} = 3$ |
| $\frac{C}{A}$: | $\frac{2.4}{1.1} = 2.18$ | > | $\frac{2}{1} = 2$ |

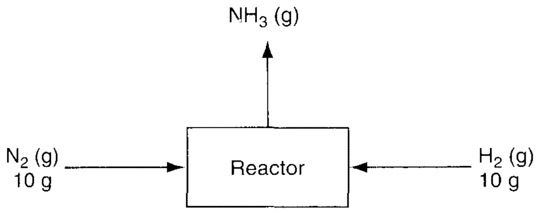
We conclude that **B** is the **limiting reactant relative to A**, and that **A** is the **limiting reactant relative** to **C**, hence **B** is the **limiting reactant** among the set of **three reactant**. In symbols we have **B < A, C > A (i.e., A < C)**, so that **B < A < C**.

**Example 19**

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 |
| Calculated g mol: | 0.357 | 4.960 | 0 |

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

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

(b) $N_2$ is the limiting reactant, and that (c) $H_2$ is the excess reactant.

The excess $H_2$ = 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**

- **Conversion** is the fraction of the feed or some key material in the feed that is converted into products.
- **Conversion** is related to the **degree of completion** of a reaction namely the percentage or fraction of the limiting reactant converted into products.

Thus, **percent conversion** is

$$\%\text{ conversion} = \frac{\text{moles (or mass) of feed (or a compound in the feed) that react}}{\text{moles (or mass) of feed (or a component in the feed) introduced}} \times 100$$

**For example**, for the reaction equation described in **Example 16**, if 14.4 kg of $CO_2$ are formed in the reaction of 10 kg of $C_7H_{16}$, you can calculate what percent of the $C_7H_{16}$ is converted to $CO_2$ (reacts) as follows:

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

$C_7H_{16}$ equivalent to $CO_2$ in the product

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$$\frac{14.4 \text{ kg } CO_2}{} \left| \frac{1 \text{ kg mol } CO_2}{44.0 \text{ kg } CO_2} \right| \frac{1 \text{ kg mol } C_7H_{16}}{7 \text{ kg mol } CO_2} = 0.0468 \text{ kg mol } C_7H_{16}$$

$$\frac{10 \text{ kg } C_7H_{16}}{} \left| \frac{1 \text{ kg mol } C_7H_{16}}{100.1 \text{ kg } C_7H_{16}} \right. = 0.0999 \text{ kg mol } C_7H_{16}$$

$C_7H_{16}$ in the reactants

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$$\%\text{ conversion} = \frac{0.0468 \text{ mol reacted}}{0.0999 \text{ kg mol fed}} 100 = 46.8\% \text{ of the } C_7H_{16}$$

☒ The conversion can also be calculated using the **extent of reaction** as follows:

**Conversion** is equal to the extent of reaction based on $CO_2$ formation (i.e., the **actual extent of reaction**) divided by the extent of reaction assuming **complete reaction** of $C_7H_{16}$ (i.e., the **maximum possible extent of reaction**).

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

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

**Selectivity**

**Selectivity** is the ratio of the moles of a particular (usually the desired) product produced to the moles of another (usually undesired or by-product) product produced in a set of reactions.

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

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

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

What is the selectivity of $C_2H_4$ relative to the $C_3H_6$ at 80% conversion of the $CH_3OH$? At 80% conversion: $C_2H_4$ 19 mole % and for $C_3H_6$ 8 mole %. Because the basis for both values is the same, **the selectivity = 19/8 = 2.4 mol $C_2H_4$ per mol $C_3H_6$**.

**Yield**

No universally agreed-upon definitions exist for **yield**—in fact, quite the contrary. Here are **three** common ones:

- **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.
- **Yield (based on reactant consumed)**—the amount (mass or moles) of desired product obtained divided by amount of the key (frequently the limiting) reactant consumed.
- **Yield (based on theoretical consumption of the limiting reactant)**—the amount (mass or moles) of a product obtained divided by the theoretical (expected) amount of the product that would be obtained based on the limiting reactant in the chemical reaction equation if it were completely consumed.

<u>**Example 20**</u>

The following overall reaction to produce biomass, glycerol, and ethanol

$$C_6H_{12}O_6(\text{glucose}) + 0.118\ NH_3 \rightarrow 0.59\ CH_{1.74}N_{0.2}O_{0.45}\ (\text{biomass})$$
$$+ 0.43\ C_3H_8O_3(\text{glycerol}) + 1.54\ CO_2 + 1.3\ C_2H_5OH\ (\text{ethanol}) + 0.03\ H_2O$$

Calculate the theoretical yield of biomass in g of biomass per g of glucose. Also, calculate the yield of ethanol in g of ethanol per g of glucose.

**Solution**

**Basis: 0.59 g mol of biomass**

$$\frac{0.59 \text{ g mol biomass}}{1 \text{ g mol glucose}}\left|\frac{23.74 \text{ g biomass}}{1 \text{ g mol biomass}}\right|\frac{1 \text{ g mol glucose}}{180 \text{ g glucose}} = 0.0778 \text{ g biomass/g glucose}$$

$$\frac{1.3 \text{ g mol } C_2H_5OH}{1 \text{ g mol glucose}}\left|\frac{46 \text{ g } C_2H_5OH}{1 \text{ g mol } C_2H_5OH}\right|\frac{1 \text{ g mol glucose}}{180 \text{ g glucose}} = 0.332 \text{ g } C_2H_5OH\text{/g glucose}$$

**Example 21**

For this example, large amounts of single wall carbon nanotubes can be produced by the catalytic decomposition of ethane over Co and Fe catalysts supported on silica

$$C_2H_6 \rightarrow 2\,C + 3\,H_2 \qquad (a)$$
$$\searrow C_2H_4 + H_2 \qquad (b)$$

If you collect 3 g mol of $H_2$ and 0.50 g mol of $C_2H_4$, what is the selectivity of C relative to $C_2H_4$?

**Solution**

Basis: 3 g mol $H_2$ by Reaction (a)

0.50 g mol $C_2H_4$ by Reaction (b)

The 0.5 g mol of $C_2H_4$ corresponds to 0.50 g mol of $H_2$ produced in Reaction (b).

The $H_2$ produced by Reaction (a) = 3 - 0.50 = 2.5 g mol.

The nanotubes (the C) produced by Reaction (a) = (2/3)(2.5) = 1.67 g mol C

The selectivity = 1.67/0.50 = 3.33 g mol C/g mol $C_2H_4$

**Example 22**

The two reactions of interest for this example are

$$Cl_2(g) + C_3H_6(g) \rightarrow C_3H_5Cl(g) + HCl(g) \qquad (a)$$

$$Cl_2(g) + C_3H_6(g) \rightarrow C_3H_6Cl_2(g) \qquad (b)$$

$C_3H_6$ 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 E9.8.

| **species** | $Cl_2$ | $C_3H_6$ | $C_3H_5C1$ | $C_3H_6Cl_2$ | HCl |
|---|---|---|---|---|---|
| **g 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 g 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**

Figure E9.8 illustrates the process as an open-flow system. A batch process could alternatively be used.

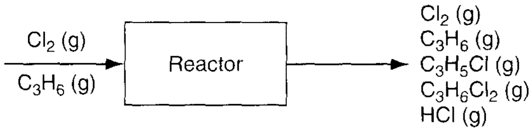


**Figure E9.8**

A convenient **basis** is what is given in the product list in Table E9.8.

**Reaction (a)**

$$\frac{4.6 \text{ g mol } C_3H_5C1}{} \left| \frac{1 \text{ g mol } Cl_2}{1 \text{ g mol } C_3H_5Cl} \right. = 4.6 \text{ g mol } Cl_2 \text{ reacts}$$

**Reaction (b)**

$$\frac{24.5 \text{ g mol } C_3H_6Cl_2}{} \left| \frac{1 \text{ g mol } Cl_2}{1 \text{ g mol } C_3H_6Cl_2} \right. = 24.5 \text{ g mol } Cl_2 \text{ reacts}$$

Total = 4.6 + 24.5 = 29.1 g mol $Cl_2$ reacts

$Cl_2$ in product = 141.0 from Table E9.8

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

Total $C_3H_6$ fed = 651.0 + 29.1 = 680.1 g 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

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

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

Thus, $\mathbf{C_3H_6}$ was the **excess reactant** and $\mathbf{Cl_2}$ the **limiting reactant**.

(d) The fraction conversion of $C_3H_6$ to $C_3H_5C1$ was

$$\frac{4.6 \text{ g mol } C_3H_6 \text{ that reacted}}{680.1 \text{ g mol } C_3H_6 \text{ fed}} = 6.76 \times 10^{-3}$$

(e) The selectivity was

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

(f) The yield was

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

(g) Because $\mathbf{C_3H_5C1}$ is produced only by the **first reaction**, the **extent of reaction** of the first reaction is

$$\xi_1 = \frac{n_i - n_{io}}{v_i} = \frac{4.6 - 0}{1} = 4.6$$

Because $\mathbf{C_3H_6C_{12}}$ is produced only by the **second reaction**, the **extent of reaction** of the second reaction is

$$\xi_2 = \frac{n_i - n_{io}}{v_i} = \frac{24.5 - 0}{1} = 24.5$$

يجب الحساب على اساس المادة الفريدة
حتى لا يسبب اشكالات في الحسابات

**Example 23**

Five pounds of bismuth (MW=209) is heated along with one pound of sulfur (MW=32) to form $Bi_2S_3$ (MW=514). At the end of the reaction, the mass is extracted and the free sulfur recovered is 5% of the reaction mass. Determine

5% من كتلة التفاعل الكلية

$2\,Bi + 3\,S \longrightarrow Bi_2S_3$

1. The limiting reactant.
2. The percent excess reactant.
3. The percent conversion of sulfur to $Bi_2S_3$

**Solution**

**a.** Find the Limiting reactant

اذا كانت النسبة فى ال feed اكبر فالمقام هو Limiting

اذا كانت النسبة في ال معادلة الكيميائية اكبر فالبسط هو Limiting

Ratio in the feed

$$\frac{Bi}{S} = \frac{\frac{5.00\text{ lb Bi}}{} \Big| \frac{1\text{ lb mol Bi}}{209\text{ lb Bi}}}{\frac{1.00\text{ lb S}}{} \Big| \frac{1\text{ lb mol S}}{32\text{ lb S}}} = \frac{0.0239\text{ mol Bi}}{0.0313\text{ mol S}} = 0.774$$

$$\text{Ratio in the chemical equation} = \frac{2\text{ lb mol Bi}}{3\text{ lb mol S}} = 0.667$$

Compare the two ratios; **S is the limiting reactant.**

**b.** % Excess reactant

$$\text{Bi required} = \frac{1\text{ lb S}}{} \Big| \frac{1\text{ lb mol S}}{32\text{ lb S}} \Big| \frac{2\text{ mol Bi}}{3\text{ mol S}} = 0.0208\text{ lb mol Bi}$$

$$\%\text{ excess Bi} = \frac{(0.0239 - 0.028)}{0.028} \times 100 = \mathbf{14.9\ \%}$$

**c.** We will assume that no gaseous products are formed, so that the total mass of the reaction mixture is conserved at 6 lb (5 lb Bi + 1 lb S). The free sulfur at the end of the reaction = 5%.

$$\frac{6.00\text{ lb rxn mass}}{} \Big| \frac{5.00\text{ lb S}}{100\text{ lb rxn mass}} \Big| \frac{1\text{ lb mol S}}{32.0\text{ lb S}} = 0.00938\text{ lb mol S}$$

$$\%\text{ Conversion} = \frac{\text{moles of feed that react}}{\text{moles of feed introduced}} \times 100$$

$$= \frac{0.0313 - 0.00938}{0.0313} \times 100 = \mathbf{70.0\ \%}$$

**Questions**

1. What is a limiting reactant?
2. What is an excess reactant?
3. How do you calculate the extent of reaction from experimental data?

**Answers:**

Q.3 Reactant present in the least stoichiometric quantity.

Q.4 All other reactants than the limiting reactant.

Q.5 For a species in

Open system: $\xi = \dfrac{n_{\text{out},i} - n_{\text{in},i}}{v_i}$ Closed system: $\xi = \dfrac{n_{\text{final},i} - n_{\text{initial},i}}{v_i}$

**Problems**

1. Write balanced reaction equations for the following reactions:
   a. $C_9H_{18}$ and oxygen to form carbon dioxide and water.
   b. $FeS_2$ and oxygen to form $Fe_2O_3$ and sulfur dioxide.
2. 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 $H_2O$?
3. The electrolytic manufacture of chlorine gas from a sodium chloride solution is carried out by the following reaction:

$$2\ NaCl + 2\ H_2O \rightarrow 2\ NaOH + H_2 + Cl_2$$

How many kilograms of $Cl_2$ can be produced from 10 $m^3$ of brine solution containing 5% by weight of NaCl? The specific gravity of the solution relative to that of water at 4°C is 1.07.

4. Can you balance the following chemical reaction equation?

$$a_1NO_3 + a_2HClO \rightarrow a_3HNO_3 + a_4HCl$$

5. For the reaction in which stoichiometric quantities of the reactants are fed

$$2\ C_5H_{10} + 15\ O_2 \rightarrow 10\ CO_2 + 10\ H_2O$$

and the reaction goes to completion, what is the maximum extent of reaction based on $C_5H_{10}$? On $O_2$? Are the respective values different or the same? Explain the result.

6. Calcium oxide (CaO) is formed by decomposing limestone (pure $CaCO_3$). In one kiln the reaction goes to 70% completion.
   a. What is the composition of the solid product withdrawn from the kiln?
   b. What is the yield in terms of pounds of $CO_2$ produced per pound of limestone fed into the process?
7. Aluminum sulfate can be made by reacting crushed bauxite ore with sulfuric acid, according to the following chemical equation:

$$Al_2O_3 + 3\ H_2SO_4 \rightarrow Al_2(SO_4)_3 + 3\ H_2O$$

The bauxite ore contains 55.4% by weight of aluminum oxide, the remainder being impurities. The sulfuric acid solution contains 77.7% pure sulfuric acid, the remainder being water. To produce crude aluminum sulfate containing 1798 lb of pure aluminum sulfate, 1080 lb of bauxite ore and 2510 lb of sulfuric acid solution are reacted.
   a. Identify the excess reactant.
   b. What percentage of the excess reactant was consumed?
   c. What was the degree of completion of the reaction?

8. 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 $C_2H_6$?

**Answers:**

1. (a) $C_9H_{18} + \frac{27}{2}O_2 \rightarrow 9\,CO_2 + 9\,H_2O$; $4\,FeS_2 + 11\,O_2 \rightarrow 2Fe_2O_3 + 8\,SO_2$
2. 3.08
3. 323
4. No
5. (a) 1,
   (b) 1,
   (c) The same,
   (d) The extent of reaction depends on the reaction equation as a whole and not on one species in the equation.
6. $CaCO_3$: 43.4%, CaO: 56.4%; (b) 0.308
7. (a) $H_2SO_4$
   (b) 79.2%;
   (c) 0.89
8. (a) $C_2H_6$ (the hydrogen is from reaction No.2, not the feed);
   (b) None;
   (c) Fraction conversion = 0.184;
   (d) 0.45;
   (e) 1.22
   (f) Based on reactant in the feed: 0.45, based on reactant consumed: 0.84, based on theory: 0.50;
   (g) Reaction (a) is 33 mol reacting and reaction (b) is 13.5 mol reacting, both based on 100 mol product.

**2.5 Material Balances for Processes Involving Reaction**

**Species Material Balances**

**Processes Involving a Single Reaction**

The material balance for a **species** must be augmented to include **generation** and **consumption** terms when **chemical reactions** occur in a process.

$$\left\{\begin{matrix}\text{moles of } i\\ \text{at } t_2\\ \text{in the system}\end{matrix}\right\} - \left\{\begin{matrix}\text{moles of } i\\ \text{at } t_1\\ \text{in the system}\end{matrix}\right\} = \left\{\begin{matrix}\text{moles of } i\\ \text{entering}\\ \text{the system}\end{matrix}\right\} - \left\{\begin{matrix}\text{moles of } i\\ \text{leaving}\\ \text{the system}\end{matrix}\right\} + \left\{\begin{matrix}\text{moles of } i\\ \text{generated}\\ \text{by reaction}\end{matrix}\right\} - \left\{\begin{matrix}\text{moles of } i\\ \text{consumed}\\ \text{by reaction}\end{matrix}\right\}$$