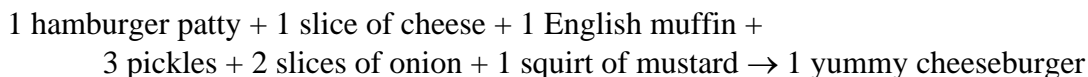# Chem 170

Stoichiometric Calculations

Module Six

Limiting Reagents, Theoretical Yields, and Percent Yields

Introduction to Module Six

The introduction to Module 4 includes the following balanced recipe for a cheeseburger

   1 hamburger patty + 1 slice of cheese + 1 English muffin +
        3 pickles + 2 slices of onion + 1 squirt of mustard $\rightarrow$ 1 yummy cheeseburger

In Module 5 we learned how to use stoichiometry to ask and answer questions such as "How many cheeseburgers can you make if you have 15 pickles?" and "How many onions will you need?".[†] There is, however, a hidden assumption in these two questions; specifically, we are assuming that you refrigerator has enough hamburger patties, cheese, English muffins, onion, and mustard to go along with the 15 pickles. Stated another way, we are assuming that we will run out of pickles before we run out of the other ingredients. In the language of stoichiometry, the pickles are the "limiting reagent" whose quantity determines the maximum, or "theoretical yield" of five cheeseburgers that can be made. The remaining ingredients are considered "excess reagents." If you drop a cheeseburger on the floor, where it is gobbled up by your dog, then you actual yield of cheeseburgers is less than the theoretical yield, giving a "percent yield" of 80% (four cheeseburgers successfully made out of an expected five).

Of course, the concepts of limiting reagents, theoretical yields, and percent yields also apply to chemical reactions. In this module you will learn how to determine which of several reactants is the limiting reagent, and how to determine a reaction's theoretical and percent yields.

Objectives for Module Six

In completing this module you will master the following objectives:

   • to identify which of several reactants is the limiting reagent

   • to determine the remaining amounts of excess reagents

   • to determine the theoretical yield of a chemical reaction

   • to determine a reaction's percent yield

[†] The answers are 5 cheeseburgers and 10 onions.

## Determining the Limiting Reagent and Excess Reagent

One of the methods used to synthesize urea, $(NH_2)_2CO$, is to react ammonia, NH_3, with carbon dioxide, CO_2. The balanced reaction for this process is shown here

$$2NH_3 + CO_2 \rightarrow (NH_2)_2CO + H_2O$$
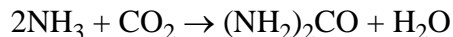
Suppose we carry out this reaction by combining 7.481 g NH_3 and 7.992 g CO_2 and wish to know the theoretical yield of urea? Because we are provided with the mass of each reactant, we first must determine which reactant is the limiting reagent. Although there are several approaches we can use to determine the limiting reagent, each uses only the basic stoichiometric calculations from Module 5. Three approaches are illustrated below for the synthesis of urea. Study these examples and use the approach that works best for you.

First Approach. One method for identifying the limiting reagent is to calculate the minimum moles or grams of one reactant (let's call it reactant A) needed to completely consume a second reactant (which we will call reactant B). If the available amount of reactant A exceeds what is needed, then it is the excess reagent; if not, then reactant B is the limiting reagent.

Example 1. Determine the limiting reagent and excess reagent for the synthesis of urea

$$2NH_3 + CO_2 \rightarrow (NH_2)_2CO + H_2O$$
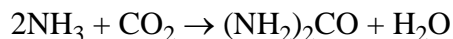
given 7.481 g NH_3 and 7.992 g CO_2.

Solution. Starting with NH_3, we calculate the minimum grams of CO_2 needed to completely consume the 7.481 g of NH_3

$$7.481 \text{ g } NH_3 \times \frac{1 \text{ mol } NH_3}{17.03 \text{ g } NH_3} \times \frac{1 \text{ mol } CO_2}{2 \text{ mol } NH_3} \times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2} = 9.666 \text{ g } CO_2$$

Because the 7.992 g CO_2 available to us is less than the 9.666 g needed, CO_2 is the limiting reagent and NH_3 is the excess reagent.

Second Approach. Another method for identifying the limiting reagent is to first calculate the moles of each reactant and then calculate the resulting mole ratio

$$\text{calculated mole ratio} = \frac{\text{moles reactant A}}{\text{moles reactant B}}$$

This calculated mole ratio is then compared to the theoretical mole ratio derived from the balanced chemical reaction's stoichiometry

$$\text{theoretical mole ratio} = \frac{\text{stoichiometric coefficient for reactant A}}{\text{stoichiometric coefficient for reactant B}}$$

If the calculated mole ratio exceeds the theoretical mole ratio, then reactant A is present in excess and reactant B is the limiting reagent. On the other hand, if the calculated mole ratio is less than the theoretical mole ratio, then reactant A is the limiting reagent and reactant B is the excess reagent.

Example 2. Determine the limiting reagent and excess reagent for the synthesis of urea

$$2NH_3 + CO_2 \rightarrow (NH_2)_2CO + H_2O$$
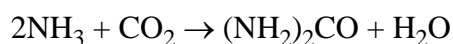
given 7.481 g NH_3 and 7.992 g CO_2.

Solution. The moles of NH_3 and CO_2 are

$$7.481 \text{ g } NH_3 \times \frac{1 \text{ mol } NH_3}{17.03 \text{ g } NH_3} = 0.4393 \text{ mol } NH_3$$

$$7.992 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} = 0.1816 \text{ mol } CO_2$$

The calculated and theoretical mole ratios are

$$\text{calculated mole ratio} = \frac{0.4393 \text{ mol } NH_3}{0.1816 \text{ mol } CO_2} = 2.419$$

$$\text{theoretical mole ratio} = \frac{2 \text{ mol } NH_3}{1 \text{ mol } CO_2} = 2$$

Because the calculated mole ratio exceeds the theoretical mole ratio, we have more NH_3 than needed to completely consume the available CO_2. The limiting reagent, therefore, is CO_2 and NH_3 is the excess reagent.

Third Approach. Finally, a third method for identifying the limiting reagent is to calculate the moles or grams of product that can be obtained if each reactant is completely consumed; that is, we assume that each reactant is the limiting reagent and calculate the amount of product obtained. The actual limiting reagent is the reactant producing the least amount of product.

Example 3. Determine the limiting reagent and excess reagent for the synthesis of urea

$$2NH_3 + CO_2 \rightarrow (NH_2)_2CO + H_2O$$
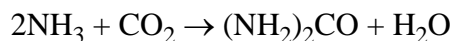
given 7.481 g NH_3 and 7.992 g CO_2.

Solution. If NH_3 is the limiting reagent, then we expect to obtain

$$7.481 \text{ g } NH_3 \times \frac{1 \text{ mol } NH_3}{17.03 \text{ g } NH_3} \times \frac{1 \text{ mol } (NH_2)_2CO}{2 \text{ mol } NH_3} = 0.2196 \text{ mol } (NH_2)_2CO$$

On the other hand, if CO_2 is the limiting reagent we obtain

$$7.992 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol } (NH_2)_2CO}{1 \text{ mol } CO_2} = 0.1816 \text{ mol } (NH_2)_2CO$$

Because 7.992 g CO_2 generates less urea than 7.481 g NH_3, CO_2 is the limiting reagent and NH_3 is the excess reagent.

Determining the Limiting Reagent for More Complex Reactions

Determining whether NH_3 or CO_2 is the limiting reagent for the synthesis of urea is relatively straightforward because there are only two reactants. Many reactions involve more than two reactants. For example, aluminum chloride, $AlCl_3$, is made by reacting aluminum oxide, Al_2O_3, carbon, C, and chlorine, Cl_2, as shown here

$$Al_2O_3 + 3C + 3Cl_2 \rightarrow 2AlCl_3 + 3CO$$
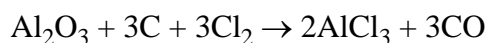
Suppose we have 10.3 g Al_2O_3, 15.9 g Cl_2, and 4.08 g C; how do we go about finding the limiting reagent? Any of the three approaches described above can be used if we first compare two reactants, determining which is the limiting reagent. This reactant is then compared to the third reactant to determine the reaction's overall limiting reagent.

Example 4. Determine the limiting reagent for the synthesis of $AlCl_3$

$$Al_2O_3 + 3C + 3Cl_2 \rightarrow 2AlCl_3 + 3CO$$
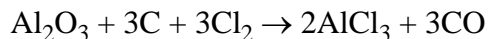
given 10.3 g Al_2O_3, 15.9 g Cl_2, and 4.08 g C.

Solution. Using the third approach to finding the limiting reagent, we first calculate the moles of $AlCl_3$ assuming, in turn, that each reactant is the limiting reagent.

$$10.3 \text{ g } Al_2O_3 \times \frac{1 \text{ mol } Al_2O_3}{101.96 \text{ g } Al_2O_3} \times \frac{2 \text{ mol } AlCl_3}{1 \text{mol } Al_2O_3} = 0.202 \text{ mol } AlCl_3$$

$$15.9 \text{ g } Cl_2 \times \frac{1 \text{ mol } Cl_2}{70.90 \text{ g } Cl_2} \times \frac{2 \text{ mol } AlCl_3}{3 \text{ mol } Cl_2} = 0.150 \text{ mol } AlCl_3$$

$$4.08 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} \times \frac{2 \text{ mol } AlCl_3}{3 \text{ mol C}} = 0.226 \text{ mol } AlCl_3$$

Because 15.9 g Cl_2 yields the fewest moles of $AlCl_3$, it is the limiting reagent and Al_2O_3 and C are present in excess.

Theoretical Yields and Percent Yields

A reaction's theoretical yield is the maximum amount of product expected when the limiting reagent is completely used up. In essence, the examples from Module 5 in which we calculated the amount of product formed during a reaction were determinations of theoretical yield.[†] It is rare, however, for a reaction to actually produce the amount of product predicted by the theoretical yield. There are many reasons why a reaction's actual yield might be less than its theoretical yield. For example, some reactions stop before the limiting reagent is completely used up; such reactions are said to reach a position of equilibrium. In other cases, there are one or more side reactions in which a portion of the limiting reagent is used up. And, of course, even if we successfully convert the entire limiting reagent to product, some of the product may be lost during the process of recovering it from the reaction mixture (sort of analogous to your dog swiping a cheeseburger!).

To indicate the efficiency of a chemical reaction, we typically report both the amount of product obtained (the actual yield) and the percent yield, which we define as

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

[†] See Examples 1, 4, and 6 in Module 5. See, also, Problems 1, and 3-10 in Module 5.

where the actual and theoretical yields may be expressed in grams or moles (provided that the same unit is used for each).

Example 5. Nitrobenzene, $C_6H_5NO_2$, is an important raw material for the preparation of dyes. It is prepared from benzene, C_6H_6, and nitric acid, HNO_3

$$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$$
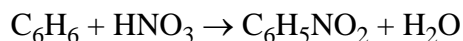
When 22.4 g benzene reacts with an excess of nitric acid, 28.7 g of nitrobenzene are obtained. What is the reaction's percent yield?

Solution. To find the reaction's percent yield we first need to know the actual yield and the theoretical yield. The actual yield is given, but we must calculate the theoretical yield in grams.

$$22.4 \text{ g } C_6H_6 \times \frac{1 \text{ mol } C_6H_6}{78.11 \text{ g } C_6H_6} \times \frac{1 \text{ mol } C_6H_5NO_2}{1 \text{ mol } C_6H_6}$$

$$\times \frac{123.1 \text{ g } C_6H_5NO_2}{1 \text{ mol } C_6H_5NO_2} = 35.30 \text{ g } C_6H_5NO_2$$

The percent yield, therefore, is

$$\% \text{yield} = \frac{28.7 \text{ g } C_6H_5NO_2}{35.3 \text{ g } C_6H_5NO_2} \times 100 = 81.3\%$$

Determining the Final Composition for a Reaction Mixture

Suppose you place a mixture of ferrous oxide, FeO, and powdered aluminum metal, Al, in a crucible and heat the mixture in a furnace. At the high temperature maintained in the furnace the ferrous oxide and aluminum react to make iron metal, Fe, and aluminum oxide, Al_2O_3

$$3FeO + 2Al \rightarrow 3Fe + Al_2O_3$$
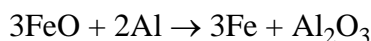
After several hours you remove the crucible from the furnace. What are the contents of the crucible? The tools that you've learned in Modules 5 and 6 can help you answer this question.

Example **6**. A mixture of 7.45 g FeO and 2.99 g Al is placed in a crucible and heated in a furnace where the following reaction takes place

$$3FeO + 2Al \rightarrow 3Fe + Al_2O_3$$
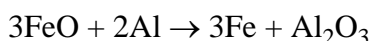
Assuming that the reaction goes to completion with a percent yield of 100%, what is the mixture's final composition?

Solution. To determine the mixture's final composition we first must find the grams of Fe and Al_2O_3 produced in the reaction, and the grams of the excess reagent (either FeO or Al) remaining. First we find the limiting reagent.

$$2.99 \text{ g Al} \times \frac{1 \text{ mol Al}}{26.98 \text{ g Al}} \times \frac{3 \text{ mol FeO}}{2 \text{ mol Al}} \times \frac{71.85 \text{ g FeO}}{1 \text{ mol FeO}} = 11.94 \text{ g FeO}$$

Because we have less FeO than needed to react with the aluminum (7.45 g FeO available vs. 11.94 g FeO needed), FeO is the limiting reagent.

Using our limiting reagent, we next determine the theoretical yields for Fe and Al_2O_3

$$7.45 \text{ g FeO} \times \frac{1 \text{ mol FeO}}{71.85 \text{ g FeO}} \times \frac{3 \text{ mol Fe}}{3 \text{ mol FeO}} \times \frac{55.85 \text{ g Fe}}{1 \text{ mol Fe}} = 5.79 \text{ g Fe}$$

$$7.45 \text{ g FeO} \times \frac{1 \text{ mol FeO}}{71.85 \text{ g FeO}} \times \frac{1 \text{ mol Al}_2O_3}{3 \text{ mol FeO}} \times \frac{101.96 \text{ g Al}_2O_3}{1 \text{ mol Al}_2O_3} = 3.52 \text{ g Al}_2O_3$$

Finally, we determine the amount of Al remaining. To do so we calculate the grams of Al consumed when reacting with the limiting reagent

$$7.45 \text{ g FeO} \times \frac{1 \text{ mol FeO}}{71.85 \text{ g FeO}} \times \frac{2 \text{ mol Al}}{3 \text{ mol FeO}} \times \frac{26.98 \text{ g Al}}{1 \text{ mol Al}} = 1.87 \text{ g Al}$$

The grams of Al remaining, therefore is

initial grams Al - grams Al consumed = grams Al remaining

2.99 g Al - 1.87 g Al = 1.12 g Al

Because FeO is the limiting reagent, none is left when the reaction is complete.

Practice Problems

The following problems provide practice in meeting this module's objectives. Answers are provided on the last page. Be sure to seek assistance if you experience difficulty with any of these problems. When you are ready, schedule an appointment for the module exam.

1. Potassium superoxide, KO_2, is used in rebreathing gas masks. As shown here

$$4KO_2 + 2H_2O \rightarrow 4KOH + 3O_2$$
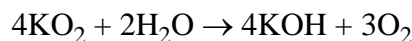
   KO_2 serves as a source of oxygen upon reacting with moist exhaled air. What is the limiting reagent if 0.25 mol KO_2 comes into contact with 0.15 mol H_2O?

2. In the first step for making nitric acid, ammonia is burned in the presence of oxygen to give nitric oxide. The balanced reaction is

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$
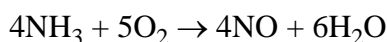
   What is the limiting reagent if 2.04 g NH_3 react with 0.140 mol O_2?

3. Methanol, CH_3OH, is prepared industrially by the following reaction

$$CO + 2H_2 \rightarrow CH_3OH$$
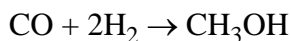
   What is the limiting reagent if 35.4 g CO react with 11.2 g H_2?

4. One source of acid rain is the conversion of SO_2, a gaseous pollutant produced during the burning of "dirty" coal, to sulfuric acid, H_2SO_4. The balanced reaction is shown here

$$2SO_2 + O_2 + 2H_2O \rightarrow 2H_2SO_4$$

   How many grams of H_2SO_4 can be made from the reaction of 5.00 mol SO_2 and 2.00 mol O_2? You may assume an unlimited supply of water.

5. The depletion of ozone, O_3, in the stratosphere is of increasing concern because ozone provides the earth with some protection from high energy UV light. One of the pathways leading to the loss of ozone is its reaction with nitric oxide, NO, which is present in the exhaust of high-altitude jets, such as the SST. The reaction is

$$O_3 + NO \rightarrow O_2 + NO_2$$
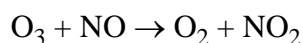
If 0.0154 mol of O_3 reacts with 0.670 g of NO, how many grams of NO_2 will be produced?

6. Sodium phosphate, Na_3PO_4, and barium nitrate, $Ba(NO_3)_2$, are soluble salts. Barium phosphate, $Ba_3(PO_4)_2$, however, is insoluble. As shown here

$$2Na_3PO_4 + 3Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + 6NaNO_3$$
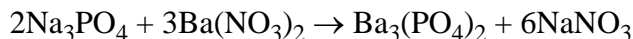
mixing together solutions of Na_3PO_4 and $Ba(NO_3)_2$ produces a precipitate of $Ba_3(PO_4)_2$. How many grams of $Ba_3(PO_4)_2$ can be made from the reaction of 3.50 g Na_3PO_4 and 6.40 g $Ba(NO_3)_2$?

7. Titanium, which is used to make airplane engines and bicycle frames, is obtained from titanium dioxide, TiO_2, in a two-step process. In the first step, TiO_2 is converted to titanium tetrachloride, $TiCl_4$; the reaction is

$$3TiO_2 + 4C + 6Cl_2 \rightarrow 3TiCl_4 + 2CO_2 + 2CO$$
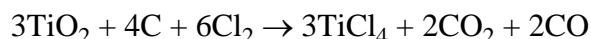
What is the theoretical yield of $TiCl_4$ upon reacting 4.15 g TiO_2, 5.67 g C, and 6.78 g Cl_2?

8. The production capacity for acrylonitrile, C_3H_3N, in the United States is over 2 billion pounds per year. "Why so much?", you ask – well, acrylonitrile is the building block for polyacrylonitrile fibers and a variety of plastics. It is synthesized using propylene, ammonia, and oxygen
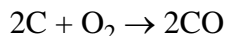
$$2C_3H_6 + 2NH_3 + 3O_2 \rightarrow 2C_3H_3N + 6H_2O$$
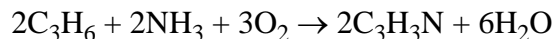
What mass of acrylonitrile can be produced from a mixture containing 5.00×10^2 g C_3H_6, 5.00×10^2 g NH_3, and 5.00×10^2 g O_2?

9. Zinc metal is obtained from zinc oxide, ZnO, by reacting it at a high temperature with carbon monoxide, CO

$$ZnO + CO \rightarrow Zn + CO_2$$
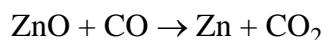
The carbon monoxide for the reaction is obtained from carbon

$$2C + O_2 \rightarrow 2CO$$

What is the theoretical yield of Zn in grams that can be obtained from 75.0 g ZnO and 50.0 g C in the presence of excess O_2?

10. Nitroglycerin, $C_3H_5N_3O_9$, is a powerful explosive. Upon detonation, it decomposes to form nitrogen, N_2, carbon dioxide, CO_2, water, H_2O, and oxygen, O_2

$$4C_3H_5N_3O_9 \rightarrow 6N_2 + 12CO_2 + 10H_2O + O_2$$
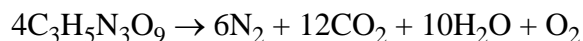
Detonation of 0.200 kg nitroglycerin produces 6.55 g O_2. What is the percent yield for oxygen?

11. Silicon carbide, SiC, is an important ceramic material that is made by reacting sand, SiO_2, with carbon at a high temperature. The balanced chemical equation for this reaction is shown here

$$SiO_2 + 3C \rightarrow SiC + 2CO$$
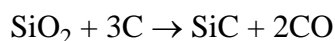
When 100.0 kg of SiO_2 reacts with 100.0 kg C, 51.4 kg of SiC are recovered. What is the reaction's percent yield?

12. Acetic acid, CH_3COOH, reacts with isopentyl alcohol, $C_5H_{12}O$, to yield isopentyl acetate, $C_7H_{14}O_2$, a fragrant substance with the odor of a banana. The balanced reaction is

$$CH_3COOH + C_5H_{12}O \rightarrow C_7H_{14}O_2 + H_2O$$
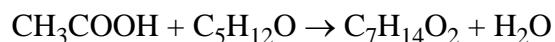
If the yield from the reaction is only 45%, how many grams of isopentyl acetate can be produced from the reaction of 3.58 g of acetic acid and 4.75 g of isopentyl alcohol?

13. Dibroane, B_2H_6, is a useful reactant for the synthesis of organic compounds. It is prepared by the following (unbalanced) reaction

$$NaBH_4 + BF_3 \rightarrow B_2H_6 + NaBF_4$$
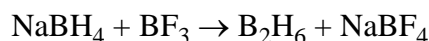
Balance the reaction and determine the yield of B_2H_6 in grams when 1.00 g $NaBH_4$ and 1.00 g BF_3 are allowed to react. Assume that the reaction proceeds with a percent yield of 75%.

14. The fizz produced when a tablet of Alka-Seltzer® dissolves in water comes from the reaction of sodium bicarbonate, $NaHCO_3$, and citric acid, $C_6H_8O_7$

$$3NaHCO_3 + C_6H_8O_7 \rightarrow 3CO_2 + 3H_2O + Na_3C_6H_5O_7$$

Suppose that a tablet containing 1.00 g of sodium bicarbonate and 1.00 g of citric acid reacts to completion. How many grams of CO_2 are produced and how many grams of the excess reagent remain when the reaction is complete?

15. Bubbling hydrogen sulfide, H_2S, through a solution of sodium hydroxide, NaOH, leads to the formation of sodium sulfide, Na_2S, and water, H_2O. Write a balanced equation for this reaction and determine the grams of Na_2S expected upon mixing 1.50 g of H_2S with 3.0 g of NaOH.

Answers to Practice Problems

1. KO_2

2. O_2

3. CO

4. 392 g H_2SO_4

5. 0.709 g NO_2

6. 4.91 g $Ba_3(PO_4)_2$

7. 9.07 g $TiCl_4$

8. 553 g C_3H_3N

9. 60.3 g Zn

10. 93.0% yield

11. 77.0% yield

12. 3.2 g $C_7H_{14}O_2$

13. $3NaBH_4 + 4BF_3 \rightarrow 2B_2H_6 + 3NaBF_4$, 0.15 g B_2H_6

14. 0.524 g CO_2, 0.238 g $C_6H_8O_7$

15. $H_2S + 2NaOH \rightarrow Na_2S + 2H_2O$, 2.9 g Na_2S