4.4 Reaction Yields

By the end of this section, you will be able to:

- Explain the concepts of theoretical yield and limiting reactants/reagents.
- Derive the theoretical yield for a reaction under specified conditions.
- Calculate the percent yield for a reaction.

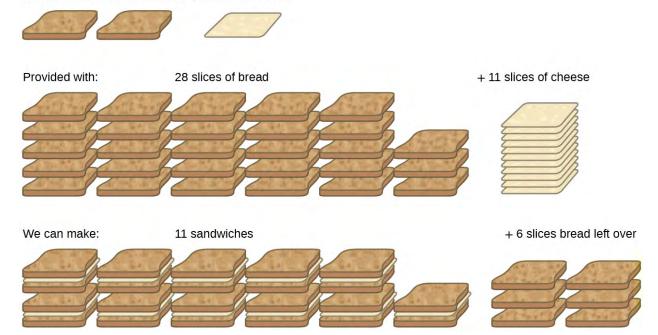
The relative amounts of reactants and products represented in a balanced chemical equation are often referred to as *stoichiometric amounts*. All the exercises of the preceding module involved stoichiometric amounts of reactants. For example, when calculating the amount of product generated from a given amount of reactant, it was assumed that any other reactants required were available in stoichiometric amounts (or greater). In this module, more realistic situations are considered, in which reactants are not present in stoichiometric amounts.

Limiting Reactant

Consider another food analogy, making grilled cheese sandwiches (Figure 4.12):

1 slice of cheese + 2 slices of bread \rightarrow 1 sandwich

Stoichiometric amounts of sandwich ingredients for this recipe are bread and cheese slices in a 2:1 ratio. Provided with 28 slices of bread and 11 slices of cheese, one may prepare 11 sandwiches per the provided recipe, using all the provided cheese and having six slices of bread left over. In this scenario, the number of sandwiches prepared has been *limited* by the number of cheese slices, and the bread slices have been provided in *excess*.



1 sandwich = 2 slices of bread + 1 slice of cheese

Figure 4.12 Sandwich making can illustrate the concepts of limiting and excess reactants.

Consider this concept now with regard to a chemical process, the reaction of hydrogen with chlorine to yield hydrogen chloride:

$$H_2(s) + Cl_2(g) \longrightarrow 2HCl(g)$$

The balanced equation shows the hydrogen and chlorine react in a 1:1 stoichiometric ratio. If these reactants are provided in any other amounts, one of the reactants will nearly always be entirely consumed, thus limiting the amount of product that may be generated. This substance is the **limiting reactant**, and the other substance is the **excess reactant**. Identifying the limiting and excess reactants for a given situation requires computing the molar amounts of each reactant provided and comparing them to the stoichiometric amounts represented in the balanced chemical equation. For example, imagine combining 3 moles of H₂ and 2 moles of Cl₂. This represents a 3:2 (or 1.5:1) ratio of hydrogen to chlorine present for reaction, which is greater than the stoichiometric ratio of 1:1. Hydrogen, therefore, is present in excess, and chlorine is the limiting reactant. Reaction of all the provided chlorine (2 mol) will consume 2 mol of the 3 mol of hydrogen provided, leaving 1 mol of hydrogen unreacted.

An alternative approach to identifying the limiting reactant involves comparing the amount of product expected for the complete reaction of each reactant. Each reactant amount is used to separately calculate the amount of product that would be formed per the reaction's stoichiometry. The reactant yielding the lesser amount of product is the limiting reactant. For the example in the previous paragraph, complete reaction of the hydrogen would yield

mol HCl produced =
$$3 \mod H_2 \times \frac{2 \mod HCl}{1 \mod H_2} = 6 \mod HCl$$

Complete reaction of the provided chlorine would produce

mol HCl produced =
$$2 \mod \text{Cl}_2 \times \frac{2 \mod \text{HCl}}{1 \mod \text{Cl}_2} = 4 \mod \text{HCl}$$

The chlorine will be completely consumed once 4 moles of HCl have been produced. Since enough hydrogen was provided to yield 6 moles of HCl, there will be unreacted hydrogen remaining once this reaction is complete. Chlorine, therefore, is the limiting reactant and hydrogen is the excess reactant (Figure 4.13).

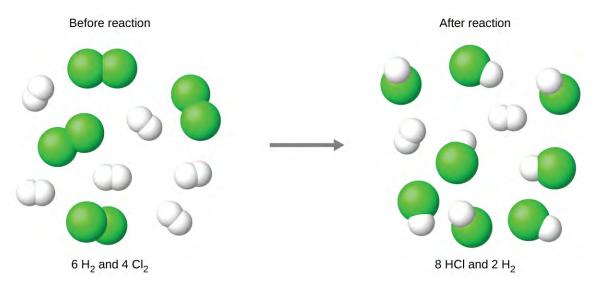


Figure 4.13 When H₂ and Cl₂ are combined in nonstoichiometric amounts, one of these reactants will limit the amount of HCl that can be produced. This illustration shows a reaction in which hydrogen is present in excess and chlorine is the limiting reactant.

Link to Learning Openstax View this interactive simulation (http://openstaxcollege.org/l/16reactantprod) illustrating the concepts of limiting and excess reactants.

Example 4.12

Identifying the Limiting Reactant

Silicon nitride is a very hard, high-temperature-resistant ceramic used as a component of turbine blades in jet engines. It is prepared according to the following equation:

$$3Si(s) + 2N_2(g) \longrightarrow Si_3N_4(s)$$

Which is the limiting reactant when 2.00 g of Si and 1.50 g of N_2 react?

Solution

Compute the provided molar amounts of reactants, and then compare these amounts to the balanced equation to identify the limiting reactant.

mol Si = 2.00
$$\frac{\text{g Si}}{\text{g Si}} \times \frac{1 \text{ mol Si}}{28.09 \frac{\text{g Si}}{\text{g Si}}} = 0.0712 \text{ mol Si}$$

mol N₂ = 1.50 $\frac{\text{g N}_2}{\text{g N}_2} \times \frac{1 \text{ mol N}_2}{28.09 \frac{\text{g N}_2}{\text{g N}_2}} = 0.0535 \text{ mol N}_2$

The provided Si:N₂ molar ratio is:

$$\frac{0.0712 \text{ mol Si}}{0.0535 \text{ mol N}_2} = \frac{1.33 \text{ mol Si}}{1 \text{ mol N}_2}$$

The stoichiometric Si:N₂ ratio is:

 $\frac{3 \operatorname{mol} \operatorname{Si}}{2 \operatorname{mol} \operatorname{N}_2} = \frac{1.5 \operatorname{mol} \operatorname{Si}}{1 \operatorname{mol} \operatorname{N}_2}$

Comparing these ratios shows that Si is provided in a less-than-stoichiometric amount, and so is the limiting reactant.

Alternatively, compute the amount of product expected for complete reaction of each of the provided reactants. The 0.0712 moles of silicon would yield

mol Si₃ N₄ produced = 0.0712 mol Si $\times \frac{1 \text{ mol Si}_3 \text{ N}_4}{3 \text{ mol Si}} = 0.0237 \text{ mol Si}_3 \text{ N}_4$

while the 0.0535 moles of nitrogen would produce

mol Si₃ N₄ produced = 0.0535 mol N₂
$$\times \frac{1 \text{ mol Si}_3 \text{ N}_4}{2 \text{ mol N}_2} = 0.0268 \text{ mol Si}_3 \text{ N}_4$$

Since silicon yields the lesser amount of product, it is the limiting reactant.

Check Your Learning

Which is the limiting reactant when 5.00 g of H₂ and 10.0 g of O₂ react and form water?

Answer: O₂

Percent Yield

The amount of product that *may be* produced by a reaction under specified conditions, as calculated per the stoichiometry of an appropriate balanced chemical equation, is called the **theoretical yield** of the reaction. In practice, the amount of product obtained is called the **actual yield**, and it is often less than the theoretical yield for a number of reasons. Some reactions are inherently inefficient, being accompanied by *side reactions* that generate other products. Others are, by nature, incomplete (consider the partial reactions of weak acids and bases discussed earlier in this chapter). Some products are difficult to collect without some loss, and so less than perfect recovery will reduce the actual yield. The extent to which a reaction's theoretical yield is achieved is commonly expressed as its **percent yield**:

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

Actual and theoretical yields may be expressed as masses or molar amounts (or any other appropriate property; e.g., volume, if the product is a gas). As long as both yields are expressed using the same units, these units will cancel when percent yield is calculated.

Example 4.13

Calculation of Percent Yield

Upon reaction of 1.274 g of copper sulfate with excess zinc metal, 0.392 g copper metal was obtained according to the equation:

 $CuSO_4(aq) + Zn(s) \longrightarrow Cu(s) + ZnSO_4(aq)$

What is the percent yield?

Solution

The provided information identifies copper sulfate as the limiting reactant, and so the theoretical yield is found by the approach illustrated in the previous module, as shown here:

$$1.274 \frac{\text{gCuSO}_{4}}{\text{gCuSO}_{4}} \times \frac{1 \frac{\text{mol} \text{CuSO}_{4}}{159.62 \frac{\text{gCuSO}_{4}}{\text{gCuSO}_{4}}} \times \frac{1 \frac{\text{mol} \text{Cu}}{1 \frac{\text{mol} \text{CuSO}_{4}}} \times \frac{63.55 \text{ gCu}}{1 \frac{\text{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{\text{mol} \text{Cu}}{1 \frac{\text{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{\text{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1 \frac{mol} \text{Cu}}{1$$

Using this theoretical yield and the provided value for actual yield, the percent yield is calculated to be

percent yield =
$$\left(\frac{\text{actual yield}}{\text{theoretical yield}}\right) \times 100$$

percent yield = $\left(\frac{0.392 \text{ g Cu}}{0.5072 \text{ g Cu}}\right) \times 100$
= 77.3%

Check Your Learning

What is the percent yield of a reaction that produces 12.5 g of the Freon CF₂Cl₂ from 32.9 g of CCl₄ and excess HF?

$$CCl_4 + 2HF \longrightarrow CF_2Cl_2 + 2HCl_3$$

Answer: 48.3%

How Sciences Interconnect

Green Chemistry and Atom Economy

The purposeful design of chemical products and processes that minimize the use of environmentally hazardous substances and the generation of waste is known as *green chemistry*. Green chemistry is a philosophical approach that is being applied to many areas of science and technology, and its practice is summarized by guidelines known as the "Twelve Principles of Green Chemistry" (see details at this website (http://openstaxcollege.org/l/16greenchem)). One of the 12 principles is aimed specifically at maximizing the efficiency of processes for synthesizing chemical products. The *atom economy* of a process is a measure of this efficiency, defined as the percentage by mass of the final product of a synthesis relative to the masses of *all* the reactants used:

atom economy = $\frac{\text{mass of product}}{\text{mass of reactants}} \times 100\%$

Though the definition of atom economy at first glance appears very similar to that for percent yield, be aware that this property represents a difference in the *theoretical* efficiencies of *different* chemical processes. The percent yield of a given chemical process, on the other hand, evaluates the efficiency of a process by comparing the yield of product actually obtained to the maximum yield predicted by stoichiometry.

The synthesis of the common nonprescription pain medication, ibuprofen, nicely illustrates the success of a green chemistry approach (Figure 4.14). First marketed in the early 1960s, ibuprofen was produced using a six-step synthesis that required 514 g of reactants to generate each mole (206 g) of ibuprofen, an atom economy of 40%. In the 1990s, an alternative process was developed by the BHC Company (now BASF Corporation) that requires only three steps and has an atom economy of ~80%, nearly twice that of the original process. The BHC process generates significantly less chemical waste; uses less-hazardous and recyclable materials; and provides significant cost-savings to the manufacturer (and, subsequently, the consumer). In recognition of the positive environmental impact of the BHC process, the company received the Environmental Protection Agency's Greener Synthetic Pathways Award in 1997.



Figure 4.14 (a) Ibuprofen is a popular nonprescription pain medication commonly sold as 200 mg tablets. (b) The BHC process for synthesizing ibuprofen requires only three steps and exhibits an impressive atom economy. (credit a: modification of work by Derrick Coetzee)

4.4 Reaction Yields

60. The following quantities are placed in a container: 1.5×10^{24} atoms of hydrogen, 1.0 mol of sulfur, and 88.0 g of diatomic oxygen.

(a) What is the total mass in grams for the collection of all three elements?

(b) What is the total number of moles of atoms for the three elements?

(c) If the mixture of the three elements formed a compound with molecules that contain two hydrogen atoms, one sulfur atom, and four oxygen atoms, which substance is consumed first?

(d) How many atoms of each remaining element would remain unreacted in the change described in (c)?

61. What is the limiting reactant in a reaction that produces sodium chloride from 8 g of sodium and 8 g of diatomic chlorine?

62. Which of the postulates of Dalton's atomic theory explains why we can calculate a theoretical yield for a chemical reaction?

63. A student isolated 25 g of a compound following a procedure that would theoretically yield 81 g. What was his percent yield?

64. A sample of 0.53 g of carbon dioxide was obtained by heating 1.31 g of calcium carbonate. What is the percent yield for this reaction?

 $CaCO_3(s) \longrightarrow CaO(s) + CO_2(s)$

65. Freon-12, CCl₂F₂, is prepared from CCl₄ by reaction with HF. The other product of this reaction is HCl. Outline the steps needed to determine the percent yield of a reaction that produces 12.5 g of CCl₂F₂ from 32.9 g of CCl₄. Freon-12 has been banned and is no longer used as a refrigerant because it catalyzes the decomposition of ozone and has a very long lifetime in the atmosphere. Determine the percent yield.

66. Citric acid, C₆H₈O₇, a component of jams, jellies, and fruity soft drinks, is prepared industrially via fermentation of sucrose by the mold *Aspergillus niger*. The equation representing this reaction is $C_{12}H_{22}O_{11} + H_2O + 3O_2 \longrightarrow 2C_6H_8O_7 + 4H_2O$

What mass of citric acid is produced from exactly 1 metric ton (1.000 \times 10³ kg) of sucrose if the yield is 92.30%?

67. Toluene, C₆H₅CH₃, is oxidized by air under carefully controlled conditions to benzoic acid, C₆H₅CO₂H, which is used to prepare the food preservative sodium benzoate, C₆H₅CO₂Na. What is the percent yield of a reaction that converts 1.000 kg of toluene to 1.21 kg of benzoic acid?

 $2C_6H_5CH_3 + 3O_2 \longrightarrow 2C_6H_5CO_2H + 2H_2O$

68. In a laboratory experiment, the reaction of 3.0 mol of H_2 with 2.0 mol of I_2 produced 1.0 mol of HI. Determine the theoretical yield in grams and the percent yield for this reaction.

69. Outline the steps needed to solve the following problem, then do the calculations. Ether, (C₂H₅)₂O, which was originally used as an anesthetic but has been replaced by safer and more effective medications, is prepared by the reaction of ethanol with sulfuric acid.

$$2C_2H_5OH + H_2SO_4 \longrightarrow (C_2H_5)_2 + H_2SO_4 H_2O_2$$

What is the percent yield of ether if 1.17 L (d = 0.7134 g/mL) is isolated from the reaction of 1.500 L of C₂H₅OH (d = 0.7894 g/mL)?

70. Outline the steps needed to determine the limiting reactant when 30.0 g of propane, C₃H₈, is burned with 75.0 g of oxygen.

percent yield = $\frac{0.8347 \text{ g}}{0.9525 \text{ g}} \times 100\% = 87.6\%$

Determine the limiting reactant.

71. Outline the steps needed to determine the limiting reactant when 0.50 g of Cr and 0.75 g of H₃PO₄ react according to the following chemical equation? $2Cr + 2H_3PO_4 \longrightarrow 2CrPO_4 + 3H_2$

Determine the limiting reactant.

72. What is the limiting reactant when 1.50 g of lithium and 1.50 g of nitrogen combine to form lithium nitride, a component of advanced batteries, according to the following unbalanced equation? $\text{Li} + \text{N}_2 \longrightarrow \text{Li}_3 \text{N}$

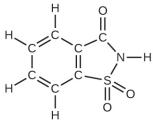
73. Uranium can be isolated from its ores by dissolving it as UO₂(NO₃)₂, then separating it as solid UO₂(C₂O₄)·3H₂O. Addition of 0.4031 g of sodium oxalate, Na₂C₂O₄, to a solution containing 1.481 g of uranyl nitrate, UO₂(NO₂)₂, yields 1.073 g of solid UO₂(C₂O₄)·3H₂O.

 $Na_2C_2O_4 + UO_2(NO_3)_2 + 3H_2O \longrightarrow UO_2(C_2O_4) \cdot 3H_2O + 2NaNO_3$

Determine the limiting reactant and the percent yield of this reaction.

74. How many molecules of C₂H₄Cl₂ can be prepared from 15 C₂H₄ molecules and 8 Cl₂ molecules?

75. How many molecules of the sweetener saccharin can be prepared from 30 C atoms, 25 H atoms, 12 O atoms, 8 S atoms, and 14 N atoms?



76. The phosphorus pentoxide used to produce phosphoric acid for cola soft drinks is prepared by burning phosphorus in oxygen.

(a) What is the limiting reactant when 0.200 mol of P4 and 0.200 mol of O2 react according to

$$P_4 + 5O_2 \longrightarrow P_4O_{10}$$

(b) Calculate the percent yield if $10.0 \text{ g of } P_4O_{10}$ is isolated from the reaction.

77. Would you agree to buy 1 trillion (1,000,000,000) gold atoms for \$5? Explain why or why not. Find the current price of gold at http://money.cnn.com/data/commodities/ (1 troy ounce = 31.1 g)