Chapter 7 – Quantitative Relationships in Chemical Reactions

As you have begun to see, chemistry is a quantitative science involving a great deal of calculations. However, the purpose of these calculations is not merely to get a number, but also to provide quantitative predictions or descriptions of how matter behaves. Correctly calculating the amount of product that is produced in a chemical reaction shows that we understand something about what is really going on in the reaction, and it allows us to use the reaction to produce a desired amount of product. Calculations are tools chemists use in understanding and using the behavior of matter.

One category of chemical calculations involves relationships between quantities of reactants and products based upon relationships given in the balanced equation for any reaction. This is why we learned how to balance chemical equations in Chapter 6 and kept it as part of our discussions of the types of reactions. Determination of quantities of reactants required for reaction, choosing the amount of reactant necessary to give a desired amount of product, calculation of the concentration of a solution (Chapter 12), determination of percent composition as a check for purity (Chapter 5), and identification of the empirical and molecular formula of an unknown product (Chapter 5) all fall into this category, which is generally called **chemical stoichiometry**.

Stoichiometry is a more formal term chemists use when they talk about the quantities involved in chemical reactions. It is also a term which is used to describe the *process* of using a chemical equation to calculate the relative masses of reactants and products involved in a reaction. Simply put, stoichiometry is the calculation of quantities in chemical equations/reactions.

Section 7-1 – Stoichiometry

1) Sec 7-1.1 – Overview of Stoichiometry
   a) The coefficients in a chemical equation carry a dual meaning: "number of formula units (particles) or molecules or atoms" at the microscopic level and "number of moles" at the macroscopic level. The coefficients of a balanced chemical equation give you the relative number of moles of reactants and products in the chemical reaction.

   b) REMEMBER: In a chemical reaction, only mass and atoms are conserved. Moles, molecules, formula units, and volumes are not generally conserved.

2) Sec 7-1.2 – The Mole Ratio (Mole-Mole Relationships)

   The relative numbers of moles of the various species participating in a reaction are provided by the chemical equation that describes the system.

   a) Consider the reaction: $2\ H_2 + O_2 \rightarrow 2\ H_2O$. This chemical equation tells us that 2 molecules of hydrogen (remember that hydrogen is diatomic!) react with 1 molecule of oxygen (ditto) to form 2 molecules of water. We can also now see that this same equation can tell us that 2 **moles** of hydrogen react with 1 **mole** of oxygen to produce 2 **moles** of water.

From this we can see several relationships:
i) 2 moles of hydrogen always produce 2 moles of water
ii) 1 mole of oxygen is needed to produce 2 moles of water
iii) 1 mole of oxygen needs 2 moles of hydrogen to react completely

b) How about the reaction: $2\ C_8H_{18} + 25\ O_2 \longrightarrow 16\ CO_2 + 18\ H_2O$?

or $N_2 + 3\ H_2 \longrightarrow 2\ NH_3$

3) <u>Sec 7-1.3 – Stoichiometry</u>

The most important aspect of stoichiometry is that by using the mole ratio, you can interconvert moles of any substance with any other substance within a reaction, given a *balanced* chemical equation. That is, if you have a balanced chemical equation and know one quantity you could calculate the amount of any reactant needed or the amount of each product you might produce, whether the reaction had a total of three reactants and products or thrity-three.

4) <u>Steps in Calculating Quantities in a Chemical Reaction (Doing a Stoichiometric Calculation)</u>

a) Write a balanced chemical equation describing the reaction that occurs.

b) Calculate the number of moles (n) of what is given.

1) Mass (convert to grams if necessary): $n = \frac{\text{mass (g)}}{\text{molar mass}}$

2) Volume of a Liquid (use density to get mass in grams): $n = \frac{\text{mass (g)}}{\text{molar mass}}$

3) Molecules: $n = \frac{\text{\# of molecules}}{6.02 \times 10^{23}\ \text{molecules/mol}}$

4) Volume of a Gas at STP (convert volume to liters if necessary): $n = \frac{\text{volume (L)}}{22.4\ \text{L/mol}}$

c) Use the reaction coefficients (a and b) and the moles of the given to calculate the moles of the unknown:

Multiply by the ratio: $\frac{\text{b (moles of unknown)}}{\text{a (moles of given)}}$

d) Convert the moles of the unknown into the desired quantity using the equations given in part b.

5) Mole-Mole and Mass-Mass Calculations – Examples
   a) How many moles of chlorine gas will be required to react with excess iron to produce 14 moles of iron(III) chloride?

   b) How many grams of hydrogen can be produced by the reaction of 5.585 g of iron reacting with excess hydrochloric acid?

   c) How many grams of aluminum must react with excess oxygen to produce 20.4 g of aluminum oxide?

6) Other Stoichiometric Calculations – Examples
   a) How many grams of glucose, $C_6H_{12}O_6$, must be burned to produce 5.6 L of CO_2 at STP?

   b) What volume of oxygen gas at STP is needed to burn 200 mL of butane, C_4H_{10}? (Butane is a liquid with a density of 0.60 g/mL.)

   c) One way to remove carbon dioxide from air in a spacecraft is to react it with LiOH. A person in one day exhales about 1.0 Kg of carbon dioxide. How many grams of LiOH are needed to remove the carbon dioxide from the air on a six-day lunar mission with three astronauts, and at the same time have 25% of the LiOH left after the mission?

7) Comparing Two Reactions – Mass and Mole Relationships in a Chemical Reaction

Have you ever listened to or read advertisements for different products, each of which says it is better in doing a certain task? Sometimes these ads can illustrate how chemical calculations can be important in everyday life. What are they talking about?

Consider two common compounds that are often used as antacids: baking soda, $NaHCO_3$ and milk of magnesia or magnesium hydroxide (in water), $Mg(OH)_2$. Both of these compounds will react with the excess hydrochloric acid which can be secreted by the stomach.

The reactions are:

a. $NaHCO_3 + HCl \rightarrow NaCl + H_2O + CO_2$

b. $Mg(OH)_2 + 2\ HCl \rightarrow MgCl_2 + H_2O$

A question we could ask is which antacid can consume the most stomach acid, 1.00 g $NaHCO_3$ or 1.00 g $Mg(OH)_2$?

Section 7-2 – Limiting Reactant

Up to this point with stoichiometry problems, we have assumed that for a given amount of one reactants the needed amounts of all other reactants are present or we have been told that a reactant or reactants is/are present in excess. The question is now how we determine the amount of product(s) produced when specific amounts of each reactant are given.

For other problems we could start with reactants or products as the given but with these limiting reactant problems we almost always start with amounts of reactants.

8) Sec 7-2.1 – The Definition of Limiting Reagent

a) Limiting Reagent limits or determines the amount of product that can be formed in a reaction.

b) Excess Reagent is present in an amount that is more than enough to react with all of the limiting reagent. Some of the excess reagent is left over.

Take one of our favorite reactions: $2\ H_2 + O_2 \rightarrow 2\ H_2O$.

The stoichiometry for this reaction tells us that 2 moles (4.04 g) of hydrogen react exactly with 1 mole (32.00 g) of oxygen to produce exactly 2 moles (36.04 g) of water. When hyrdogen and oxygen react in this 4:32 mass ratio (remember that we do not always have to have the moles represented by the balanced chemical equation) we know that all of the reactants are consumed and only product appears. *When reactants are combined in exactly the mass ratio determined by the balanced chemical equation, the reaction is said to be stoichiometric.*

But what happens if we mix 6.0 g of hydrogen with 32.0 g of oxygen, do we get 38.0 g of water? No, we still get only 36.0 g. The hydrogen is in excess but the stoichiometry tells us that only 4.0 g of hydrogen will react and 2.0 g will be left over. In this case, O_2 is the limiting reactant.

Likewise, if we mix 4.0 g hydrogen with 36.0 g oxygen we still only get 36.0 g water. All of the hydrogen is consumed and it limits the amount of water produced. Thus, H_2 is now the limiting reactant and O_2 is in excess.

9) <u>Solving Limiting Reactant Problems</u>

When we do limiting reactant problems we still have to do the type of stoichiometric calculations that we have already learned!

The difference is that we have to do **TWO** calculations, one for each reactant, and we need to make a decision as to which reactant is **limiting** and which is in **excess**.

However, we have a <u>*choice*</u> for the two calculations we do, and the decision point changes depending upon which method is used. We will use the same reaction to show both ways of doing the calculation.

Methanol (CH_3OH) is used as a fuel for racing cars. It burns in the engine according to the balanced equation:

$$2\ CH_3OH + 3\ O_2 \longrightarrow 2\ CO_2 + 4\ H_2O$$

If 40.0 g of methanol is burned with 46.0 g of O_2, which is the limiting reactant and what is the mass of CO_2 produced?

10) **<u>Calculation Option 1:</u>** (This is the more common approach.)

a. Convert the grams of methanol to grams of CO_2.

$$CH_3OH: \quad \frac{40.0\ g\ CH_3OH}{1} \times \frac{1\ mole\ CH_3OH}{32.04\ g\ CH_3OH} \times \frac{2\ mole\ CO_2}{2\ mole\ CH_3OH} \times \frac{44.01\ g\ CO_2}{1\ mole\ CO_2} = 54.9\ g\ CO_2$$

b. Convert the grams of O_2 to grams of CO_2.

$$O_2: \quad \frac{46.0\ g\ O_2}{1} \times \frac{1\ mole\ O_2}{32.00\ g\ O_2} \times \frac{2\ mole\ CO_2}{3\ mole\ O_2} \times \frac{44.01\ g\ CO_2}{1\ mole\ CO_2} = 42.2\ g\ CO_2$$

c. *Decision point:* The limiting reactant is the one that produces the smaller amount of material. The amount of product produced by the reaction is this amount.

Thus: O_2 is the limiting reactant because it produces the smaller amount and 42.2 g of CO_2 can be made in this reaction.

11) **<u>Calculation Option 2:</u>** (This one compares the two reactants.)

a. Pick one reactant and calculate how much of the other would be needed for complete reaction. ex. Convert the grams of methanol to grams of O_2.

$$CH_3OH:\ \frac{40.0\text{ g } CH_3OH}{1} \times \frac{1\text{ mole } CH_3OH}{32.04\text{ g } CH_3OH} \times \frac{3\text{ mole } O_2}{2\text{ mole } CH_3OH} \times \frac{32.00\text{ g } O_2}{1\text{ mole } O_2} = 59.9\text{ g } O_2$$

b. *Decision point:* If you **have** more of the second reactant than you need, the first reactant is the limiting reactant. If you **need** more of the second reactant than you have, then it is the limiting reactant.

The problem states that you have 46.0 g of O_2 and the calculation says that you need 59.9 g of O_2 to react with all of the methanol. Thus: you **do not have** all the oxygen you need to react with the methanol and oxygen is the limiting reactant.

[If you had started in "a." with oxygen and calculated the amount of methanol that would have reacted, you would determine that you had **more** methanol (40.0 g) than you needed (32.6 g) to react with the given amount of oxygen. This still indicates that oxygen is the limiting reactant. This might also help you to calculate how much excess methanol you had in the reaction (7.4 g).]

c. Take the limiting reactant and calculate how much of the product that will produce. For this problem: Convert the grams of O_2 to grams of CO_2 to determine the amount of CO_2 asked for.

$$O_2:\ \frac{46.0\text{ g } O_2}{1} \times \frac{1\text{ mole } O_2}{32.00\text{ g } O_2} \times \frac{2\text{ mole } CO_2}{3\text{ mole } O_2} \times \frac{44.01\text{ g } CO_2}{1\text{ mole } CO_2} = 42.2\text{ g } CO_2$$

12) <u>Summary of Calculation Options</u>

Both of these calculation options will give the correct answer. As you see, both require doing two calculations and making a decision. You choice is which calculations you do and where you have your decision point.

Both also have their uses.

a. The first is very straight-forward because you just calculate the desired product amount for both reactants.

b. The second allows you to determine the limiting reactant with only one calculation. And if that was the question ("which is the limiting reactant?") this would be an easier way to get to the answer. It also is a way to determine how much more of the limiting reactant you would need to react with all of the excess reactant, but, of course, not the only way.

You can go between the calculation options depending upon what question or questions are asked.

13) Example – How many grams of NO can be produced by the reaction of 6.35 g of copper with 18.9 g of nitric acid? What reagent is in excess, and what mass of the excess reagent will remain after the reaction?

$$3\ Cu + 8\ HNO_3 \dashrightarrow 3\ Cu(NO_3)_2 + 2\ NO + 4\ H_2O$$

14) Example – How many grams of water are needed to react with exactly 249 g of methane according to the balanced equation $CH_4 + H_2O \rightarrow 3H_2 + CO$? If the reaction produced 280.0 g CO, which reactant was limiting and which was excess?

15) Sec 7-3 – Percent Yield

a) Theoretical Yield – is the maximum amount of product that can be produced from the stated amount of reactants. It is a calculated number. Calculated from stoichiometry.

b) Actual Yield – is the amount of product obtained when the reaction is actually done in the laboratory. It is an experimentally measured value. It can never be greater than the theoretical yield. It is given or you measure it.

c) Percent Yield

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

Example – A mixture of 80g of chromium oxide and 8.0 g of carbon experimentally produces 21.7 g of chromium. What is the percent yield of the Cr? The chemical equation for this reaction is: $Cr_2O_3 + 3\ C \dashrightarrow 2\ Cr + 3\ CO$

Example – Before beginning a lab, a student read that the percent yield for a difficult reaction to be studied was likely to be only 40.0% of the theoretical yield. Her prelab stoichiometric calculations predict that the theoretical yield should be 12.5 g. What is her actual yield likely to be?

Example – Zinc and silver nitrate undergo a single replacement reaction according to the equation: $Zn + 2\ AgNO_3 \rightarrow Zn(NO_3)_2 + 2\ Ag$

When 25.0 g of zinc is added to a silver nitrate solution, the percent yield of silver is 72.3%. What mass of silver is formed?

Section 7-4 – Heat Energy in Chemical Reactions

Matter is not the only thing that is involved in chemical reactions. Energy is also an intimate part of chemical reactions.

16) Sec 7-4.1 – Thermochemical Equations

A balanced chemical equation that includes heat energy is referred to as a **thermochemical equation.**

Heat involved in a chemical reaction can be shown in two ways.

a. The heat is shown separately from the balanced equation using th symbol ***ΔH***. This is officially known as the *change in **enthalpy*** but is generally referred to as the heat of reaction. A negative sign for ***ΔH*** indicates an exothermic reaction, and a positive sign indicates an endothermic reaction.

   Written in his manner, the thermochemical equation for the combustion of two moles of hydrogen is

   $$2\ H_2 + O_2 \rightarrow 2\ H_2O \qquad \Delta H = -572\ kJ$$

   The enthalpy reported for a reaction is for the amount of moles of compounds represented by the balancing coefficients.

b. The second way shows the heat energy as if it were a reactant or a product. In exothermic reactions heat energy is a product, and in endothermic reactions heat energy is a reactant. A positive sign is used in either case.

   $$2\ H_2 + O_2 \rightarrow 2\ H_2O + 572\ kJ \qquad \text{(exothermic reaction)}$$
   $$N_2 + O_2 + 181\ kJ \rightarrow 2\ NO \qquad \text{(endothermic reaction)}$$

17) Sec 7-4.2 – Calculation of Heat Energy in a Reaction

The heat energy involved in a chemical reaction may be treated quantitatively in a manner similar to the amount of a reactant or product. The enthalpy of the reaction, with units of kJ/mole, is similar to molar mass and its units of g/mole.

Where molar mass allows us to convert between grams and moles, reaction enthalpies allow us to convert between energy and moles.

Consider the combustion of acetylene according to the thermochemical equation:

$$2\ C_2H_2 + 5\ O_2 \longrightarrow 4\ CO_2 + 2\ H_2O \qquad \Delta H = -2602\ \text{kJ}$$

If 550 kJ of heat is evolved in the combustion of a sample of C_2H_2, what is the mass of CO_2 formed?

$$\frac{550\ \text{kJ}}{1} \times \frac{4\ \text{mole}\ CO_2}{2602\ \text{kJ}} \times \frac{44.01\ \text{g}\ CO_2}{1\ \text{mole}\ CO_2} = 37.2\ \text{g}\ CO_2$$

What mass of acetylene was burned in the example?