Chapter 9 – Calculations from Chemical Equations

In this chapter, we explore the relationship between the numbers of atoms and molecules involved in chemical reactions and the amounts of the materials involved in the reaction in units that can be measured (e.g. mass and volume).

Consider the reaction of hydrogen with oxygen to form water:

$$2H_{2\,(g)} + O_{2\,(g)} \rightarrow 2\ H_2O_{(g)}$$

From what we covered in the balancing chemical equations chapter, you know this equation tells you that two molecules of hydrogen react with one molecule of oxygen to form two molecules of water.

From a practical perspective of doing the reaction, working with the reactant chemicals using the equation as written has a problem. Can you predict what it is?

Basically, counting molecules in a reaction vessel is normally impossible and even in the few cases where it can be done, the work involved is incredibly difficult. When chemists do reactions, they usually think in terms of the weight (solids) or volumes (liquids and gasses) of the reacting species because those are easy to measure. Counting out a mole of material (6.022×10^{23} items) isn't possible (but numbers can be estimated when it's useful to use them).

What is needed, then, is a method from going from the numbers of reacting particles to a method of measuring how much of the material is present and the process in reverse. We learn about this process in Chapter 9.

9.1 Introduction to Stoichiometry

Stoichiometry is the area of chemistry that addresses the quantity relationships between materials involved in chemical reactions. From earlier chapters, remember that: Molar mass (weight) is the sum of the masses of all of the component atoms in a compound. The mole is a collective counting term, similar to a dozen, but with a value of 6.022×10^{23} items. Balanced equations are chemical equations where the total number of each kind of atom is the same on each side of the reaction arrow.

Finally, your book discusses "mole ratios," which we did not cover earlier. These are simply a fraction composed of the number of moles of a reactant or product from a chemical equation divided by the number of moles of another material from that same reaction. This is a place where units are very important and a little challenging because the subscripts are very similar. We'll see this in an example in the next section.

9.2 Mole-Mole Calculations

Reactions typically occur between molecules or molecular ions (e.g. NO_3^-) when two of these species collide with one another. In the simplest reactions, two molecules collide in a single step. However, in nearly all reactions, there are a series of steps in which two molecules collide ultimately yielding products listed in the chemical equation in the relative numbers provided by the balancing coefficients. The mole-to-mole calculation describes this process mathematically.

Let's return to our hydrogen/oxygen/water example from a few paragraphs ago. In this reaction we consume hydrogen molecules at twice the rate as oxygen molecules. This can be expressed mathematically as

$$\frac{2\ \text{molecules}_{H2}}{1\ \text{molecules}_{O2}}$$

It would be read as 2 moles of molecular hydrogen **per** 1 mole of molecular oxygen. (Just like your car's speedometer records velocity in miles per hour ($\frac{\text{miles}}{\text{hour}}$)).

If one thinks on the macro scale, then two moles of hydrogen react with one mole of oxygen to produce two moles of water and the ratio changes to:

$$\frac{2\ \text{mol}_{H2}}{1\ \text{mol}_{O2}}$$

We use mole ratios like this to express mathematically relative amounts of materials in equations where the goal is to determine how much of a reactant is used or product made.

For example, how much water is produced in this reaction if 2.46 moles of hydrogen are reacted with excess oxygen?

$$\text{mol}_{H2O} = (2.46\ \text{mol}_{H2})\left(\frac{2\ \text{mol}_{H2O}}{2\ \text{mol}_{H2}}\right) = 2.46\ \text{mol}_{H2O}$$

It is important to note that the "2"s are not simplified to "1"s. That is, when writing the ratios, keep the stoichiometric coefficients, do not divide by a common denominator when setting up the equation. Similarly, how much oxygen is required to react with 2.46 moles of hydrogen gas?

$$mol_{O2} = (2.46\ mol_{H2})(\frac{1\ mol_{O2}}{2\ mol_{H2}}) = 1.23\ mol_{O2}$$

9.3 Mole-Mass Calculations

This is basically a review of section 7.1.

9.4 Mass-Mass Calculations

This type of calculation is very common in chemistry labs where materials are prepared. Here we move from what we can measure (mass) to what is counted (molecules) then do a mole-mole conversion and return to what we can measure. Returning to the water preparation equation, consider the following question: What mass of water is produced from reacting 1.00 g of hydrogen gas with excess oxygen gas?

$$mass_{H2O} = (1.00\ g_{H2})\left(\frac{1\ mol_{H2}}{2.016\ g_{H2}}\right)\left(\frac{2\ mol_{H2O}}{2\ mol_{H2}}\right)\left(\frac{18.02\ g}{1\ mol_{H2O}}\right) = 8.94\ g_{H2O}$$

9.5 Limiting Reactant and Yield Calculations

Limiting reactant is a concept that you have experience within day-to-day living. For example, if you buy a box of cereal and carton of milk, you don't expect to run out of cereal and milk at exactly the same time. The same is true of a loaf of bread and package of lunchmeat. In short, you expect to have leftovers of one or the other, right?

The same is true in chemical reactions. Under normal circumstances, when chemicals are mixed in a reaction at least some of one will be left over. Consider the reaction of hydrogen with oxygen that we have been using. If you were going to do the reaction, which would you want to use all of and which would be left over? If you were making gold(I) chloride (AuCl) by reacting gold and chlorine gas, which would you want to use all of and why?

In short, it is frequently the case that one of the reagents is relatively expensive or difficult to obtain and, in that case, the experimenter wants to avoid wasting it. A reagent that is completely consumed in a chemical reaction is called the limiting reagent because it limits the amount of product that can be made because once it's gone, the reaction stops.

You may have noticed that in examples in the notes, "excess" reagent appears occasionally. This is because when reactions are carried out, in nearly all cases all reagents but one appears in excess. Does this sound reasonable? If so, why?

Consider the hydrogen/oxygen/water reaction again. When hydrogen gas and oxygen gas burn to form water, the oxygen can come from the air, while the hydrogen comes from a tank, which has to be purchased. The oxygen in the air costs nothing, so there is a good reason to make sure all of the hydrogen is used, while having excess oxygen left over.

In some cases, like the previous example, which reagent is present in excess is obvious, but that isn't typically the case. There are two ways to use reaction stoichiometries to answer this question. The first does a better job of illustrating the rationale at the molecular level, the other is more time efficient, but is more applied.

Example: Reaction of tungsten with chlorine gas yields tungsten(VI) chloride. How much tungsten(VI) chloride is formed when 12.6 g of tungsten is treated with 13.6 g of chlorine gas?

<u>Method 1</u>: We begin by generating a balanced chemical equation.

$$W_{(s)} + 3\ Cl_{2\,(g)} \rightarrow WCl_{6\,(s)}$$

$$mol_W = 12.6\ g_W\left(\frac{1\ mol_W}{183.9\ g_W}\right) = 0.0685\ mol_W$$

$$mol_{Cl2} = 13.6\ g_{Cl2}\left(\frac{1\ mol_{Cl2}}{70.90\ g_{Cl2}}\right) = 0.192\ mol_{Cl2}$$

Now calculate how much chlorine is needed to completely react with tungsten

$(0.0685\ mol_W)\left(\frac{3\ mol_{Cl2}}{1\ mol_W}\right) = 0.206\ mol_{Cl2}$ but you only have 0.192 mol of chlorine, so it is the limiting reagent.

$$mass_{WCl6} = 13.6\ g_{Cl2}\left(\frac{1\ mol_{Cl2}}{70.90\ g_{Cl2}}\right)\left(\frac{1\ mol_{WCl6}}{3\ mol_{Cl2}}\right)\left(\frac{396.6\ g_{WCl6}}{mol_{WCl6}}\right) = 25.4\ g_{WCl6}$$

<u>Method 2</u>: Here the theoretical yields for each reagent are calculated with the smallest one indicating the limiting reagent.

$$mass_{WCl6} = 12.6\ g_W\left(\frac{1\ mol_W}{183.9\ g_W}\right)\left(\frac{1\ mol_{WCl6}}{1\ mol_W}\right)\left(\frac{396.6\ g_{WCl6}}{mol_{WCl6}}\right) = 27.2\ g_{WCl6}$$

$$mass_{WCl6} = 13.6\ g_{Cl2}\left(\frac{1\ mol_{Cl2}}{70.90\ g_{Cl2}}\right)\left(\frac{1\ mol_{WCl6}}{3\ mol_{Cl2}}\right)\left(\frac{396.6\ g_{WCl6}}{mol_{WCl6}}\right) = 25.4\ g_{WCl6}$$

Since using up all of the tungsten metal yields less product than using up all of the chlorine gas, tungsten metal is the limiting reagent.

Finally, reactions rarely produce as much product as the previous calculations predict. There are many reasons why reactions don't produce 100% of the expected amount. Three common examples include:

1) Not waiting until the reaction completes. For reactions which proceed slowly, this happens commonly. Imagine a reaction that takes two weeks to complete. Shutting it down early and collecting the product produced to that point is common.
2) Many, probably most, reactions yield secondary products. For example, when carbon compounds like methane (CH_4) burn, the expected carbon product is CO_2. If oxygen is not present in plentiful amounts, however, burning can be incomplete with some CO produced instead. This lowers the yield of carbon dioxide.
3) Impure reactants. Most commercial chemicals are 99+% pure, but not all of them. Obviously, impurities won't react to give the desired products.

The amount of product obtained as compared to the amount expected is quantified as the percent yield of a reaction and is given by the equation:

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

Where actual yield is the amount actually obtained when doing the reaction and theoretical yield is the amount calculated from the reaction stoichiometry. Interestingly, percent yields are actually quite consistent across experimenters. That is to say, two different people running a synthetic reaction typically get very similar yields, which suggests that factors reducing product yield below 100% are inherent to each reaction.

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