Introduction

We have assumed that any chemical reaction we start will go to **completion** - that is, all reactants will be converted to product up to the moment the limiting reagent runs out. In reality, this is not always the case.

Actual vs. theoretical yield

Sometimes, reactions don't always produce as much product as we think they will. There are several reasons for this:

1. Errors in transferring reagents to reaction vessels (we dropped some!)
2. The reaction is slow and we don't have enough time to wait for complete reaction
3. The chemicals react to form more than one thing. There is a main reaction which produces our desired product, and a **side reaction** that produces an unwanted by-product.
4. The reaction may precede to an **equilibrium state**, where a stable mixture containing a significant amount of the original reactants as well as products is formed.

Here is an example of a side reaction that could occur in the combustion of methane (CH_4). The side reaction would affect the amount of CO_2 formed.

Example reaction: $CH_4 + 2O_2 \text{-->} CO_2 + 2\ H_2O$ (Carbon **dioxide** production)
Side reaction: $2\ CH_4 + 3\ O_2 \text{-->} 2\ CO + 4\ H_2O$ (Carbon **monoxide** production)

The formation of carbon monoxide is favored when there is little oxygen in the environment. Burning methane in an enclosed space would lead to the production of more carbon monoxide and less carbon dioxide.

We will discuss equilibrium states in the second general chemistry course.

After we perform a chemical reaction, we're often interested in how well the amount we produced (the **actual yield**) compares with the amount we would have produced under ideal conditions (the **theoretical yield**). What's the best way to describe this to someone else?

The percentage yield

A standard way that chemists would describe how well their reaction went (in other words, how much product they produced compared to the amount they "should" have produced) is the **percentage yield**. (**Percent yield** and **percentage yield** are the same thing.)

This percentage yield is very simple to calculate. The formula is below.

$$\text{Percentage yield} = 100\% \times \frac{\textbf{Actual yield in mass units}}{\textbf{Theoretical yield in mass units}}$$

So, if the actual yield of a chemical reaction was 5.956g and the theoretical yield was 6.000g, then the percentage yield would be:

$$\text{Percentage yield} = 100\% \times \frac{5.956\text{ g}}{6.000\text{ g}} = \mathbf{99.27\%} \quad \text{(which is pretty good)}$$

Problems involving percentage yield

We've established that percentage yield isn't difficult to calculate. But how would you normally see it in an actual problem? When you do a regular stoichiometry problem, you're calculating the amount of a substance that would be produced or consumed under **ideal conditions**. If you calculate the amount of product produced using a stoichiometry calculation, you're calculating the **theoretical yield** of product.

Of course, due to Murphy's Law you won't produce exactly this amount of product. You'll have a different **actual yield** when you actually **do** the reaction. You would calculate a percent yield after doing an experiment where you have previously calculated a theoretical yield. Here is an example.

Wintergreen ($C_8H_8O_3$, FW = 152.145 g/mol) is prepared by heating salicylic acid ($C_7H_6O_3$, FW = 138.120 g/mol) with methanol (CH_3OH, FW = 32.042 g/mol). If 1.50 g salicylic acid is reacted with methanol, 1.31 g of wintergreen is produced. What is the percentage yield of wintergreen? The chemical reaction is:

$$C_7H_6O_3 + CH_3OH \rightarrow C_8H_8O_3 + H_2O$$

The first thing to do is to examine the problem and see what type it is. You're given the amount of a reagent (the 1.50 g salicylic acid) and the amount of a product produced (the 1.31 g wintergreen). It's **not** a limiting reagent problem, as you're **not given the amounts of two or more reactants**. So, it's just a stoichiometry problem with a percentage yield calculation tacked on the end.

Why is it a regular stoichiometry problem? Because to calculate the percentage yield we first need to calculate the **theoretical yield**! The theoretical yield in this problem is the amount of wintergreen produced if all 1.50 grams of salicylic acid reacts to form wintergreen. So now we solve a simple stoichiometry problem.

First, convert the amount of salicylic acid to moles using **formula weight**:

$$1.50\,\text{g}\,C_7H_6O_3 \times \frac{1\,\text{mol}\,C_7H_6O_3}{138.12\,\text{g}\,C_7H_6O_3} = 0.01086\,\text{mol}\,C_7H_6O_3$$

The ratio of wintergreen to salicylic acid is **1:1** In other words, 1 mol salicylic acid reacts to give 1 mole of wintergreen.

$$0.01086\ \text{mol}\ C_7H_6O_3 \times \frac{1\ \text{mol}\ C_8H_8O_3}{1\ \text{mol}\ C_7H_6O_3} = 0.01086\ \text{mol}\ C_8H_8O_3$$

Now that we have moles of wintergreen, simply convert to mass using the formula weight.

$$0.01086\ \text{mol}\ C_8H_8O_3 \times \frac{152.15\ \text{g}\ C_8H_8O_3}{1\ \text{mol}\ C_8H_8O_3} = 1.65\ \text{g}\ C_8H_8O_3$$

1.65 g is our **theoretical yield** of wintergreen. To finish the problem (and answer the question asked), we need to calculate the percentage yield. Since we actually produced only 1.31 grams of wintergreen,

$$\text{Percentage yield} = 100\% \times \frac{1.31\ \text{g}}{1.65\ \text{g}} = \mathbf{79.4\%\ yield\ of\ wintergreen}$$

(This yield is typical of many synthetic organic reactions where side reactions occur.)

To sum up, you'd deal with a percentage yield problem by first solving a regular stoichiometry problem to find the **theoretical yield**, then use the actual yield (which is given in the problem statement, or that you find experimentally in the lab) to find the percentage yield.

You'll be given an opportunity to work with wintergreen and calculate percentage yields of your own chemical reaction in the lab. You will use wintergreen as a starting material, and you'll prepare salicylic acid from it. In other words, you'll do this example backwards. Salicylic acid is the active ingredient in the commercial product *Compound W*, so this lab will involve the preparation of wart remover. Sometimes this experiment is part of the first semester course, and sometimes it is part of the second semester course.

Summary

In this note pack, we discussed the fact that in most chemical reactions we usually don't produce all of the product we could theoretically produce. Instead, we get an actual yield of product that is less than the amount a simple stoichiometric calculation says we could get. When we describe our results to others, we calculate a percentage yield, expressing what we actually got as a percentage of what we could theoretically have gotten if everything went perfectly. You should now know how to calculate this percentage yield.