Theoretical Yield and Percent Yield

key concepts:

- **Theoretical yield** is the maximum amount of **product** that can be made from a given amount of **reactants**.
- **Percent yield** is the **actual yield** expressed as a percentage of the theoretical yield.

How many grams of ethyl acetate should we expect from the reaction of 20.0 grams of ethanol and 60.0 grams of acetic anhydride?

ethanol		acetic anhydride		ethyl acetate		acetic acid
CH_3CH_2OH	+	$(CH_3CO)_2O$	→	$CH_3CH_2OC(O)CH_3$	+	CH_3COOH
0.435 mol		0.588 mol		0.435 mol		

Convert the theoretical yield from moles to grams.

$$\frac{0.435 \text{ mol ethyl acetate}}{} \times \frac{88.0 \text{ g ethyl acetate}}{1 \text{ mol ethyl acetate}} = 38.3 \text{ g ethyl acetate}$$

Theoretical yield is the maximum amount of product that can be made from a given amount of reactants.

To calculate theoretical yield, first determine the **limiting reactant**. Convert the **masses** of the reactants into **moles**. Use the amount of each reactant and the coefficients from the balanced **chemical equation** to determine the limiting reactant. In this example, because the reactants are in a 1:1 ratio, the limiting reactant is ethanol (0.435 moles).

Finally, calculate the theoretical yield of ethyl acetate by determining the moles produced (using the molar ratio with ethanol, a simple 1:1 in this case). Convert the moles of ethyl acetate to grams using the **molar mass**, as shown, to obtain the theoretical yield of ethyl acetate in grams (38.3 g).

20.0 grams of ethanol reacted with 60.0 grams of acetic anhydride and produced 34.2 grams of ethyl acetate. What is the percent yield?

$$\text{percent yield} = \frac{34.2 \text{ g ethyl acetate}}{38.3 \text{ g ethyl acetate}} \cdot 100\% = 89.3\%$$

Often, chemical reactions do not produce their maximum yield. The amount of product produced in an experiment is the actual yield.

Percent yield is the actual yield expressed as a percentage of the theoretical yield. Divide the actual yield by the theoretical yield and multiply by 100 to obtain the percent yield.

The value of the actual yield is always less than the value of the theoretical yield and thus the percent yield is always less than 100 %.

However, good chemists get higher percent yields.

Problem Using Combined Concepts of Stoichiometry

key concepts:

- Several tools can be brought together to solve a **stoichiometry** problem.

$$\_\,Al(s) + \_\,NaOH(s) + \_\,H_2O(l) \rightarrow \_\,NaAl(OH)_4(aq) + \_\,H_2(g)$$

$$1\,Al(s) + 1\,NaOH(s) + 3\,H_2O(l) \rightarrow 1\,NaAl(OH)_4(aq) + \tfrac{3}{2}H_2(g)$$

$$2\cdot(1\,Al(s) + 1\,NaOH(s) + 3\,H_2O(l) \rightarrow 1\,NaAl(OH)_4(aq) + \tfrac{3}{2}H_2(g))$$

Steps for calculating the percent yield of hydrogen gas

1. Balance the reaction.
2. Do mass-mass conversions for the reagents.
3. Determine the limiting reagent.
4. Find the theoretical yield.
5. Calculate the percent yield.

Problem: 7.75 g of aluminum, 8.00 g of sodium hydroxide, and 100 g of water were reacted. 0.541 g of hydrogen **gas** was collected. What was the **percent yield**?

First, the **chemical equation** must be balanced. In the balanced chemical equation, 2 **mol** Al react with 2 mol NaOH and 6 mol H_2O to produce 2 mol $NaAl(OH)_4$ and 3 mol H_2.

$$\text{moles of Al} = \frac{7.75\text{ g Al}}{} \left| \frac{1\text{ mol Al}}{27.0\text{ g Al}} \right. = 0.287\text{ mol Al}$$

$$\text{moles of NaOH} = \frac{8.00\text{ g NaOH}}{} \left| \frac{1\text{ mol NaOH}}{40.0\text{ g NaOH}} \right. = 0.200\text{ mol NaOH}$$

$$\text{moles of } H_2O = \frac{100\text{ g } H_2O}{} \left| \frac{1\text{ mol } H_2O}{18.0\text{ g } H_2O} \right. = 5.56\text{ mol } H_2O$$

Steps for calculating the percent yield of hydrogen gas

1. Balance the reaction.
2. Do mass-mass conversions for the reagents.
3. Determine the limiting reagent.
4. Find the theoretical yield.
5. Calculate the percent yield.

Second, the **masses** of **reagents** given must be converted to moles. The **molar mass** of each **reactant** is multiplied by the mass of each reactant to give moles.

For example, 7.75 g Al is equivalent to 0.287 mol Al.

$$\text{moles of } H_2 \;\; \frac{0.287\text{ mol Al}}{} \left| \frac{3\text{ mol } H_2}{2\text{ mol Al}} \right. = 0.430\text{ mol } H_2$$

$$\text{moles of } H_2 \;\; \frac{0.200\text{ mol NaOH}}{} \left| \frac{3\text{ mol } H_2}{2\text{ mol NaOH}} \right. = 0.300\text{ mol } H_2$$

NaOH is the limiting reagent.

This is the theoretical yield of H_2.

$$\text{moles of } H_2 \;\; \frac{5.56\text{ mol } H_2O}{} \left| \frac{3\text{ mol } H_2}{6\text{ mol } H_2O} \right. = 2.78\text{ mol } H_2$$

Steps for calculating the percent yield of hydrogen gas

1. Balance the reaction.
2. Do mass-mass conversions for the reagents.
3. Determine the limiting reagent.
4. Find the theoretical yield.
5. Calculate the percent yield.

Next, the **limiting reagent** must be determined.

To determine the limiting reagent, calculate how much hydrogen gas could be produced from each reactant. The reactant that results in the lowest number of moles of hydrogen gas is the limiting reagent. In this problem, NaOH is the limiting reagent.

Next, the **theoretical yield** must be determined. Using the reactants given, 0.300 mol H_2 can be produced. This is the theoretical yield of hydrogen gas.

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

$$= \frac{0.268\text{ mol } H_2}{0.300\text{ mol } H_2} \cdot 100\% = 89.3\%$$

Steps for calculating the percent yield of hydrogen gas

1. Balance the reaction.
2. Do mass-mass conversions for the reagents.
3. Determine the limiting reagent.
4. Find the theoretical yield.
5. Calculate the percent yield.

Finally, the percent yield must be calculated. The percent yield is the **actual yield** divided by the theoretical yield and multiplied by 100%. In this problem, the actual yield is 0.541 g H_2 • 1 mol H_2 / 2.0158 g H_2 = 0.268 mol H_2. The percent yield is 89.3%. This percent yield means that 89.3% of the hydrogen gas that could have been produced was collected.