Chemical Equations and Stoichiometry

❖The word "stoichiometry" comes from the Greek stoikheion "element" and metriā "measure."

❖The term stoichiometry means, literally, to measure the elements but from a practical standpoint, it includes all the quantitative relationships involving atomic and formula masses, chemical formulas, and chemical equations.

❖Stoichiometry calculations are about calculating the amounts of substances that react and form in a chemical reaction.

❖Based on the balanced chemical equation, we can calculate the amount of a product substance that will form if we begin with a specific amount of one or more reactants.

❖Or, you may have a target amount of product to prepare. How much starting compounds are needed to prepare this amount? These are practical calculations that are done frequently by chemists.

❖The coefficients in the chemical equation

$$2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l)$$

mean that

$$2x \text{ molecules } H_2 + x \text{ molecules } O_2 \rightarrow 2x \text{ molecules } H_2O$$

❖ Suppose we let x=6.02214 x 10^{23}(Avogadro's number). Then x molecules represents 1 mole.

❖ Thus the chemical equation also means that

$$2\text{mol } H_2 + 1\text{mol } O_2 \rightarrow 2\text{mol } H_2O$$

❖ The coefficients in the chemical equation allow us to make statements such as

❖ Two moles of H_2O are produced for every two moles of consumed.
❖ Two moles of H_2O are produced for every one mole of consumed.
❖ Two moles of H_2 are consumed for every one mole of consumed.

❖For practically all stoichiometry calculations can be solved using a four-step approach.

❖Step 1: **Write the balanced chemical equation for the reaction.**

❖Step 2: **Calculate the moles of "given" substance.** If more than one reactant amount is given, calculate the moles of each to determine which is the limiting reactant.

❖Step 3: **Calculate the moles of "desired" substance from your answer in Step 2 using the coefficients from the balanced chemical equation.** If more than one reactant was given originally, you can calculate the moles of product twice, based on the moles of each reactant. The reactant that gives the smaller moles of product is the limiting reactant.

❖Step 4: **Convert your answer in Step 3 to the units the problem asks for.** Usually this is grams, but it could be volume (for gases or liquid solutions) or concentration (such as molarity, for solutions).

❖EXAMPLE 1. How many grams of iron(III) oxide (ferric oxide), Fe_2O_3, are formed from the reaction of 5.00 g of iron metal with excess oxygen gas?

❖Step 1: Balanced reaction.

$$4\ Fe\ (s) + 3\ O_2\ (g) \rightarrow 2\ Fe_2O_3\ (s)$$

❖ Step 2: Moles of "given" substance. For this reaction Iron is the '1 "given" substance . 1 mol of Fe is equals to 55.847 grams, therefore 5 g of Fe equals to 0.08953353 mol (do not round the numbers yet).

55.847 g — 1 mol Fe
5 g Fe — x mol Fe

X= 0.08953353 mol

❖ Step 3: Moles of "desired" substance. This is the product, ferric oxide. 4 moles of Fe, produce 2 moles of ferric oxide, therefore 0,08953353 mol Fe produce 0.044766765 mol Fe_2O_3.

4 moles Fe — 2 moles Fe_2O_3
0.08953353 mol Fe — x moles Fe_2O_3
X= 0.044766765 mol Fe_2O_3

- Step 4: Convert your answer in Step 3 to the units the problem asks for, which is grams of Fe2O3. 0.044766765 mol Fe_2O_3 equals to 7.15 g.

1 mol Fe_2O_3 — 159.6882 g
0.044766765 mol Fe_2O_3 — x mol Fe
X= 7.148724123 mol Fe_2O_3

- At last, round your answer to significant number which is 7.15 g.
- When working stoichiometry problems, always do the following:
- a) Write the units on all numbers. b) Check that the units cancel properly. c) Give the correct unit for the answer. d) Avoid rounding numbers too much during the calculation, or you will have roundoff error in your answer. e) Round your final answer to the correct number of significant figures.

- EXAMPLE 2. How many grams of carbon dioxide are produced in the combustion of 2.72 mol of triethylene glycol, with an excess oxygen gas?

- Step 1: Balanced reaction.

$$2\ C_6H_{14}O_4 + 15\ O_2 \rightarrow 12\ CO_2 + 14\ H_2O$$

- Step 2: Moles of "given" substance. It is given as 2.72 mol.
- Step 3: Moles of desired substance, CO_2

2 moles of $C_6H_{14}O_4$ — produce 12 moles of CO_2
2.72 moles of $C_6H_{14}O_4$ — produce x moles of CO_2
X= 16.32 mol CO_2

- Step 4: Convert your answer in Step 3 to the units the problem asks for, which is grams of CO_2
- If 1 mol of CO_2 equals to 44.01 g 16.32 mol of CO_2 equals to 718.24 g.

- EXAMPLE 3. If 10.0 g of iron metal is reacted with 15.0 g of Cl2 gas, how many grams of ferric chloride, FeCl3, will form?
- In this problem, the amounts of both reactants are given, so we will have to determine which reactant is the limiting reactant (the one that "limits" the amount of product that is formed). The other reactant is in excess amount.
- The reactant that is completely consumed the limiting reactant determines the quantities of products formed.
- We'll use the Fab Four Steps just as before.
- Step 1: Balanced reaction.

$$2\ Fe\ (s) + 3\ Cl_2\ (g) \rightarrow 2\ FeCl_3\ (s)$$

- Step 2: Moles of given substances.

moles of Fe = 10.0 g / 55.845 g/mol = 0.17906706 mol
moles of Cl_2 = 15.0 g / 70.906 g/mol = 0.211547682 mol

- Step 3: Moles of desired substance, $FeCl_3$.

Since we have two given amounts, a straightforward approach to this step is to calculate the moles of $FeCl_3$ twice, first based on the moles of Fe and second based on the moles of Cl_2.

- Keep the smaller answer. The reactant that gives this smaller answer is the limiting reactant. The other reactant is in excess amount.
- From the equation 2 moles of Fe produce 2 moles of $FeCl_3$ therefore 0.17906706 mol Fe produce (same amount of) 0.17906706 mol $FeCl_3$
- From the equation 3 moles of Cl_2 produce 2 moles of $FeCl_3$ therefore 0.211547682 mol Cl_2 produce 0.141031788 mol $FeCl_3$
- Since the moles of $FeCl_3$ based on moles of Cl_2 is the smaller answer, Cl_2 is the limiting reactant.
- Iron metal is therefore in excess amount, so there will be some Fe left over as unreacted excess.

❖Note that we might have reasonably assumed that iron metal was the limiting reactant since it was present in lesser amount in grams initially (10.0 g of Fe and 15.0 g of Cl_2).

❖But it turned out that Cl_2 was the limiting reactant.

❖The molar masses of the substances and the reaction stoichiometry come into play also, so we can't automatically assume which substance is the limiting reactant until we go through the steps as we did above.

❖Step 4: Finally! Convert moles of $FeCl_3$ to grams.

1 mol of Fe $FeCl_3$ is 162.204 g

0.141031788 mol of Fe $FeCl_3$ is x g

X=22.87592014 g rounded to significant number 22.9 g

Practice Makes Perfect

❖There are few additional factors in reaction stoichiometry that we need to consider both in the laboratory and in the manufacturing plant.

❖First, the calculated outcome of a reaction may not be what is actually observed. Specifically, the amount of product may be, unavoidably, less than expected.

❖Second, the route to producing a desired chemical may require several reactions carried out in sequence.

❖And third, in some cases two or more reactions may occur simultaneously.

❖The **theoretical yield** of a reaction is the calculated quantity of product expected from given quantities of reactants. The quantity of product that is actually produced is called the **actual yield**. The **percent yield** is defined as

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

❖In many reactions the actual yield almost exactly equals the theoretical yield, and the reactions are said to be quantitative. Such reactions can be used in quantitative chemical analyses.

❖In other reactions the actual yield is less than the theoretical yield, and the percent yield is less than 100%.

❖The reduced yield may occur for a variety of reasons.

❖(1) The product of a reaction rarely appears in a pure form, and some product may be lost during the necessary purification steps, which reduces the yield.

❖(2) In many cases the reactants may participate in reactions other than the one of central interest. These are called side reactions, and the unintended products are called by-products. To the extent that side reactions occur, the yield of the main product is reduced.

❖(3) If a reverse reaction occurs, some of the expected product may react to re-form the reactants, and again the yield is less than expected.

❖At times, the apparent yield is greater than 100%. Because we cannot get something from nothing, this situation usually indicates an error in technique.

❖Some products are formed as a precipitate from a solvent. If the product is weighed when it is wet with solvent, the result will be a larger-than-expected mass. More thorough drying of the product would give a more accurate yield determination. Another possibility is that the product is contaminated with an excess reactant or a by-product. This makes the mass of product appear larger than expected. In any case, a product must be purified before its yield is determined.

❖EXAMPLE 4. What is the percent yield if the reaction of 25.0g P_4 and 91.5 g Cl_2 produces 104 g PCl_3?

❖Step 1: Balanced reaction

$P_4(s) + 6\ Cl_2(g) \rightarrow 4\ PCl_3(l)$

❖Step 2: Moles of given substances.

❖For P_4 25.0g / 123.89 g/ mol = 0.201791912 mol P_4

❖For Cl_2 91.5g/ 70.9 g/ mol = 1.290550071 mol Cl_2

❖Step 3: Moles of desired substance, PCl_3

❖From the equation 1 mol of P_4 produce 4 moles of PCl_3 therefore 0.201791912 mol P_4 produce 0.807167648 mol PCl_3 **(since its smaller, keep this answer)**

From the equation 6 moles of Cl_2 produce 4 moles of PCl_3 therefore 1.290550071 mol Cl_2 produce 0.860366714 mol PCl_3

❖Since the moles of PCl_3 based on moles of P_4 is the smaller answer, P_4 is the limiting reactant. Cl_2 is therefore in excess amount, so there will be some Cl_2 left over as unreacted excess.

❖Step 4: Convert moles of PCl_3 to grams.

Grams of PCl3 = 0.807167648 mol x 137.33 g/mol = 110.848333 g

This is our **theoretical yield!**

Actual yield is given in the problem and it is 104 g. Thus percent yield in this reaction is:

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

percent yield = 104/110.848333 x 100 = %93.821889 rounded to %94.

❖Both in laboratory work and in manufacturing, the preferred processes are those that yield a product through a single reaction.

❖Often such processes give a higher yield because there is no need to remove products from one reaction mixture for further processing in subsequent reactions.

❖However, in many cases a multistep process is unavoidable.

❖**Consecutive reactions** are reactions carried out one after another in sequence to yield a final product.

❖In **simultaneous reactions**, two or more substances react independently of one another in separate reactions occurring at the same time.

❖Often, we can combine a series of chemical equations for consecutive reactions to obtain a single equation to represent the overall reaction.

❖The equation for this overall reaction is the overall equation. At times we can use the overall equation for solving problems instead of working with the individual equations.

❖This strategy does not work, however, if the substance of interest is not a starting material or final product but appears only in one of the intermediate reactions.

❖Any substance that is produced in one step and consumed in another step of a multistep process is called an **intermediate**.

❖As an example production of titanium dioxide could be given.

❖Titanium dioxide, is the most widely used white pigment for paints, having displaced most lead-based pigments, which are environmental hazards.

❖Before it can be used, however, naturally occurring TiO_2 must be freed of colored impurities.

❖One process for doing this converts impure $TiO_2(s)$ to $TiCl_4$ (g) which is then converted back to pure TiO_2 (s) The process is based on the following reactions, the first of which generate $TiCl_4$.

$$2\,TiO_2\,(impure) + 3\,C(s) + 4\,Cl_2(g) \longrightarrow 2\,TiCl_4(g) + CO_2(g) + 2\,CO(g)$$
$$TiCl_4(g) + O_2(g) \longrightarrow TiO_2(s) + 2\,Cl_2(g)$$

❖To write an overall equation for , multiply the coefficients in the second equation by the factor 2, add the second equation to the first, and cancel any substances that appear on both sides of the overall equation.

$$2\,\cancel{TiO_2}\,(impure) + 3\,C(s) + 4\,\cancel{Cl_2}(g) \longrightarrow 2\,\cancel{TiCl_4}(g) + CO_2(g) + 2\,CO(g)$$
$$2\,\cancel{TiCl_4}(g) + 2\,O_2(g) \longrightarrow 2\,\cancel{TiO_2}(s) + 4\,\cancel{Cl_2}(g)$$
$$\textit{Overall equation:}\quad 3\,C(s) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,CO(g)$$

❖The result suggests that (1) we should obtain as much TiO_2 in the second reaction as we started with in the first, (2) the $Cl_2(g)$ produced in the second reaction can be recycled back into the first reaction, and (3) the only substances actually consumed in the overall reaction are C(s) and O_2 (g).

❖In the general chemistry laboratory we will investigate stoichiometry the synthesis of metallic copper.

❖Safety Note: Hydrochloric acid is a strong acid that is harmful to the skin and especially to your eyes.

❖Wear your safety glasses or goggles during the entire procedure.

❖The reaction also produces flammable hydrogen gas (H2), so reaction should be carried out under the hood and Bunsen burners should not be used while the reaction is in progress.

❖Procedure

❖1) Weigh a clean, dry 150 mL beaker and record its weight on the report form.

❖2) Carefully add copper(II) sulfate pentahydrate, CuSO4 • 5 H2O, until 2.00 g have been added.

❖Note: A hydrate is a solid compound that contains “trapped” water molecules in the solid. In copper(II) sulfate pentahydrate, one mole of the solid CuSO4 has 5 moles of water molecules trapped in it. The water molecules are included in the molar mass of CuSO4 • 5 H2O, which is 249.69 g/mol.

❖3) Measure 10 mL of deionized water in a small graduated cylinder and add the water to the beaker to dissolve the copper(II) sulfate pentahydrate with the aid of a glass stirring rod. Record the color of the solution on the report sheet.

❖4) Measure 2.0 mL of 6 M HCl in your graduated cylinder, add it to the solution, and mix well.

❖Note: Chloride ion facilitates the reaction of Al with CuSO4 • 5 H2O. A convenient source of chloride ion is from hydrochloric acid, and in addition, the hydrochloric acid will react with any excess aluminum, allowing it to be separated from the solid copper product.

❖The relevant reactions are, a) The reaction of aluminum with copper(II) sulfate in aqueous solution. This reaction ordinarily occurs rather slowly, but when chloride ion is present, the reaction rate increases dramatically.

$$2\,Al\,(s) + 3\,CuSO_4\,(aq) \longrightarrow 3\,Cu\,(s) + Al_2(SO_4)_3\,(aq)$$

❖b) The competing reaction of aluminum with hydrochloric acid. This reaction still occurs more slowly than the above chloride-aided reaction with the reactant concentrations that are used. This reaction thus has a minimal effect on the percent yield, so the maximum amount of copper should be able to form if excess aluminum is used.

$$2\,Al\,(s) + 6\,HCl\,(aq) \longrightarrow 3\,H_2\,(g) + 2\,AlCl_3\,(aq)$$

❖Both of these reactions are single replacement reactions. Al is a more active element than Cu in the first reaction, and in the second reaction, Al is more active than the element H2.

❖(the activity series: Li > K > Ba > Sr > Ca > Na > Mg > Al > Mn > Zn > Fe > Cd > Co > Ni > Sn > Pb > H2 > Cu > Ag > Hg > Au).

❖On the other hand, as seen from the series, the element Cu is less active than H2, so the copper metal product will not react with the hydrochloric acid that is present.

$$Cu\,(s) + 2\,HCl\,(aq) \nrightarrow H_2\,(g) + CuCl_2\,(aq)$$

❖5) Weigh 0.25 g of dry aluminum foil in small pieces and record the weight on the report sheet.

❖6) Add the pieces of Al foil a little at a time. Use the stirring rod to mix the solution during the reaction. (CAUTION: Exothermic reaction!) Note the color of the solution after the added piece of aluminum no longer darkens on its surface.

❖Add the remaining few pieces of aluminum foil, and add an additional 5 mL of 6 M HCl to facilitate the reaction of any excess aluminum with the hydrochloric acid.

❖7) After all of the aluminum foil has reacted, allow the solid particles of copper product to settle, and carefully decant the solution from the solid (leaving the copper behind in the beaker). Add 20 mL of deionized water to the solid, stir well with the stirring rod, and decant again. Repeat this washing with 20 mL of water once more. Finally, add 10 mL of methanol to the solid, stir, and decant.

❖Note: The methanol (methyl alcohol) wash removes additional water, facilitating complete drying of the product.

❖8) Heat the beaker on a electric hot plate at medium heat (a setting of about 1 out of 4) until the solid and beaker are thoroughly dry. Allow the beaker and its contents to cool, and then weigh and record the weight on the report form.

❖Note: Heating the copper particles at too high of a temperature in air results in an undesirable darkening and a gain in weight, apparently due to the formation of black cupric oxide, CuO. During heating, the dry particles of copper should remain loose when stirred and should not darken in color.

❖9) On the report sheet, record the moles of Al and CuSO4 • 5 H2O used, and determine which is the limiting reactant. Based on the limiting reactant, calculate the theoretical yield of copper metal product. From your actual yield of copper, calculate the percent yield of copper product obtained from the reaction.

❖10) Place your copper metal in the collection container on the front desk (do not wash it down the sink!), rinse your glassware well, and return it and your other equipment to their proper storage locations.

A student reacted 1.5 g of $K_2Cr_2O_7$ with 2.5 g of $CuSO_4.5H_2O$ according to the reaction,

$$K_2Cr_2O_7 + CuSO_4 \rightarrow CuCr_2O_7 + K_2SO_4$$

If the student obtained 0.987 grams of $CuCr_2O_7$ product after collecting it by filtration and drying it, what was the percent yield of $CuCr_2O_7$ obtained?

$K_2Cr_2O_7$ MW 294.18 mol/g
CuSO4 MW 159.61 mol/g
$CuCr_2O_7$ MW 279.534 mol/g
K_2SO_4 MW 174.26 mol/g

A student reacted 0.500 g of $Pb(NO_3)_2$ with 0.750 g of K_I according to the reaction,

$$Pb(NO_3)_2\ (aq) + 2\ KI\ (aq) \rightarrow PbI_2\ (s) + 2\ KNO_3\ (aq)$$

If the student obtained 0.583 grams of PbI_2 product after collecting it by filtration and drying it, what was the percent yield of PbI_2 obtained?

$Pb(NO_3)_2$ MW 331.21 mol/g
KI MW 166.0 mol/g
PbI_2 MW 461.01 mol/g
KNO_3 MW 101.1 mol/g