The Mole Concept

Counting by weighing

The size of molecule is so small that it is physically difficult if not impossible to directly count out molecules. this problem is solved using a common trick. Atoms and molecules are counted indirectly by weighing.

Here is a practical example. You need to estimate the number of nails in a box. You weigh an empty box, 213. g. The weight of the box plus nails is 1340. g. The weight of one nail is 0.450 g.

I hope you aren't going to tear open the package and count the nails. We agree that

mass of nails = 1340 g - 213 g = 1227. g

Number of nails = (1227. grams nails)(1 nail/ 0.450 grams)

= 2726.6 nails = **2730 nails**

You can count the nails by weighing them.

Avogadro's Number and the Mole

To calculate real chemical reactions in the laboratory, chemists use a special unit called a mole (abbreviated mol). One mole of a substance is the amount of the substance that is equal in molar mass of the molecular or formula mass of the substance in grams. Thus for ethylene, C_2H_4, its molecular weight is 28 and its molar mass is 28 g. In other words, 28 g represents 1 mol of ethylene. One mole contains 6.022×10^{23} molecules or formula units. The number 6.022×10^{23} is called Avogadro's number.

For ethylene, C_2H_4,
Molecular mass C_2H_4 = 28.
Molar mass C_2H_4 = 28.0 g
1 mol C_2H_4 contains 6.022×10^{23} molecules

The coefficients of a balanced chemical equation indicate the number of moles of each substance in the
reaction. Thus, at the level of moles:

$$C_3H_8 + 5O_2 \text{ --------}\rightarrow 3CO_2 + 4H_2O$$

One mole of propane reacts with five moles of oxygen to form three moles of carbon dioxide and four moles of water.

Avogadro's number is an accident of nature. It is the number of particles that delivers a mole of a substance. **Avogadro's number = 6.022×10^{23}**.

The reason why the value is an accident of nature is that the mole is tied to the gram mass unit.

The gram is a convenient mass unit because it matches human sizes. If we were a thousand times greater in size (like Paul Bunyan) we would find it handy to use kilogram amounts. This means the kilogram mole would be convenient. The number of particles handled in a kilogram mole is 1000

times greater. The kilo Avogadro number for the count of particles in a kilomole is 6.022 x 10^{26}.
If humans were tiny creatures (like Lilliputians) only 1/1000 our present size, milligrams would be more convenient. This means the milligram mole would be more useful. The number of particles handled in a milligram mole (millimole) would be 1/1000 times smaller. The milli Avogadro number for the count of particles in a millimole is 6.022 x 10^{20}.

Molecular Mass and Mass Percent Activity

It is very helpful to think about chemical reactions in molecular terms. However, it is not practical to carry out reactions at the molecular level.

1 C_2H_4 molecule + 1 HCl molecule 1 C_2H_5Cl molecule

Because it is not practical to count individual molecules, chemists use ratios of the masses of molecules to carry out reactions. Mass ratios are determined by using the molecular masses of the substances involved in a reaction.

Molecular mass provides the mass ratio we need for carrying out reactions. The mass ratio of one HCl molecule to one ethylene molecule is 36.5 to 28 in the following equation.

$$C_2H_4 \quad + \quad HCl \quad \text{-------------}\rightarrow \quad C_2H_5Cl$$

More useful, however, is the fact that the mass ratio in grams is also 36.5 to 28.0. If we were to combine 36.5 g HCl with 28 g ethylene in the laboratory, they would react in a 1:1 molecular ratio.

Molar mass for elements

You are able to read the periodic table and determine the average atomic mass for an element like carbon. The average mass is 12. This is a ridiculously tiny number of grams. It is too small to handle normally.

The molar mass of carbon is defined as the mass in grams that is numerically equal to the average atomic weight. This means

1 mole carbon = 12.0 grams carbon.

This is the mass of carbon that contains 6.022 x 10^{23} carbon atoms. Avogadro's number is 6.022 x 10^{23} particles.

This same process gives us the molar mass of any element.

1 mole neon = 20 grams neon, Ne

1 mole sodium = 23 grams sodium, Na

Molar Mass for Compound

The formulas for compounds are familiar to you. You know the formula for water is H_2O. It should be reasonable that the weight of a formula unit can be calculated by adding up the weights for the atoms in the formula.

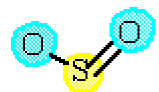
The formula weight for water = weight from hydrogen + weight from oxygen

The formula weight for water = 2 H atoms x 1. + 1 O atom x 16. = 18.

The molar mass for water = 18. grams water.

Example 1.

What is the molar mass for sulfur dioxide, SO_2 (g), a gas used in bleaching and disinfection processes.



1. Look up the atomic weight for each of the elements in the formula.
   1 sulfur atom = 32 1 oxygen atom = 16
2. Count the atoms of each element in the formula unit. .
   one sulfur atom ; two oxygen atoms
3. The formula weight = weight from sulfur + weight from oxygen
4. The formula weight = 1 sulfur atom x (32) + 2 oxygen atoms x (16)
5. The formula weight SO_2 = 32 + 32. = 64

6. The molar mass SO_2 = 64 grams SO_2

Example 2: The formula for methane the major component in natural gas is CH_4.

The formula weight for methane = weight from hydrogen + weight from carbon

The formula weight for methane = 4 H atoms x 1. + 1 C atom x 12. = 16.

The molar mass for methane = 16.0 grams methane

Example 3: The formula for ethyl chloride is CH_3 CH_2Cl.

The formula weight = weight from hydrogen + weight from carbon + weight from chlorine

The formula weight = 5 H atoms x 1.0 + 2 C atom x 12.0 + 1 Cl atom x 35.5 = 64.5

The molar mass for ethyl chloride = 64.5 grams

Mole, Molar Mass and Mass Conversions

Example.

How many grams of hydrogen are needed to give 3. moles of hydrogen?

1. Calculate the molar mass for hydrogen. Look up the atomic weight/mass in the periodic table

The molar mass for hydrogen is 1 mole H_2 = 2 grams H_2

2. determine the mass needed to provide 3. moles of hydrogen.

1 mole H_2 = 2.0 grams H_2;

2 mole H_2 = 4.0 grams H_2

3 mole H_2 = 6.0 grams H_2

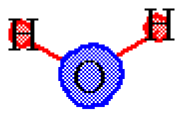
The practical way is to multiply the molar mass by the number of moles. This converts mole to grams

(3 mole H_2)(2 grams H_2/ 1 mole H_2) = 6 grams H_2

Example.

How many moles of water are in a liter of water? Assume 1 liter = 1 kilogram water

1. Calculate the formula weight(mass) for water, H_2O.



Look up the atomic weights in the periodic table for H and O.
The atomic weight for hydrogen is 1
The atomic weight for oxygen is 16
2. Add up the masses from all the atoms in the formula

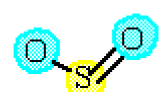
The formula weight for water is 1 + 1 + 16 = 18
3. Determine the molar mass for water. Molar mass is a mass in grams that is numerically the same as the formula weight.

1 mole H_2O = 18.0 grams H_2O
4. Convert 1000 grams of water to moles. The "conversion factor" is the molar mass.

(1000 grams H_2O)(1 mole H_2O/ 18. grams H_2O) = **55.55 moles H_2O**

Example.

How many moles of sulfur dioxide, SO_2 (g), are in 2000 grams of the gas?



1. Look up the atomic weights in the periodic table for S and O.

The atomic weight for sulphur is 32
The atomic weight for oxygen is 16
2. Calculate the formula weight for SO_2 . Add up the masses from all the atoms in the formula

The formula weight for sulfur dioxide is 32 S + 2 x (16 O) = 64 SO_2
3. Determine the molar mass. Molar mass is a mass in grams that is numerically the same as the formula weight.

1 mole SO_2 = 64. grams SO_2

4. Convert 2000 grams of SO_2 to moles. The "conversion factor" is the molar mass.

(2000 grams SO_2)(1 mole SO_2 /64. grams SO_2) = **31.25 moles SO_2,**

Chemical Equations and Mole Relationships

The balanced equations are a chemists recipe for producing a product from reactants. The equation tell us the amounts of reactants needed and the amount of product formed. Balanced equations can be viewed at three levels. The first is the molecular level. The second is the mole level. The third is in terms of masses. We will look at mole relationships here.

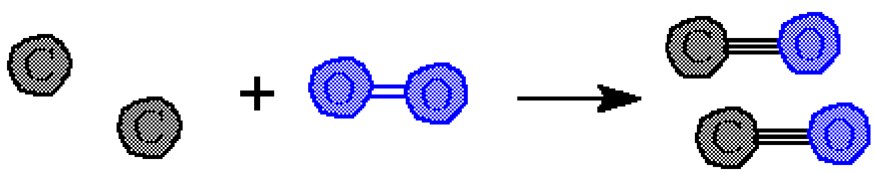
These interpretations of chemical equations are of value because they enable us to make predictions about the outcome of reactions.

Example:

Burning carbon and carbon containing compounds in air can produce carbon monoxide. Carbon monoxide is poisonous. It is cumulative and even if it doesn't kill it can cause chronic illness and brain damage.

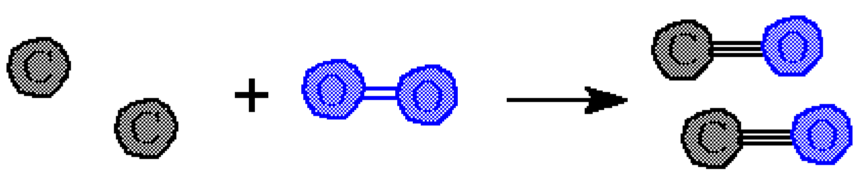
$$2\ C(s) + O_2(g) \text{ -----> } 2\ CO(g)$$

This equation can be viewed in terms of the atomic and molecular level. Two atoms of carbon must react with one molecule of oxygen. Two molecules of carbon monoxide are produced.



The coefficients in the balanced equation tell the moles of each substance involved in the equation

2 moles C   1 mole O_2 2 moles CO



The mole ratios for this equation are

C	:	O	:	CO
2moles	:	1 mole	:	2moles

The reaction between nitrogen and oxygen to produce nitrogen dioxide is analyzed here.

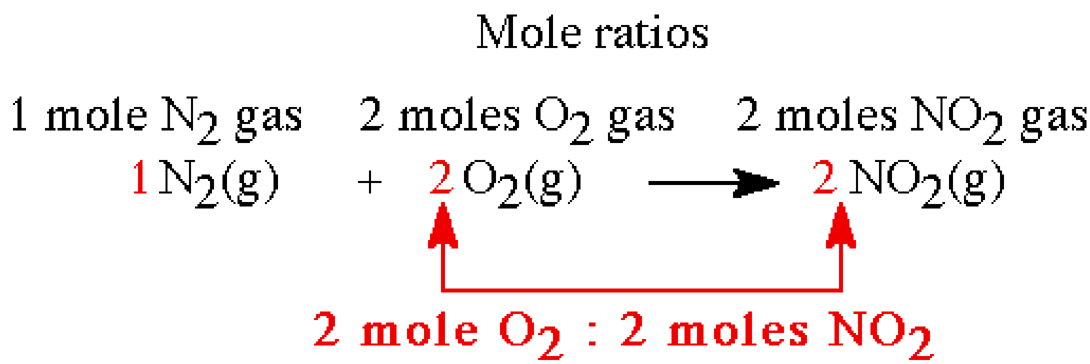
The equation is $N_2(g) + 2\ O_2(g)\text{--->}\ 2\ NO_2(g)$

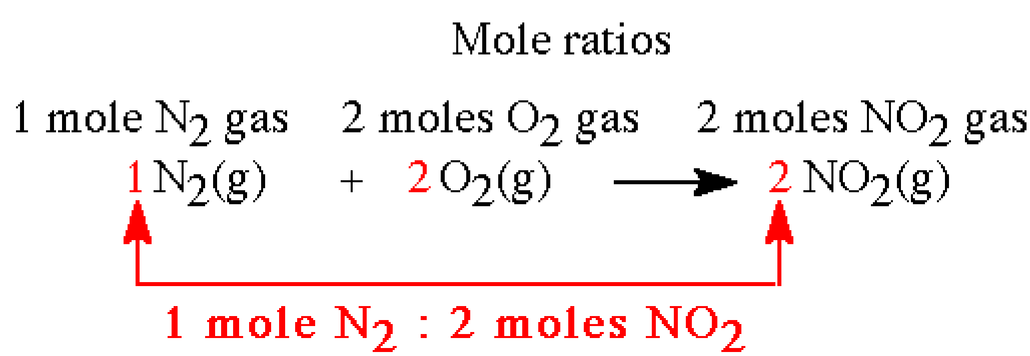
Balanced equation

Nitrogen gas		Oxygen gas		Nitrogen dioxide gas
$1\,N_2(g)$	+	$2\,O_2(g)$	$\longrightarrow$	$2\,NO_2(g)$

Mole view of equation

1 mole N_2 gas		2 moles O_2 gas		2 moles NO_2 gas
$1\,N_2(g)$	+	$2\,O_2(g)$	$\longrightarrow$	$2\,NO_2(g)$





Exercise: What is the mol ratio for nitrogen to oxygen? **Answer: 1 mole N_2 : 2 moles O_2**

Stoichiometry: Chemical Arithmetic

In the laboratory, it is often necessary to convert between moles and mass of a substance. This relationships is called stoichiometry.

Example:

How many grams of carbon are required to react completely with 100 g Fe_2O_3?

$$Fe_2O_3(s) + 3C(s)\ \ 2Fe(l) + 3CO(g)$$

Step 1: Write a balanced chemical equation (or check to see that a given equation is balanced). In this case, a balanced chemical equation was given. Organize the information in the problem. It's often helpful to write the amounts given underneath the balanced chemical equation.

$$Fe_2O_3(s) + 3C(s) \text{ ------------}\rightarrow 2Fe(l) + 3CO(g)$$

100 g ? g

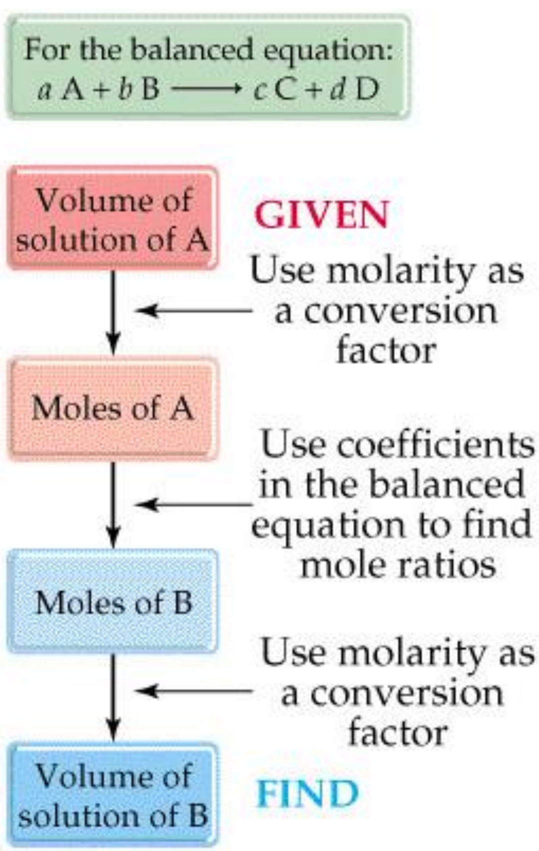
Step 2: Convert grams of a given substance to moles. Remember that substances react in terms of their mole ratios, not their mass ratios. To convert grams of Fe_2O_3 to moles, we need to know the molar mass of this compound.

2 x 56. g for each mol Fe + 3 x 16.0 g for each mol O

= 160 g/mol

Step 3: Use coefficients in the balanced chemical equation to find the mole ratio. Relate moles of what you were given to moles of what you are determining using the mole ratio.

Step 4: Convert moles to grams using molar mass as a conversion factor. It's always a good idea to check to make sure you have answered the question you were asked. Here you were asked to calculate grams of carbon. Another step or two would be necessary if you had been asked to report your answer in some other unit, such as kg.



Reactions with Limiting Amount of Reactants

In actual chemical reactions, one or more reactants may be in excess. The limiting reactant will be consumed completely and limit the amount of product formed. The following exercise provides a simplified view of how limiting reactants affect a chemical reaction.

Example:

30 g NO_2 and 10 g H_2O react as shown below.

$$3\,NO_2(g) + H_2O(l) \text{ ----------------}\rightarrow 2\,HNO_3(l) + NO(g)$$

What is the limiting reactant?

When two or more reactants are present, one reactant must be limiting. To determine which reactant is limiting, we need to look at the mole ratio of the reactants involved.

$$30.0\text{ g }NO_2\left(\frac{1\text{ mol }NO_2}{46.0\text{ g}}\right) = 0.652\text{ mol }NO_2$$

$$10.0\text{ g }H_2O\left(\frac{1\text{ mol }H_2O}{18.0\text{ g}}\right) = 0.555\text{ mol }H_2O$$

The mole ratio of the two reactants is

0.652 mol NO_2/0.555 mol H_2O = 1.17

According to the stoichiometry of the balanced equation, the mole ratio should be

3 mol NO_2/1 mol H_2O = 3.

We see that there is not enough NO_2, and thus NO_2 is the limiting reactant. H_2O is the excess reactant.

b. What amount of HNO_3 forms under these conditions?

Once the limiting reactant is consumed, no additional product can be formed. We therefore use the limiting reactant to calculate the amount of product.

$$0.652\text{ mol }NO_2\left(\frac{2\text{ mol }HNO_3}{3\text{ mol }NO_2}\right)(63.05\text{ g/mol }HNO_3) = 27.4\text{ g }HNO_3$$

c. What amount of NO_2 and H_2O remain?

All of the limiting reactant is consumed, so no NO_2 remains. Stoichiometry will allow us to calculate the amount of H_2O remaining by first determining how much H_2O reacts.

$$0.652\text{ mol }NO_2\left(\frac{1\text{ mol }H_2O}{3\text{ mol }NO_2}\right)(18.0\text{ g/mol }H_2O) = 3.91\text{ g }H_2O\text{ reacts with 30 g }NO_2$$

$$10.0\text{ g }H_2O\text{ available} - 3.91\text{ g reacted} = 6.09\text{ g }H_2O\text{ remaining}$$

3.5 Yields of Chemical Reactions

In the previous section, it was assumed that the reactions proceed "to completion,"—in other words, that all reactants are converted to products. However, this is not always the case. Side reactions can result in the formation of secondary products. Chemists calculate the percent yield of a reaction by comparing the amount of product formed to the theoretical yield predicted from stoichiometry.

$$\textbf{Percent yield} = \frac{\text{Actual yield of product}}{\text{Theoretica yield of product}} \times 100\%$$

Example: What is the theoretical yield of Al_2S_3 when 10.0 g of aluminum is reacted with excess sulfur according to the equation below?

$$2Al(s) + 3\ S(s)\ \ Al_2S_3(s)$$

First, we need to convert grams of aluminum to moles:

$$10.0\text{g Al}\left(\frac{1\text{ mol Al}}{26.98\text{ g}}\right) = 0.3706\text{ mol Al}$$

Next, we relate moles of aluminum to moles of product using the stoichiometric coefficients as a mole ratio:

$$0.3706\text{ mol Al}\left(\frac{1\text{ mol }Al_2S_3}{2\text{ mol Al}}\right) = 0.1853\text{ mol }Al_2S_3$$

Finally, we calculate our theoretical yield of Al2S3 in grams.

$$0.1853\text{ mol }Al_2S_3\left(\frac{150.17\text{ g}}{1\text{ mol }Al_2S_3}\right) = 27.8\text{ g }Al_2S_3$$

Example: A student performing the reaction above collected 18.7 g Al2S3. What is her percent yield?

$$\text{Percent yield} = \left(\frac{18.7\text{ g}}{27.8\text{ g}}\right) \times 100 = 62.7\%\text{ yield}$$

Percent Yield

The percent yield is defined as

$$\text{Percent yield} = 100\left[\frac{\text{Actual mass of product}}{\text{Predicted mass of product}}\right]$$

The predicted yield is determined by the masses used in a reaction and the mole ratios in the balanced equation. This predicted yield is the "ideal". It is not always possible to get this amount of product. Reactions are not always simple. There often are competing reactions. For example, if you burn carbon in air you can get carbon dioxide and carbon monoxide formed. The two reactions occur simultaneously. Some carbon atoms end up in CO and others end up in CO_2

Example:

What is the percent yield for a reaction if you predicted the formation of 21. grams of C_6H_{12} and actually recovered only 3.8 grams?

1. Recall definition of percent yield.

$$\text{Percent yield} = 100\left[\frac{\text{actual yield}}{\text{predicted yield}}\right]$$

2. Substitute the actual and predicted yields.

$$\text{Percent yield} = 100\left[\frac{3.8\ \text{g}}{21\ \text{g}}\right]$$

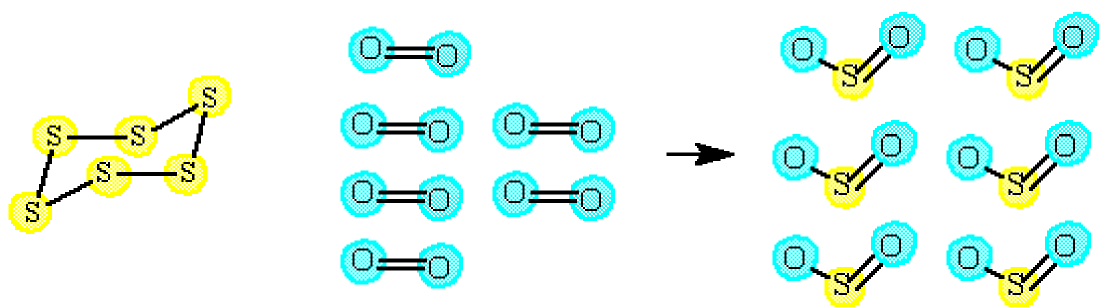
3. **Answer: The percent yield is 18 %.**

Example:

A reaction between solid sulfur and oxygen produces sulfur dioxide.

The reaction started with 384 grams of S_6 (s). Assume an unlimited supply of oxygen. What is the predicted yield and the percent yield if only 680 grams of sulfur dioxide are produced?

$1\ S_6\ (s) \qquad 6\ O_2\ (g) \longrightarrow 6\ SO_2\ (g)$



Step 1 : Calculate the molar masses for S_6 (s) and SO_2(g). The oxygen has no effect on the answer because there is more than you need.

1 mole S_6 (s)= 193 grams S_6 (s); 1 mole SO_2(g) = 64 grams SO_2(g)

Step 2 : Mole ratio method

Determine the mole ratio for 1 mole S_6 (s) to mole SO_2(g)

The balanced equation indicates 1 mole S_6 (s) to 6 mole SO_2(g)

Step 3: Calculate the number of moles of S_6 (s) moles S_6 (s) = [384 g S_6 (s)][1 mole S_6 (s)/ 192 g S_6 (s)] = 2 moles S_6 (s)

Step 4: Calculate the moles of SO_2(g) expected using the mole ratio 6 SO_2(g) / 1 S_6 (s)

moles SO_2(g) = 2 moles S_6 (s)[6 SO_2(g) / 1 S_6 (s)] = 12 moles SO_2(g)

Step 5: Calculate the grams of SO_2(g) predicted using 1 mole SO_2(g) = 64 grams SO_2(g)

grams SO_2(g) = 12 moles SO_2(g)[64 grams SO_2(g)/1 mole SO_2(g)] = **768 g SO_2(g)**

Step 6: Calculate the percent yield using the definition

Percent yield = 100[actual yield/ predicted yield] = 100[680 grams SO_2(g)/ 768 g SO_2(g)]= **89%**

Concentrations of Reactants in Solution: Moles/dm^3 (Molarity)

Many chemical reactions occur in solution. In order to make stoichiometric calculations for these reactions, we need to be able to express the concentration of reactants in solution. One of the most useful concentration units is moles/dm^3 (molarity abbreviated M). Using moles/dm^3 as a conversion factor is quite useful.

$$\textbf{Molarity (M)} = \frac{\text{Moles of solute}}{\text{Liters of solution}}$$

In the laboratory, solutions are prepared according to several steps. Let's prepare 250 mL of a 0.100 M solution of NaCl. (Unless otherwise noted, solutions are aqueous and water is the solvent.)

First, we have to do a calculation. We need to know how many grams of NaCl to weigh.

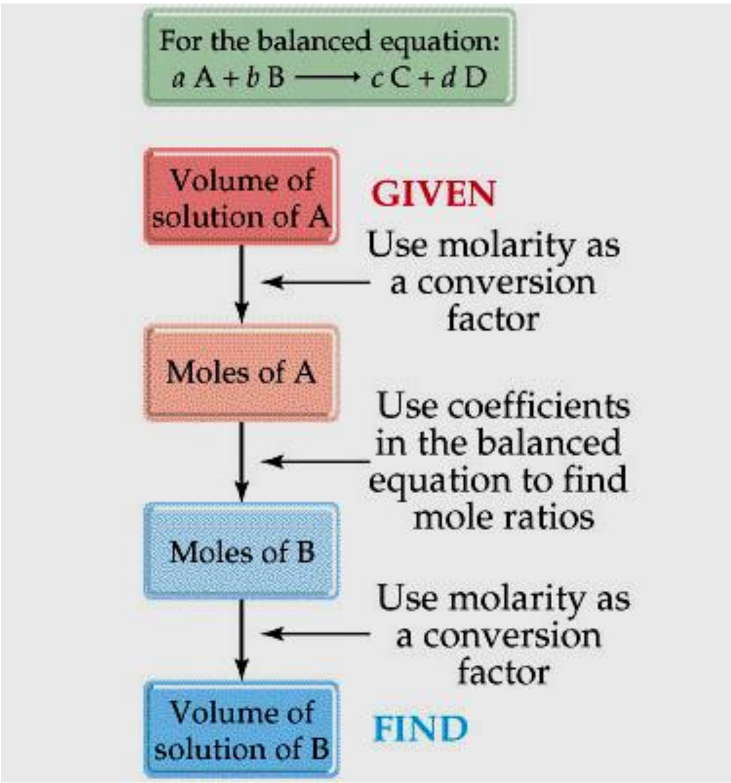
0.250 L (0.100 mol NaCl/dm^3 solution)
= 0.0250 mol NaCl (58.5 g/mol)
= 1.46 g NaCl.

Next, we weigh this amount on a balance and transfer the solid to a 250 mL volumetric flask—a very precise piece of glassware designed to contain only a specific volume of liquid.

Finally, we add our solvent—in this case, water—to the flask. First, we add a small amount to dissolve the solute. Then we add water up to the calibration mark on the flask and mix well.

Solution Stoichiometry

Moles/dm^3 serves as a useful link between the volume of a solution and the number of moles of a solute. The flow diagram below summarizes the steps in stoichiometry calcuations involving solutions.



Example:
How many mL of a 0.90 M solution of HCl is required to react with 4.16 g $CaCO_3$, according to the equation below?

$$CaCO_3(s) + 2\,HCl(aq) \text{-------}\rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$

In this problem, we are given the concentration of the HCl solution. We are given a mass in grams of one of the reactants. So our first step is to convert mass to moles.

$$4.16\text{ g } CaCO_3\ (1\text{ mol}/100\text{ g}) = 4.16 \times 10^{-2}\text{ mol } CaCO_3$$

Next, we relate moles of $CaCO_3$ to moles of HCl required using the coefficients in the balanced equation. The reaction ratio is 2:1 respectively

$$4.16 \times 10^{-2}\text{ mol } CaCO_3\ (2\text{ mol HCl} / 1\text{ mol } CaCO_3) = 8.31 \times 10^{-2}\text{ mol HCl}$$

Now we can convert moles of HCl to volume of HCl using the moles/dm^3.

$$8.31 \times 10^{-2}\text{ mol HCl } (1\text{ dm}^3\text{ solution} / 0.90\text{ mol HCl}) = 9.23 \times 10^{-2}\text{ L HCl solution}$$

$$9.23 \times 10^{-2}\text{ L } (1000\text{ mL} / \text{L}) = 92.3\text{ mL HCl solution}$$