Molar Calculations

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November 2, 2020

1 Introduction

If we have a simple reaction like burning magnesium in air we have:

$$Mg + O_2 \longrightarrow MgO$$

Adding balancing numbers we get:

$$2\,Mg + O_2 \longrightarrow 2\,MgO$$

Balancing numbers are useful, they give us several ways to read this equation:

1. 2 atoms of Mg + 1 molecule of $O_2 \rightarrow$ 2 molecules of MgO.
2. 2 moles of Mg + 1 mole of $O_2 \rightarrow$ 2 moles of MgO.
3. n atoms of Mg and $\frac{n}{2}$ molecules of O_2 produce n molecules of MgO.
4. n moles of Mg and $\frac{n}{2}$ moles of O_2 produce n moles of MgO.

The balancing numbers tell us the *ratios* between the various reactants and products in the reaction. For example looking at the above equation we know that:

1. There are as many atoms of Mg before the reaction as there are molecules of MgO after the reaction. Because they both have a 2 in front of them.
2. For every molecule of O_2 before the reaction there are two atoms of Mg. Because O_2 has a 1 (hidden) in front but Mg has a 2.
3. For every molecule of O_2 before the reaction there are two molecules of MgO after.

Let's look at a more complex reaction, the combustion (burning) of methane in air/oxygen:

$$CH_4 + O_2 \longrightarrow CO_2 + 2\,H_2O$$

A few tasks

1. Draw a molecular diagram of this reaction.
2. If we started with 1 mole of methane how many moles of carbon dioxide would we produce?
3. If we started with 1 mole of methane how many moles of water would we produce?
4. If we produce 4 moles of Carbon dioxide how many moles of O_2 did we start with?
5. If we produce 6 moles of water how many moles of O_2 did we produce?

2 Moles and mass

A mole is simply a very large number, it's 6.023×10^{23}, just like all numbers it is used for counting, we could have a mole of people of a mole of shoes or a mole of moles[1]. The mole was devised for counting how many atoms or molecules are involved in chemical reactions, since the numbers are usually incredibly large and it gets boring writing them out.

A moles is defined like this

1 Mole A sample contains 1 mole atoms/molecules of an element/compound when the mass of the sample in grammes is equal to the element's relative atomic mass or the compound's relative formula mass.

For example:

1. There's 1 mole of Hydrogen atoms in 1 gram of Hydrogen.
2. There's 1 mole of Helium atoms in 4 grams of Helium.
3. There's 1 mole of Carbon atoms in 12 grams of Carbon.
4. There's 1 mole of water molecules in 18 grams of water[2].
5. There's 1 mole of methane molecules in 16 grams of methane.

This suggests a useful equation

$$\text{Mass in Grams} = \text{number of moles} \times \text{relative formula mass}$$

Have a look at the periodic table. We can see that Helium has four times the mass of Hydrogen, this means that gram for gram a hydrogen sample has four times as many atoms because each atom is a quarter the mass of a Helium atom.

[1] see `https://what-if.xkcd.com/4/`

[2] because the RFM for water is $16 + 1 + 1 = 18$

2.1 Example

We can use this formula along with balanced equations to figure out the masses involved. For instance take the following equation:

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O\cdot$$

Suppose we start with 32g of methane and an excess of Oxygen.

The RFM of methane is 16 so our equation tells us we have

$$\text{number of moles} = \text{mass of methane} \div \text{RFM of methane} = 32 \div 16 = 2 \text{ moles}$$

Now look at the chemical equation, we can see that we must have the same number of moles of methane as Carbon dioxide so we can immediately find its mass using our equation:

$$\text{mass of } CO_2 = 2 \text{ moles} \times 44 = 88\text{g}$$

Now we also know we have twice as many moles of O_2 as CH_4 i.e. 4 so we find:

$$\text{mass of } O_2 = 4 \text{ moles} \times 32 = 128\text{g}$$

and finally the mass of water:

$$\text{mass of } H_2O = 4 \text{ moles} \times 18 = 72\text{g}$$

To check our work let's plug these numbers into the equation:

$$32 + 128 = 88 + 72$$

which works.

This is an important point which we have assumed: For any chemical reaction if we add up all the masses of the reactants we put in and then add up all the masses of the products we get out we will find these masses are exactly equal. More succinctly:

Chemical reactions conserve mass.

2.2 A Better Method

These are easier if we lay them out in a table. Table 1 lays out the equation with 3 extra rows. The second row simply restates the balancing numbers, the third row will hold the RFMs of the compounds we're interested in and the last row holds the masses in grams.

Table 1:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM							
mass(g)	32						
moles							

If we want to find out the mass of Carbon dioxide and water first we follow these steps. First fill in the RFMs

Table 2:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32						
moles							

Next look for columns for which we have 2 of the 3 terms from our mole equation. In this case the CH_4 column. calculate the number of moles

$$\text{number of moles} = \text{mass of methane} \div \text{RFM of methane} = 32 \div 16 = 2 \text{ moles}$$

giving

Table 3:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32						
moles	2						

Now look at the moles row. Once you have one number you can fill in all the others using the ratio numbers.

Table 4:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32						
moles	2		4		2		4

Now we can fill in all the masses using the usual equation.

$$\text{mass of } CO_2 = 2 \text{ moles} \times 44 = 88\text{g}$$

and finally the mass of water:

$$\text{mass of } H_2O = 4 \text{ moles} \times 18 = 72\text{g}$$

giving

Table 5:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32				88		72
moles	2		4		2		4

we can even figure out how much oxygen that was used from the air:

$$\text{mass of } O_2 = 4 \text{ moles} \times 32 = 128\text{g}$$

Table 6:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32		128		88		72
moles	2		4		2		4

a final check that mass is conserved:

Table 7:

	CH_4	+	$2\,O_2$	$\rightarrow$	CO_2	+	$2\,H_2O$
ratio	1		2		1		2
RFM	16		32		44		18
mass(g)	32	+	128	=	88	+	72
moles	2		4		2		4

Notice we could also have figured out the mass of Oxygen by simply doing

$$160 - 32 = 128$$

due to conservation of mass.