2: Quantities in Chemical Reactions

So far, we have dealt with chemical reactions in terms of counting atoms and molecules. Even though this works, measuring the number of particles (atoms, molecules, ions, *etc.*) is not something we can easily do. Instead, we would like to quantify the reactants and products of a reaction by parameters such as mass or volume, which can be measured more easily.

Let's look at the reaction we have considered in the previous subtopic (glucose reacts with oxygen to form carbon dioxide and water). The masses of the molecules in the reaction can be determined on the atomic mass scale, as the sum of the masses of the atoms making up the molecule: the **molecular weight**.

	$C_6H_{12}O_6$	+	$6\ O_2$	→	$6\ CO_2$	+	$6\ H_2O$
Molecular weight:	72 +12 +96 =180		6 x 32 = 192		6x(12 + 32)= 264		6x18 = 108

We see that the sum of the molecular weights on both sides is equal: 372. (If you ask yourself where all these numbers come from, please read the following excursus.)

Excursus: Molecular Weight

Since a molecule consists of a minimum of 2 atoms, its molecular weight is calculated as the sum of the atomic weights of the atoms which form the molecule. For example the atomic weight of one oxygen atom (O) is 16.00 (see periodic table). Consequently, the molecular weight of an oxygen molecule (O_2) consisting of 2 oxygen atoms is (2 x 16.00 =) 32.00.

If you want to figure out the molecular weight of glucose ($C_6H_{12}O_6$), proceed as follows:

1) Look up the atomic weights of the elements that make up the molecule in the periodic table (let's round to whole numbers):
    - Atomic weight of carbon (C): 12
    - Atomic weight of hydrogen (H): 1
    - Atomic weight of oxygen (O): 16

2) From the chemical formula of glucose ($C_6H_{12}O_6$) we know that the glucose molecule contains 6 atoms of C, 12 atoms of H and 6 atoms of O. Now, we can figure out the molecular weight of glucose:

6 x C +	12 x H +	6 x O	
6 x 12 +	12 x 1 +	6 x 16	= 72 + 12 + 96 = 180

The Mole Concept and Avogadro Constant

In practice we are dealing with an immense number of atoms and molecules, all with very small weights. The SI unit for the amount of substance is called the **mole**; it stands for a certain number of particles (atoms, molecules, ions, *etc.*).

This number is called **Avogadro constant**; its value is **6.022×10^{23} mol^{-1}**. In other words, one mole of any substance contains **6.022×10^{23} particles**.

The size of a mole is chosen in a particular way. **If we take one mole of atoms (or molecules), the mass of that mole in grams has a numerical value that is equal to the atomic (or molecular) weight. It also contains, in all cases, 6.022×10^{23} atoms (or molecules).**

For example:

The atomic weight of carbon (C) is 12.01.

1 atom of carbon weighs: $12.01 \times \frac{1}{6.022 \times 10^{23}}$ g = $12.01 \times 1.661 \times 10^{-24}$g; then

1 <u>mole</u> of carbon weighs: $12.01 \times 1.661 \times 10^{-24} \times 6.022 \times 10^{23}$g = 12.01 g.

Another example:

Similarly, one mole of sodium (Na) atoms weighs 22.99 g and one mole of chlorine (Cl) atoms weighs 35.45 g (see periodic table). The weight of one mole of sodium chloride (NaCl) is then 58.44 g.

We can immediately see the great importance of the mole concept, looking at the reaction discussed earlier between glucose and oxygen:

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$

By multiplying with the Avogadro constant, we can now say that

- **1 mole of glucose** reacts with **6 moles of O_2** to form **6 moles of CO_2** and **6 moles of H_2O**,
- or, in grams: **180 g of glucose** reacts with **192 g of O_2** to form **264 g of CO_2** and **108 g of H_2O.**

Molar Mass

The mass of one mole of a substance is called **molar mass (M)**. It is expressed in **g/mol**. The molar mass equals the atomic or molecular weight multiplied by 1 g/mol. For carbon this means, its molar mass is 12.01 g/mol. For glucose it means its molar mass is 180 g/mol.

The formula expression of the molar mass is very useful when it comes to converting between the **amount of substance (n)** in mol and the **mass of substance (m)** in g, without getting the units confused.

$$M = \frac{m}{n} \qquad \text{(formula 1)}$$

Example: How many moles are in 100 g of phosphorous (P)?

$$n = \frac{m}{M} = \frac{100\cancel{g}}{30.97\,\cancel{g}/_{mol}} = 3.23\ mol$$

Question 1:

How much do 5 mole of aluminum (Al) weigh?

Question 2:

How many moles are in 270 g of aluminum oxide (Al_2O_3)? (two digits)→ 2.65 mol

Answers: *see p. 5*

Molar Volume

Avogadro derived another important law, now for ideal gases[1]:

1 mole of each gas, measured at the same temperature and pressure, occupies the same volume.

$$V_m = \frac{V}{n} \qquad \text{(formula 2.1)}$$

in which: V_m - molar volume [L/mol]
V - volume of substance [L]
n - amount of substance [mol]

At standard temperature and pressure (STP: 0°C and 1 atm), this volume = 22.4 L (liters).

At STP (0°C, 1 atm): $$V_m = 22.4\ {}^{L}/_{mol} = \frac{V}{n} \qquad \text{(formula 2.2)}$$

Using the molar volume (V_m) and molar mass (M) you can convert between volume and mass of a given substance.

Example:

1 mole of chlorine gas (Cl_2) weighs 35.45 g x 2 = 70.90 g. At STP it occupies 22.4 L.

Question 3:

How much volume does 1 g of Cl_2 occupy at STP?

Answer: *see p. 5*

Adaptations for non-STP conditions can be made with the help of the general gas law of Boyle - Gay Lussac:

$$\frac{pV}{T} = \text{Constant} \qquad \text{(formula 3)}$$

in which: p = pressure (atm)
V = volume (L)
T = temperature (Kelvin, K = °C + 273).

Thus, at 25°C, one gram of Cl_2 occupies (p is constant):

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \quad ; \quad \frac{0.32L}{273K} = \frac{V_2}{(273+25)K} \rightarrow V_2 = 0.35\text{ L.}$$

[1] An ideal gas is defined as a dilute gas without interaction between the gas molecules.

Question 4:

How much volume does one mole of Cl_2 occupy at 20°C (p is constant)?

Answer: *see p. 5*

Sum-up Example:

Suppose 3.5 million inhabitants in the river Schelde basin (Belgium) discharge per day a wastewater containing, per inhabitant, 100 grams organic compounds of a composition equivalent to $C_6H_{12}O_6$ (glucose).

What is the theoretical amount of oxygen from the air (liters O_2 at 25 °C and 1 atm), necessary per day to fully convert this waste stream to CO_2 and H_2O?

- First set up the balanced equation:

$$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$$

→ So: 1 mole (= 180g) of glucose reacts with 6 moles of O_2.

- Estimate the actual load of glucose; from this calculate the moles of O_2 needed:

Discharge per day of glucose in grams:

$$3.5\ x\ 10^6 \cancel{inhabitants}\ x\ 100\ {}^{g}/_{(\cancel{inhabitant})} = 3.5\ x\ 10^8 g$$

Discharge per day of glucose in moles (the molar mass of glucose is 180 g/mol): see formula 1

$$n = \frac{m}{M} = \frac{3.5\ x\ 10^8 \cancel{g}}{180\ {}^{\cancel{g}}/_{mol}} = 1.9\ x\ 10^6 mol$$

→ Moles of O_2 needed:

1.9×10^6 moles of glucose react with 1.9×10^6 x 6 moles of O_2 .

- Convert the moles of O_2 into liters O_2 at 0^0C and 1 atm, then calculate the liters of O_2 at non-STP conditions, using the Boyle-Gay Lussac law:

Volume of 0_2 needed at 0^oC (1 mole of O_2 = 22.4 L): see formula 2.2

$$V = n\ x\ V_m = 1.9\ x\ 10^6\ x\ 6\ \cancel{mol}\ x\ 22.4\ {}^{L}/_{\cancel{mol}} = 2.6\ x\ 10^8 L\ of\ O_2$$

- Then, finally, at 25^0C: see formula 3

$$\frac{pV}{T} = \text{Constant, or: } \frac{V_1}{T_1} = \frac{V_2}{T_2}\ ;$$

$$V_2 = \frac{2.6\ x\ 10^8 L\ x\ (273 + 25)\cancel{K}}{273\cancel{K}} = \mathbf{2.9\ x\ 10^8 L\ of\ O_2}$$

(N.B. this amount of oxygen needed is a common measure to express the waste loads, *viz.* in the terms Chemical and Biochemical Oxygen Demand (COD, BOD)).

Sources:

- *D.W. Ball et al., 2016. The Basics of General, Organic, and Biological Chemistry, ch. 6: Quantities in Chemical Reactions. Libre Texts/UC Davis.* http://chem.libretexts.org/Textbook_Maps/Introductory_Chemistry_Textbook_Maps/Map%3A_The_Basics_of_GOB_Chemistry_(Ball_et_al.)/06%3A_Quantities_in_Chemical_Reactions
- *CK-12 Foundation (S. Bewick et al.), 2016. Map: Introductory Chemistry (CK-12), ch. 10: The Mole. Libre Texts/UC Davis.* *http://chem.libretexts.org/Textbook_Maps/Introductory_Chemistry_Textbook_Maps/Map%3A_Introductory_Chemistry_(CK-12)/10%3A_The_Mole*
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Answers to Questions

Q1: ***Answer:*** 134.90 g

Explanation: $m = n \; x \; M = 5\cancel{mol} \; x \; 26.98 \, {}^{g}/_{\cancel{mol}} = 134.90g$

Q2: ***Answer:*** 2.65 mol

Explanation: The molar mass of Al_2O_3 is

$$(2 \; x \; 26.98 + 3 \; x \; 16.00) \, {}^{g}/_{mol} = 101.96 \, {}^{g}/_{mol}$$

$$n = \frac{m}{M} = \frac{270\cancel{g}}{101.96 \, {}^{\cancel{g}}/_{mol}} = 2.65 \; mol$$

Q3: ***Answer:*** 0,32 L

Explanation: Applying formula 1 and formula 2.2 you will find that

$$V = \frac{m}{M} \; x \; V_m = \frac{1\cancel{g}}{70.9 \, {}^{\cancel{g}}/_{\cancel{mol}}} \; x \; 22.4 \, {}^{L}/_{\cancel{mol}} = 0.32L$$

→ 1 gram of Cl_2 occupies 0.32 L at STP conditions.

Q4: ***Answer:*** 24.0 L

Explanation: At standard temperature (0°C) 1 mole of Cl_2 occupies 22.4 L. If the pressure is constant, at 20°C, 1 mole of Cl_2 occupies

$\frac{V_1}{T_1} = \frac{V_2}{T_2}$; $\frac{22.4L}{273K} = \frac{V_2}{(273+20)K}$ → V_2 = 24.0 L.