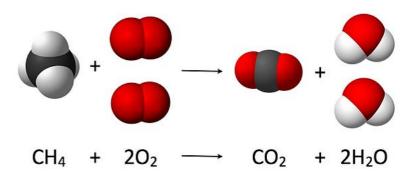
# **Stoichiometry**

**Stoichiometry** / stoiki omitri/ is the calculation of reactants and products in chemical reactions in chemistry.

Stoichiometry is founded on the <u>law of conservation of mass</u> where the total mass of the reactants equals the total mass of the products, leading to the insight that the relations among quantities of reactants and products typically form a ratio of positive integers. This means that if the amounts of the separate reactants are



A stoichiometric diagram of the <u>combustion</u> reaction of <u>methane</u>.

known, then the amount of the product can be calculated. Conversely, if one reactant has a known quantity and the quantity of the products can be empirically determined, then the amount of the other reactants can also be calculated.

This is illustrated in the image here, where the balanced equation is:

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

Here, one molecule of methane reacts with two molecules of oxygen gas to yield one molecule of carbon dioxide and two molecules of water. This particular chemical equation is an example of complete combustion. Stoichiometry measures these quantitative relationships, and is used to determine the amount of products and reactants that are produced or needed in a given reaction. Describing the quantitative relationships among substances as they participate in chemical reactions is known as *reaction stoichiometry*. In the example above, reaction stoichiometry measures the relationship between the quantities of methane and oxygen that react to form carbon dioxide and water.

Because of the well known relationship of <u>moles</u> to <u>atomic weights</u>, the ratios that are arrived at by stoichiometry can be used to determine quantities by weight in a reaction described by a balanced equation. This is called *composition stoichiometry*.

Gas stoichiometry deals with reactions involving gases, where the gases are at a known temperature, pressure, and volume and can be assumed to be <u>ideal gases</u>. For gases, the volume ratio is ideally the same by the <u>ideal gas law</u>, but the mass ratio of a single reaction has to be calculated from the <u>molecular masses</u> of the reactants and products. In practice, due to the existence of <u>isotopes</u>, <u>molar masses</u> are used instead when calculating the mass ratio.

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# **Etymology**

The term *stoichiometry* was first used by Jeremias Benjamin Richter in 1792 when the first volume of Richter's *Stoichiometry or the Art of Measuring the Chemical Elements* was published. The term is derived from the Ancient Greek words στοιχεῖον *stoicheion* "element" and μέτρον *metron* "measure". In patristic Greek, the word *Stoichiometria* was used by Nicephorus to refer to the number of line counts of the canonical New Testament and some of the Apocrypha.

### **Definition**

A **stoichiometric amount**[2] or **stoichiometric ratio** of a <u>reagent</u> is the optimum amount or ratio where, assuming that the reaction proceeds to completion:

- 1. All of the reagent is consumed
- 2. There is no deficiency of the reagent
- 3. There is no excess of the reagent.

Stoichiometry rests upon the very basic laws that help to understand it better, i.e., <u>law of conservation of mass</u>, the <u>law of definite proportions</u> (i.e., the <u>law of constant composition</u>), the <u>law of multiple proportions</u> and the <u>law of reciprocal proportions</u>. In general, chemical reactions combine in definite ratios of chemicals. Since chemical reactions can neither create nor destroy matter, nor <u>transmute</u> one element into another, the amount of each element must be the same throughout the overall reaction. For example, the number of atoms of a given element X on the reactant side must equal the number of atoms of that element on the product side, whether or not all of those atoms are actually involved in a reaction.

Chemical reactions, as macroscopic unit operations, consist of simply a very large number of <u>elementary reactions</u>, where a single molecule reacts with another molecule. As the reacting molecules (or moieties) consist of a definite set of atoms in an integer ratio, the ratio between reactants in a complete reaction is also in integer ratio. A reaction may consume more than one molecule, and the **stoichiometric number** counts this number, defined as positive for products (added) and negative for reactants (removed). The unsigned coefficients are generally referred to as the *stoichiometric coefficients*. [4]

Different elements have a different <u>atomic mass</u>, and as collections of single atoms, molecules have a definite <u>molar mass</u>, measured with the unit mole  $(6.02 \times 10^{23} \text{ individual molecules}, \underline{\text{Avogadro's constant}})$ . By definition, carbon-12 has a molar mass of 12 g/mol. Thus, to calculate the stoichiometry by mass, the number of molecules required for each reactant is expressed in moles and multiplied by the molar mass of each to give the mass of each reactant per mole of reaction. The mass ratios can be calculated by dividing each by the total in the whole reaction.

Elements in their natural state are mixtures of <u>isotopes</u> of differing mass, thus <u>atomic masses</u> and thus molar masses are not exactly integers. For instance, instead of an exact 14:3 proportion, 17.04 kg of ammonia consists of 14.01 kg of nitrogen and  $3 \times 1.01$  kg of hydrogen, because natural nitrogen includes a small amount of nitrogen-15, and natural hydrogen includes hydrogen-2 (deuterium).

A **stoichiometric reactant** is a reactant that is consumed in a reaction, as opposed to a <u>catalytic reactant</u>, which is not consumed in the overall reaction because it reacts in one step and is regenerated in another step.

# Converting grams to moles

Stoichiometry is not only used to balance chemical equations but also used in conversions, i.e., converting from grams to moles using molar mass as the conversion factor, or from grams to milliliters using density. For example, to find the amount of NaCl (sodium chloride) in 2.00 g, one would do the following:

$$\frac{2.00~g~NaCl}{58.44~g~NaCl~mol^{-1}} = 0.0342~mol$$

In the above example, when written out in fraction form, the units of grams form a multiplicative identity, which is equivalent to one (g/g = 1), with the resulting amount in moles (the unit that was needed), as shown in the following equation,

$$\left(rac{2.00~\mathrm{g~NaCl}}{1}
ight)\left(rac{1~\mathrm{mol~NaCl}}{58.44~\mathrm{g~NaCl}}
ight) = 0.0342~\mathrm{mol}$$

# **Molar proportion**

Stoichiometry is often used to balance chemical equations (reaction stoichiometry). For example, the two <u>diatomic</u> gases, <u>hydrogen</u> and <u>oxygen</u>, can combine to form a liquid, water, in an <u>exothermic</u> reaction, as described by the following equation:

$$2 H_2 + O_2 \rightarrow 2 H_2O$$

Reaction stoichiometry describes the 2:1:2 ratio of hydrogen, oxygen, and water molecules in the above equation.

The molar ratio allows for conversion between moles of one substance and moles of another. For example, in the reaction

$$\textrm{2 CH}_{\textrm{3}}\textrm{OH} + \textrm{3 O}_{\textrm{2}} \rightarrow \textrm{2 CO}_{\textrm{2}} + \textrm{4 H}_{\textrm{2}}\textrm{O}$$

the amount of water that will be produced by the combustion of 0.27 moles of  ${\rm CH_3OH}$  is obtained using the molar ratio between  ${\rm CH_3OH}$  and  ${\rm H_2O}$  of 2 to 4.

$$\left(\frac{0.27 \text{ mol CH}_3\text{OH}}{1}\right) \left(\frac{4 \text{ mol H}_2\text{O}}{2 \text{ mol CH}_3\text{OH}}\right) = 0.54 \text{ mol H}_2\text{O}$$

The term stoichiometry is also often used for the  $\underline{\text{molar}}$  proportions of elements in stoichiometric compounds (composition stoichiometry). For example, the stoichiometry of hydrogen and oxygen in  $H_2O$  is 2:1. In stoichiometric compounds, the molar proportions are whole numbers.

## **Determining amount of product**

Stoichiometry can also be used to find the quantity of a product yielded by a reaction. If a piece of solid <u>copper</u> (Cu) were added to an aqueous solution of <u>silver nitrate</u> (AgNO<sub>3</sub>), the <u>silver</u> (Ag) would be replaced in a <u>single displacement reaction</u> forming aqueous <u>copper(II) nitrate</u> (Cu(NO<sub>3</sub>)<sub>2</sub>) and solid silver. How much silver is produced if 16.00 grams of Cu is added to the solution of excess silver nitrate?

The following steps would be used:

- 1. Write and balance the equation
- 2. Mass to moles: Convert grams of Cu to moles of Cu
- 3. Mole ratio: Convert moles of Cu to moles of Ag produced
- 4. Mole to mass: Convert moles of Ag to grams of Ag produced

The complete balanced equation would be:

$$Cu + 2 AgNO_3 \rightarrow Cu(NO_3)_2 + 2 Ag$$

For the mass to mole step, the mass of copper (16.00 g) would be converted to moles of copper by dividing the mass of copper by its molecular mass: 63.55 g/mol.

$$\left(\frac{16.00 \text{ g Cu}}{1}\right) \left(\frac{1 \text{ mol Cu}}{63.55 \text{ g Cu}}\right) = 0.2518 \text{ mol Cu}$$

Now that the amount of Cu in moles (0.2518) is found, we can set up the mole ratio. This is found by looking at the coefficients in the balanced equation: Cu and Ag are in a 1:2 ratio.

$$\left(\frac{0.2518 \ mol \ Cu}{1}\right) \left(\frac{2 \ mol \ Ag}{1 \ mol \ Cu}\right) = 0.5036 \ mol \ Ag$$

Now that the moles of Ag produced is known to be 0.5036 mol, we convert this amount to grams of Ag produced to come to the final answer:

$$\left(rac{0.5036 ext{ mol Ag}}{1}
ight)\left(rac{107.87 ext{ g Ag}}{1 ext{ mol Ag}}
ight) = 54.32 ext{ g Ag}$$

This set of calculations can be further condensed into a single step:

$$m_{\mathrm{Ag}} = \left(rac{16.00 \mathrm{~g~Cu}}{1}
ight) \left(rac{1 \mathrm{~mol~Cu}}{63.55 \mathrm{~g~Cu}}
ight) \left(rac{2 \mathrm{~mol~Ag}}{1 \mathrm{~mol~Cu}}
ight) \left(rac{107.87 \mathrm{~g~Ag}}{1 \mathrm{~mol~Ag}}
ight) = 54.32 \mathrm{~g}$$

### Further examples

For propane (C<sub>3</sub>H<sub>8</sub>) reacting with oxygen gas (O<sub>2</sub>), the balanced chemical equation is:

$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$$

The mass of water formed if 120 g of propane (C<sub>3</sub>H<sub>8</sub>) is burned in excess oxygen is then

$$m_{
m H_2O} = \left(rac{120.~{
m g~C_3H_8}}{1}
ight) \left(rac{1~{
m mol~C_3H_8}}{44.09~{
m g~C_3H_8}}
ight) \left(rac{4~{
m mol~H_2O}}{1~{
m mol~C_3H_8}}
ight) \left(rac{18.02~{
m g~H_2O}}{1~{
m mol~H_2O}}
ight) = 196~{
m g}$$

### Stoichiometric ratio

Stoichiometry is also used to find the right amount of one <u>reactant</u> to "completely" react with the other reactant in a <u>chemical reaction</u> – that is, the stoichiometric amounts that would result in no leftover reactants when the reaction takes place. An example is shown below using the <u>thermite</u> reaction,

$$\mathrm{Fe_2O_3} + 2\,\mathrm{Al} \longrightarrow \mathrm{Al_2O_3} + 2\,\mathrm{Fe}$$

This equation shows that 1 mole of <u>iron(III)</u> oxide and 2 moles of <u>aluminum</u> will produce 1 mole of <u>aluminium</u> oxide and 2 moles of <u>iron</u>. So, to completely react with 85.0 g of iron(III) oxide (0.532 mol), 28.7 g (1.06 mol) of aluminium are needed.

$$m_{
m Al} = \left(rac{85.0~{
m g~Fe_2O_3}}{1}
ight) \left(rac{1~{
m mol~Fe_2O_3}}{159.7~{
m g~Fe_2O_3}}
ight) \left(rac{2~{
m mol~Al}}{1~{
m mol~Fe_2O_3}}
ight) \left(rac{26.98~{
m g~Al}}{1~{
m mol~Al}}
ight) = 28.7~{
m g}$$

# Limiting reagent and percent yield

The limiting reagent is the reagent that limits the amount of product that can be formed and is completely consumed when the reaction is complete. An excess reactant is a reactant that is left over once the reaction has stopped due to the limiting reactant being exhausted.

Consider the equation of roasting  $\underline{lead(II)}$  sulfide (PbS) in oxygen (O<sub>2</sub>) to produce  $\underline{lead(II)}$  oxide (PbO) and  $\underline{sulfur}$  dioxide (SO<sub>2</sub>):

2 PbS + 3 
$$\mathrm{O_2} \rightarrow$$
 2 PbO + 2  $\mathrm{SO_2}$ 

To determine the theoretical yield of lead(II) oxide if 200.0 g of lead(II) sulfide and 200.0 g of oxygen are heated in an open container:

$$m_{ ext{PbO}} = \left(rac{200.0 ext{ g PbS}}{1}
ight) \left(rac{1 ext{ mol PbS}}{239.27 ext{ g PbS}}
ight) \left(rac{2 ext{ mol PbO}}{2 ext{ mol PbS}}
ight) \left(rac{223.2 ext{ g PbO}}{1 ext{ mol PbO}}
ight) = 186.6 ext{ g}$$

$$m_{
m PbO} = \left(rac{200.0~{
m g~O_2}}{1}
ight) \left(rac{1~{
m mol~O_2}}{32.00~{
m g~O_2}}
ight) \left(rac{2~{
m mol~PbO}}{3~{
m mol~O_2}}
ight) \left(rac{223.2~{
m g~PbO}}{1~{
m mol~PbO}}
ight) = 930.0~{
m g}$$

Because a lesser amount of PbO is produced for the 200.0 g of PbS, it is clear that PbS is the limiting reagent.

In reality, the actual yield is not the same as the stoichiometrically-calculated theoretical yield. Percent yield, then, is expressed in the following equation:

$$percent\ yield = \frac{actual\ yield}{theoretical\ yield}$$

If 170.0 g of lead(II) oxide is obtained, then the percent yield would be calculated as follows:

$$ext{percent yield} = rac{170.0 ext{ g PbO}}{186.6 ext{ g PbO}} = 91.12\%$$

#### **Example**

Consider the following reaction, in which <u>iron(III) chloride</u> reacts with <u>hydrogen sulfide</u> to produce iron(III) sulfide and hydrogen chloride:

```
2 FeCl<sub>3</sub> + 3 H<sub>2</sub>S \rightarrow Fe<sub>2</sub>S<sub>3</sub> + 6 HCl
The stoichiometric masses for this reaction are: 324.41 g FeCl<sub>3</sub>, 102.25 g H<sub>2</sub>S, 207.89 g Fe<sub>2</sub>S<sub>3</sub>, 218.77 g HCl
```

Suppose 90.0 g of  $FeCl_3$  reacts with 52.0 g of  $H_2S$ . To find the limiting reagent and the mass of HCl produced by the reaction, we change the above amounts by a factor of 90/324.41 and obtain the following amounts:

```
90.00 g FeCl<sub>3</sub>, 28.37 g H<sub>2</sub>S, 57.67 g FeS<sub>3</sub>, 60.69 g HCl
```

The limiting reactant (or reagent) is FeCl<sub>3</sub>, since all 90.00 g of it is used up while only 28.37 g H2S are consumed. Thus, 52.0 - 28.4 = 23.6 g H2S left in excess. The mass of HCl produced is 60.7 g.

Note: By looking at the stoichiometry of the reaction, one might have guessed FeCl<sub>3</sub> being the limiting reactant; three times more FeCl<sub>3</sub> is used compared to H<sub>2</sub>S (324 g vs 102 g).

# Different stoichiometries in competing reactions

Often, more than one reaction is possible given the same starting materials. The reactions may differ in their stoichiometry. For example, the <u>methylation</u> of <u>benzene</u> ( $C_6H_6$ ), through a <u>Friedel-Crafts reaction</u> using <u>AlCl<sub>3</sub></u> as a catalyst, may produce singly methylated ( $C_6H_5CH_3$ ), doubly methylated ( $C_6H_4(CH_3)_2$ ), or still more highly methylated ( $C_6H_{6-n}(CH_3)_n$ ) products, as shown in the following example,

```
C_6H_6 + CH_3CI \rightarrow C_6H_5CH_3 + HCI

C_6H_6 + 2 CH_3CI \rightarrow C_6H_4(CH_3)_2 + 2 HCI

C_6H_6 + n CH_3CI \rightarrow C_6H_{6-n}(CH_3)_n + n HCI
```

In this example, which reaction takes place is controlled in part by the relative <u>concentrations</u> of the reactants.

### Stoichiometric coefficient and stoichiometric number

In lay terms, the *stoichiometric coefficient* of any given component is the number of molecules and/or <u>formula units</u> that participate in the reaction as written. A related concept is the *stoichiometric number* (using IUPAC nomenclature), wherein the stoichiometric coefficient is multiplied by +1 for all products and by -1 for all reactants.

For example, in the reaction  $CH_4 + 2 O_2 \rightarrow \underline{CO_2} + 2 H_2O$ , the stoichiometric number of  $CH_4$  is -1, the stoichiometric number of  $O_2$  is -2, for  $CO_2$  it would be +1 and for  $H_2O$  it is +2.

In more technically precise terms, the stoichiometric number in a <u>chemical reaction</u> <u>system</u> of the *i*th component is defined as

$$u_i = rac{\Delta N_i}{\Delta \xi}$$

or

$$\Delta N_i = 
u_i \, \Delta \xi$$

where  $N_i$  is the number of molecules of i, and  $\xi$  is the progress variable or extent of reaction. [5] [6]

The stoichiometric number  $v_i$  represents the degree to which a chemical species participates in a reaction. The convention is to assign negative numbers to *reactants* (which are consumed) and positive ones to *products*, consistent with the convention that increasing the extent of reaction will correspond to shifting the composition from reactants towards products. However, any reaction may be viewed as going in the reverse direction, and in that point of view, would change in the negative direction in order to lower the system's Gibbs free energy. Whether a reaction actually *will* go in the arbitrarily selected forward direction or not depends on the amounts of the <u>substances</u> present at any given time, which determines the <u>kinetics</u> and <u>thermodynamics</u>, i.e., whether <u>equilibrium</u> lies to the *right* or the *left* of the initial state,

In reaction mechanisms, stoichiometric coefficients for each step are always integers, since elementary reactions always involve whole molecules. If one uses a composite representation of an overall reaction, some may be rational fractions. There are often chemical species present that do not participate in a reaction; their stoichiometric coefficients are therefore zero. Any chemical species that is regenerated, such as a catalyst, also has a stoichiometric coefficient of zero.

The simplest possible case is an isomerization

$$A \rightarrow B$$

in which  $v_B = 1$  since one molecule of B is produced each time the reaction occurs, while  $v_A = -1$  since one molecule of A is necessarily consumed. In any chemical reaction, not only is the total <u>mass conserved</u> but also the numbers of <u>atoms</u> of each <u>kind</u> are conserved, and this imposes corresponding constraints on possible values for the stoichiometric coefficients.

There are usually multiple reactions proceeding simultaneously in any <u>natural</u> reaction system, including those in <u>biology</u>. Since any chemical component can participate in several reactions simultaneously, the stoichiometric number of the ith component in the kth reaction is defined as

$$u_{ik} = rac{\partial N_i}{\partial \xi_k}$$

so that the total (differential) change in the amount of the ith component is

$$dN_i = \sum_k 
u_{ik} \, d\xi_k.$$

Extents of reaction provide the clearest and most explicit way of representing compositional change, although they are not yet widely used.

With complex reaction systems, it is often useful to consider both the representation of a reaction system in terms of the amounts of the chemicals present  $\{N_i\}$  (state variables), and the representation in terms of the actual compositional degrees of freedom, as expressed by the extents of reaction  $\{\xi_k\}$ . The transformation from a vector expressing the extents to a vector expressing the amounts uses a rectangular matrix whose elements are the stoichiometric numbers  $[v_{ik}]$ .

The <u>maximum and minimum</u> for any  $\xi_k$  occur whenever the first of the reactants is depleted for the forward reaction; or the first of the "products" is depleted if the reaction as viewed as being pushed in the reverse direction. This is a purely <u>kinematic</u> restriction on the reaction <u>simplex</u>, a <u>hyperplane</u> in composition space, or *N*-space, whose <u>dimensionality</u> equals the number of <u>linearly-independent</u> chemical reactions. This is necessarily less than the number of chemical components, since each reaction manifests a relation between at least two chemicals. The accessible region of the hyperplane depends on the amounts of each chemical species actually present, a contingent fact. Different such amounts can even generate different hyperplanes, all sharing the same algebraic stoichiometry.

In accord with the principles of chemical kinetics and thermodynamic equilibrium, every chemical reaction is *reversible*, at least to some degree, so that each equilibrium point must be an interior point of the simplex. As a consequence, extrema for the  $\xi$ s will not occur unless an experimental system is prepared with zero initial amounts of some products.

The number of *physically*-independent reactions can be even greater than the number of chemical components, and depends on the various reaction mechanisms. For example, there may be two (or more) reaction *paths* for the isomerism above. The reaction may occur by itself, but faster and with different intermediates, in the presence of a catalyst.

The (dimensionless) "units" may be taken to be molecules or moles. Moles are most commonly used, but it is more suggestive to picture incremental chemical reactions in terms of molecules. The Ns and  $\xi s$  are reduced to molar units by dividing by Avogadro's number. While dimensional mass units may be used, the comments about integers are then no longer applicable.

# Stoichiometry matrix

In complex reactions, stoichiometries are often represented in a more compact form called the stoichiometry matrix. The stoichiometry matrix is denoted by the symbol  $\mathbf{N}$ . [7][8][9]

If a reaction network has n reactions and m participating molecular species then the stoichiometry matrix will have correspondingly m rows and n columns.

For example, consider the system of reactions shown below:

$$S_1 \rightarrow S_2$$
  
 $5 S_3 + S_2 \rightarrow 4 S_3 + 2 S_2$   
 $S_3 \rightarrow S_4$   
 $S_4 \rightarrow S_5$ 

This system comprises four reactions and five different molecular species. The stoichiometry matrix for this system can be written as:

$$\mathbf{N} = egin{bmatrix} -1 & 0 & 0 & 0 \ 1 & 1 & 0 & 0 \ 0 & -1 & -1 & 0 \ 0 & 0 & 1 & -1 \ 0 & 0 & 0 & 1 \end{bmatrix}$$

where the rows correspond to  $S_1$ ,  $S_2$ ,  $S_3$ ,  $S_4$  and  $S_5$ , respectively. Note that the process of converting a reaction scheme into a stoichiometry matrix can be a lossy transformation: for example, the stoichiometries in the second reaction simplify when included in the matrix. This means that it is not always possible to recover the original reaction scheme from a stoichiometry matrix.

Often the stoichiometry matrix is combined with the rate vector,  $\mathbf{v}$ , and the species vector,  $\mathbf{x}$  to form a compact equation describing the rates of change of the molecular species:

$$\frac{d\mathbf{x}}{dt} = \mathbf{N} \cdot \mathbf{v}.$$

# **Gas stoichiometry**

Gas stoichiometry is the quantitative relationship (ratio) between reactants and products in a chemical reaction with reactions that produce gases. Gas stoichiometry applies when the gases produced are assumed to be <u>ideal</u>, and the temperature, pressure, and volume of the gases are all known. The ideal gas law is used for these calculations. Often, but not always, the <u>standard</u> temperature and pressure (STP) are taken as 0 °C and 1 bar and used as the conditions for gas stoichiometric calculations.

Gas stoichiometry calculations solve for the unknown <u>volume</u> or <u>mass</u> of a gaseous product or reactant. For example, if we wanted to calculate the volume of gaseous  $NO_2$  produced from the combustion of 100 g of  $NH_3$ , by the reaction:

$$4 \text{ NH}_3(g) + 7 \text{ O}_2(g) \rightarrow 4 \text{ NO}_2(g) + 6 \text{ H}_2\text{O(I)}$$

we would carry out the following calculations:

$$100\,\mathrm{g\,NH_3}\cdotrac{1\,\mathrm{mol\,NH_3}}{17.034\,\mathrm{g\,NH_3}}=5.871\,\mathrm{mol\,NH_3}$$

There is a 1:1 molar ratio of NH<sub>3</sub> to NO<sub>2</sub> in the above balanced combustion reaction, so 5.871 mol of NO<sub>2</sub> will be formed. We will employ the <u>ideal gas law</u> to solve for the volume at 0 °C (273.15 K) and 1 atmosphere using the gas law constant of R = 0.08206 L·atm·K<sup>-1</sup>·mol<sup>-1</sup>:

$$egin{aligned} PV &= nRT \ V &= rac{nRT}{P} \ &= rac{5.871 \cdot 0.08206 \cdot 273.15}{1} \ &= 131.597 \, \mathrm{L \, NO_2} \end{aligned}$$

Gas stoichiometry often involves having to know the <u>molar mass</u> of a gas, given the <u>density</u> of that gas. The ideal gas law can be re-arranged to obtain a relation between the <u>density</u> and the <u>molar mass</u> of an ideal gas:

$$ho = rac{m}{V}$$
 and  $n = rac{m}{M}$ 

and thus:

$$ho = rac{MP}{RT}$$

#### where:

- P = absolute gas pressure
- V = gas volume
- *n* = amount (measured in moles)
- R = universal ideal gas law constant
- *T* = absolute gas temperature
- $\rho$  = gas density at T and P
- $\blacksquare$  m = mass of gas
- *M* = molar mass of gas

### Stoichiometric air-to-fuel ratios of common fuels

In the <u>combustion</u> reaction, oxygen reacts with the fuel, and the point where exactly all oxygen is consumed and all fuel burned is defined as the stoichiometric point. With more oxygen (overstoichiometric combustion), some of it stays unreacted. Likewise, if the combustion is incomplete due to lack of sufficient oxygen, fuel remains unreacted. (Unreacted fuel may also remain because of slow combustion or insufficient mixing of fuel and oxygen – this is not due to stoichiometry). Different hydrocarbon fuels have different contents of carbon, hydrogen and other elements, thus their stoichiometry varies.

Fuel	Ratio by mass	Ratio by volume	Percent fuel by mass	Main reaction
Gasoline	14.7 : 1	_	6.8%	$2 C_8 H_{18} + 25 O_2 \rightarrow 16 CO_2 + 18 H_2 O$
Natural gas	17.2 : 1	9.7 : 1	5.8%	$CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$
Propane (LP)	15.67 : 1	23.9 : 1	6.45%	$C_3H_8 + 5 O_2 \rightarrow 3 CO_2 + 4 H_2O$
Ethanol	9:1	_	11.1%	$C_2H_6O + 3 O_2 \rightarrow 2 CO_2 + 3 H_2O$
Methanol	6.47 : 1	_	15.6%	2 CH <sub>4</sub> O + 3 O <sub>2</sub> → 2 CO <sub>2</sub> + 4 H <sub>2</sub> O
<i>n</i> -Butanol	11.2 : 1	_	8.2%	$C_4H_{10}O + 6 O_2 \rightarrow 4 CO_2 + 5 H_2O$
Hydrogen	34.3 : 1	2.39 : 1	2.9%	2 H <sub>2</sub> + O <sub>2</sub> → 2 H <sub>2</sub> O
Diesel	14.5 : 1	_	6.8%	$2 C_{12}H_{26} + 37 O_2 \rightarrow 24 CO_2 + 26 H_2O$
Methane	17.19 : 1	9.52 : 1	5.5%	$CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$
Acetylene	13.26 : 1	11.92 : 1	7.0%	2 C <sub>2</sub> H <sub>2</sub> + 5 O <sub>2</sub> → 4 CO <sub>2</sub> + 2 H <sub>2</sub> O
Ethane	16.07 : 1	16.68 : 1	5.9%	2 C <sub>2</sub> H <sub>6</sub> + 7 O <sub>2</sub> → 4 CO <sub>2</sub> + 6 H <sub>2</sub> O
Butane	15.44 : 1	30.98 : 1	6.1%	$2 C_4H_{10} + 13 O_2 \rightarrow 8 CO_2 + 10 H_2O$
Pentane	15.31 : 1	38.13 : 1	6.1%	$C_5H_{12} + 8 O_2 \rightarrow 5 CO_2 + 6 H_2O$

Gasoline engines can run at stoichiometric air-to-fuel ratio, because gasoline is quite volatile and is mixed (sprayed or carburetted) with the air prior to ignition. Diesel engines, in contrast, run lean, with more air available than simple stoichiometry would require. Diesel fuel is less volatile and is effectively burned as it is injected. [12]

### See also

Non-stoichiometric compound

#### References

- 1. Richter, J.B. (1792). Anfangsgründe der Stöchyometrie ... (in 3 vol.s) (https://books.google.com/books?id=NhFQAAAAcAAJ&pg=RA1-PA121) [Rudiments of Stoichiometry ...] (in German). vol. 1. Breslau and Hirschberg, (Germany): Johann Friedrich Korn der Aeltere. p. 121. From p. 121: "Die Stöchyometrie (Stöchyometria) ist die Wissenschaft die quantitativen oder Massenverhältnisse ... zu messen, in welchen die chemischen Elemente ... gegen einander stehen." (Stoichiometry (stoichiometria) is the science of measuring the quantitative or mass relations in which the chemical "elements" exist in relation to each other.) [Note: On pp. 3–7, Richter explains that an "element" is a pure substance, and that a "chemical element" (chymisches Element (Elementum chymicum)) is a substance that cannot be resolved into dissimilar substances by known physical or chemical means. Thus, for example, aluminium oxide was a "chemical element" because in Richter's time, it couldn't be resolved further into its component elements.]
- 2. What's in a Name? Amount of Substance, Chemical Amount, and Stoichiometric Amount Carmen J. Giunta Journal of Chemical Education 2016 93 (4), 583-586 <a href="mailto:doi:10.1021/acs.jchemed.5b00690">doi:10.1021/acs.jchemed.5b00690</a> (https://doi.org/10.1021%2Facs.jchemed.5b00690)
- 3. IUPAC, <u>Compendium of Chemical Terminology</u>, 2nd ed. (the "Gold Book") (1997). Online corrected version: (2006–) "<u>stoichiometric number</u>, <u>v</u> (https://goldbook.iupac.org/S06025.html)". doi:10.1351/goldbook.S06025 (https://doi.org/10.1351%2Fgoldbook.S06025)
- 4. Nijmeh, Joseph; Tye, Mark (2 October 2013). "Stoichiometry and Balancing Reactions" (https://chem.libretexts.org/Bookshelves/Inorganic\_Chemistry/Modules\_and\_Websites\_(Inorganic\_Chemistry)/Chemical\_Reactions/Stoichiometry\_and\_Balancing\_Reactions#:~:text=The%20stoichiometric%20coefficient%20is%20the,product%20sides%20of%20the%20equation.). LibreTexts. Retrieved 5 May 2021.
- 5. Prigogine & Defay, p. 18; Prigogine, pp. 4-7; Guggenheim, p. 37 & 62
- IUPAC, Compendium of Chemical Terminology, 2nd ed. (the "Gold Book") (1997). Online corrected version: (2006–) "extent of reaction, ξ (https://goldbook.iupac.org/E02283.html)". doi:10.1351/goldbook.E02283 (https://doi.org/10.1351%2Fgoldbook.E02283)
- 7. Ghaderi, Susan; Haraldsdóttir, Hulda S.; Ahookhosh, Masoud; Arreckx, Sylvain; Fleming, Ronan M.T. (August 2020). "Structural conserved moiety splitting of a stoichiometric matrix" (https://doi.org/10.1016%2Fj.jtbi.2020.110276). Journal of Theoretical Biology. 499: 110276. doi:10.1016/j.jtbi.2020.110276 (https://doi.org/10.1016%2Fj.jtbi.2020.110276). PMID 32333975 (https://pubmed.ncbi.nlm.nih.gov/32333975).
- 8. Hofmeyr, Jan-hendrik S. (2001). "Metabolic control analysis in a nutshell" (https://citeseerx.ist.ps u.edu/viewdoc/summary?doi=10.1.1.324.922&rank=1). In Proceedings of the 2 Nd International Conference on Systems Biology: 291–300. CiteSeerX 10.1.1.324.922 (https://citeseerx.ist.psu.ed u/viewdoc/summary?doi=10.1.1.324.922).
- 9. Reder, Christine (21 November 1988). "Metabolic control theory: A structural approach". *Journal of Theoretical Biology*. **135** (2): 175–201. doi:10.1016/s0022-5193(88)80073-0 (https://doi.org/10.1016%2Fs0022-5193%2888%2980073-0). PMID 3267767 (https://pubmed.ncbi.nlm.nih.gov/3267767).
- 10. John B. Heywood: "Internal Combustion Engine Fundamentals page 915", 1988
- 11. North American Mfg. Co.: "North American Combustion Handbook", 1952
- 12. "Air-fuel ratio, lambda and engine performance" (https://x-engineer.org/automotive-engineering/int ernal-combustion-engines/performance/air-fuel-ratio-lambda-engine-performance/). Retrieved 2019-05-31.
  - Zumdahl, Steven S. *Chemical Principles*. Houghton Mifflin, New York, 2005, pp 148–150.
  - Internal Combustion Engine Fundamentals, John B. Heywood

### **External links**

- Engine Combustion primer (https://web.archive.org/web/20070206060439/http://www.tech.plym.a c.uk/sme/ther305-web/Combust1.PDF) from the University of Plymouth
- Free Stoichiometry Tutorials (http://www.chemcollective.org/tutorials.php) from Carnegie Mellon's ChemCollective
- Stoichiometry Add-In for Microsoft Excel (http://chemistry-in-excel.jimdo.com/) for calculation of molecular weights, reaction coëfficients and stoichiometry.
- Reaction Stoichiometry Calculator (http://www.thermobook.net/stoichiometry/) a comprehensive free online reaction stoichiometry calculator.
- Stoichiometry Plus (https://play.google.com/store/apps/details?id=net.thermobook.thermostoichiometryplus) a stoichiometry calculator and more for Android.

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