Combustion

Combustion is a chemical reaction in which certain element of the fuel combine with oxygen and releasing a large quantity of energy causing an increase in temperature of gases. There are many thousands of different hydrocarbon fuel components, which consist mainly of hydrogen and carbon but may also contain oxygen, nitrogen, and/or sulphur, etc. The main combustible elements are carbon and hydrogen; another combustible element often present in fuels, although rather undesirable, is sulphur. Except this, combustible of solid and liquid fuels consists of passive elements N and O.

The oxygen necessary for combustion is obtained from air, which is oxygen diluted chiefly by nitrogen. Table gives proportion of oxygen and nitrogen by volume of dry air. In combustion, oxygen is the reactive component of air. The properties of air vary geographically, with altitude and with time.

Gas	Volume %
O_2	21.00
N_2	78.05
A	0.92
CO_2	0.03
Dry air	100.00

Direct combustion by atmospheric oxygen is a reaction mediated by radical intermediates. The conditions for radical production are naturally produced by thermal runaway, where the heat generated by combustion is necessary to maintain the high temperature necessary for radical production. In a complete combustion reaction, a compound reacts with oxygen, and the products are oxydes of each combustible element in the fuel. A simpler example can be seen in the combustion of carbon and oxygen. The result is simply CO_2.

$$\mathbf{C} + \mathbf{O_2} \rightarrow \mathbf{CO_2} + \textbf{heat}$$

The objective of combustion is to retrieve energy from the burning of fuels in the most efficient way possible. To maximize combustion efficiency, it is necessary to burn all fuel material with the least amount of losses. The more efficiently fuels are burned and energy is gathered, the cheaper the combustion process becomes.

Complete Combustion

Complete combustion occurs when all combustible 100% of the energy in the fuel is extracted. It is important to strive for complete combustion to preserve fuel and improve the cost efficiency of the combustion process. There must be enough air in the combustion chamber for complete combustion to occur. The balance of complete combustion of carbon in solid state is as follows

C	+	$\mathbf{O_2}$	→	$\mathbf{CO_2}$	**+ heat**
1 kmol		1 kmol		1 kmol	
12.01 kg		22.39 Nm^3		22.27 Nm^3	
1 kg		$\frac{22.39}{12.01} Nm^3$		$\frac{22.27}{12.01} Nm^3$	+ 33828,5 kJ/kg of Carbon

Necessary volume of oxygen in normal m^3 (Nm^3) for complete combustion of 1 kg of carbon and resulted volume of CO_2 can be evaluated from this balance. Similar balances for combustion of H and S is possible to write:

$\mathbf{2H_2}$	+	$\mathbf{O_2}$	→	$\mathbf{2H_2O}$	**+ heat**
2 kmol		1 kmol		2 kmol	
4.032 kg		22.39 Nm^3		44.81 Nm^3	
1 kg		$\frac{22.39}{4.032} Nm^3$		$\frac{44.81}{4.032} Nm^3$	121094 kJ/kg of Hydrogen

S	+	$\mathbf{O_2}$	→	$\mathbf{SO_2}$	**+ heat**
1 kmol		1 kmol		1 kmol	
32.06 kg		22.39 Nm^3		21.89 Nm^3	
1 kg		$\frac{22.39}{32.06} Nm^3$		$\frac{22.89}{32.06} Nm^3$	9312 kJ/kg of Sulphur

Complete stoichiometric combustion

The maximum amount of chemical energy that can be released (heat) from the fuel is when it reacts (combust) with a minimal necessary (=stoichiometric) amount of oxygen. Stoichiometric oxygen (sometimes also called theoretical oxygen) is just enough to burn all combustible in the fuel with no oxygen left over.

Stoichiometric calculations for complete combustion of solid and liquid fuels

Stoichiometry calculations can predict volume of necessary air for combustion of 1kg of fuel and volume and composition of resulted flue gas.

Volume of oxygen necessary for complete combustion of 1 kg of fuel is possible evaluate with use of above mentioned balances as follows

$$V_{O_2\,\min} = 22{,}39 \cdot \left(\frac{C^r}{12{,}01} + \frac{H^r}{4{,}032} + \frac{S^r}{32{,}06} - \frac{O^r}{32} \right) \quad [\mathrm{Nm^3/kg}]$$

It is assumed that oxygen contained in combustible of fuel takes part in oxidant reactions, therefore the volume of air oxygen is proportionally reduced.

Volume of dry air necessary for complete combustion of 1 kg of fuel is

$$V_{DA\min} = \frac{V_{O_2\,\min}}{0{,}21} \quad [\mathrm{Nm^3/kg}]$$

Share of vapor falling on 1 Nm^3 of dry aid can be quantified by coefficient χ_v [-] which can be calculated by following equation

$$\chi_v = 1 + \frac{\varphi}{100} \cdot \frac{p''}{p_t - \frac{\varphi}{100} \cdot p''} \quad [-] \qquad (0.1)$$

where φ [%] je relative air humidity, p'' [MPa] is partial pressure of saturated vapor for air temperature t_a by following table and p_t [MPa] is total pressure which usually is 0,1 MPa.

t_a [°C]	0	10	20	30	40	50
p'' [MPa]	0,000 610 8	0,001 227 7	0,002 336 8	0,004 241 6	0,007 374 2	0,012 331 6

In design practice χ_v = 1,016 is commonly used. The value is related to φ = 70% and t_a = 20°C.

Then volume of humid air necessary for complete combustion of 1 kg of fuel is

$$V_{HA\min} = \chi_v \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}]$$

and volume of vapor in air is

$$V_{H_2O}^{A} = V_{HA\min} - V_{DA\min} = (\chi_v - 1) \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}]$$

Volume of flue gas resulted from combustion with necessary air can be evaluated similarly. Stoichiometric flue gas from complete combustion of fuel consists from combustion products and gases from combustion air except the oxygen which was completely consumed within combustion process.

Volume of dry flue gas from complete combustion of 1 kg of fuel is

$$V_{DFG\min} = V_{CO_2} + V_{SO_2} + V_{N_2} + V_{Ar} \quad [\mathrm{Nm^3/kg}]$$

Volumes of components in dry flue gas are

$$V_{CO_2} = \frac{22{,}26}{12{,}01} \cdot C^r + 0{,}0003 \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}$$

$$V_{SO_2} = \frac{21{,}89}{32{,}06} \cdot S^r \quad [\mathrm{Nm^3/kg}]$$

$$V_{N_2} = \frac{22{,}4}{28{,}016} \cdot N^r + 0{,}7805 \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}]$$

$$V_{Ar} = 0{,}0092 \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}]$$

Volume of vapor in flue gas consists from combustion of hydrogen, vaporized water form fuel and from air humidity

$$V_{H_2O}^{FG} = \frac{44,8}{4,032} \cdot H^r + \frac{22,4}{18,016} \cdot W^r + V_{H_2O}^{A} \quad [\mathrm{Nm^3/kg}]$$

Volume of humid stoichiometric flue gas from complete combustion of 1 kg of fuel is

$$V_{HFG\,\min} = V_{DFG\,\min} + V_{H_2O}^{FG} \quad [\mathrm{Nm^3/kg}]$$

Excess Air Factor

The stochiometric air would completely combust the fuel to CO_2, H_2O and SO_2. If the fuel does not get enough air for combustion, it will be incomplete, generate smoke and a potential unhealthy mixture of stack gas products. If too much air is used for combustion the heat loss in flue gas leaving a boiler increases. A less trivial issue in combustion technology is therefore to ensure the proper amount of air that minimizes environmental impact and fuel consumption. For convenience we define the excess air factor as the ratio of the actual volume of air, in which fuel is burned, to the volume required for complete combustion of fuel (stoichiometric air):

$$\lambda = \frac{V_{HA}}{V_{HA\min}} = \frac{V_{DA}}{V_{DA\min}} \quad [-]$$

In order to obtain complete combustion, it is usually necessary to provide more air than it is apparent from the stoichiometric equations. For instance saying a burner requires 20 % excess air to correctly combust fuel oil, is the same as saying the burner operates at an excess air factor of 1.2. A ideal combustion process would require 0 % excess air or has an excess air factor of 1. A combustion process requiring 100 % excess air uses twice as much air as necessary, or in other words has an excess air factor of two.
Most modern fuel efficient cars have therefore Lambda sensors (= Oxygen sensors) to control the fuel efficiency. In boilers and furnaces they are called an "oxygen trim".
As mentioned, the excess air factor of a burner furnace or boiler is depends on fuel, combustion technology as well as the skill of the operator. Standard average figures are

- Gas burners, forced draft 1.1 - 1.3
- Atmospheric gas burners 1.25 - 1.5
- Oil burners 1.15 - 1.3
- Coal dust burners 1.15 - 1.3
- Coal grate firing (mechanical) 1.2 - 1.5
- Coal grate firing (hand) 1.5 - 2.5

These are best values that can be achieved with careful monitoring and constant adjustment of the combustion air at varying loads. In reality energy auditors may see much higher numbers.

Volume of humid flue gas resulted from complete combustion with air excess is

$$V_{HFG} = V_{HFG\,\min} + (\lambda - 1) \cdot V_{HA\min} \quad [\mathrm{Nm^3/kg}]$$

Derivation of excess air factor

The amount of excess air can not be measured directly, but is rather derived from a measurement of either the O_2 or CO_2 content of the stack gas. Whether one measures O_2 or CO_2 is irrelevant for the calculation of the excess air, or λ, as long as one has obtained an accurate measurement of either O_2 or CO_2. Various sensors and methods exist to measure O_2 or CO_2. There is no simply and also accurate equation to calculate λ if O_2 or CO_2 is known. The correct equation based on a CO_2 measurement is

$$\lambda = 1 + \left(\frac{\mathrm{CO_{2\,max}}}{\mathrm{CO_2}} - 1 \right) \cdot \frac{\mathrm{V_{DFG\,min}}}{\mathrm{V_{DA\,mim}}}$$

where $CO_{2\,max}$ is the maximum CO_2 content of the dry flue gas at stochiometric combustion given in volume %

The equation based on a O_2 measurement is

$$\lambda = \frac{21 + \left(\frac{V_{DFG\min}}{V_{DA\min}} - 1 \right) \cdot O_{O_2}}{21 - O_{O_2}}$$

It is best to calculate λ as a function of either O_2 or CO_2 in the flue gas by computer software. The factor f = $\frac{V_{DFG\ \min}}{V_{DA\ \min}}$ is between 0.93 to 0.97 for fuel oils, between 0.98 and 1 for solid fuels and between 0.9 and 1.9 for gases. One should appreciate the complexity involved, that has resulted in quite a number of simplistic equations. Most commonly used equations are

$$\lambda = \frac{CO_{2\max}}{CO_2}$$

$$\lambda = \frac{21}{21 - O_2}$$

Stoichiometric calculations for complete combustion of gaseous fuels

Composition of gaseous fuels is done by volume fractions v_i of component gases. Stoichiometric volumes are related to 1 Nm^3 of combusted gas. Various hydrocarbons contained in gaseous fuel will be generally described by formula C_mH_n, where m is the number of carbon atoms and n is the number of hydrogen atoms in hydrocarbon.

Volume of oxygen necessary for complete combustion of 1 Nm^3 of gas is possible evaluate as follows

$$V_{O_2\min} = 0{,}5 \cdot v_{H_2} + 0{,}5 \cdot v_{CO} + \sum \left(m + \frac{n}{4} \right) \cdot v_{C_mH_n} - v_{O_2} \quad [Nm^3/Nm^3]$$

Volume of dry air necessary for complete combustion of 1 Nm^3 of gas is

$$V_{DA\min} = \frac{V_{O_2\min}}{0{,}21} \quad [Nm^3/Nm^3],$$

volume of humid air is

$$V_{HA\min} = \chi_v \cdot V_{DA\min} \quad [Nm^3/Nm^3]$$

and volume of vapor in air is

$$V_{H_2O}^A = V_{HA\min} - V_{DA\min} = (\chi_v - 1) \cdot V_{DA\min} \quad [Nm^3/Nm^3]$$

Volume of dry flue gas from complete combustion of 1 kg of fuel is

$$V_{DFG\min} = V_{CO_2} + V_{SO_2} + V_{N_2} + V_{Ar} \quad [Nm^3/Nm^3]$$

Volumes of components in dry flue gas are

$$V_{CO_2} = v_{CO_2} + 0{,}994 \cdot \left(v_{CO} + \sum m \cdot v_{C_mH_n} \right) + 0{,}0003 \cdot V_{DA\min} \quad [Nm^3/Nm^3]$$

$$V_{SO_2} = v_{SO_2} \quad [Nm^3/Nm^3]$$

$$V_{N_2} = v_{N_2} + 0{,}7805 \cdot V_{DA\min} \quad [Nm^3/Nm^3]$$

$$V_{Ar} = v_{Ar} + 0{,}0092 \cdot V_{DA\min} \quad [Nm^3/Nm^3]$$

Volume of vapor in flue gas consists from combustion of hydrogen, vapor form fuel and from air humidity

$$V_{H_2O}^{FG} = v_{H_2O} + v_{H_2} + \sum \frac{n}{2} \cdot v_{C_mH_n} + V_{H_2O}^{A} \quad [\mathrm{Nm^3/Nm^3}]$$

Volume of humid stoichiometric flue gas from complete combustion of 1 kg of fuel is

$$V_{HFG\,\min} = V_{DFG\,\min} + V_{H_2O}^{FG} \quad [\mathrm{Nm^3/Nm^3}]$$

Volume of humid flue gas resulted from complete combustion with air excess is

$$V_{HFG} = V_{HFG\,\min} + (\lambda - 1) \cdot V_{HA\min} \quad [\mathrm{Nm^3/Nm^3}]$$

Incomplete combustion of solid fuels

When too little air is supplied to the boiler, there is not enough oxygen to completely form CO_2 with all the carbon in the fuel. Instead, some part of carbon marked as *a* does not burn and some part of carbon marked as *b* combines with oxygen to form carbon monoxide (CO). Unburned carbon increases mass of solid residues after combustion (ash, sludge, fly ash). CO is a highly toxic gas associated with incomplete combustion and efforts must be made to minimize its formation. Incomplete combustion decrease efficiency of fuel utilization.
Incomplete combustion of carbon to CO is described by following balance:

C	**+**	**1/2 O_2**	**→**	**CO_2**	**+ heat**
1 kmol		1/2 kmol		1 kmol	
12.01 kg		$\frac{22.39}{2}$ Nm^3		22.40 Nm^3	
1 kg		$\frac{22.39}{2 \cdot 12.01}$ Nm^3		$\frac{22.40}{12.01}$ Nm^3	+ 10334 kJ/kg of Carbon

Incomplete combustion results in change od stoichiometric flue gas composition. Volume of CO_2 decreases and CO and O_2 as new components appear. These changes are described as follows

$$V_{CO_2}^{i} = (1 - a - b) \cdot \frac{22{,}26}{12{,}01} \cdot C^r + 0{,}0003 \cdot V_{DA\min} \quad [\mathrm{Nm^3/kg}]$$

$$V_{CO}^{i} = b \cdot \frac{22{,}40}{12{,}01} \cdot C^r \quad [\mathrm{Nm^3/kg}]$$

$$V_{O_2}^{i} = \left(a + \frac{b}{2} \right) \cdot \frac{22{,}39}{12{,}01} \cdot C^r \quad [\mathrm{Nm^3/kg}]$$

Volume of dry flue gas from incomplete combustion of 1 kg of fuel with stoichiometric air is

$$V_{DFG\,\min}^{i} = V_{CO_2}^{i} + V_{SO_2} + V_{N_2} + V_{Ar} + V_{CO}^{i} + V_{O_2}^{i} \quad [\mathrm{Nm^3/kg}]$$

Difference in flue gas volumes from complete and incomplete combustion is negligible and it is not necessary to take it into account.