Combustion

It is a rapid chemical reaction between fuel and oxygen, it is usually accompanied by a flame, heat is released during the reaction (exothermic reaction).

- Combustion may be classified to:
  - Complete combustion.
  - Incomplete combustion.
  - Stoichiometric (theoretical) combustion.

1. Complete Combustion:

This type of combustion occurs when the amount of air (oxygen) available is more or enough to convert all carbon to carbon dioxide (CO_2).

Example:

$$C + O_2 \longrightarrow CO_2$$

$$CH_4 + 3\,O_2 \longrightarrow CO_2 + 2\,H_2O + O_2$$

2. Incomplete Combustion:

This combustion occurs when the amount of air (oxygen) available is not enough to convert all carbon to carbon dioxide, therefore a carbon monoxide (CO) is present in the product as a result of incomplete combustion.

Example:

$$C + \frac{1}{2}\,O_2 \longrightarrow CO$$

$$CH_4 + d\,O_2 \longrightarrow a\,CO_2 + b\,CO + 2\,H_2O$$

3. Stoichiometric Combustion:

This combustion occurs when the amount of air (oxygen) available is just enough to convert all carbon in the fuel to CO_2, with no oxygen left over.

Example:

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

$$C_8H_{18} + 12.5O_2 \longrightarrow 8CO_2 + 9H_2O$$

The maximum amount of chemical energy (heat) that can be released from the fuel is when it reacts stoichiometric amount of oxygen.

Fuel:

Fuel may be solid, liquid or gas, solid such as coal, wood, ….etc. , liquid such as benzene, gasoil ….etc. , gases such as natural gas and methane … etc.

Chemical Equation:

It shows how the atoms of the reactants are arranged to form the products. It expresses the principle of conservation of mass. It can be written in the form of atoms, mass, mole and volume.

Reactants				***Products***
C	+	O_2	$\longrightarrow$	CO_2
1 atom		2 atom		3 atom
12 kg		32 kg		44 kg
1 mole		1 mole		1 mole
0 volume		1 volume		1 volume

Note: Volume of solid is normally neglected compared with gases volume.

It will be assumed that (N_2) does not react hence it appears on both sides of the equation.

Molecular Weight:

Molecular weights for basic elements can be found in following table:

Substance		Molecular weights (kg/kg.mole)
Air		
Carbon	C	12
Carbon Monoxide	CO	28
Carbon Dioxide	CO_2	44
Hydrogen	H_2	2
Water vapor	H_2O	18
Nitrogen	N_2	28
Oxygen	O_2	32

Composition of Air:

The following composition of air is used:

Type of Analysis	$\mathbf{O_2}$	$\mathbf{N_2}$
Volumetric(Molar) Analysis	21 %	79 %
Mass(Gravimetric) Analysis	23.3 %	76.7 %

∴ One mole of air consist of 0.21 mole of O_2 and 0.79 mole of N_2 . Also one kg of air consist of 0.233 kg of O_2 and 0.767 kg of N_2 .

Example:

$$C + O_2 + 1\times\frac{79}{21}N_2 \longrightarrow CO_2 + 1\times\frac{79}{21}N_2$$

$$H_2 + \frac{1}{2}O_2 + \frac{1}{2}\times\frac{79}{21}N_2 \longrightarrow H_2O + \frac{1}{2}\times\frac{79}{21}N_2$$

Air – Fuel Ratio:

It is the ratio of the amount of the air used in combustion to the amount of fuel burnt. A mixture which has excess air is called "Weak Mixture" and one which has less air is called "Rich Mixture".

$$A/F = \frac{m_a}{m_f} = \frac{\dot{m}_a}{\dot{m}_f}$$

Mixture Strength(Equivalence Ratio), $\emptyset = \frac{stoichiometric\ A/F\ ratio}{actual\ A/F\ ratio}$

$\emptyset = 1$ Stoichiometric Mixture (maximum energy released from fuel).

$\emptyset <$ Weak (lean) Mixture (excess air, oxygen in exhaust).

$\emptyset > 1$ Rich Mixture (less air, CO and fuel in exhaust).

<u>Dissociation:</u>

Chemical phenomenon takes place at high engine temperatures that affects the overall combustion process in the engine and dissociate the stable components through the combustion to another components, such as CO_2 dissociates to CO and O, O_2 dissociates to monatomic O, N_2 dissociates to monatomic N, .. etc.

Even when the flow of air and fuel into an engine is controlled exactly at stoichiometric conditions, combustion will not be "perfect," and components other than CO_2, H_2O, and N_2 are found in the exhaust products. Major reasons for this are: **1.** Extremely short time available for each engine cycle, which often means that less than complete mixing of the air and fuel is obtained. Some fuel molecules do not find an oxygen molecule to react with, and small quantities of both fuel and oxygen end up in the exhaust. **2.** Dissociation phenomenon, occur to dissociate some quantities of CO_2 to CO and O, N_2 to N then react with O to form nitrogen oxides, NO and NO_2, a major pollutant from automobiles.

Example:

Find the stoichiometric A/F ratio of ethyl-Alcohol (C_2H_6O) in a petrol engine, and calculate the actual A/F ratio for the mixture strength of 90% and 120% .

Solution:

Stoichiometric combustion equation is:

$$C_2H_6O + 3(O_2 + \frac{79}{21} N_2) \longrightarrow 2CO_2 + 3H_2O + 3\times\frac{79}{21} N_2$$

mass of fuel = 2×12 + 6×1 + 16 = 46 kg

O_2 required = 3×32 = 96 kg

air required = $\frac{96}{0.233}$ = 412 kg   or   air required = $3\times32+3\times\frac{79}{21}\times28$ = 412 kg

$\therefore$ stoichiometric A/F ratio $= \frac{412}{46} = 8.96$

$$\emptyset = \frac{stoichiometric\ A/F\ ratio}{actual\ A/F\ ratio}$$

$\emptyset$ = 90% = 0.9

$$(actual\ A/F\ ratio) = \frac{stoichiometric\ \ A/F\ \ ratio}{\emptyset} = \frac{8.96}{0.9} = 9.95$$

$\emptyset$ = 120% = 1.2

$$(actual\ A/F\ ratio) = \frac{8.96}{1.2} = 7.46$$

Combustion – Problems

Q1/ An internal combustion engine is fuelled with hexane (C_6H_{14}). Calculate the gravimetric exhaust analysis when the air-fuel ratio is:

A- 16:1, **B-**14:1, **C-** Stoichiometric.

Q2/ An internal combustion engine is fuelled with heptane (C_7H_{16}). Calculate:

1- The stoichiometric air-fuel ratio.
2- The volumetric exhaust analysis when 20 % excess air is used.
3- The volumetric and gravimetric analysis when 10 % less air is used.

Q3/ The four-cylinder engine of a light truck owned by a utility company has been converted to run on propane fuel (C_3H_8). A dry analysis of the engine exhaust gives the following volumetric percentages: CO_2=4.9%, CO=9.79% , O_2=2.45% . Calculate the mixture strength at which the engine is operating.

Q4/ Isooctane (C_8H_{18}) is burned with 120 % theoretical air in a small three cylinder turbocharged automobile engine. Calculate: 1- Air/Fuel ratio, 2- Fuel/Air ratio, 3- Equivalence ratio.

Q5/ A taxicab is equipped with a flexible-fuel four-cylinder SI engine running on a mixture of methanol(CH_3OH) and gasoline(C_8H_{15}) at an equivalence ratio of 0.95. How must the air-fuel ratio change as the fuel flow to the engine shifts from 10 % methanol (M10) to 85 % methanol (M85).

Combustion – Problems

Q1/ The four-cylinder engine of a light truck owned by a utility company has been converted to run on propane fuel (C_3H_8). A dry analysis of the engine exhaust gives the following volumetric percentages: CO_2=4.9%, CO=9.79% , O_2=2.45% . Calculate the mixture strength at which the engine is operating.

Calculate the equivalence ratio at which the engine is operating. The three components identified sum up to 4.90 + 9.79 + 2.45 = 17.14% of the total, which means that the remaining gas (nitrogen) accounts for 82.86% of the total. Volume percent equals molar percent, so if an unknown amount of fuel is burned with an unknown amount of air, the resulting reaction is:

$$x\,C_3H_8 + y\,O_2 + y(3.76)\,N_2 \rightarrow 4.90\,CO_2 + 9.79\,CO + 2.45\,O_2 + 82.86\,N_2 + z\,H_2O$$

where: z = number of moles of water vapor removed before dry analysis

Conservation of nitrogen during reaction gives:

$$y(3.76) = 82.86 \quad \text{or} \quad y = 22.037$$

Conservation of carbon:

$$3x = 4.90 + 9.79 \quad \text{or} \quad x = 4.897$$

Conservation of hydrogen:

$$8x = 8(4.897) = 2z \quad \text{or} \quad z = 19.588$$

The reaction is:

$$4.90\,C_3H_8 + 22.037\,O_2 + 22.037(3.76)\,N_2 \rightarrow$$
$$4.90\,CO_2 + 9.79\,CO + 2.45\,O_2 + 82.86\,N_2 + 19.588\,H_2O$$

Dividing by 4.90:

$$C_3H_8 + 4.50\,O_2 + 4.50(3.76)N_2 \rightarrow CO_2 + 2\,CO + 0.50\,O_2 + 16.92\,N_2 + 4\,H_2O$$

Actual air–fuel ratio:

$$AF_{act} = m_a/m_f = [(4.50)(4.76)(29)]/[(1)(44)] = 14.12$$

Stoichiometric combustion:

$$C_3H_8 + 5\,O_2 + 5(3.76)\,N_2 \rightarrow 3\,CO_2 + 4\,H_2O + 5(3.76)\,N_2$$

Stoichiometric air–fuel ratio:

$$AF_{stoich} = m_a/m_f = [(5)(4.76)(29)]/[(1)(44)] = 15.69$$

Equivalence ratio using Eq. (4-2):

$$\phi = (AF)_{stoich}/(AF)_{act} = 15.69/14.12 = \underline{1.11}$$

Q2/ Isooctane (C_8H_{18}) is burned with 120 % theoretical air in a small three cylinder turbocharged automobile engine. Calculate: 1- Air/fuel ratio, 2- fuel/air ratio, 3- Equivalence ratio

Isooctane is burned with 120% theoretical air in a small three-cylinder turbocharged automobile engine.
Calculate:

1. air–fuel ratio
2. fuel–air ratio
3. equivalence ratio

Stoichiometric reaction:

$$C_8H_{18} + 12.5\,O_2 + 12.5(3.76)\,N_2 \rightarrow 8\,CO_2 + 9\,H_2O + 12.5(3.76)\,N_2$$

With 20% excess air:

$$C_8H_{18} + 15\,O_2 + 15(3.76)\,N_2 \rightarrow 8\,CO_2 + 9\,H_2O + 15(3.76)\,N_2 + 2.5\,O_2$$

With 20% excess air, all the fuel gets burned, and the same amount of CO_2 and H_2O is found in the products. In addition, there is some oxygen and additional nitrogen in the products (the excess air).

1) Equations (2-55) and (4-1) are used to find the air–fuel ratio:

$$AF = m_a/m_f = N_a M_a / N_f M_f = [(15)(4.76)(29)]/[(1)(114)]$$

$$= \underline{18.16}$$

2) Equation (2-56) is used to find fuel–air ratio:

$$FA = m_f/m_a = 1/AF = 1/18.16 = \underline{0.055}$$

3) Fuel–air ratio of stoichiometric combustion:

$$(FA)_{stoich} = [(1)(114)]/[(12.5)(4.76)(29)] = 0.066$$

Equivalence ratio is obtained using Eq. (4-2):

$$\phi = (FA)_{act}/(FA)_{stoich} = (0.055)/(0.066) = \underline{0.833}$$

Q3/ A taxicab is equipped with a flexible-fuel four-cylinder SI engine running on a mixture of methanol(CH_3OH) and gasoline(C_8H_{15}) at an equivalence ratio of 0.95. How must the air-fuel ratio change as the fuel flow to the engine shifts from 10 % methanol (M10) to 85 % methanol (M85).

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Change masses of fuel to moles at M10:

FUEL	MASS, m (kg)	MOLECULAR WEIGHT, M	MOLES $N = m/M$ (kgmoles)	MOLE FRACTION
CH_3OH	0.10	32	0.003125	0.278
C_8H_{15}	0.90	111	0.008108	0.722
	1.00		0.011233	1.000

For one kgmole of fuel reacting with stoichiometric air:

$$0.278\ CH_3OH + 0.722\ C_8H_{15} + 8.9005\ O_2 + 8.9005(3.76)\ N_2 \rightarrow$$
$$6.054\ CO_2 + 5.971\ H_2O + 8.9005(3.76)\ N_2$$

For one kgmole of fuel reacting with an equivalence ratio $\phi = 0.95$:

$$0.278\ CH_3OH + 0.722\ C_8H_{15} + (8.9005/0.95)\ O_2 + (8.9005/0.95)(3.76)\ N_2$$
$$\rightarrow 6.054\ CO_2 + 5.971\ H_2O + (8.9005/0.95)(3.76)\ N_2 + 0.468\ O_2$$

Air–fuel ratio:

$$AF = m_a/m_f$$
$$= [(8.9005/0.95)(1 + 3.76)(29)]/[(0.278)(32) + (0.722)(111)]$$
$$= 14.53$$

Repeating calculations for M85:

FUEL	MASS, m (kg)	MOLECULAR WEIGHT, M	MOLES $N = m/M$ (kgmoles)	MOLE FRACTION
CH_3OH	0.85	32	0.026563	0.952
C_8H_{15}	0.15	111	0.001351	0.048
	1.00		0.027914	1.000

Stoichiometric reaction:

$$0.952\ CH_3OH + 0.048\ C_8H_{15} + 1.992\ O_2 + 1.992(3.76)\ N_2 \rightarrow$$
$$1.336\ CO_2 + 2.264\ H_2O + 1.992(3.76)\ N_2$$

Reaction with an equivalence ratio $\phi = 0.95$:

$$0.952\ CH_3OH + 0.048\ C_8H_{15} + (1.992/0.95)\ O_2 + (1.992/0.95)(3.76)\ N_2$$
$$\rightarrow 1.336\ CO_2 + 2.264\ H_2O + (1.992/0.95)(3.76)\ N_2 + 0.105\ O_2$$

Air–fuel ratio:

$$AF = m_a/m_f$$

$$= [(1.992/0.95)(1 + 3.76)(29)]/[(0.952)(32) + (0.048)(111)]$$

$$\underline{= 8.09}$$

As the fuel flow composition is changed, the engine management system (EMS) must adjust the AF from 14.53 to 8.09.

Q4/ C_4H_2 is burned in an engine with a fuel-rich air-fuel ratio. Dry analysis of the exhaust gives the following volume percentages: CO_2 = 14.95%, C_4H_2 = 0.75%, CO = 0%, H_2 = 0%, O_2 = 0%, with the rest being N_2. Higher heating value of this fuel is QHHV = 46.9 MJ/kg. Write the balanced chemical equation for one mole of this fuel at these conditions.

Calculate:

(a) Air-fuel ratio.

(b) Equivalence ratio.

(c) Lower heating value of fuel. [MJ/kg]

(d) Energy released when one kg of this fuel is burned in the engine with a combustion efficiency of 98%. [MJ]