

UNIT -5

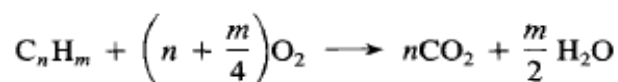
COMBUSTION & ANALYSIS

Stoichiometry - calculation of theoretically correct air required for combustion of liquid and gaseous fuels, volumetric and gravimetric analysis of the dry products of combustion, mass of dry gas per kg of fuel burnt, mass of carbon in the exhaust gas, mass of carbon burnt to carbon-monoxide per kg of fuel, heat loss due to incomplete combustion, exhaust gas analysis by Orsat apparatus.

STOICHIOMETRY

This section develops relations between the composition of the reactants (fuel and air) of a combustible mixture and the composition of the products. Since these relations depend only on the conservation of mass of each chemical element in the reactants, only the relative elemental composition of the fuel and the relative proportions of fuel and air are needed.

Complete oxidation of simple hydrocarbon fuels forms carbon dioxide (CO₂) from all of the carbon and water (H₂O) from the hydrogen, that is, for a hydrocarbon fuel with the general composition C_nH_m ,



Even in the idealized case of complete combustion, the accounting of all species present in combustion exhaust involves more than simply measuring the CO₂ and H₂O. Since fuels are burned in air rather than in pure oxygen, the nitrogen in the air may participate in the combustion process to produce nitrogen oxides. Also, many fuels contain elements other than carbon, and these elements may be transformed during combustion. Finally, combustion is not always complete, and the effluent gases contain unburned and partially burned products in addition to CO₂ and H₂O. Air is composed of oxygen, nitrogen, and small amounts of carbon dioxide, argon, and other trace species. Since the vast majority of the diluent in air is nitrogen, for our purposes it is perfectly reasonable to consider air as a mixture of 20.9% (mole basis) O₂ and 79.1% (mole basis) N₂. Thus for every mole of oxygen required for combustion, 3.78 mol of nitrogen must be introduced as well. Although nitrogen may not significantly alter the oxygen balance, it does have a major impact on the thermodynamics, chemical kinetics, and formation of pollutants in combustion systems. For this reason it is useful to carry the "inert" species along in the combustion calculations. The stoichiometric relation for complete oxidation of a hydrocarbon fuel, C_nH_m , becomes



Thus for every mole of fuel burned, $4.78(n + m/4)$ mol of air are required and $4.78(n + m/4) + m/4$ mol of combustion products are generated. The molar *fuel/air* ratio for stoichiometric combustion is $1/[4.78(n + m/4)]$.

Gas compositions are generally reported in terms of mole fractions since the mole fraction does not vary with temperature or pressure as does the concentration (moles/unit volume). The product mole fractions for complete combustion of this hydrocarbon fuel are

$$y_{\text{CO}_2} = \frac{n}{4.78(n + m/4) + m/4}$$

$$y_{\text{H}_2\text{O}} = \frac{m/2}{4.78(n + m/4) + m/4}$$

$$y_{\text{N}_2} = \frac{3.78(n + m/4)}{4.78(n + m/4) + m/4}$$

Calculation of theoretically correct air required for combustion of liquid Fuels

Air is a mixture of about 21% oxygen, 78% nitrogen, and 1% other constituents by volume. For combustion calculations it is usually satisfactory to represent air as a 21% oxygen, 79% nitrogen mixture, by volume. Thus for every 21 moles of oxygen that react when air oxidizes a fuel, there are also 79 moles of nitrogen involved. Therefore, $79/21 = 3.76$ moles of nitrogen are present for every mole of oxygen in the air. At room temperature both oxygen and nitrogen exist as diatomic molecules, O₂ and N₂, respectively. It is usually assumed that the nitrogen in the air is non reacting at combustion temperatures; that is, there are as many moles of pure nitrogen in the products as there were in the reactants. At very high temperatures small amounts of nitrogen react with oxygen to form oxides of nitrogen, usually termed NO_x. These small quantities are important in pollution analysis because of the major role of even small traces of NO_x in the formation of smog. However, since these NO_x levels are insignificant in energy analysis applications, nitrogen is treated as inert here. The molecular weight of a compound or mixture is the mass of 1 mole of the substance. The average molecular weight, M , of a mixture, as seen earlier, is the linear combination of the products of the mole fractions of the components and their respective molecular weights. Thus the molecular weight for air, M_{air} , is given by the sum of the products of the molecular weights of oxygen and nitrogen and their respective mole fractions in air. Expressed in words:

$M_{\text{air}} = \text{Mass of air/Mole of air} = (\text{Moles of } N_2 / \text{Mole of air})(\text{Mass of } N_2 / \text{Mole of } N_2) + (\text{Moles of } O_2 / \text{Mole of air}) (\text{Mass of } O_2 / \text{Mole of } O_2)$

Or $M_{\text{air}} = 0.79 M_{\text{nitrogen}} + 0.21 M_{\text{oxygen}} = 0.79(28) + 0.21(32) = 28.84$

The mass fractions of oxygen and nitrogen in air are then $mf_{\text{oxygen}} = (0.21)(32)/28.84 = 0.233$, or 23.3%

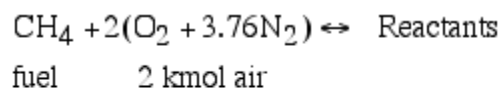
and $mf_{\text{nitrogen}} = (0.79)(28)/28.84 = 0.767$, or 76.7%

Theoretical Air and Air-Fuel Ratio -The minimum amount of air which will allow the complete combustion of the fuel is called the Theoretical Air (also referred to as Stoichiometric Air). In this case the products do not contain any oxygen. If we supply less than theoretical air then the products could include carbon monoxide (CO), thus it is normal practice to supply more than theoretical air to prevent this occurrence. This **Excess Air** will result in oxygen appearing in the products.

The standard measure of the amount of air used in a combustion process is the Air-Fuel Ratio (AF), defined as follows:

$$AF = \frac{m_{\text{air}}}{m_{\text{fuel}}}$$

Thus considering only the reactants of the methane combustion with theoretical air presented above, we obtain:



$$AF = \frac{m_{\text{air}}}{m_{\text{fuel}}} = \frac{2(4.76) \text{ [kmol]} \cdot 29 \left[\frac{\text{kg}}{\text{kmol}} \right]}{1 \text{ [kmol]} (12 + 4) \left[\frac{\text{kg}}{\text{kmol}} \right]}$$

$$AF = 17.3 \frac{\text{kg-air}}{\text{kg-fuel}}$$

Analysis of the Products of Combustion - Combustion always occurs at elevated temperatures and we assume that all the products of combustion (including the water vapor) behave as ideal gases. Since they have different gas constants, it is convenient to use the ideal gas equation of state in terms of the universal gas constant as follows:

$$P \cdot V = m \cdot R \cdot T = \frac{m}{M} R \cdot M \cdot T$$

where: m is mass [kg], V is volume [m^3], P is pressure [kPa] and T is temperature [K]

$R \left[\frac{\text{kJ}}{\text{kg} \cdot \text{K}} \right]$ is the gas constant

$M \left[\frac{\text{kg}}{\text{kmol}} \right]$ is the molar mass of the substance

thus: $P \cdot V = N \cdot R_u \cdot T$

where: $R_u = R \cdot M = 8.314 \left[\frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \right]$ is the Universal Gas Constant

$N = \frac{m}{M}$ is the number of kmols

volumetric and gravimetric analysis

Fuels are generally comprised of a number of different elements in a vast array of molecular forms. The main elements in flammable materials are Carbon C, Hydrogen, H, Oxygen, O, Nitrogen, N, and Sulphur with other trace elements to boot.

The components of a mixture (whether liquid, solid or gas) can take be expressed in many ways: volumetric, gravimetric, dry, wet, ash free, as supplied etc. etc. It is important right from the start to know exactly what these mean so that, when combustion calculations are carried out, we have the right numbers.

Gravimetric and Volumetric Ratios

The two fundamental methods of defining the quantities of mixture are by weight (gravimetric) or by volume (molar). For clarity, the following symbols are often (but not exclusively) used.

c_i = the gravimetric fraction (mass fraction) of element / molecule i

y_i = the volumetric fraction (molar fraction) of element / molecule i

Of course, the sum of mass or mole fractions for all species in a mixture will be unity:

$$\sum_N w_i = \sum_N x_i = 1$$

To convert from mole fraction to mass fraction we must know the molecular weight, M (kg/kmol), of the individual chemical species. We then calculate the mass of all species by multiplying the volume fraction by the molecular weight. Then we divide the mass of the individual element/molecule by the total mass.

$$\chi_i = \frac{\psi_i M_i}{\sum_N \psi_i M_i} \quad \text{- Molar to mass}$$

$$\psi_i = \frac{\chi_i / M_i}{\sum_N \chi_i / M_i} \quad \text{- Mass to molar}$$

So, if we are given a coal of composition C 95%, H 4%, Cl 0.5%, S 0.5% by weight. Then the molar composition is calculated thus:

Element	χ_i (mass)	χ_i / M_i	ψ_i (volumetric)
C	95	7.917	66.25
H	4	4.0	33.47
Cl	0.5	0.014286	0.195
S	0.5	0.015625	0.131
Total	100	11.95	100.046

Mass of dry gas per kg of fuel

Mass of carbon in the exhaust gas

The mass emission of pollutants are calculated by means of the following equation :

$$M_i = \frac{V_{mix} * Q_i * k_H * C_i * 10^{-6}}{d}$$

M_i = Mass emission of the pollutant i in g/km

V_{mix} = Volume of the diluted exhaust gas expressed in m³/test and corrected to standard conditions 293 K and 101.33 kPa

Q_i = Density of the pollutant i in kg/m³ at normal temperature and pressure (293 K and 101.33 kPa)

k_H = Humidity correction factor used for the calculation of the mass emissions of oxides of

nitrogen. There is no humidity correction for HC and CO.

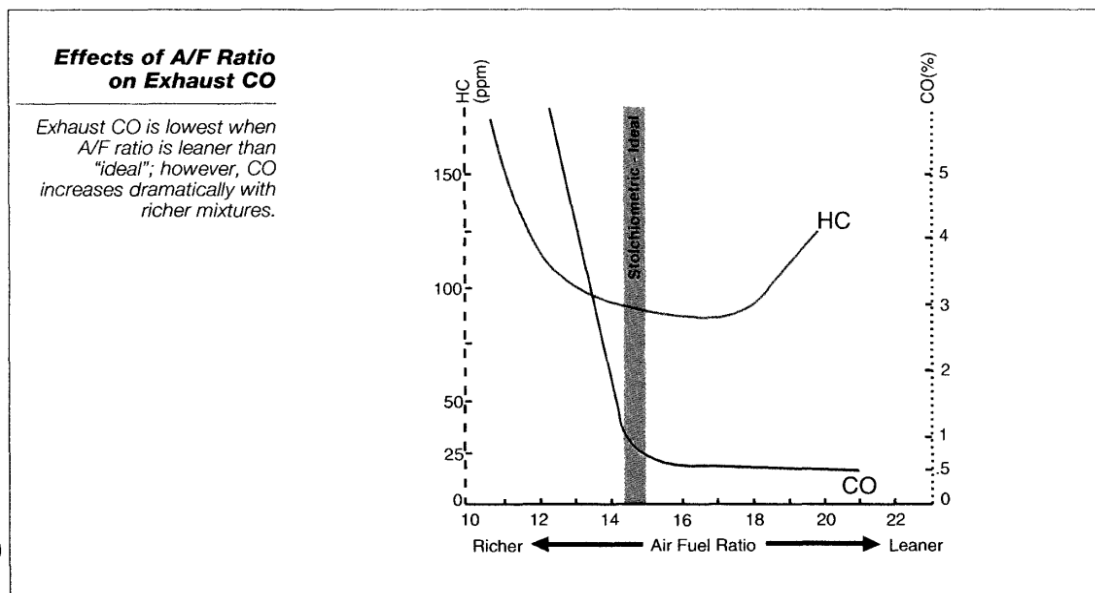
C_i = Concentration of the pollutant i in the diluted exhaust gas expressed in ppm and corrected by the amount of the pollutant i contained in the dilution air.

d = distance covered in km

Mass of carbon burnt to carbon-monoxide

Carbon monoxide (CO) is a byproduct of incomplete combustion and is essentially partially burned fuel. If the air/fuel mixture does not have enough oxygen present during combustion, it will not burn completely. When combustion takes place in an oxygen starved environment, there is insufficient oxygen present to fully oxidize the carbon atoms into carbon dioxide (CO₂). When carbon atoms bond with only one oxygen atom carbon monoxide (CO) forms.

An oxygen starved combustion environment occurs as a result of air/fuel ratios which are richer than stoichiometry (14.7 to 1). There are several engine operating conditions when this occurs normally. For example, during cold operation, warm-up, and power enrichment. It is, therefore, normal for higher concentrations of carbon monoxide to be produced under these operating conditions. Causes of excessive carbon monoxide includes leaky injectors, high fuel pressure, improper closed loop control, etc



Heat loss due to incomplete combustion

The gasoline-powered internal combustion engine takes air from the atmosphere and gasoline, a hydrocarbon fuel, and through the process of combustion releases the chemical energy stored in the fuel. Of the total energy released by the combustion process, about 20% is used to propel the vehicle, the remaining 80% is lost to friction, aerodynamic drag, accessory operation, or simply wasted as heat transferred to the cooling system.

The heat transfer from cycle to cycle varies for different points in an engine. Below figure shows the heat transfer at three different locations in the combustion chamber for a single cylinder during one cycle. There is significant variation in the heat transfer for these points.

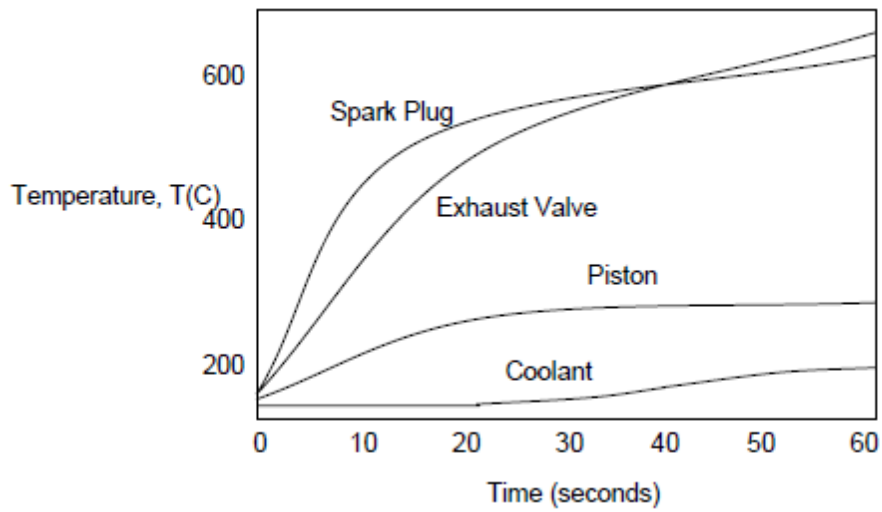
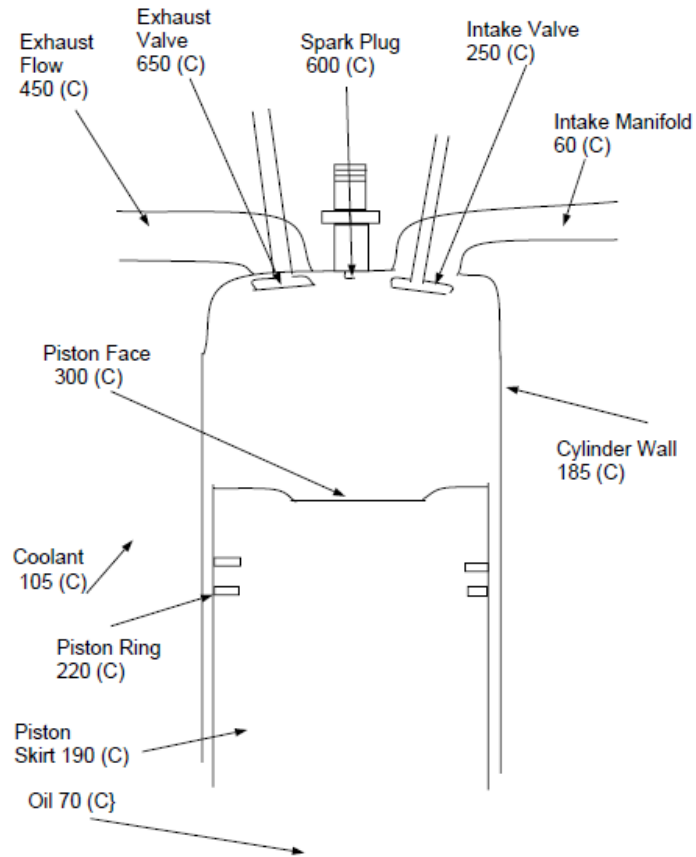


Fig: Temperaturer vs. time

❖ **Areas where heat transfer is important**

- Intake system: manifold, port, valves
- In-cylinder: cylinder head, piston, valves, liner
- Exhaust system: valves, port, manifold, exhaust pipe
- Coolant system: head, block, radiator
- Oil system: head, piston, crank, oil cooler, sump

❖ **Information of interest**

- Heat transfer per unit time (rate)
- Heat transfer per cycle (often normalized by fuel heating value)
- Variation with time and location of heat flux (heat transfer rate per unit area)

❖ Heat transfer mostly from hot burned gas

- That from unburned gas is relatively small
- Flame geometry and charge motion/turbulence level affects heat transfer rate

❖ Order of Magnitude

- SI engine peak heat flux $\sim 1\text{-}3 \text{ MW/m}^2$
- Diesel engine peak heat flux $\sim 10 \text{ MW/m}^2$

For SI engine at part load, a reduction in heat losses by 10% results in an improvement in fuel consumption by 3%

– Effect substantially less at high load

ORSAT APPARATUS.

An Orsat gas analyser is a piece of laboratory equipment used to analyse a gas sample (typically fossil fuel flue gas) for its oxygen, carbon monoxide and carbon dioxide content. Although largely replaced by instrumental techniques, the Orsat remains a reliable method of measurement and is relatively simple to use.

The apparatus consists essentially of a calibrated water-jacketed gas burette connected by glass capillary tubing to two or three absorption pipettes containing chemical solutions that absorb the gasses it is required to measure. For safety and portability, the apparatus is usually encased in a wooden box.

The absorbents are:

Potassium Hydroxide (Caustic Potash)

Alkaline pyrogallol

Ammoniacal Cuprous chloride

The base of the gas burette is connected to a levelling bottle to enable readings to be taken at constant pressure and to transfer the gas to and from the absorption media. The burette contains slightly acidulated water with a trace of chemical indicator (typically methyl orange) for coloration.

By means of a rubber tubing arrangement, the gas to be analyzed is drawn into the burette and flushed through several times. Typically, 100ml is withdrawn for ease of calculation. Using the stopcocks that isolate the absorption burettes, the level .

The gas is then passed into the caustic potash burette, left to stand for about two minutes and then withdrawn, isolating the remaining gas via the stopcock arrangements. The process is repeated to ensure full absorption. After leveling the liquid in the bottle and burette, the remaining volume of gas in the burette indicates the percentage of carbon dioxide absorbed.

The same technique is repeated for oxygen, using the pyrogallol, and carbon monoxide using the ammoniacal cuprous chloride.

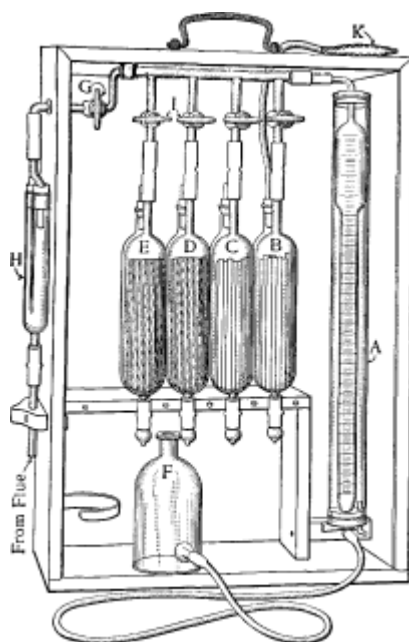


Fig: ORSAT APPARATUS