Internal Combustion Engine 1

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Thermo-chemistry

Thermo-chemistry

- Most internal combustion (IC) engines obtain their energy from the combustion of a hydrocarbon (HC) fuel with air.
- This combustion process converts the chemical energy of the fuel into internal energy in the gases within the engine.
- This topic deals with the composition and thermodynamic properties of pre- and post-combustion gases.

Combustion Process

- Combustion is an exothermic process involving the oxidation of a fuel, typically with oxygen from air.
- Combustion is defined as the oxidation of a 'Fuel', with large amounts of released energy. The oxidizers in most cases air (or more specifically, O_2 in air) because of its abundance which effects power, efficiency and emission.
- Energy stored in the bonds between consistent atoms of fuel and air (form internal energy) and in the combustion process it will transformed to new molecules of lower energy level combustion products plus release heat (exothermic reaction).
- The thermodynamic aspects of combustion are crucial in understanding chemical reactions in this process.

Combustion Process

- Controls the engine power.
- Efficiency.
- Controls the emissions.
- Different for SI and CI engines.

What is a Flame?

- A subsonic combustion reaction moving relative to unburned gas, characterized by:
  - Reaction Zone
  - Thermo-chemical properties
- A region of burning gas or vapor fuel that maintains a consistent shape due to a continuous fuel supply.
- Fuel can start as a solid, liquid, or gas, but ultimately burns in its gaseous form.
- The presence of flame motion indicates that the reaction occurs in a thin zone, commonly referred to as the flame front, compared to the combustion chamber.

Types of Flame

- Flames can be categorised as:
    - Premixed
    - Non-premixed (Diffusion)
- Flames also categorized as;
    - Laminar
    - Turbulent
- Flames also categorized by whether the flow is;
    - Steady
    - Unsteady

Premixed

- Mixed before combustion
- Characteristics
    - Reacts rapidly
    - Constant pressure
    - Propagates as thin zone at velocities slightly a few m/sec
- Example: Spark Ignition Engine

Diffusion

- Mixed during combustion
- Characteristic
    - Reacts occurs at Fuel/Air interface
    - Controlled by the mixing of the reactants
- Example: Diesel Engine

Laminar

- Premixed
  - Simplest flame type
  - Flame moves at fairly low velocity
  - Mechanically created laminar conditions
  - Example: Bunsen burner

- Diffusion
  - Characterized by smooth and steady flow
  - Fuel and oxidizer diffuse into each other and react at the interface
  - Flame has a well-defined, stable shape
  - Example: Candle

Turbulent

- Premixed
    - Faster heat release than laminar
    - Increase flame propagation
    - No definite theories to predict behaviour
    - Example: Indirect fuel injection engines in diesel engine

- Diffusion
    - Can obtain high rates of combustion energy release per unit volume
    - Modeling is very complex, no well established approach
    - Example: Direct fuel injection engines in diesel engine

Engine Flames

- Premixed (SI) or Diffusion (CI) turbulent unsteady gas-phase flames.
  - Turbulence increases mixing and flame speed.
  - Diffusion (motion due to concentration gradient) of species is slower Than connection (motion due to bulk velocity)
  - In flame propagation there is strong coupling between chemical reactions and mass and heat transport process.

Ideal Gas Model

- Usually, IC engine working fluids can be ”modeled” as ideal gases (or a mixture of ideal gases)

- The ideal gas law:

$$PV = nRT$$

- P : pressure
- V : volume
- n : number of moles
- R : universal gas constant
- T : absolute temperature

- Another form of the ideal gas equation:

$$PV = mR_sT$$

- P : pressure
- V : volume
- m : mass
- R_s : specific gas constant
- T : absolute temperature

Air Composition

Air is primarily composed of the following gases on a molar (or volume) basis:

Component	**Percentage**
Nitrogen (N_2)	78.09%
Oxygen (O_2)	20.95%
Argon (Ar)	0.93%
Carbon Dioxide (CO_2)	0.04%
Neon (Ne)	0.0018%
Helium (He)	0.0005%
Methane (CH_4)	0.0002%

- Nitrogen (78.08%): relatively inert and stable due to the triple bond $N \equiv N$.
- Oxygen (20.95%): the reactive component in air.
- Carbon dioxide, Argon, Helium, Neon, Hydrogen, and traces of other gases (0.97%).
- A good approximation is: 21% oxygen, 79% nitrogen.
- Thus, each mole of O_2 is accompanied by $0.79/0.21 = 3.76$ moles of N_2.

Air Composition - cont.

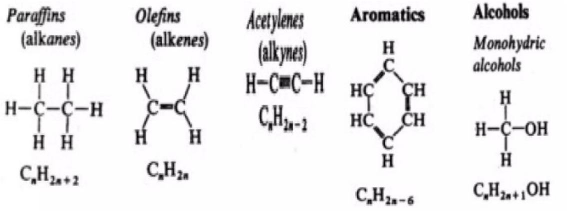
- At ordinary combustion temperatures, N_2 is inert, but nonetheless greatly affects the combustion process because its abundance, and hence its enthalpy change, plays a large part in determining the reaction temperatures.
  - This, in turn , affects the combustion chemistry.
  - At higher temperatures, N_2 does react, forming species such as oxides of nitrogen NO_x, which are a significant pollutant.
- Actually air inducted into an IC engine contains some water vapor. The water vapor is the inlet air, increases the specific heats $(c_p \& c_v)$ of air. Thus $\gamma = \frac{c_p}{c_v}$ is decreased, thus end of compression temperature decreases.

Fuels

- A fuel is any material (mostly Hydrocarbons "HCs") that store energy in their chemical bonds. Highest energy storage per unit mass or unit volume (in liquid form) that can be burned to release energy. HC fuels of the form C_xH_y are the most common.
- Many HC fuels are mixtures of many different HCs although they mainly consist of the following:
  - Gasoline $\sim$ Octane: C_8H_{18}
  - Diesel $\sim$ Dodecane: $C_{12}H_{26}$
  - Methanol $=$ Methyl alcohol: CH_3OH
  - LNG (liquefied natural gas) $\sim$ methane CH_4
  - LPG (liquefied petroleum gas) $\sim$ Propane C_3H_8

Classes of Organic Compounds

- **Paraffins:** Also known as alkanes, these are saturated hydrocarbons with single bonds between carbon atoms.
- **Olefins:** Also known as alkenes, these are unsaturated hydrocarbons with at least one double bond between carbon atoms.
- **Acetylenes:** Also known as alkynes, these are unsaturated hydrocarbons with at least one triple bond between carbon atoms.
- **Aromatics:** These compounds contain benzene rings or similar structures with alternating double bonds.
- **Alcohols:** Organic compounds with one or more hydroxyl (-OH) groups attached to a carbon atom.



Combustion Stoichiometry

- Develops relations between the composition of the reactants (fuel and air) of a combustible mixture and the composition of the product by using the conservation of mass of atomic species.

$$\text{Fuel} + \text{Air} \longrightarrow \text{Products}$$

- Air contains molecular nitrogen N_2, but when the products are low temperatures the nitrogen is not significantly affected by the reaction, it is considered inert.
- The above equation defines the Stoichiometric proportions of fuel and air.

Combustion Stoichiometry - cont.

- Stoichiometric air is defined as the theoretical amount of air required to completely burn a fuel to products with no dissociation.
- In stoichiometric combustion of hydrocarbons (HCs), if sufficient oxygen is available, the fuel is completely oxidized, producing carbon dioxide (CO_2) from carbon and water (H_2O) from hydrogen.
- This process adheres to the principle of conservation of mass, where elements are neither created nor destroyed, necessitating careful consideration of element balances.
- The overall complete combustion equation is:

$$\boldsymbol{C_aH_b + (a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow aCO_2 + \frac{b}{2}H_2O + 3.76(a + \frac{b}{2})N_2}$$

Combustion Stoichiometry for Propane

- Example: The balanced chemical equation for the complete combustion of one mole of Propane (C_3H_8) is:

$$C_3H_8 + \left(a + \frac{b}{4}\right)(O_2 + 3.76N_2) \rightarrow aCO_2 + \frac{b}{2}H_2O + 3.76\left(a + \frac{b}{2}\right)N_2$$

$$a = 3 \text{ and } b = 8$$

- Since the conservation of elements must be maintained, the equation can be simplified to:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

Stoichiometric air-fuel ratio

- The Stoichiometric of theoretical A/F is defined as the minimum amount of air that supplies sufficient oxygen for the complete combustion of all the carbon, hydrogen, and any other elements in the fuel that may oxidize.
- On a molar basis:

$$\boldsymbol{(A/F)_{mole}} = \frac{\text{moles of air}}{\text{moles of fuel}} = \frac{\text{moles of } \boldsymbol{O_2} + \text{moles of } \boldsymbol{N_2}}{\text{mole of fuel}} = \frac{\mathbf{1}}{\boldsymbol{(F/A)_{mole}}}$$

- On a mass basis:

$$\boldsymbol{(A/F)_{mass}} = \frac{\text{mass of air}}{\text{mass of fuel}} = \frac{\text{mass of } \boldsymbol{O_2} + \text{mass of } \boldsymbol{N_2}}{\text{mass of fuel}} = \frac{\mathbf{1}}{\boldsymbol{(F/A)_{mass}}}$$

- Air-Fuel ratio on mass basis is different from Air-Fuel ratio on mole basis

Stoichiometric air-fuel ratio for Propane

- For example, the Stoichiometric A/F for the ideal combustion of Propane can be calculated as follows:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

- On a molar basis:

$$(A/F)_{mole} = \frac{5 \text{ moles of } O_2 + 18.8 \text{ moles of } N_2}{1 \text{ mole of fuel}} = \frac{23.8 \text{ moles of air}}{1 \text{ mole of fuel}} = 23.8$$

- On a mass basis:

$$(A/F)_{mass} = \frac{23.8 \text{ moles of air}}{1 \text{ mole of fuel}} \times \frac{28.97 \text{ g/mole air}}{44.097 \text{ g/mole fuel}} = 15.64$$

Stoichiometric air-fuel ratio

- The ratio of the number of moles of hydrogen to carbon in the fuel can be expressed as $y = \frac{b}{a}$.

$$C_aH_b + (a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow aCO_2 + \frac{b}{2}H_2O + 3.76(a + \frac{b}{2})N_2$$

$$(A/F)_s = (F/A)_s^{-1} = \frac{\left(1 + \frac{y}{4}\right)(32 + 3.76 \times 28.16)}{12.011 + 1.008y}$$

$$(A/F)_s = (F/A)_s^{-1} = \frac{34.47(4 + y)}{12.011 + 1.008y}$$

Stoichiometric air-fuel ratio for Propane

- For example, the Stoichiometric A/F for the ideal combustion of Propane can be calculated as follows:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

- $y = \frac{8}{3}$

$$(A/F)_s = (F/A)_s^{-1} = \frac{34.47(4 + \frac{8}{3})}{12.011 + 1.008\frac{8}{3}} = 15.64$$

Equivalences ratio

- The equivalence ratio, ϕ, is commonly used to indicate if a mixture is Stoichiometric, fuel lean or fuel rich.

$$\phi = \frac{\text{Actual fuel-air mass ratio}}{\text{Stoichiometric fuel-air ratio}}$$

$$\phi = \frac{(F/A)_a}{(F/A)_s} = \frac{(m_f/m_a)_a}{(m_f/m_a)_s}$$

$$\begin{aligned} \text{Stoichiometric:} \quad & \phi = 1 \\ \text{Fuel-lean:} \quad & \phi < 1 \\ \text{Fuel-rich:} \quad & \phi > 1 \end{aligned}$$

Equivalences ratio

- Another parameter that is used with reference to engine is the relative air/fuel ratio (λ)
- The inverse of (ϕ), the relative air/fuel ratio (λ)

$$\boldsymbol{\lambda} = \frac{\text{Stoichiometric fuel-air mass ratio}}{\text{Actual fuel-air ratio}}$$

$$\boldsymbol{\lambda = \frac{1}{\phi} = \frac{(F/A)_s}{(F/A)_a}}$$

$$\text{If } \phi < 1, \quad \lambda > 1, \quad \text{Fuel-lean mixture}$$

$$\text{If } \phi > 1, \quad \lambda < 1, \quad \text{Fuel-rich mixture}$$

Fuel Lean Mixture

- Fuel-air mixtures with more than stoichiometric air, excess air, can burn.
- With excess air you get fuel lean combustion, the extra air appears in the product in unchanged form.

$$C_aH_b + \lambda(a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow aCO_2 + \frac{b}{2}H_2O + dN_2 + eO_2$$

- where for fuel lean mixture have excess air so $\lambda > 1$
- Above reaction equation has two unknowns (d, e) and we have two atom balance equations (O, N) so can solve for the unknowns.

Fuel Lean Mixture - Propane

- Example: Consider a reaction of Propane with 10% excess air that is ϕ.
- We know the Stoichiometric reaction is:

$$C_aH_b + (a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow aCO_2 + \frac{b}{2}H_2O + 3.76(a + \frac{b}{2})N_2$$

- The stoichiometric reaction for Propane is:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

- In case of 10% excess air The stoichiometric reaction for Propane is:

$$C_3H_8 + (1.1)(5)(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + aO_2 + bN_2$$

Fuel Lean Mixture - Propane

$$\boldsymbol{C_3H_8 + (1.1)(5)(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + aO_2 + bN_2}$$

$$\begin{aligned} &\text{Oxygen balance gives:} && 1.1(5)(2) = 6 + 4 + 2a && \Rightarrow && a = 0.5 \\ &\text{Nitrogen balance gives:} && 1.1(5)(3.76) = b && \Rightarrow && b = 20.68 \end{aligned}$$

$$\boldsymbol{C_3H_8 + (1.1)(5)(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 0.5O_2 + 20.68N_2}$$

Off-stoichiometric conditions:

110% Stoichiometric air = 110% therorictal air = 10% excees air.

$\lambda = 1.1 \rightarrow$ fuel lean mixture

Fuel Rich Mixture

- Fuel-air mixtures with less than stoichiometric air can also burn.
- With less air you get fuel rich combustion, there is insufficient oxygen to oxidize all the C and H in the fuel to CO_2 and H_2O.
- Get incomplete combustion where carbon monoxide (CO) and molecular hydrogen (H_2) also appear in the products

$$\boldsymbol{C_aH_b + \lambda(a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow cCO_2 + dH_2O + eN_2 + fCO + gH_2}$$

- where for fuel rich mixture have less air so $\lambda < 1$

Fuel Rich Mixture

$$C_aH_b + \lambda(a + \frac{b}{4})(O_2 + 3.76N_2) \rightarrow cCO_2 + dH_2O + eN_2 + fCO + gH_2$$

- where for fuel rich mixture have less air so $\lambda < 1$
- Above reaction equation has five unknowns (c, d, e, f, g) and we only have four atoms balance equations (C, H, O, N) so can not solve for the unknowns unless additional information about the products is given.

End of Lecture 7

End of Lecture 7