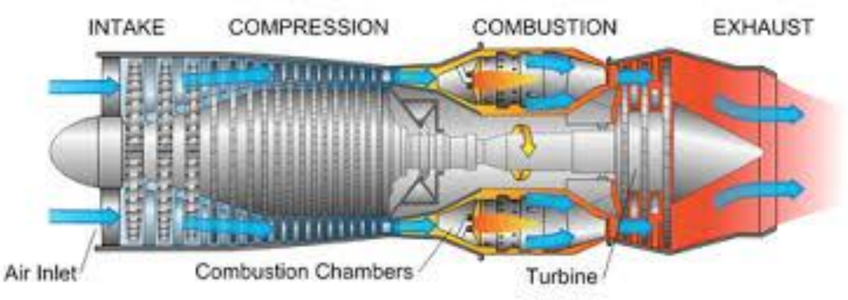
TIKRIT UNIVERSITY

COLLEGE OF ENGINEERING

MECHNICAL DEPARTMENT

INTERNAL COMBUSTION ENGINE



Chapter 5

Fuel Chemistry and Combustion Analysis

Course Instructor

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Introduction

In IC engines, the chemical energy contained in the fuel is converted into mechanical power by burning (oxidizing) the fuel inside the combustion chamber of the engine.

As a result of the chemical reactions which occur inside the cylinder, heat is released. The fuel-air mixture (the working fluid before combustion) must stay in the cylinder for a sufficient time so that the chemical reactions can be completed.

Generally, the fuel is classified into the following:

1) Solid Fuel

2) Liquid Fuel

3) Gaseous Fuel

Fuels suitable for fast chemical reaction have to be used in IC engines.

Hydrocarbons in liquid form

Alcohols (methanol, ethanol)

LPG (propane and butane)

Natural gas (methane)

Hydrogen

Liquid hydrocarbons $C_n H_m$ **Or** $C_x H_y$ **Or** $C_\alpha H_\beta$

Fuels are mainly mixtures of hydrocarbons, with bonds between carbon atoms and between hydrogen and carbon atoms.

During combustion these bonds are broken and new bonds are formed with oxygen atoms, accompanied by the release of chemical energy. Principal products are carbon dioxide and water vapour.

Fuels also contain small amounts of O_2 , N_2 , S , H_2O

So, the general form of hydrocarbons fuel is: $C_\alpha H_\beta O_\gamma N_\delta$

The different constituents of crude petroleum which are available in liquid hydrocarbons are:- paraffins, naphthenes, olefins, aromatics.

Alkanes or Paraffins can in general be represented by $C_n H_{2n+2}$

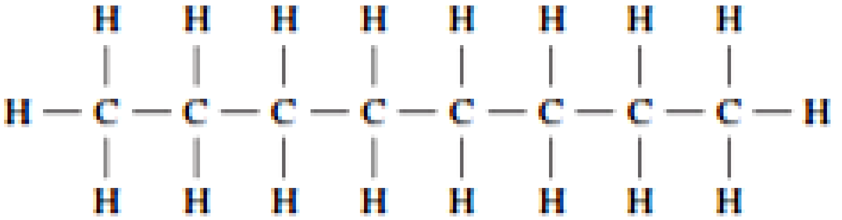
all the carbon bonds are single bonds – they are "saturated"

high number of H atoms, high heat content and low density ($620 – 770\ kg/m^3$)

The carbon atoms can be arranged as, a straight chain or as branched chain compounds.

Straight chain group (normal paraffins)

- shorter the chain, stronger the bond
- not suitable for SI engines – high tendancy for autoignition
- according to the value of “n” in the formula, they are in gaseous (1 to 4), liquid (5 to 15) or solid (>16) state.



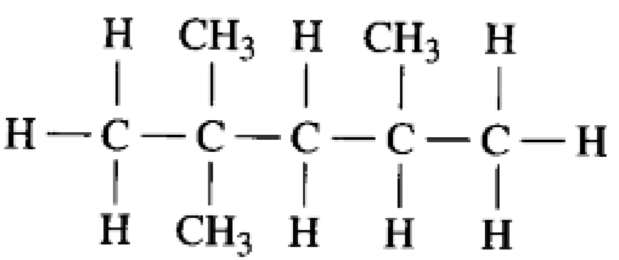
Octane, C_8H_{18}

Branched chain compounds (isoparaffins)

when four or more C atoms are in a chain molecule it is possible to form isomers – they have the same chemical formula but different structures, which often leads to very different chemical properties.

example : iso-octane $C_8 H_{18}$

2. 2 .4 trimethyl pentane



Isooctane, C_8H_{18} or 2,2,4-trimethylpentane

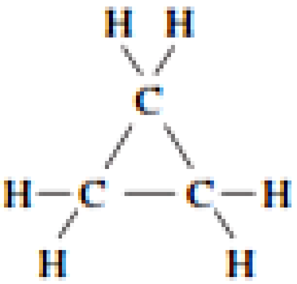
Naphthenes Also called cycloparaffins $C_n H_{2n}$

saturated hydrocarbons which are arranged in a circle

have stable structure and low tendancy to autoignite compared to alkanes (normal paraffins)

can be used both in SI-engines and CI-engines

low heat content and high density (740 – 790 kg / m^3)



Cyclopropane

Alkenes Also called olefins

mono-olefins $C_n H_{2n}$ or dio-olefins $C_n H_{2n-2}$

have the same C-to-H ratio and the same general formula as naphthenes, their behavior and characteristics are entirely different

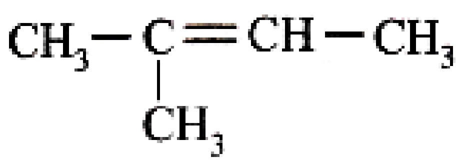
can be used in SI-engines, obtained by cracking of large molecules

low heat content and density in the range 620 – 820 kg / m^3

Alkenes

they are straight or branch chain compounds with one or more double bond. The position of the double bond is indicated by the number of first C atom to which it is attached, ie,

CH2=CH.CH2.CH2.CH3 called pentene-1



called butene-2

olefinic compounds are easily oxidized, have poor oxidation stability

Hexen (mono-olefin)

```
    H    H    H    H    H    H
H – C – C – C – C – C = C - H
    H    H    H    H
```

Butadien (dio-olefin)

```
     H    H    H    H
H – C = C – C = C – H
```

Aromatics

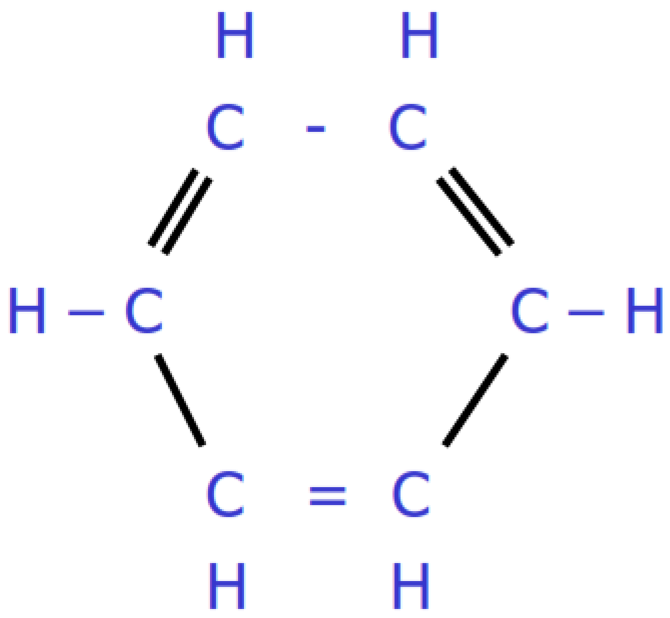
Aromatic hydrocarbons are so called because of their "aromatic" odor

$$C_n H_{2n-6}$$

Aromatics

- they are based on a six-membered ring having three conjugated double bonds
- aromatic rings can be fused together to give polynuclear aromatics, PAN, also called polycyclic aromatic hydrocarbons, PAH
- simplest member is benzene $C_6 H_6$
  - can be used in SI-engines, to increase the resistance to knock
  - not suitable for CI-engines due to low cetene number

Benzen C6 H6



Hydrocarbon Group	General Formula	Molecular Structure	Saturation	Stability
Paraffins	C_nH_{2n+2}	Chain	Saturated	Stable
Naphthene	C_nH_{2n}	Ring	Saturated	Stable
Olefins	C_nH_{2n} C_nH_{2n-2}	Chain	Unsaturated	Unstable
Aromatics	C_nH_{2n-6}	Ring	Highly unsaturated	Most unstable

Gaseous Fuels

due to storage and transportation problems they are not widely used

reduce volumetric efficiency and power output of engine (5 – 10 %)

have low tendancy to knock and low emissions

Alcohols (monohydric alcohols)

these include methanol (methyl alcohol), ethanol (ethyl alcohol), propanol (propyl alcohol), butanol (butyl alcohol) as compounds

the OH group which replaces one of the H atoms in an alkane, gives these compounds their characteristic properties.

Methanol CH_3OH

can be obtained from natural gas – has near and long-term potential

has high octane quality (130 RON, 95 MON)

can be used in low-concentration (5-15 %) in gasoline to increase octane number of the mixture

Ethanol C_2H_5OH

produced from biomass

has high octane number – can be used in low–concentrations in gasoline

specific heating value is lower than gasoline (42 – 43 MJ/kg)

methanol (19.7 MJ/kg) and ethanol (26.8 MJ/kg)

Fuel Specifications

Relative density (specific gravity): **is the ratio of fuel density to the density of water at STP (20 ^{O}C and 1atm).**

$$SG = \frac{\rho_f}{\rho_w}$$

American Petrolium Institute, also defines degrees API as,

$$\text{Specific Gravity} = \frac{141.5}{131.5 + API}$$

For gasoline, the relative density is around 0.72 to 0.78 - which is equivalent to an API range of 65 to 50

$$\rho = 700 - 800 \text{ [kg/m}^3\text{]}$$

for unleaded gasoline this value is higher due to the aromatics

For diesel fuel, $\rho = 830 - 950 \text{ [kg/m}^3\text{]}$

Fuel Composition most petroleum, however, on a mass basis, consists chiefly of the following elements:

Element	Mass fraction, %
Carbon	84–87
Hydrogen	11–14
Sulfur	0–2
Nitrogen	0–0.2

Composition of a typical unleaded gasoline	
Alkenes	30 – 45 %
Aromatics	30 – 45 %
Alkanes	20 – 30 %
Cycloalkanes	5 %

Additional impurities, such as water, gum deposits, sulfur, lead, manganese and metals like vanadium can influence or even limit use of liquid fuels unless they do not exceed defined concentrations.

Manganese: used for antiknock in gasoline, max 0.00025 to 0.03 (g/L).

Lead: cause pollution and destroys catalytic converters.

Sulfur: it has low ignition temp., promote knock in SI engines. Max 250 ppm.

Heat (or calorific) value is defined as the amount of energy generated by burning 1 g of fuel in the presence of oxygen measured as kJ/kg

in IC engines lower heating value is given as the combustion products contain water in vapour form.

For gasoline and diesel fuel

$$LHV = 42000 - 44000 \ \text{[kJ/kg]}$$

$$LHV = 10200 - 10500 \ \text{[kcal/kg]}$$

Surface tension is a parameter which effects the formation of fuel droplets in sprays

increasing the surface tension will reduce mass flow and air-fuel ratio in gasoline engines

lower the value, smaller the droplet diameter

diesel fuel	0.023 – 0.032 N/m
gasoline	0.019 – 0.023 N/m

Flashpoint: It is the temperature at which the surface of the liquid fuel generates enough vapors to ignite. It very important in terms of auto ignition characteristics.

For gasoline it is 25 ^{O}C, diesel fuel 35 ^{O}C and heavy diesel 65 ^{O}C

Freezing point

the precipitation of paraffin crystals in winter can lead to clogged filters. It can be prevented by either removing paraffins from the fuel or adding flow improvers (additives).

For gasoline freezing point is –65 ^{O}C and for diesel fuel –10 ^{O}C

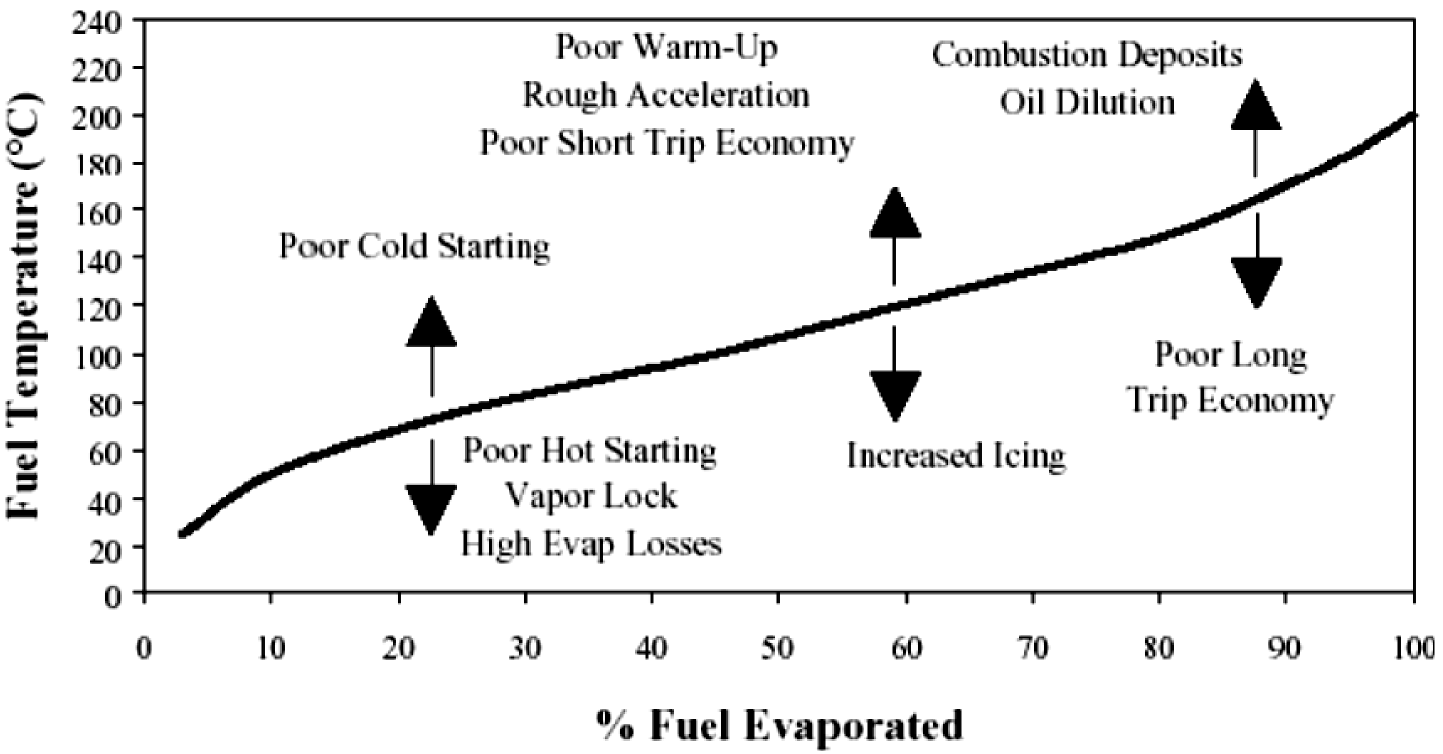
Viscosity is an important parameter for CI engines, also influences fuel metering orifices since Re is an inverse function of fuel viscosity

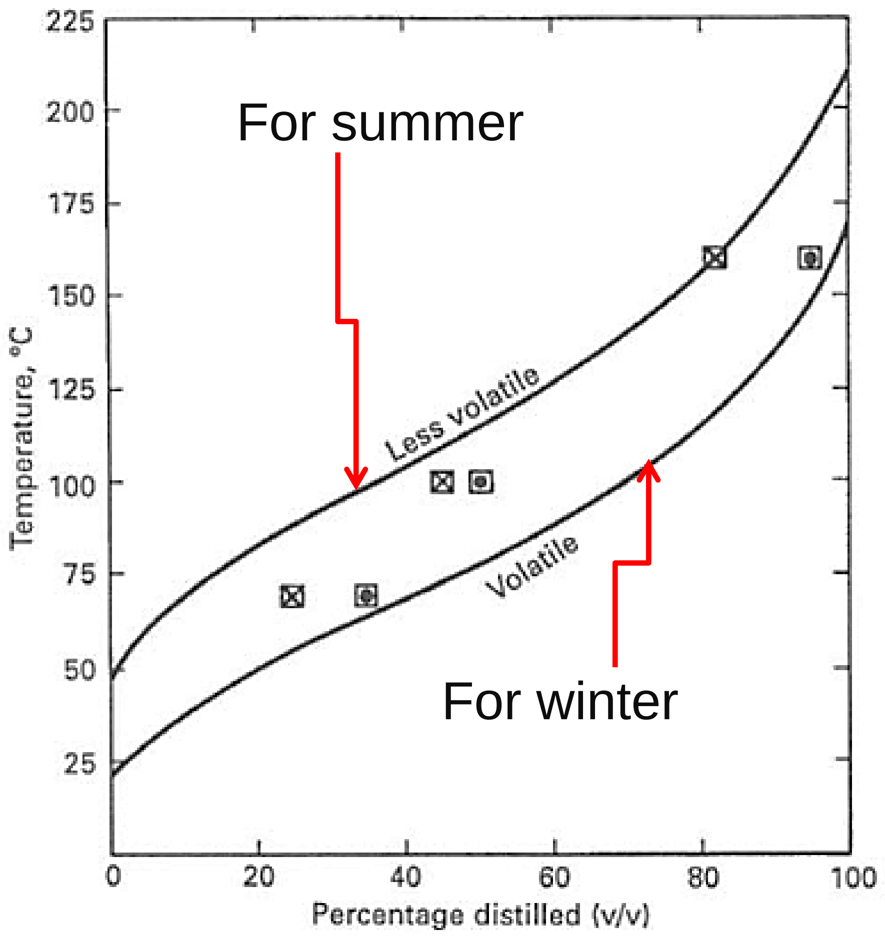
lower the viscosity, smaller the diameter of the droplets in the spray.

Below certain limits, low viscosity increases the leaks in the fuel system. It is a strong function of T – must be given at certain T values

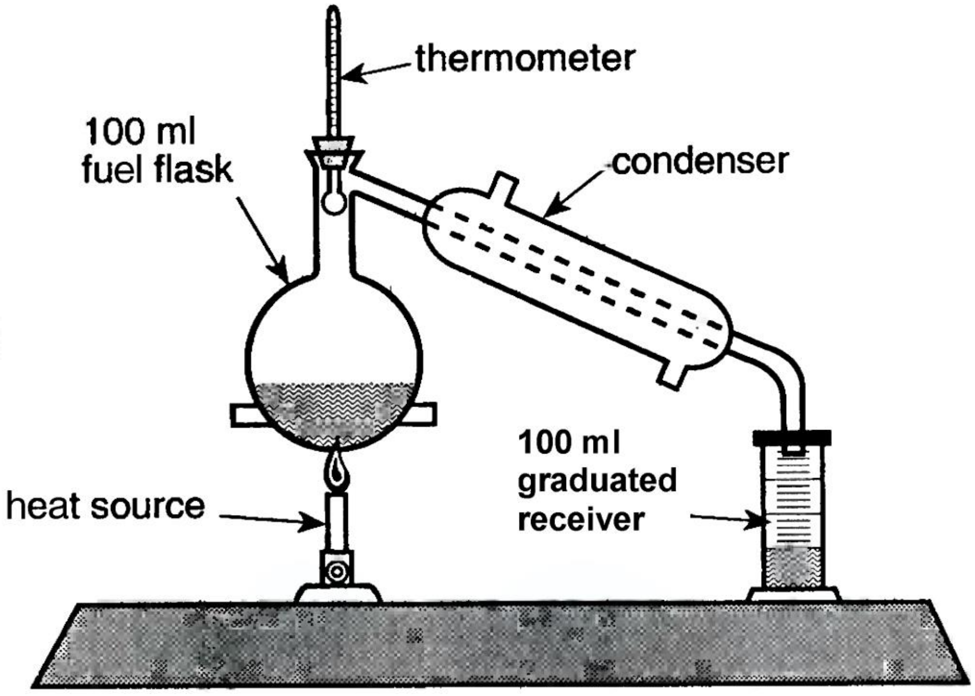
Volatility is defined as the tendency of a liquid to evaporate, which is the liquid fuel characteristic will affect its suitability in particular combustion systems. Volatility is expressed in terms of the volume percentage that is distilled at or below fixed temperatures.

***Distillation Curve*:** Figure below illustrates the effect of changing the shape of the distillation curve.





Distillation curves for petrol



Typical ASTM petroleum distillation test facility and distillation curves.

Octane/CetaneRating: The octane rating defines a gasoline's ignition quality (engine "knock resistance") for gasoline engines. The cetane number carries similar meaning but for diesel engines. However, the two numbers have inverse relationships with respect to knock resistance; the resistance to engine knock increases with increasing octane number and decreasing cetane number.

Driveability Index: The driveability index (DI) is used often by engineers to predict engine performance based on three points from a fuel's distillation curve. These points are referred to as the T10, T50 and T90 temperatures, and correspond to temperatures in °F at which 10%, 50%, and 90% of the volume of a fuel has evaporated. The index is calculated using Eq. 5.1:

$$DI = 1.5\,T_{10} + 3.0\,T_{50} + T_{90} \qquad (5.1)$$

ADDITIVES: Chemicals are added to gasoline in very small quantities to improve and maintain gasoline quality.

Examples include: detergents (مطهرات) which prevent or clean up carburetor and fuel injector deposits, corrosion inhibitors, antioxidants to reduce gum formation in storage, acetone or similar water absorbents, and ethers such as methyl tertiary butyl ether (MTBE) for increased octane levels.

Effects of Fuel Additives

Fuel additive serve two distinct purposes.

- to improve combustion and pollutant emissions,
- to ensure reduced wear and limit deposit formation during the engine life cycle of several hundreds of thousands of miles.