FUELS AND EFFECTS ON ENGINE EMISSIONS

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TRANSPORT FUELS AND QUALITY REQUIREMENTS

Petroleum crude is presently the main source of automotive fuels although alternative fuels like natural gas, LPG are also being used in large numbers of road vehicles in some countries. The renewable fuels like ethyl alcohol and biodiesel too are being used in the form of blends with the petroleum derived gasoline and diesel fuels. Petroleum crude contains over 25000 compounds mainly the hydrocarbons composed of hydrogen and carbon elements. A number of these compounds also contain sulphur in varying amounts and, nitrogen and oxygen in small quantities. The commercial liquid engine fuels are the mixtures of a few hundred different hydrocarbons.

Typically, the petroleum transport fuels contain about 85 - 86 percent carbon and 14 – 15 percent hydrogen by mass. Sulphur containing compounds are also present in significant amounts.

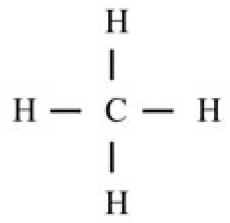
In this module at first chemical composition and key characteristics of petroleum derived fuels and how they influence engine combustion and emissions are covered. Later, the most promising alternative fuels are also discussed.

Fuel Hydrocarbons and Other Components

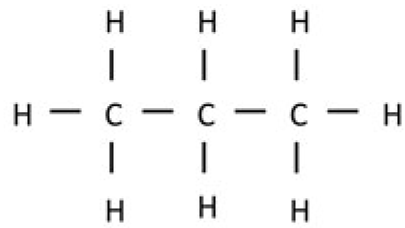
Hydrocarbons are broadly grouped into paraffins, cycloparaffins (naphthenes), olefins and aromatics. The olefins are not present in the crude petroleum but are generated during processing and refining of crude when the practical transport fuels are being produced.

Paraffins

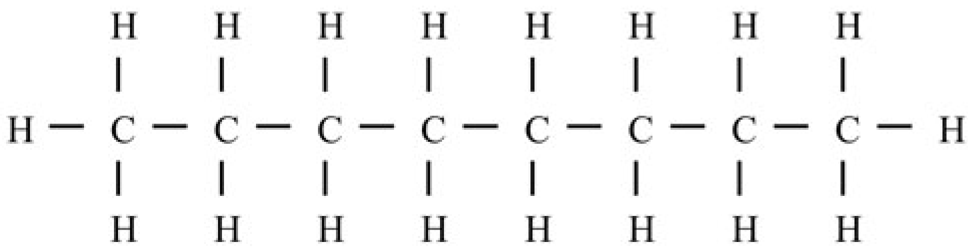
The paraffins are saturated hydrocarbons which are also known as *alkanes*. The carbon atoms have single bond between them. The large *alkane* molecules are either straight chain or branched chain. The empirical formula for the paraffin family is C_nH_{2n+2}. Methane (CH_4) is the first member of this family, the higher members being ethane (C_2H_6), propane (C_3H_8), ……n-heptane, n-octane, isooctane (C_8H_{18}), n- hexadecane (n-cetane) and so on. The straight chain paraffins are called normal- (n-) and branched chain are called iso- paraffins. Structures of some paraffins are given below. There are several isomers of isooctane depending upon the position of the branches. The isooctane that is most commonly referred to is 2-2-4 trimethyl pentane having five carbon atoms in straight chain and three methyl groups in 2, 2 and 4 carbon atom positions.



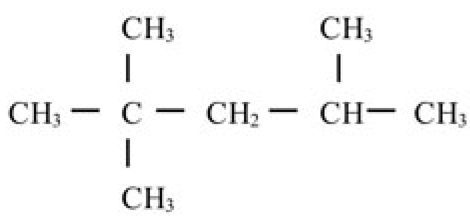
methane, CH_4



propane, C_3H_8



n-octane , C_8H_{18}



2,2,4 - trimethylpentane (isooctane), $C_8 H_{18}$

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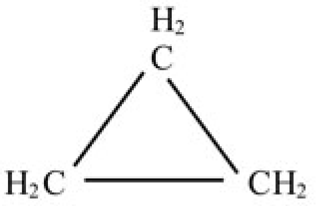
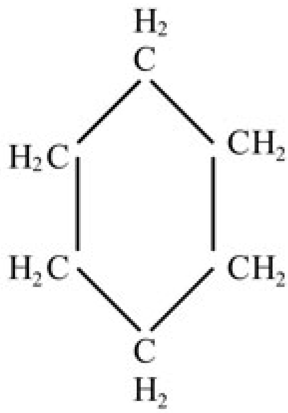
Cycloparaffins

The carbon atoms are present in a ring structure and a single bond exists between carbon atoms. Cycloparaffins or naphthenes have the formula, C_nH_{2n} and cyclopropane (C_3H_6), cyclobutane (C_4H_8), cyclohexane (C_6H_{12}) etc., are its examples. The cycloparaffins having more than 6 carbon atoms are not common.



cyclopropane, C_3H_6



cyclohexane, C_6H_{12}

Olefins

Olefins or *alkenes* are open chain hydrocarbons having one or more carbon-carbon double bonds. The compounds having one double bond are called mono-olefins and their empirical formula is C_nH_{2n}. The examples are ethylene, propylene, butene, octene etc. Those having two double bonds are called as diolefins or dienes, the chemical formula being C_nH_{2n-2}. The position of the double bond (s) is indicated by a prefix like 1-octene, 1, 3- butadiene etc. The diolefins are highly unstable during storage and therefore, are undesirable compounds in the engine fuels. Another family of unsaturated hydrocarbons has triple carbon-carbon bond. These compounds are known as acetylenes or alkynes. The empirical chemical formula for alkynes is C_nH_{2n-2} and the first member of the series is acetylene (C_2H_2). Higher alkynes are similar to higher alkenes with each double bond replaced by triple bond

$CH_2 = CH - CH_2 - CH_3$

1-butene, C_4H_8

$CH_2 = CH - \quad H = CH_2$

1,3- butadiene, C_4H_6

$H - C \equiv C - H$

acetylene, C_2H_2

Aromatics

Aromatics are double bonded hydrocarbons arranged in a ring structure of carbon atoms. Each ring of aromatics has 6 carbon atoms. Benzene (C_6H_6) is the first member of the family. Benzene structure has three double bonds which alternate in position between carbon atoms. Other aromatics are formed when hydrogen atom(s) attached to carbon in the aromatic ring is substituted by an alkyl radical such as methyl-, ethyl-, propyl- etc. Some examples of aromatics having side chains attached to ring are toluene (methylbenzene), ethyl benzene, xylene (dimethyl benzene) etc. Many aromatic hydrocarbons have two or more aromatic rings such as naphthalene, anthracene, benzo(a)pyrene. These compounds are known as polycyclic aromatic hydrocarbons (PAH).

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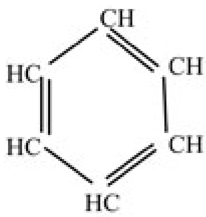
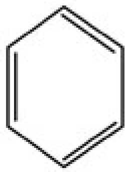
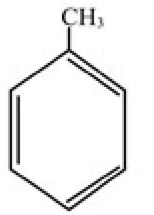


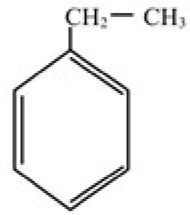
benzene, C_6H_6



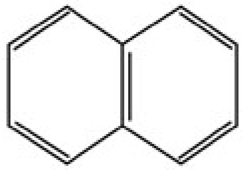
representation of benzene



toluene, C_7H_8



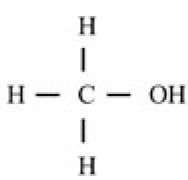
ethylbenzene



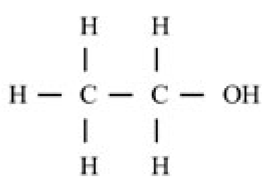
naphthalene

Alcohols and Ethers

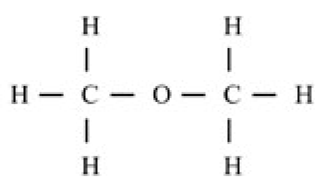
Alcohols as engine fuel have been of interest for a long time. In the hydrocarbons when a hydrogen atom is substituted with hydroxyl radical (OH), alcohols are formed. Among the alcohols, methyl alcohol (CH_3OH) and ethyl alcohol (C_2H_5OH) are considered as alternative fuels. Ethers, such as di-methyl ether (DME) has been investigated as diesel engine fuel and methyl teriary butyl ether (MTBE) is being used as a high octane blending component in gasoline.



methanol, CH_3OH



ethanol, C_2H_5OH



di-methyl ether, $(CH_3)_2O$

General Fuel Quality Requirements

Many properties of the fuels influence engine performance and emissions. The most important properties of liquid fuels, gasoline and diesel most of which are specified in the fuel quality standards are given in Table 8.1

Table 8.1

Important Characteristics of Liquid Petroleum Fuels

Gasoline	Diesel
Distillation	Ignition quality (Cetane index, Cetane number)
Reid vapour pressure	Distillation (volatility), 90% boiling point

Heat of combustion*	Heat of combustion*
Density	Density
Antiknock quality (Research and Motor octane number)	Viscosity
Oxidation stability	Aromatic content
Gum content, mg/100ml	Sulphur content
Lead content	Storage stability
Sulphur	Injection system cleanliness
Benzene	
Sediments	Sediments

* Heat of combustion is not specified in the fuel quality standards

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cont....

Properties specific to gasoline and diesel are measured by a variety of test methods described in the relevant ASTM, ISO and other standards. The properties of engine fuel have been changing since the first engine was developed. A number of factors, most important being the vehicle emission control, have been responsible for changes in the fuel properties over the last few decades. The relationship of fuel properties with engine performance are qualitatively described in Table 8.2.

Table 8.2

Requirements of Automotive Fuels

Fuel Quality	Relationship with Engine and Vehicle Performance
Combustion characteristics	Better ignition and combustion properties result in higher fuel efficiency and lower emission of pollutants. High octane number for SI engine and a high cetane number for CI engines is necessary for good combustion
High heat of combustion	For the same mass of fuel on board a higher operation range of vehicle is obtained.
High volumetric energy content	A smaller fuel tank improving vehicle space utilization and packaging. Liquid fuels being sold on volume basis, it results in better economics for the operators.
Low temperature performance	A significant fraction of fuel is required to evaporate at low engine temperatures for better engine cold start and warm-up, good low-temperature drivability and better fuel economy and emissions.
High temperature drivability	For ease of hot starting, good hot weather drivability and low evaporative emissions, volatility of fuels is appropriately controlled to meet the needs of seasonal and geographical variations in ambient temperature.
Oxidation stability	Good low temperature oxidation stability reduces fuel deterioration during storage and deposit formation in the fuel system and engine combustion chamber.
Deposit formation control	Deposit control additives are now widely used for minimizing deposit formation and maintenance to get better fuel economy and low emissions during the vehicle service life.
Material Compatibility	It is essential to prevent corrosion of metallic and deterioration of fuel system rubber and elastomeric components
Flow characteristics	Fuel has to be in fluid condition at low ambient temperatures. It is particularly critical for diesel fuels. Also, appropriate diesel fuel viscosity is essential for flow as well as for good injection characteristics

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Fuel Quality Relationship with Emissions

Fuel properties can affect emissions directly as well as indirectly. Some fuel components by themselves may pose health hazards or adversely influence the environment. Some other fuel properties influence engine combustion and engine durability, while some other properties accelerate deterioration in the performance of emission control devices and systems. These fuel quality-emission interactions are given in Table 8.3

Table 8.3

Fuel Quality Interactions with Emissions

Type of Interactions	Gasoline characteristics	Diesel characteristics
Direct emission of pollutants	Lead content, Front end volatility, vapour pressure, benzene content	Sulphur, Poly aromatic hydrocarbon content
Effect on combustion	Octane number, volatility, oxygen content, final boiling point	Cetane number, Viscosity, Density, Volatility (mid – and tail-end boiling points), aromatic content
Effect on engine cleanliness and maintenance	Lead content, Final boiling point, Oxidation stability, Storage stability, Corrosion resistance	Tail-end volatility and final boiling point, Carbon residue, Sulphur content, Oxidation and storage stability, Sediments
Durability of emission control devices	Lead content, Sulphur, Sediments	Sulphur

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