ME 417: Engine Fuels

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ME 417: Internal Combustion Engines

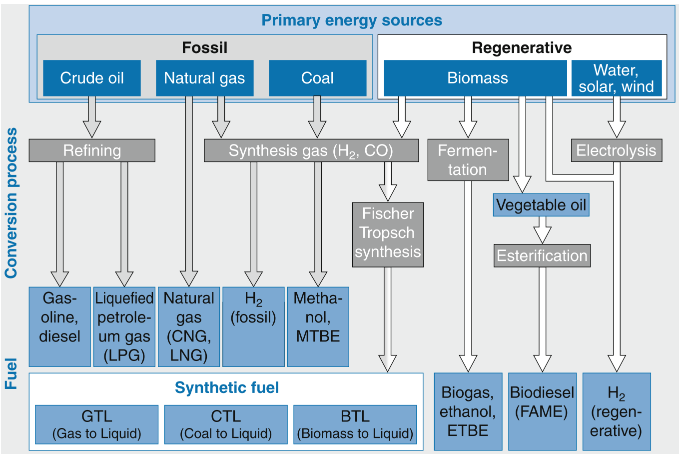
`http://zahurul.buet.ac.bd/ME417/`

Why Fuels?

Reservoirs	Requirements to hold/release 42 MJ
Kinetic energy	84,000 tons at 36 km/h
	10 m wide lead disk, 1 m thick, at 27 rpm
	1 ton of water losing 10°
	364 L of gas at 700 bar and 20 °C
Gravitation	43 tons of water falling from 100 m
Electromagnetic force	
Oil combustion	1 kg
Wood combustion	3 kg
Batteries	84 kg (best state-of-the-art technology)
Hydrogen @ 700 bar	4.7 L
Hydrogen @ −255 °C	14 L
Nuclear forces	Fission of 0.5 mg of Ur-235
	Fusion of 0.05 mg of D with 0.07 mg of T

T1718 Requirements to store 42 MJ of energy, i.e., 1 L of oil. "D" stands for deuterium, "T" for tritium

Primary Energy Sources



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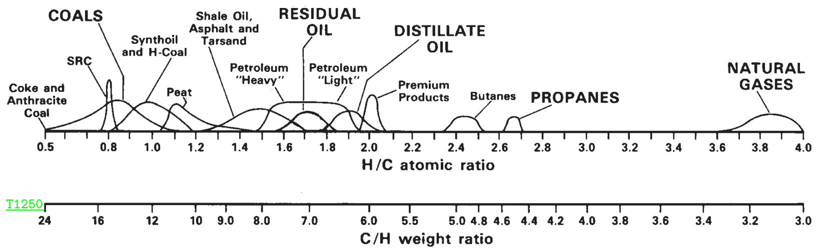
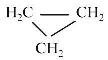
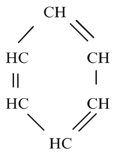
Fuels & Desirable Characteristics of Fuels



T1250

- High energy density (content)
- High heat of combustion (release)
- Good thermal stability (storage)
- Low vapour pressure (volatility)
- Non-toxicity (environmental impact)

Naming Conventions for HC Fuels

Family Name	Formula	C-C	Structure	Example
Alkanes (saturated, Paraffins)	$C_\alpha H_{2\alpha+2}$	Single	Straight or branched	Ethane CH_3-CH_3
Alkenes (olefins)	$C_\alpha H_{2\alpha}$	One double bond remaining single	Straight or branched	Ethene CH_2=CH_2
Alkynes (Acetylenes)	$C_\alpha H_{2\alpha-2}$	One triple bond remaining single	Straight or branched	Ethyne HC≡CH
Cyclanes (cycloalkanes)	$C_\alpha H_{2\alpha}$	Single bond	Closed rings	Cyclopropane 
Aromatics (benzene family)	$C_\alpha H_{2\alpha-6}$	Aromatic bond	Closed ring	Benzene 

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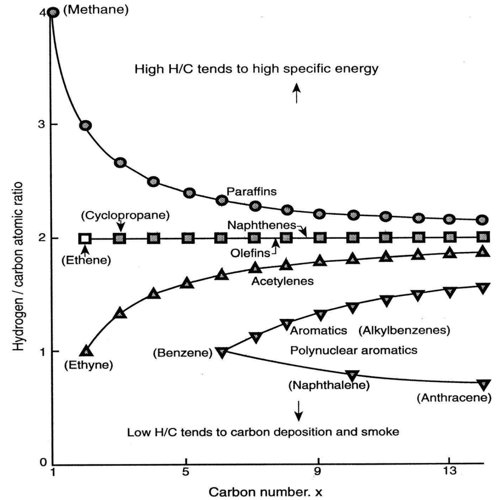


T1236

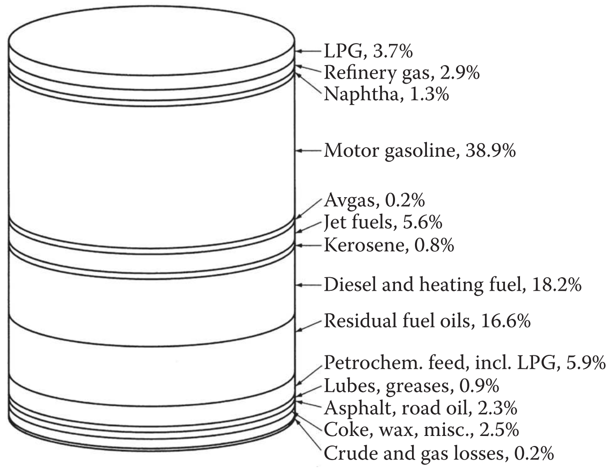
H:C atomic ratio of various inorganic hydrocarbon compounds

A comparison of some alternative fuels to the traditional petroleum-based fuels used in transportation

Fuel	Energy content kJ/L	Gasoline equivalence,* L/L-gasoline
Gasoline	31,850	1
Light diesel	33,170	0.96
Heavy diesel	35,800	0.89
LPG (Liquefied petroleum gas, primarily propane)	23,410	1.36
Ethanol (or ethyl alcohol)	29,420	1.08
Methanol (or methyl alcohol)	18,210	1.75
CNG (Compressed natural gas, primarily methane, at 200 atm)	8,080	3.94
LNG (Liquefied natural gas, primarily methane)	20,490	1.55

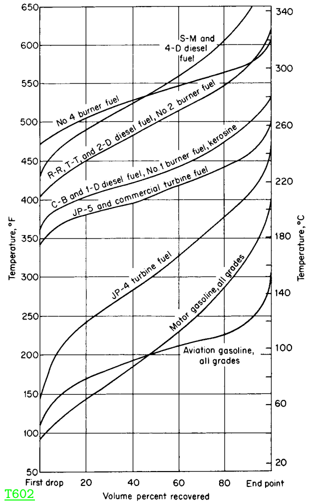
T301 **Amount of fuel whose energy content is equal to the energy content of 1-L gasoline.*

Typical Crude Oil Refinery Products



T1170

Typical ASTM Petroleum Distillation Curves



T602

- The 10% and 90% evaporation temperatures, T_{10} and T_{90} , are used in the volatility specifications.
- T_{10}: indicates the start of vaporization, is used to characterize the cold starting behaviour,
- T_{90}: indicates the finish of vaporization, is used to characterize the possibility of unburned hydrocarbons.
- The **ASTM drivability index (DI)** is a measure of fuel volatility and is defined as: $DI = 1.5T_{10} + 3T_{50} + T_{90}$

Octane Number

Steps to measure the octane number of a test fuel is as follows:

1. Run the CFR engine on the test fuel at either the motor or the research operating conditions.
2. Slowly increase the compression ratio until the standard amount of knock occurs.
3. At that compression ratio, run the engine on blends of the reference fuels isooctane and n-heptane.
4. The octane number is the percentage of isooctane in the blend that produces the standardized knock at that compression ratio.

Two sets of CFR engine operating conditions for engines are employed to define two octane numbers:

1. Research Octane Number (RON) (ASTM D908)
2. Motor Octane Number (MON) (ASTM D357)

Diesel Cetane Number

- The Cetane number characterizes the ability of the fuel to auto-ignite, the opposite of octane number.
- For high Cetane numbers, ignition delay is short. Hence, combustion is initiated while the fuel is being injected, so the burning rate is controlled by the rate of fuel–air mixing.
- For low Cetane numbers, fuel will not ignite until late in the injection process. Hence, fuel is well mixed so that once combustion is initiated, the burning rate is very high, causing diesel knock to occur.
- Cetane numbers for vehicular diesel range from about 40 to 55.
- The Cetane number of n-cetane is assigned a value of 100, as it is one of the fastest-igniting hydrocarbon.
- Isocetane (heptamethylnonane) ignites slowly & its CN = 15.

Typical Composition of Gasoline Fuels

	Average gasoline	Gasohol	Phase 1 RFG	Phase 2 RFG
Aromatics, vol%	28.6	23.9	23.4	25.4
Olefins, vol%	10.8	8.7	8.2	4.1
Benzene, vol%	1.60	1.6	1.3	0.93
Reid vapor pressure, kPa	60-S	67-S	50-S	46
(S: summer and W: winter)	79-W	79-W	79-W	
T_{50}, K	370	367	367	367
T_{90}, K	440	431	431	418
Sulfur, mass ppm	338	305	302	31
Ethanol, vol%	0	10	4	0

T580 *Source:* Adapted from EPA 420-F-95-007.

Diesel Fuel Specifications (ASTM D975)

	ASTM Method	No. 1-D	No. 2-D	No. 4-D
Minimum cetane number	D613	40	40	30
Minimum flash point, °C	D93	38	52	55
Cloud point, °C	D2500	Local	Local	Local
Maximum water and sediment, vol%		0.05	0.05	0.05
Maximum carbon residue	D524	0.15	0.35	
Maximum ash, wt%	D482	0.01	0.01	0.10
T_{90}, K	D86	561 max	555–611	
Kinematic viscosity at 40 °C (mm^2/s)	D445	1.3–2.4	1.9–4.1	5.5–24
Maximum copper strip corrosion		No. 3	No. 3	

T590

- 1-D: is a light distillate ($\sim C_{12}H_{22}$) for cold weather.
- 2-D: is a middle distillate ($\sim C_{15}H_{25}$) diesel fuel of lower volatility and is the most common for vehicles.
- 4-D: is a heavy distillate fuel used for stationary applications.

Typical Properties of Automotive Fuels

Property	Automotive Gasoline	No. 2 Diesel Fuel	Ethanol	B100 Biodiesel
Chemical formula	C_4 to C_{12}	C_8 to C_{25}	C_2H_5OH	C_{12} to C_{22}
Molecular weight	100–105	~200	32	~292
Specific gravity at 16°C	0.72–0.78	0.85	0.794	0.88
Kinematic viscosity at 20°C (m^2/s)	0.8×10^{-6}	2.5×10^{-6}	1.4×10^{-6}	–
Boiling point range (°C)	30–225	210–235	78	182–338
Reid vapor pressure (kPa)	48–69	<2	148	<0.3
Flash point (°C)	–43	60–80	13	100–170
Autoignition temp (°C)	257	~315	423	–
Octane No. (Research)	88–98	–	109	–
Octane No. (Motor)	80–88	–	90	–
Cetane No.	<15	40–55	–	48–65
Stoichiometric air-fuel ratio by weight	14.7	14.7	9.0	13.8
Carbon content (wt %)	85–88	87	52.2	77
Hydrogen content (wt %)	12–15	13	13.1	12
Oxygen content (wt %)	2.7–3.5	0	34.7	11
Heat of vaporization (kJ/kg)	380	375	920	–
LHV (MJ/kg)	43.5	45	28	42

T1171

Typical Aviation Turbine Fuel Properties

Property	Units	Jet A	Jet B
Naphthalenes	% vol max	3	3
Aromatics	% vol max	20	20
Specific gravity	°API	37–51	45–57
LHV	MJ/kg, min	42.8	42.8
Viscosity	cST at –4°F, max	8	–
Freezing point	°C, max	−40	−50
Existent gum	mg/100 mL, max	7	7
Total sulfur	wt %, max	0.3	0.3
Flash point	°C, min	38	–

T1172

Combustion Stoichiometry

$$\underbrace{C_\alpha H_\beta O_\gamma N_\delta}_{fuel} + \underbrace{a_s\ (O_2 + 3.76 N_2)}_{air} \longrightarrow \underbrace{n_1 CO_2 + n_2 H_2O + n_3 N_2}_{complete\ \ combustion\ \ product}$$

- $a_s \equiv$ stoichiometric molar air-fuel ratio
- $(A/F)_s \equiv$ stoichiometric air-fuel ratio

$$a_s = \alpha + \frac{\beta}{4} - \frac{\gamma}{2} \Rightarrow \left(\frac{A}{F}\right)_s = \left(\frac{F}{A}\right)_s^{-1} = \frac{28.85(4.76 a_s)}{12\alpha + \beta + 16\gamma + 14\delta}$$

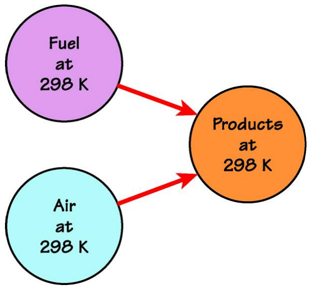
- $\phi \equiv$ fuel-air equivalence ratio, simply equivalence ratio
- $\lambda \equiv$ relative air-fuel ratio or excess-air factor

$$\phi = \lambda^{-1} = \frac{(A/F)_s}{(A/F)_a} = \frac{(F/A)_a}{(F/A)_s} : \quad \phi \begin{cases} < 1 & : \text{lean mixture} \\ = 1 & : \text{stoichiometric mixture} \\ > 1 & : \text{rich mixture} \end{cases}$$

- $(A/F)_a \equiv$ actual air-fuel ratio

Homework: Heywood: Ex. 3.1

Heating Values of Fuels



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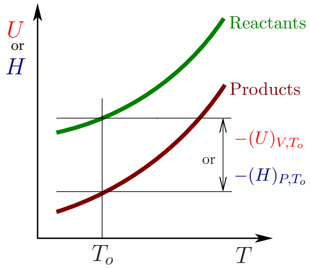

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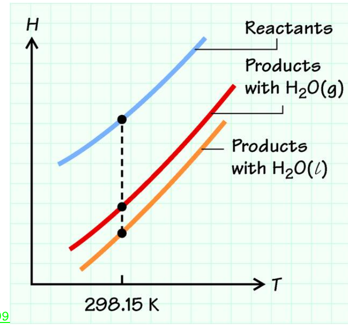
- The **heating value** is the heat release per unit mass of the fuel initially at 25°C reacts completely with oxygen (or air) and the products are returned to 25°C.
- Heating value at constant pressure $\equiv Q_{HV,P} = -(\Delta H)_{P,T_o}$
- Heating value at constant volume $\equiv Q_{HV,V} = -(\Delta U)_{V,T_o}$



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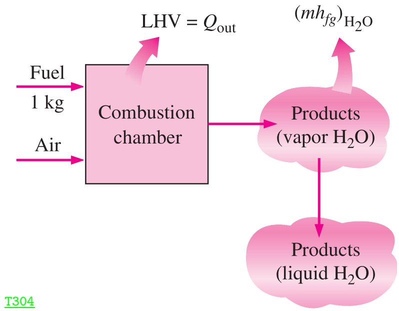
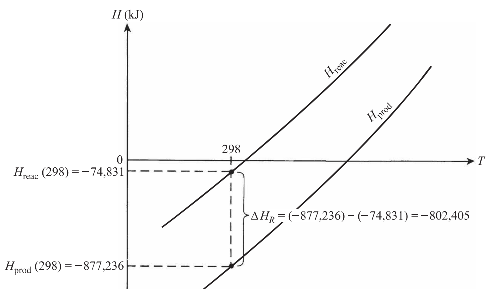


T304

$$Q_{HHV,P} = Q_{LHV,P} + \left[\frac{m_{H_2O}}{m_{fuel}}\right] h_{fg,H_2O}$$

- $Q_{HHV,P} \equiv$ Higher (Gross) Heating Value
- $Q_{LHV,P} \equiv$ Lower (Net) Heating Value
- $m_{H_2O}/m_{fuel} \equiv$ mass ratio of water produced to fuel burned.
- $h_{fg,H_2O,298K} = 2.445$ MJ/kg for water

Example: Methane-Air Combustion



T839

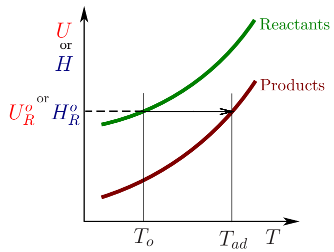
- $CH_4 + a_s\,(O_2 + 3.76N_2) \longrightarrow n_1 CO_2 + n_2 H_2O + n_3 N_2$
- $a_s = 2.0,\ n_1 = 1.0,\ n_2 = 2.0,\ n_3 = 7.52$

⇒ LHV = (802.33/16.0) MJ/kg = 50.14 MJ/kg

⇒ HHV = 50.14 + 2 × 18 /16 ×2.445 = 55.64 MJ/kg

Homework: Estimate HHV of CH_4 at constant volume.

Adiabatic Flame Temperature, T_{ad}



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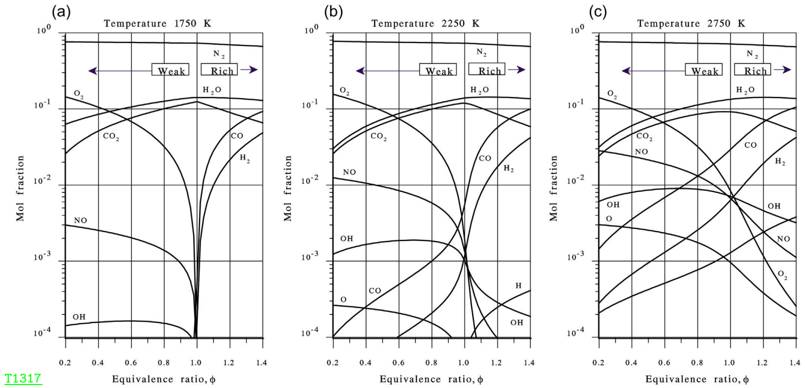
$$U_R^o = U_{prod}(T_{ad}, V = \text{constant})$$

$$H_R^o = H_{prod}(T_{ad}, P = \text{constant})$$

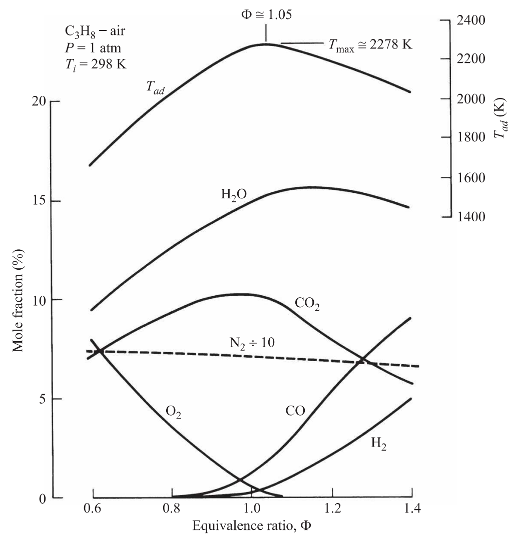
Adiabatic Flame Temperature is the product temperature in an ideal adiabatic combustion process. Actual peak temperatures in engines are several hundred degrees less due to:

- heat loss from the flame,
- combustion efficiency is less than 100%: a small fraction of fuel does not get burned, and some product components dissociate (endothermic reaction) at high temperatures.

Equilibrium Composition: iso-octane at 30 bar



T1317



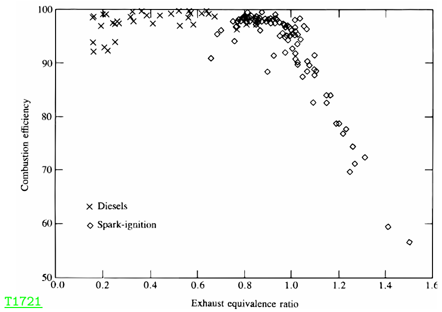
T840

- Major products of lean combustion are H_2O, CO_2, O_2 and N_2; while, for rich combustion these are H_2O, CO_2, CO, H_2 and N_2.
- Maximum flame temperature is at slightly rich condition ($\phi \simeq 1.05$) as a result of both the heat of combustion, ΔH_c and heat capacity of products decaying beyond $\phi = 1.0$.
- Between $1.0 \leqq \phi \leqq \phi(T_{max})$ heat capacities decays more rapidly with ϕ than ΔH_c and beyond $\phi(T_{max})$, ΔH_c falls more rapidly than does the heat capacity.
- Increase in temperature promotes dissociation (endothermic) reactions and increase in pressure decreases dissociation.

Fuel	Symbol	$(A/F)_s$	a_s	LHV (MJ/kg)	$T_{ad,P}$ (K)	SIT (K)
Hydrogen	H_2(g)	34.01	0.5	119.95	2383	673
Methane	CH_4(g)	17.12	2.0	50.0	2227	810
Methanol	CH_4O(l)	6.43	1.5	19.9	2223	658
Gasoline	C_7H_{17}(l)	15.27	11.25	44.5	2257	519
Octane	C_8H_{18}(l)	15.03	12.50	44.4	2266	691
Diesel	$C_{14.4}H_{24.9}$(l)	14.3	20.63	42.94	2283	483

Combustion Efficiency in ICEs

- Exhaust gas of an ICE contains incomplete combustion products (e.g. CO, H_2, unburned hydrocarbon, soot) as well as complete combustion products (CO_2 and H_2O). The amounts of incomplete combustion products are small in case of lean mixture, however these amounts become more substantial under fuel-rich conditions.



T1721

$$\eta_c = \frac{H_R(T_o) - H_P(T_o)}{m_f Q_{HV}}$$

η_c ≡ combustion efficiency
T_o ≡ ambient temperature
H_R ≡ enthalpy of reactants
H_P ≡ enthalpy of products
m_f ≡ mass of fuel
Q_{HV} ≡ heating value of fuel