M2-1: Fuels & Combustion

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Capacity Development Training Program on
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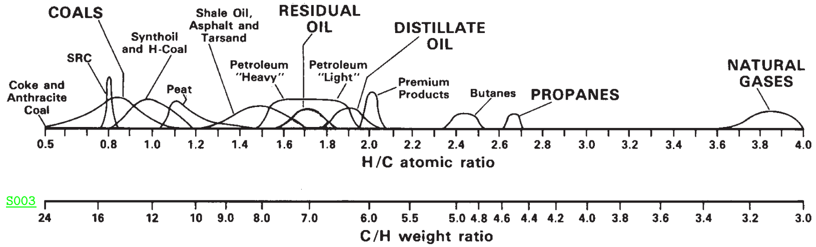
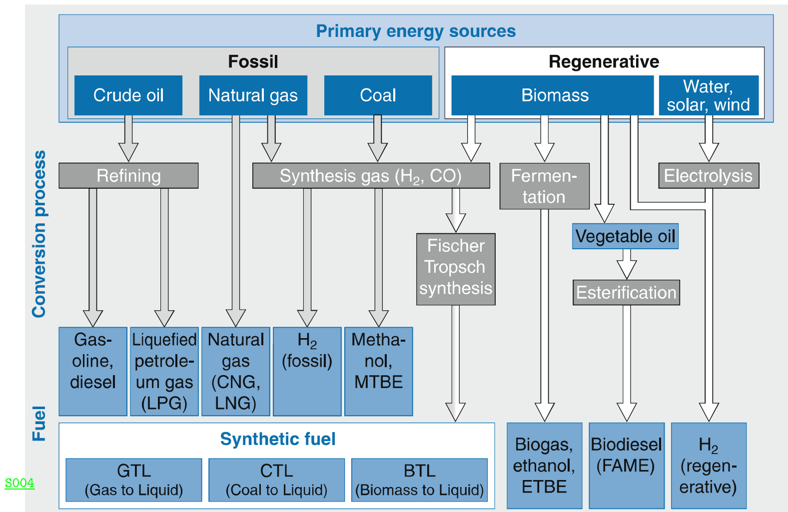
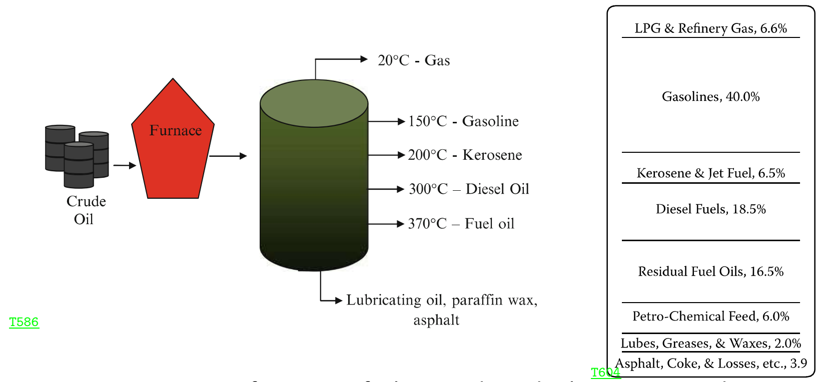
Fuels & Desirable Characteristics of Fuels



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



Petroleum Distillation Refinery



For proper engine performance, fuels must have boiling points within approximate ranges: from 30 °Cto 230 °Cfor gasoline, and for 230 °Cto 370 °Cfor diesel etc.

Properties 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

T592 *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 (mm²/s)	D445	1.3–2.4	1.9–4.1	5.5–24
Maximum copper strip corrosion		No. 3	No. 3	

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- **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 where the engine speed is low and more or less constant.

Coal Ranking & Analysis

ASTM (American Society for Testing Materials) Classifications:

1. Anthracitic coals (class I)
2. Bituminous coals (class II)
3. Subbituminous coals (class III)
4. Lignitic coals (class IV)

Analysis of coal:

- As-burned mass fraction = [dry, ash-free mass fraction][1-M-A]
- As-burned HHV = [dry, ash-free HHV][1-M-A]
  - FC ≡ mass fraction of fixed carbon
  - VM ≡ mass fraction of volatile matter
  - A ≡ mass fraction of ash
  - M ≡ mass fraction of moisture
- $HHV - LHV = 2400(M + 9H_2) \quad (kJ/kg)$
- $HHV = 33950C + 144200\left(H_2 - \frac{O_2}{8}\right) + 9400S \quad (kJ/kg)$

Combustion

- **Combustion** of fuel-air mixture inside engine cylinder is one of the processes that controls engine power, efficiency and emissions.
- Combustion commonly observed involves **flame**, which is a thin region of rapid exothermic chemical reaction.
- Flame propagation is the result of strong coupling between chemical reaction, transport processes of mass diffusion, heat conduction and fluid flow.
- Conventional spark-ignition (SI) flame is premixed unsteady turbulent flame, and the fuel-air mixture through which it propagates is in the gaseous state.
- Diesel engine (CI) combustion process is predominantly an unsteady turbulent diffusion flame, and the fuel is initially in the liquid phase.

Combustion Stoichiometry

$$\underbrace{C_\alpha H_\beta O_\gamma S_\delta}_{fuel} + \underbrace{a_s\,(O_2 + 3.76 N_2)}_{air} \longrightarrow \underbrace{\alpha CO_2 + n_1 H_2O + \delta SO_2 + n_2 N_2}_{complete\ \ combustion\ \ product}$$

$$a_s = \alpha + \frac{\beta}{4} + \delta - \frac{\gamma}{2}$$

$$M_{fuel} = 12\alpha + \beta + 16\gamma + 32\delta$$

Stoichiometric or theoretical air-fuel ratio (A/F):

$$\left(\frac{A}{F}\right)_{T,M,D} = 4.76 a_s, \qquad \left(\frac{A}{F}\right)_{T,G,D} = \frac{28.85\left(\frac{A}{F}\right)_{T,M,D}}{M_{fuel}}$$

T : theoretical or stroichiometric

M : molar basis

G : gravimetric or mass basis

D : dry

- Generalized form of $(A/F)_{T,G,D}$ from ultimate analysis:

$$\left(\frac{A}{F}\right)_{T,G,D} = \frac{2.66C + 7.94H_2 + 0.998S - O_2}{0.232}[1 - M - A]$$

where, the moisture and ash values are as-burned values and all other values are dry, ash-free values.

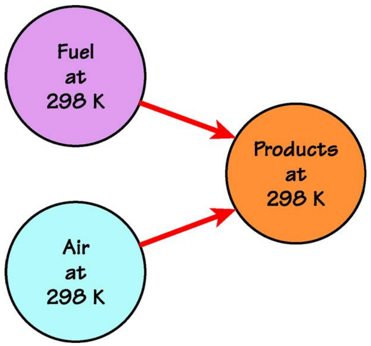
- $\lambda \equiv$ relative air-fuel ratio or excess-air factor

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

- 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.
- For lean combustion:

$$C_\alpha H_\beta O_\gamma S_\delta + \lambda\, a_s(O_2 + 3.76N_2) \rightarrow \alpha CO_2 + n_1 H_2O + \delta SO_2 + n_2 N_2 + (\lambda - 1) a_s O_2$$

Heating Values of Fuels



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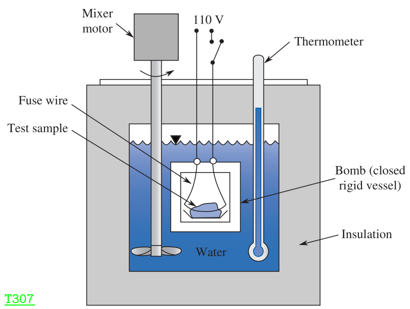
- The **heating value** is the heat release per unit mass of the fuel initially at 25 °Creacts completely with oxygen (or air) and the products are returned to 25 °C.



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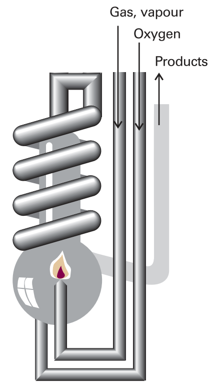
Constant Volume Bomb Calorimeter



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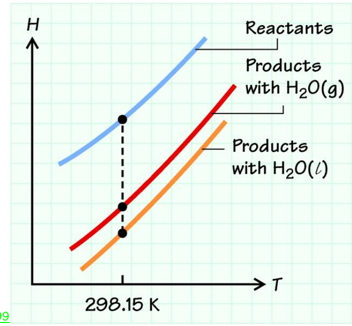
Constant Pressure Flame Calorimeter



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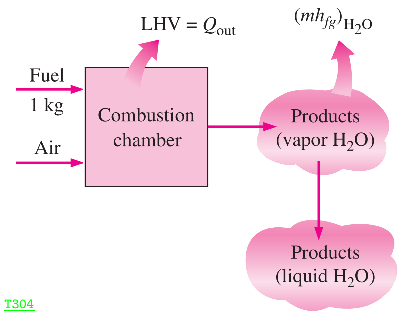

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$$Q_{HHV,P} = Q_{LHV,P} + \left[\frac{m_{H_2O}}{m_f}\right] h_{fg,H_2O}$$

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

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

Example – Methane-Air Combustion

- $CH_4 + a_s\,(O_2 + 3.76N_2) \longrightarrow n_1\,CO_2 + n_2 H_2O + n_3 N_2$
- $a_s = 2.0,\ \ n_1 = 1.0,\ \ n_2 = 2.0,\ \ n_3 = 7.52$
- $\left(\frac{A}{F}\right)_{T,M,D} = 4.76a_s = 9.52$ mole-air/mole-fuel
- $\left(\frac{A}{F}\right)_{T,G,D} = \frac{28.85\left(\frac{A}{F}\right)_{T,M,D}}{M_{fuel}} = 17.17$ kg-air/kg-fuel

⇒ Higher Heating Value (HHV): when water is in liquid form.

- $HHV = LHV + \frac{m_{H2O}}{m_f} h_{fg} = 55.5$ MJ/kg ◀

• Estimate $A/F)_{T,G,D}$ for Diesel-air combustion using two formulas.

[14.32 kg-air/kg-fuel]

Propane is used as fuel in heaters for preheating paints. Calculate the Air to Fuel ratio for complete combustion of C_3H_8 (Propane) and CO_2 released per kg of propane, if 15% excess air is supplied to the heater.

[17.95 kg-air/kg-fuel, 3 kg CO_2 per kg of fuel.]

For combustion of 500 litre/hr of furnace oil, estimate combustion air quantity per hr with 20% excess air. Sp.Gr. of furnace oil is 0.95.
(Fuel analysis: C - 84%, H_2 - 12%, S - 3%, O_2 - 1%).

[7877 kg-air/hr]

Calculate $(A/F)_{T,G,D}$ for burning LPG, composes of 40% propane and 60% butane.

[15.56 kg-air/kg-fuel]

Excess air supplied (EA)

- If $O_2\%$ of flue gas is known:

$$EA = 100 \frac{O_2\%}{21 - O_2\%} (\%)$$

- If $[CO_2\%]$ of flue gas is known:

$$EA = 7900 \frac{[CO_2\%]_t - [CO_2\%]}{[CO_2\%] \times \{100 - [CO_2\%]_t\}} (\%)$$

- $[CO_2\%]_t = 100 \frac{\text{C mole}}{\text{C mole+S mole+N mole}}$
- If ultimate analysis of fuel is known:

$C\ mole = \frac{\%C}{12}$

$S\ mole = \frac{\%S}{32}$

$N\ mole = \frac{\%N}{28} + 2.75 \left(\frac{A}{F}\right)$

Estimate EA for the combustion of coal (Ultimate analysis: C - 36%, H_2 - 2.6%, S - 0.6%, O_2 - 7.3%, N_2 - 1.1%, ash - 48% and moisture = 4.4%).
Flue gas contains: 14% CO_2 and 0.55% CO.

[32.5%]