Week 5 – Combustion and energy

EGR3030 – Energy systems and conversion 2024/25

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Reference text: Thermodynamics: An Engineering Approach. By Cengel and Boles **Chapter 15** (especially for calculation parts)

Outline

Fuels

Combustion basics

- Combustion in oxygen
- Combustion in air
- Stoichiometric ratios and air-fuel ratios

Flames and flame temperatures

Fuels

- Solid
  - Coal
  - Wood
  - Charcoal

biomass


- Liquid
  - Hydrocarbons - mostly petroleum based – kerosene, petrol, diesel
  - Spirits
- Gaseous
  - Mostly hydrocarbons – also petroleum based
    - Methane
    - Butane
    - Ethane
    - Propane, etc

Solid fuels - coal

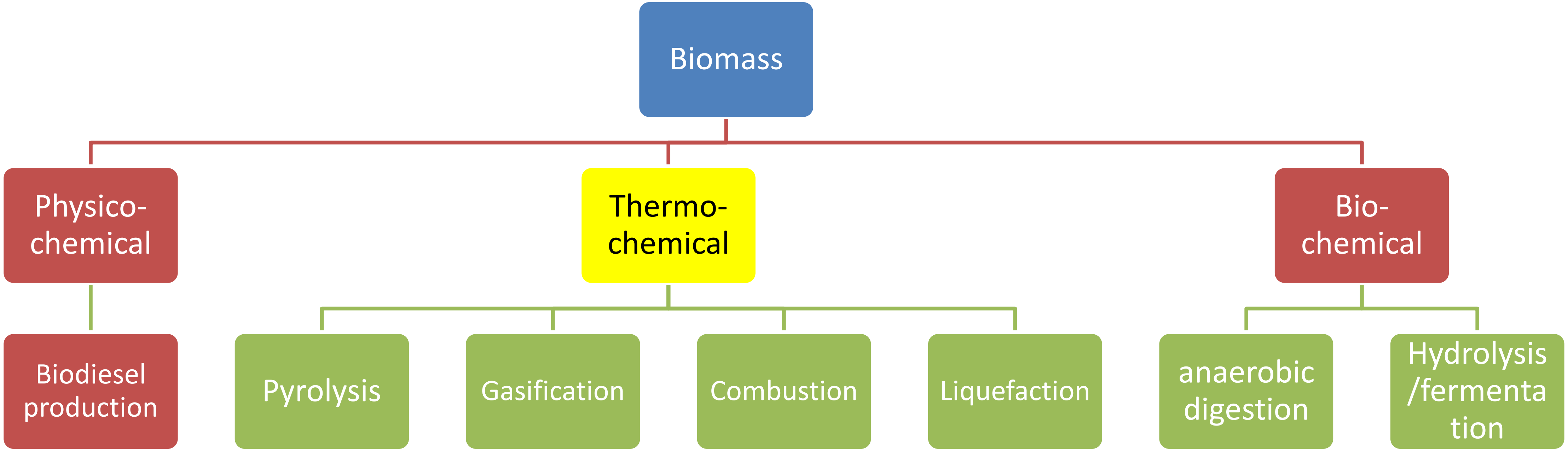
- **Coal** is a sedimentary rock that can be ignited & combusted.
- Formed by the decomposition of plant matter. It is a complex substance that can be found in many forms, mostly:
  - Anthracite
  - bituminous,
  - sub-bituminous, and
  - lignite.
- Elemental analysis gives empirical formulas such as
  - $C_{137}H_{97}O_9NS$ for bituminous coal and
  - $C_{240}H_{90}O_4NS$ for high-grade anthracite.

Solid fuels - coal

Coal composition

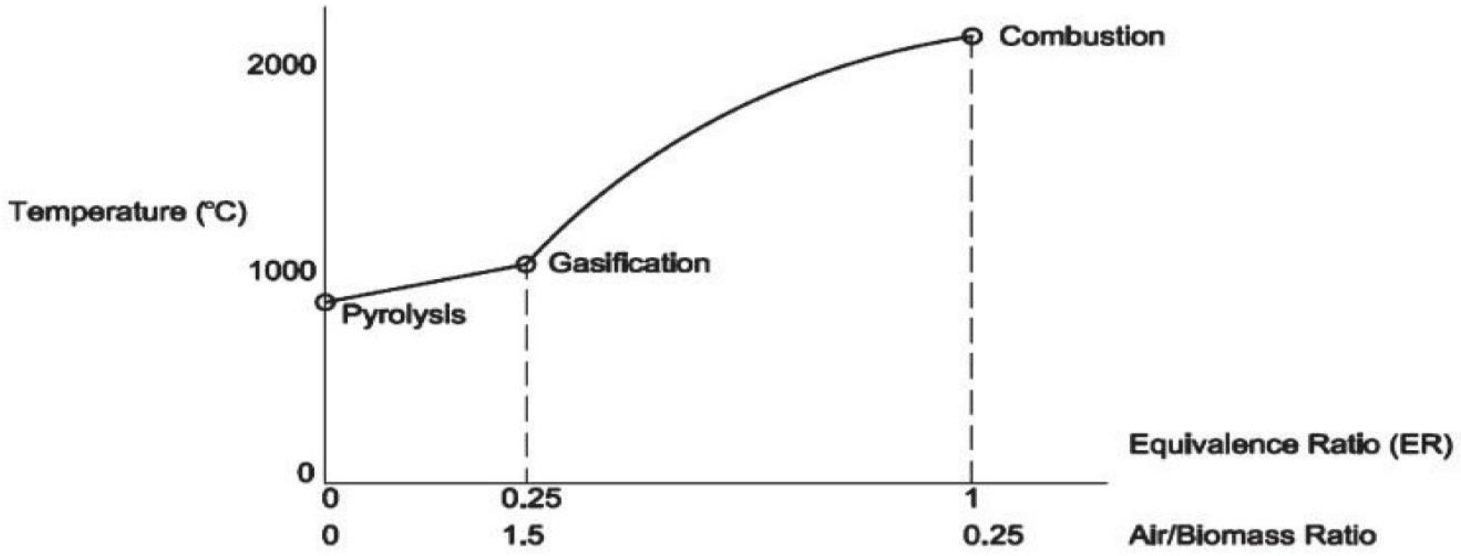
Type	Anthracite	Bituminous	Sub-bituminous	Lignite (brown coal)
Composition	Carbon 86–97%, sulphur and nitrogen, < 1%, 5-15% moisture, 10-20% ash.	84.4% carbon, 5.4% hydrogen, 6.7% oxygen, 1.7% nitrogen, and 1.8% sulphur (% w/w)	Carbon 35-35%, 15-30% moisture, sulphur <1%	Carbon 25-35%, moisture up to 66%, and ash 6% to 19%
Calorific value	26 to 35 MJ/kg	26 - 33 MJ/kg	19 – 27 MJ/kg	10 MJ/kg
Availability	Rare, mostly found in Pennsylvania in the United States	Most abundant found around the world	Attractive for steam electric power plants due to low SOx production	Mostly used for steam electric power generation

Thermochemical conversion processes for the gasification of biomass



Non-combustion thermo-chemical conversion processes are used to produce useful gases for fuels.
*Note liquid volatiles and tars are also produced

Gasification process



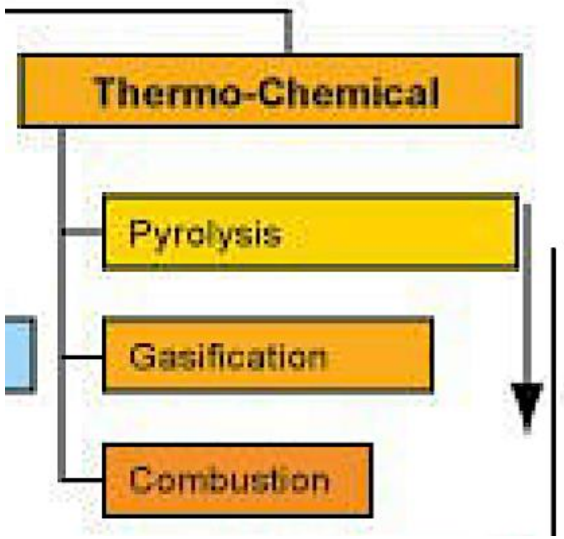
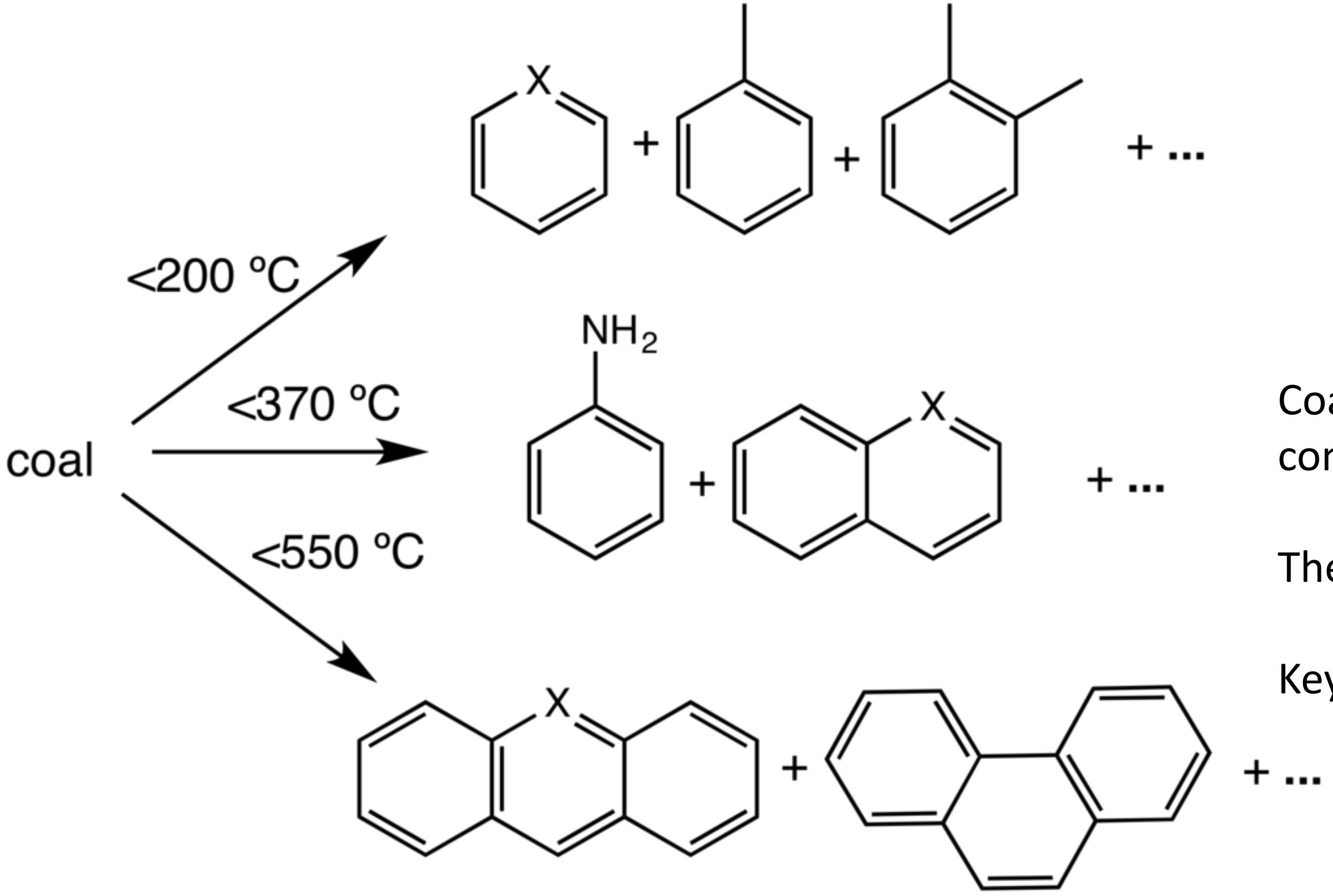


Figure 9: ER and Temperature differentiating between Pyrolysis, Gasification and Combustion.

Pyrolysis example – coal pyrolysis products



Coal pyrolysis releases volatile organic compounds without combusting them

These can be collected and used as fuel

Key: X = CH, N

Biomass in the UK

List of 100% Biomass Based Power Plants in UK:

Power Plant Name:	**Plant Capacity: (MW)**
Barton-upon-Irwell	20
Blackburn Meadows Biomass.	25
Blyth Biomass.	100
Drax Ouse.	300
Brigg Biomass.	40
Glanford.	13.5
Immingham Heron.	290
Portbury Dock.	150
Stallingborough Biomass.	65
Teesport.	300
Wilton 10.	30

Drax Power Station

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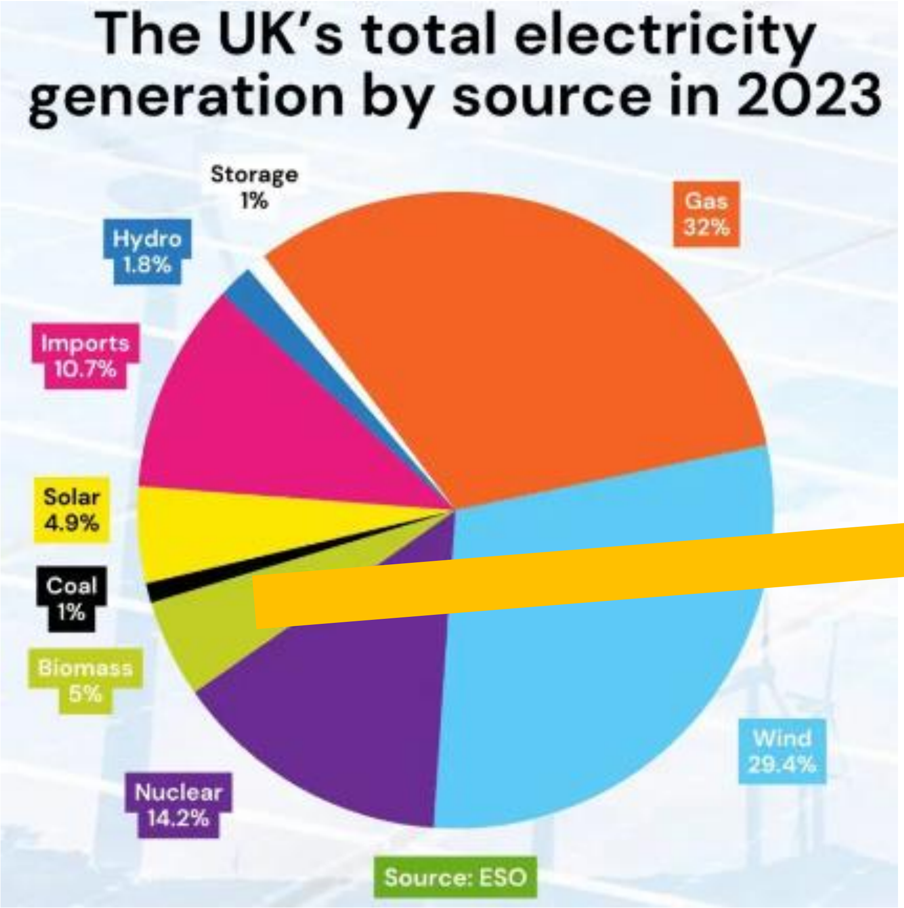
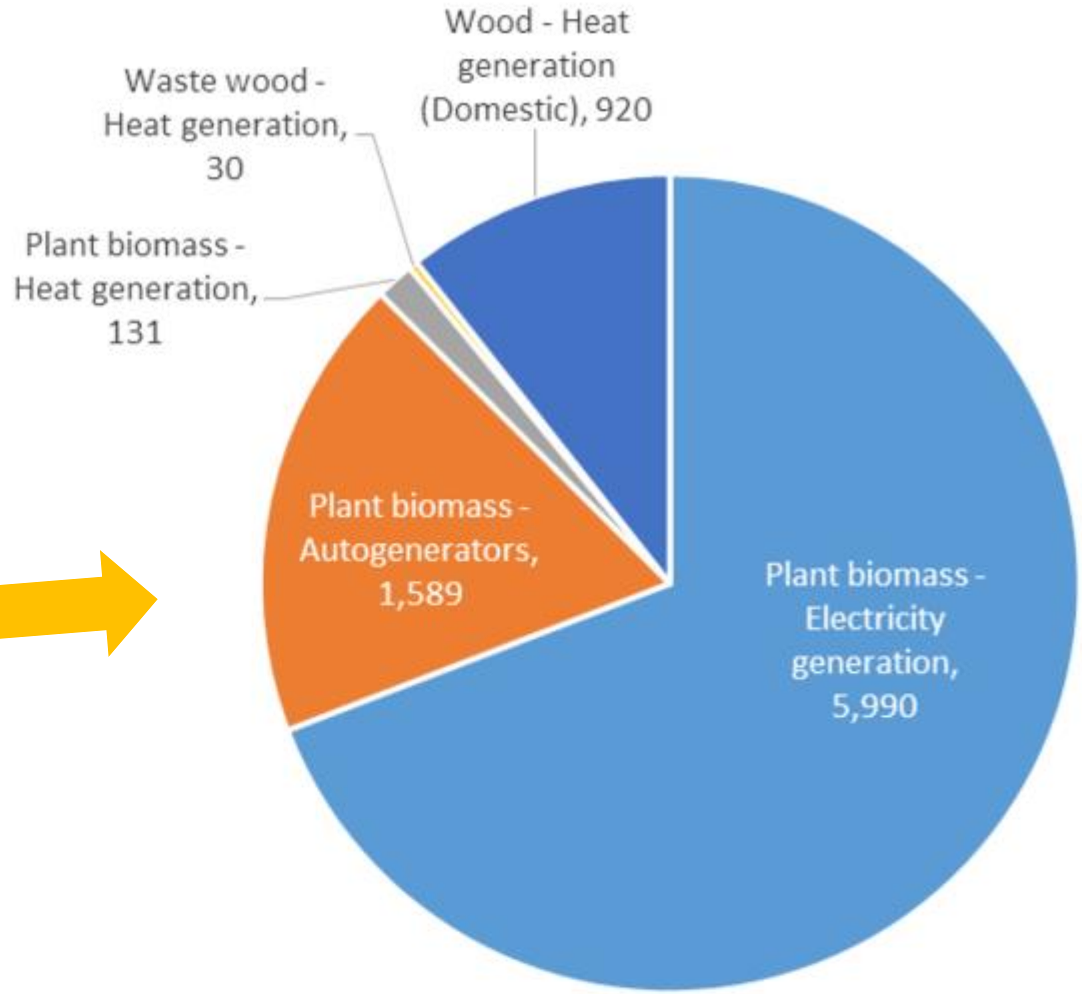
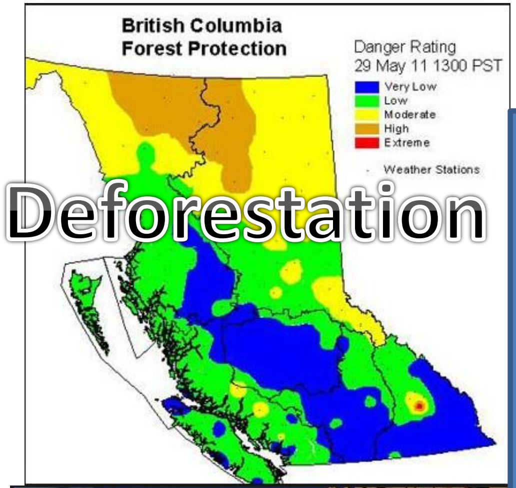
Current State of Biomass Power





Solid fuels - biomass



Current system

Logging

Transport

Chipping
& pellets

Shipping across the globe
Fossil fuel based

Combustion
&
Power
Generation

Biomass – suggestion for improvements

- Generate power where biomass is grown
- Small scale plants <1MW (so no need of transporting to large sites)
- Use process waste heat to prepare biomass
- Use engine exhaust as medium for gasification of biomass for combustion in an internal combustion engine.

Liquid fuels

Mostly used for transportation

Petroleum liquids

- Gasoline
- Diesel
- Kerosene
- Liquefied petroleum gas (LPG)

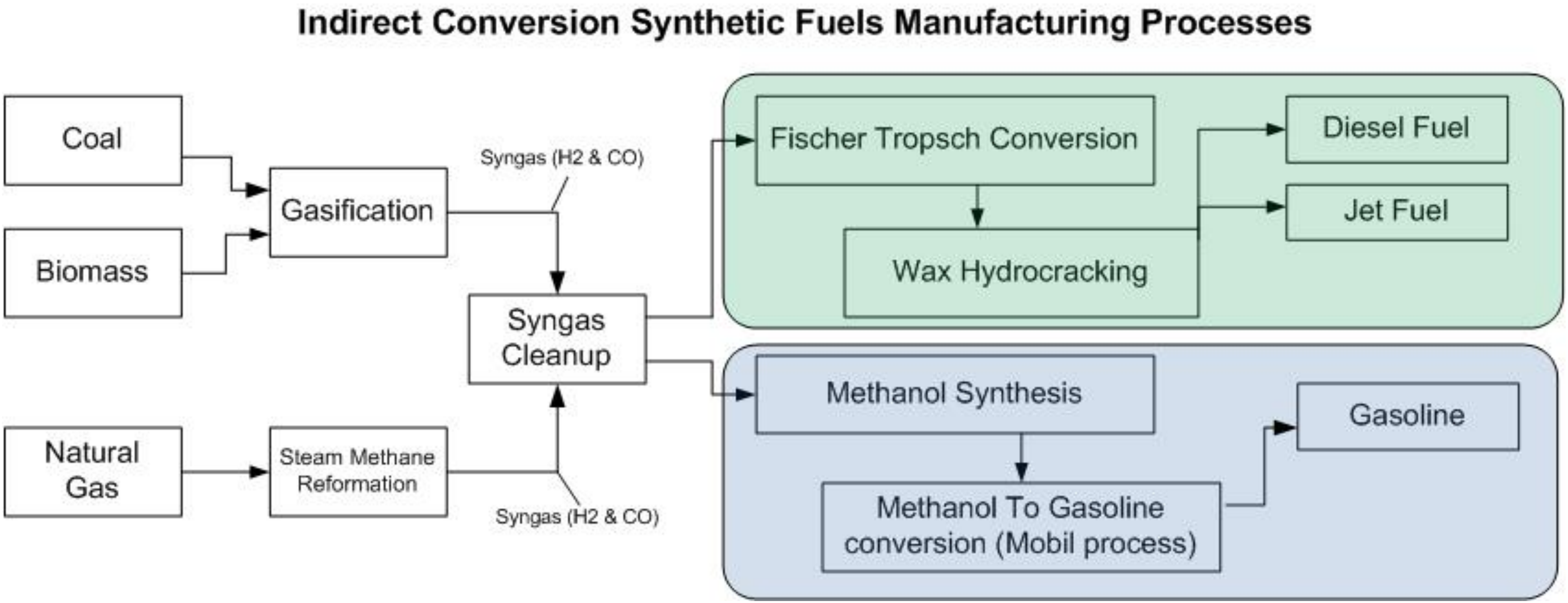
Non-petroleum liquid fossil fuels

- Synthetic fuels
- Liquefied natural gas
- Hydrogen
- Ammonia

Biofuels

- Biodiesel
- Alcohols
  - Methanol
  - (bio) Ethanol
  - Butanol

Liquid fuels – synthetic liquid fuels



Gaseous fuels

Density, molar mass and volume of, gas constant of technical gases

Name	Chemical Formula	Density $kg\,m^{-3}$	Molar Mass $kg\,kmol^{-1}$	Molar Volume $m^3\,kmol^{-1}$	Gas Constant $J\,kg^{-1}\,K^{-1}$
Acetylene	C_2H_2	1.171	26.038	22.24	319.3
Argon	Ar	1.784	39.948	22.39	208.1
Benzene	C_6H_6	3.478	78.115	22.46	106.4
Isobutane	C_4H_{10}	2.668	58.12	21.78	143.1
n-Butane	C_4H_{10}	2.703	58.12	21.50	143.1
Ethane	C_2H_6	1.356	30.07	22.17	276.5
Ethylene	C_2H_4	1.261	28.054	22.25	296.4
n-Heptane	C_7H_{16}	4.459	100.21	22.47	83.0
n-Hexane	C_6H_{14}	3.840	86.178	22.44	96.5
Hydrogen	H_2	0.090	2.016	22.43	4124.7
Sulfur dioxide	SO_2	2.928	64.06	21.88	129.8
Hydrogen sulfide	H_2S	1.539	34.08	22.14	244.0
Air	-	1.293	28.96	22.40	287.1
Methane	CH_4	0.718	16.043	22.38	518.3
Nitrogen	N_2	1.206	28.013	22.40	296.8
Oxygen	O_2	1.429	31.999	22.39	295.8
n-Pentane	C_5H_{12}	3.457	72.151	20.87	115.2
Propane	C_3H_8	2.019	44.097	21.84	178.6
Propylene	C_3H_6	1.915	42.081	21.97	197.6
Carbon dioxide	CO_2	1.977	44.01	22.26	188.9
Carbon monoxide	CO	1.25	28.01	22.41	296.8
Steam	H_2O	0.804	18.015	23.46	461.5

Gaseous fuels – natural gas

- The most common gaseous fuel for industry
- Typical composition:

Name	Formula	Amount (vol.%)
Methane	CH_4	70–90
Ethane	C_2H_6	0–20
Propane	C_3H_8	
Butane	C_4H_{10}	
Carbon dioxide	CO_2	0–8
Oxygen	O_2	0–0.2
Nitrogen	N_2	0–5
Hydrogen sulfide	H_2S	0–5
Rare gases	Ar, He, Ne, Xe	trace

Cost of fuels for power generation in terms of CO_2 emissions

FUEL:	**CO2 EMISSIONS :** kg CO2 **(PER KWH*)**
Coal.	0.390
Gas oil.	0.327
Wood Pellets.	0.044
Seasoned Wood.	0.025

Combustion basics

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What is combustion

- Combustion is the exothermic reaction of an oxidising agent and a fuel, Generally a hydrocarbon ($C_x H_y$)
- The heat release is accompanied in most cases by light in the form of glowing or flame.
- Combustion requires:
  – Fuel
  – Oxidising agent (oxidant)

  It is a complex process depending on the fuel or oxidising agent

Combustion basics – stoichiometry of combustion in O_2

Fundamental definitions

Chemical Reaction

The exchange and/or rearrangement of atoms between colliding molecules.

Methane combustion in the presence of pure oxygen

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

What about:

- Ethane
- Propane
- Ethene
- Propyne?

Recall that

Alkanes: C_nH_{2n+2}

Alkenes: C_nH_{2n}

Alkynes C_nH_n

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O$$

Combustion basics – stoichiometry of combustion in air

- Combustion in air implies the presence of nitrogen. By volume: 21% O_2 and 79% N_2
  i.e., for every 1 mole of O_2 there are 3.76 moles N_2

$$C_xH_y + a(O_2 + 3.76N_2) \rightarrow xCO_2 + \left(\frac{y}{2}\right)H_2O + 3.76aN_2$$

- Example Methane CH_4 (Main component of natural gas)

$$CH_4 + a(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 3.76aN_2$$

- Hence $a = \left[x + \frac{y}{4}\right] = 2$ from Oxygen (O_2) balance.
- This is the volumetric stoichiometric balance.
- But Stoichiometric balance (hence ratio) is normally mass based.
  - This is calculated using atomic weights (basic whole numbers)
  - C= 12 H =1 O=16 N=14
  - Hence Methane = 12+4 = 16
  - Air used = 2*(32 + 3.76 *28) = 274.56
  - Stoichiometric ratio (mass based) = 274.56/16 = 17.16 m/m

Combustion basics

Fundamental definitions

Stoichiometric ratio

- The ideal (theoretical) air-fuel ratio, for a **complete combustion**, is called **stoichiometric air fuel ratio (AFR)**.

- For a petrol engine, the stoichiometric AFR $\cong$ 14.7:1. This means to completely burn 1 kg of fuel, we'll need 14.7 kg of air. Combustion is possible even if the actual AFR $\neq$ stoichiometric. Minimum AFR is around 6:1 and the maximum can go up to 20:1.

- When:
  - actual AFR > stoichiometric ratio, the air fuel mixture is called **lean**. Actual AFR
  - actual AFR < stoichiometric ratio, the air fuel mixture is called **rich**.

  For example, for a petrol engine, an AFR of 16.5:1 is lean and 13.7:1 is rich.

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Consequences of non ideal AFR

- Lean AFR: a lean mixture can simply shut the engine down, either because the fuel/air ratio gets too small to be combustible, or because the amount of fuel becomes too small to give any power

- Rich AFR: if the engine is fed too much fuel, combustion is incomplete, it produces excessive smoke, wears out quickly and is expensive to run.

Combustion basics – stoichiometric ratio class tutorial

Calculate the stoichiometric ratio for the combustion in air of:

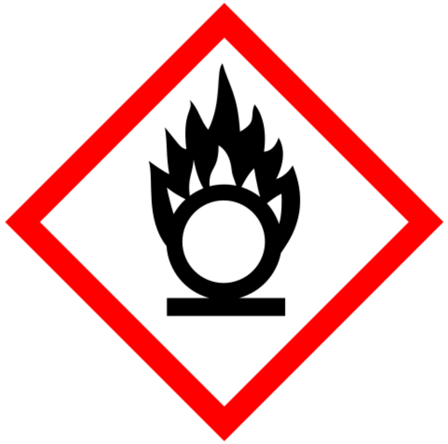
- Ethane C_2H_6
- Propane C_3H_8
- Butane C_4H_{10}
- Benzene C_6H_6
- Diesel Fuel $C_{15}H_{28}$

Stoichiometry in air

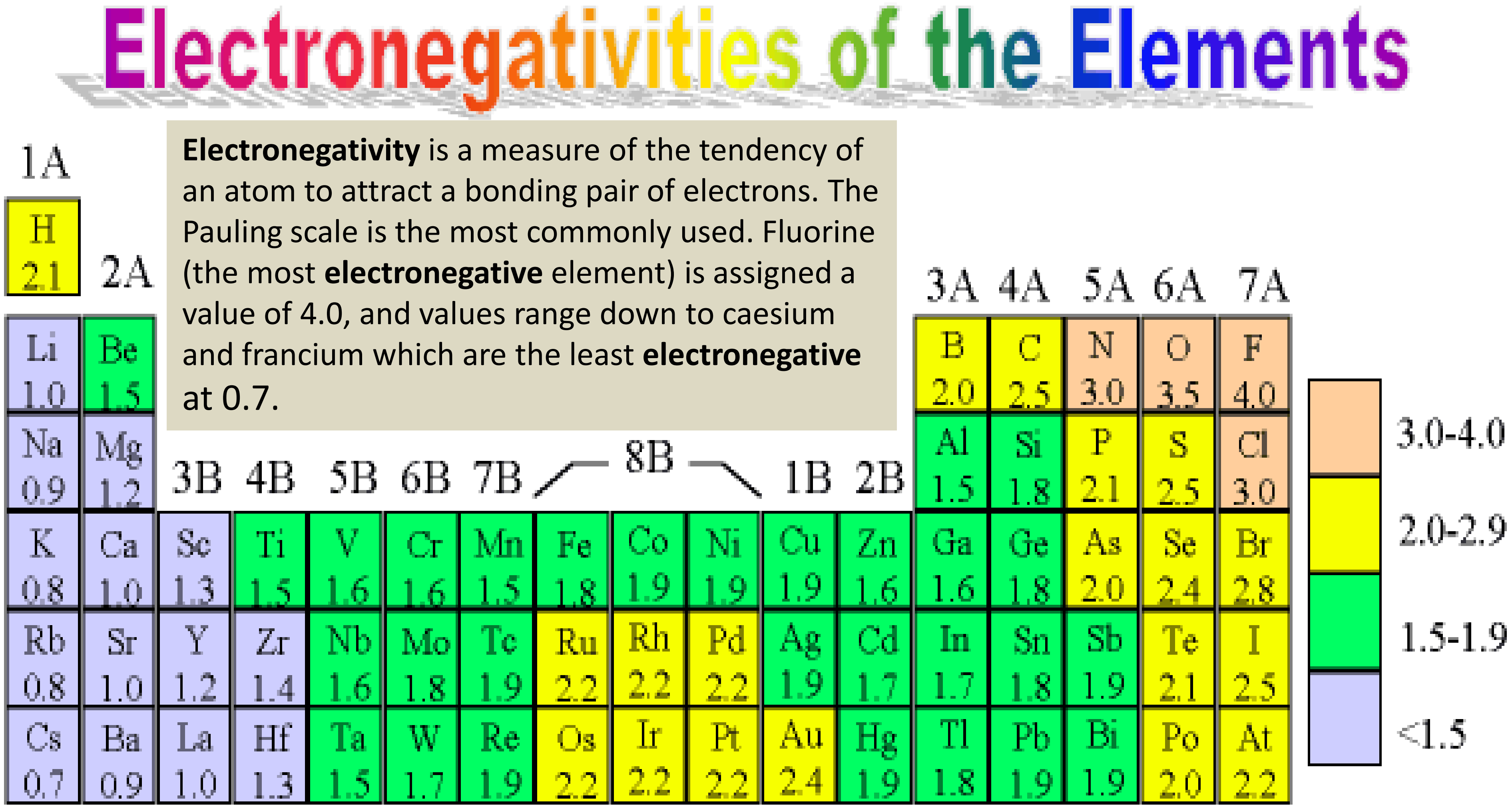
Fuel	Ratio by mass [6]	Ratio by volume [7]	Percent fuel by mass	Main Reaction
Gasoline	14.7 : 1	—	6.8%	$2\ C_8H_{18} + 25\ O_2 \rightarrow 16\ CO_2 + 18\ H_2O$
Natural gas	17.2 : 1	9.7 : 1	5.8%	$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$
Propane (LP)	15.67 : 1	23.9 : 1	6.45%	$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$
Ethanol	9 : 1	—	11.1%	$C_2H_6O + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$
Methanol	6.47 : 1	—	15.6%	$2\ CH_4O + 3\ O_2 \rightarrow 2\ CO_2 + 4\ H_2O$
n-Butanol	11.2 : 1	—	8.2%	$C_4H_{10}O + 6\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$
Hydrogen	34.3 : 1	2.39 : 1	2.9%	$2\ H_2 + O_2 \rightarrow 2\ H_2O$
Diesel	14.5 : 1	—	6.8%	$2\ C_{12}H_{26} + 37\ O_2 \rightarrow 24\ CO_2 + 26\ H_2O$
Methane	17.19 : 1	9.52 : 1	5.5%	$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$
Acetylene	13.26 : 1	11.92 : 1	7.0%	$2\ C_2H_2 + 5\ O_2 \rightarrow 4\ CO_2 + 2\ H_2O$
Ethane	16.07 : 1	16.68 : 1	5.9%	$2\ C_2H_6 + 7\ O_2 \rightarrow 4\ CO_2 + 6\ H_2O$
Butane	15.44 : 1	30.98 : 1	6.1%	$2\ C_4H_{10} + 13\ O_2 \rightarrow 8\ CO_2 + 10\ H_2O$
Pentane	15.31 : 1	38.13 : 1	6.1%	$C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$

Oxidants

- An **oxidising agent** (oxidant, oxidiser) is a substance that has the ability to oxidize other substances (cause them to lose electrons).
- Common oxidising agents are oxygen O_2, Ozone O_3, hydrogen peroxide H_2O_2, and the halogens Br, Cl, Fl.
- In one sense, an oxidizing agent is a chemical species that undergoes a chemical reaction that removes one or more electrons from another atom.



Oxidising agents – periodic table



Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons. The Pauling scale is the most commonly used. Fluorine (the most **electronegative** element) is assigned a value of 4.0, and values range down to caesium and francium which are the least **electronegative** at 0.7.

Flames

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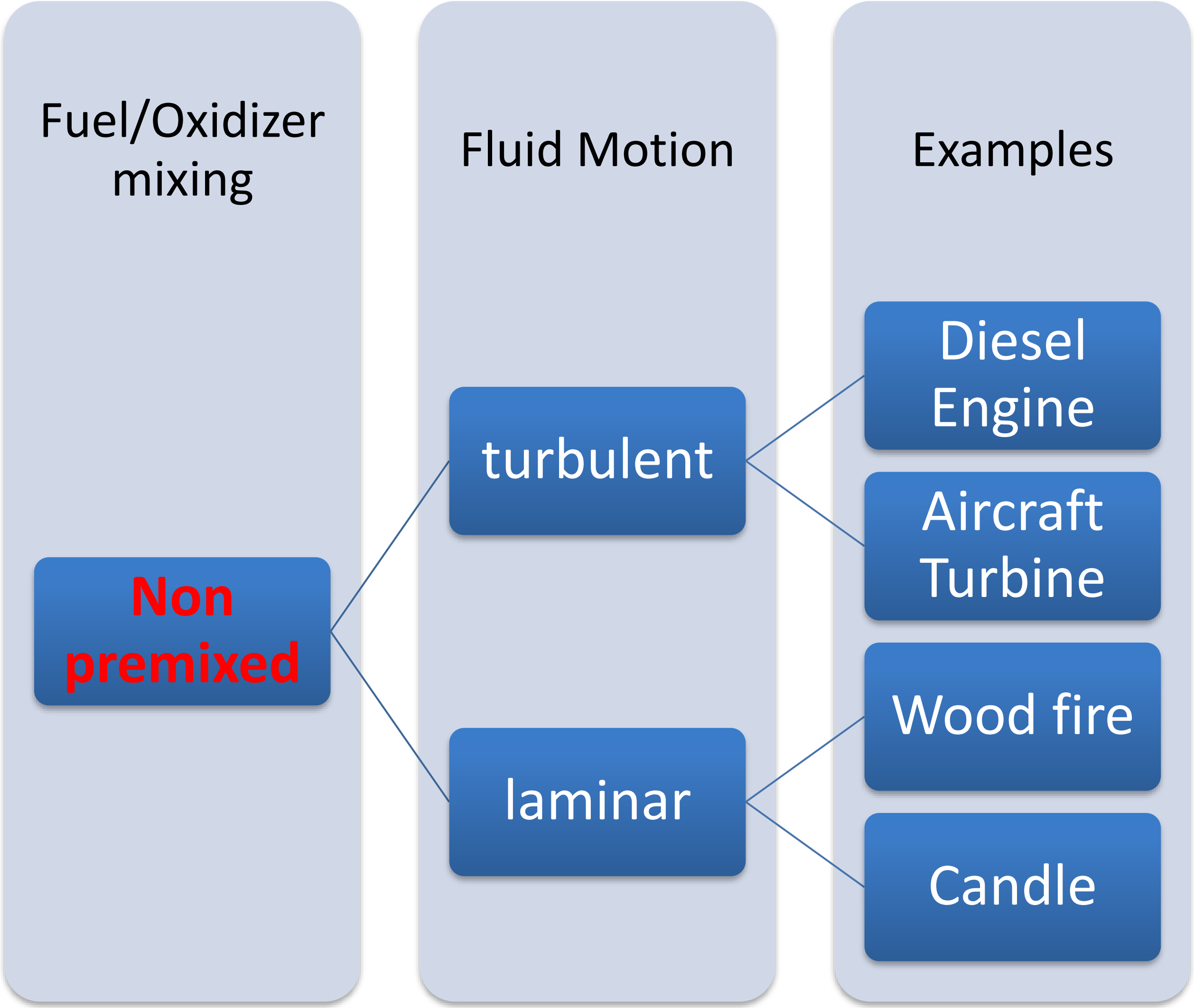
Basic Flame Types

Fuel/Oxidizer mixing	Fluid Motion	Examples

- **Premixed**
  - turbulent
    - SI gasoline engine
    - Low Nox stationary GT
  - laminar
    - Flat flame
    - Bunsen flame

Basic Flame Types



The adiabatic flame temperature (AFT)

- The *adiabatic flame* or *adiabatic combustion temperature* is the temperature during combustion, when no heat is lost to the surroundings ($Q = 0$) such that the temperature of the products reaches a maximum.

- In combustion chambers, the highest temperature to which a material can be exposed is limited by metallurgical considerations. Therefore, the adiabatic flame temperature is an important consideration in the design of combustion nozzles & chambers, IC engines, and gas turbines.

- The maximum temperature in a combustion chamber can be controlled by adjusting the amount of excess air, which serves as a coolant.

- The adiabatic flame temperature of a fuel is not unique. Its value depends on (1) the state of the reactants, (2) the degree of completion of the reaction, and (3) the amount of air used.

Calculation of AFT

From the first law,

$$Q - W \ = \ \Delta H = \ H_{prod} \ - \ H_{reactants}$$

As Q = 0 for AFT, with no work done:

$$H_{prod} = \ H_{reactants}$$

or

$$\sum N_p\left(h^\circ{}_f \ + \ h \ - \ h^\circ\right)_p \ = \sum N_r\left(h^\circ{}_f \ + \ h \ - \ h^\circ\right)_r \quad (kJ/kmol\ fuel)$$

where Nr, Np = number of moles of the reactant r and the product p, per mole of fuel. Note:

Nr and Np are picked directly from the balanced combustion equation;

h = the sensible enthalpy at the specified state

h° = sensible enthalpy at the standard reference state of 25°C and 1 atm

$h^\circ{}_f$ is the standard heat of formation of the compound (reactant or product)

Calculation of AFT procedure

1. Once the reactants and their states are specified, the enthalpy of the reactants H_{react} can be easily determined.

2. The calculation of the enthalpy of the products H_{prod} is not so straightforward, because the temperature of the products is not known prior to the calculations.

3. Hence, calculating AFT requires iteration – a temperature is assumed for the product gases, and H_{prod} is determined for this temperature. If it is not equal to H_{react}, calculation is repeated with another temperature. The AFT is then determined from these two results by interpolation.

4. When the oxidant is air, the product gases mostly consist of N_2, and a good first guess for the adiabatic flame temperature is obtained by treating the product gases as N_2.

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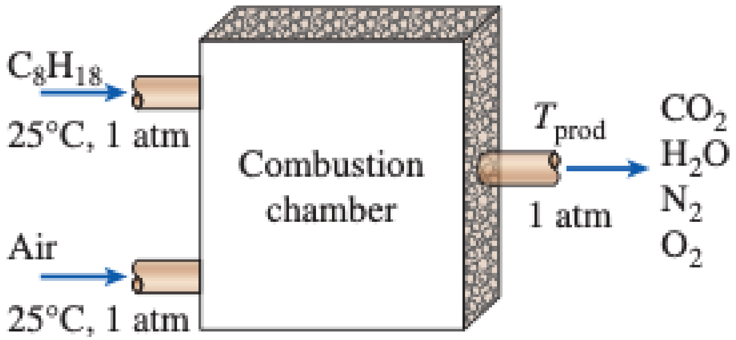
Calculation of AFT – tutorial

Liquid octane (C_8H_{18}) enters the combustion chamber of a gas turbine steadily at 1 atm and 25°C, and it is burned with air that enters the combustion chamber at the same state. Determine the adiabatic flame temperature for:



(a) complete combustion with 100 percent theoretical air

(b) complete combustion with 400 percent theoretical air, and

(c) incomplete combustion (some CO in the products) with 90% theoretical air.

Substance	$\bar{h}_f^\circ$ kJ/kmol	$\bar{h}_{298\text{ K}}$ kJ/kmol
$C_3H_{18}(l)$	–249,950	—
O_2	0	8682
N_2	0	8669
$H_2O(g)$	–241,820	9904
CO_2	–393,520	9364

Calculation of AFT – tutorial Matlab code – using the Cp method

```
clc; clear;
format short g;

T_init = 1000;
fun = @enthalpy_equations;

[T_final, fval] = fsolve(@enthalpy_equations, T_init)

function eqn = enthalpy_equations(T_init)
%please check the values of cp coefficients, I may have made errors
%entering some of them, but this is the method using fsolve.
%cp = a + bT + cT^2 + dT^3; ; and then H_total = sum(cp*T)

hCO2 = 22.26 + (5.981*1e-2)*T_init + (-3.501*1e-5)*T_init^2 + (7.469*1e-9)*T_init^3;
hH2O = 32.24 + (0.1923*1e-2)*T_init + (1.055*1e-5)*T_init^2 + (-3.595*1e-9)*T_init^3;
hN2 = 28.9 + (-0.1571*1e-2)*T_init + (0.8081*1e-5)*T_init^2 + (-2.873*1e-9)*T_init^3;
eqn = T_init*(8*hCO2 + 9*hH2O + 47*hN2) – sum_nh;

end
```

Additional questions to try

1. Propane (C_3H_8) is burned with 75 percent excess air during a combustion process. Assuming complete combustion, determine the air–fuel ratio.

    Answer: 27.5 kg air/kg fuel

2. In a combustion chamber, ethane (C_2H_6) is burned at a rate of 8 kg/h with air that enters the combustion chamber at a rate of 176 kg/h. Determine the percentage of excess air used during this process.

    Answer: 37 percent

3. Determine the enthalpy of combustion of methane (CH_4) at 25°C and 1 atm, using the enthalpy of formation data from Table A–26. Assume that the water in the products is in the liquid form. Compare your result to the value listed in Table A–27.

    Answer: –890,330 kJ/kmol

4. Acetylene gas (C_2H_2) at 25°C is burned during a steady-flow combustion process with 30 percent excess air at 27°C. It is observed that 75,000 kJ of heat is being lost from the combustion chamber to the surroundings per kmol of acetylene. Assuming combustion is complete, determine the exit temperature of the product gases. (AFT question)

    Answer: 2301 K

Recap

- Fuels
- Combustion basics
  - ➢ Combustion in oxygen
  - ➢ Combustion in air
  - ➢ Stoichiometric ratios and air-fuel ratios
- Flames and flame temperatures