Aalto University
School of Engineering

EEN-E2002 Combustion Technology

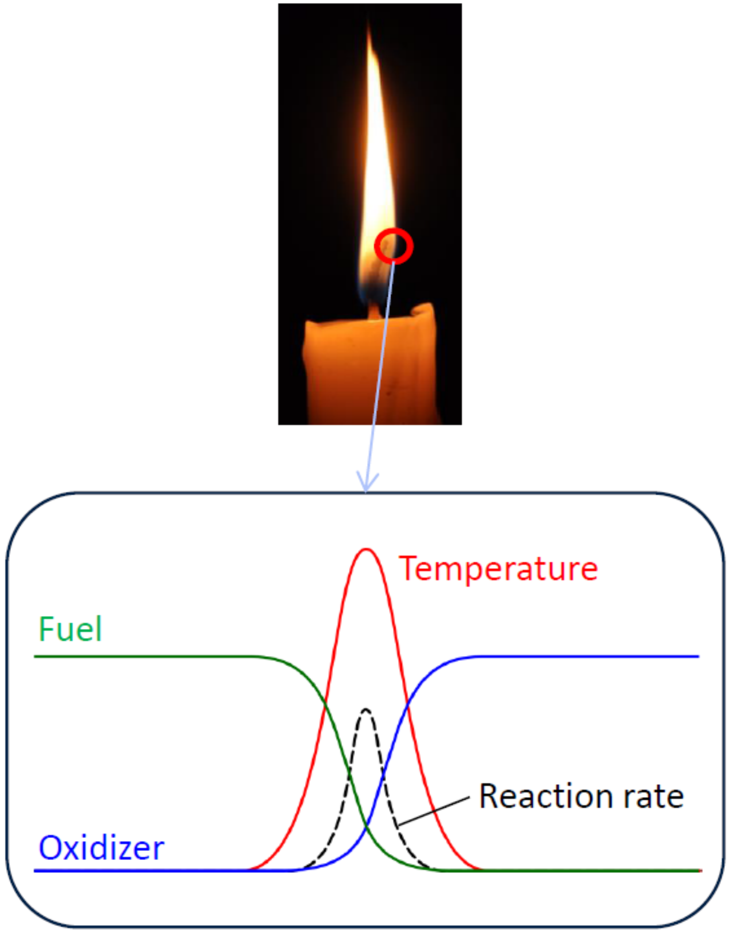
LE1 advice session

21.01.2019, Jonny

Basic combustion types- Diffusion (non-premixed) flame

Laminar diffusion flames

- Fuel and Oxidizer: Seperate feeding of fuel and oxidizer
- Mixing: Convection and diffusion
  On a molecular level
  (locally) stoichiometric mixture
- Simple example for a diffusion flame:
  Candle flame
  Paraffin vaporizes at the wick →
  diffuses into the surrounding air
- Simultaneously: Air flows towards the flame due to free convection and forms a mixture with the vaporized paraffin



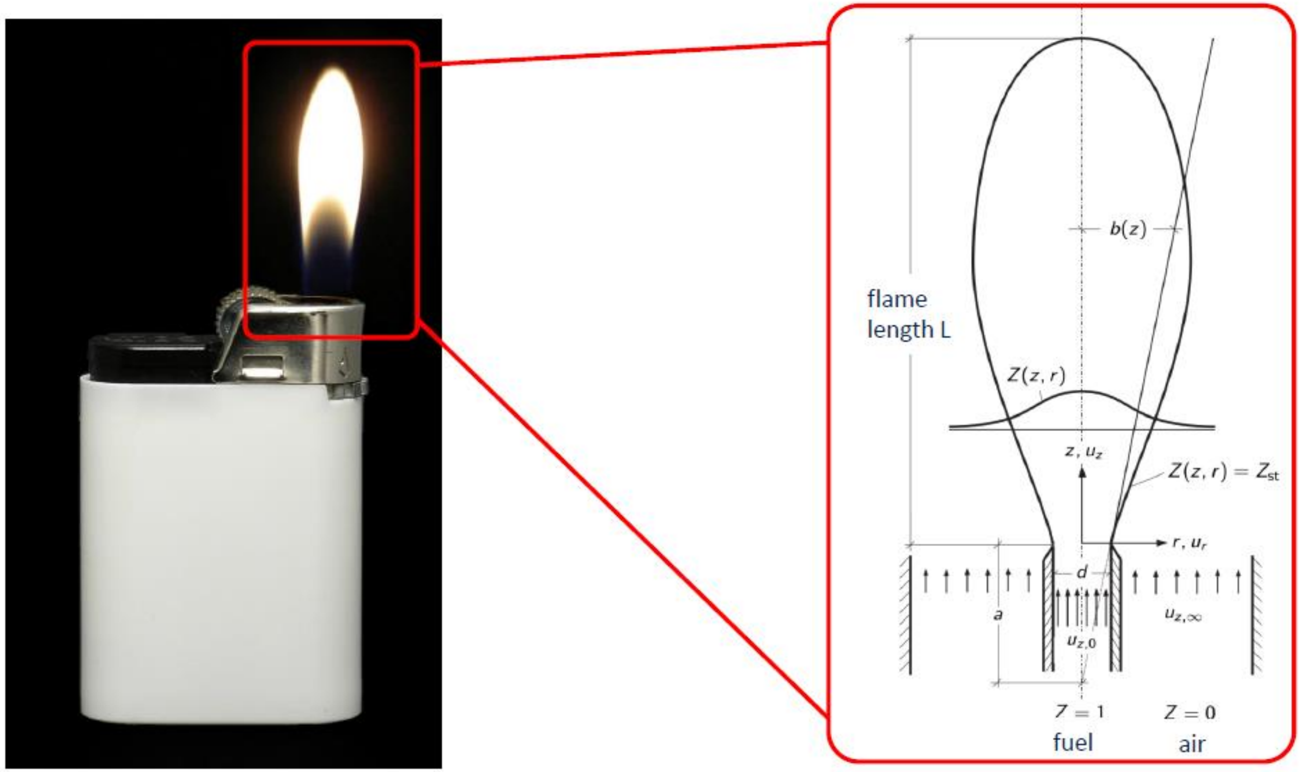
Structure of a diffusion flame (schematic)

Basic combustion types- Diffusion (non-premixed) flame

Laminar Jet Diffusion Flames

- Fuel enters into the combustion chamber as a round jet
- Forming mixture is ignited
- Example: Flame of a gas lighter
    - Only stable if dimensions are small
    - Dimensions too large: flickering due to influence of gravity
    - Increasing the jet momentum → Reduction of the relative importance of gravity (buoyancy) in favor of momentum forces

At high velocities, hydrodynamic instabilities gain increasing importance: laminar-turbulent transition



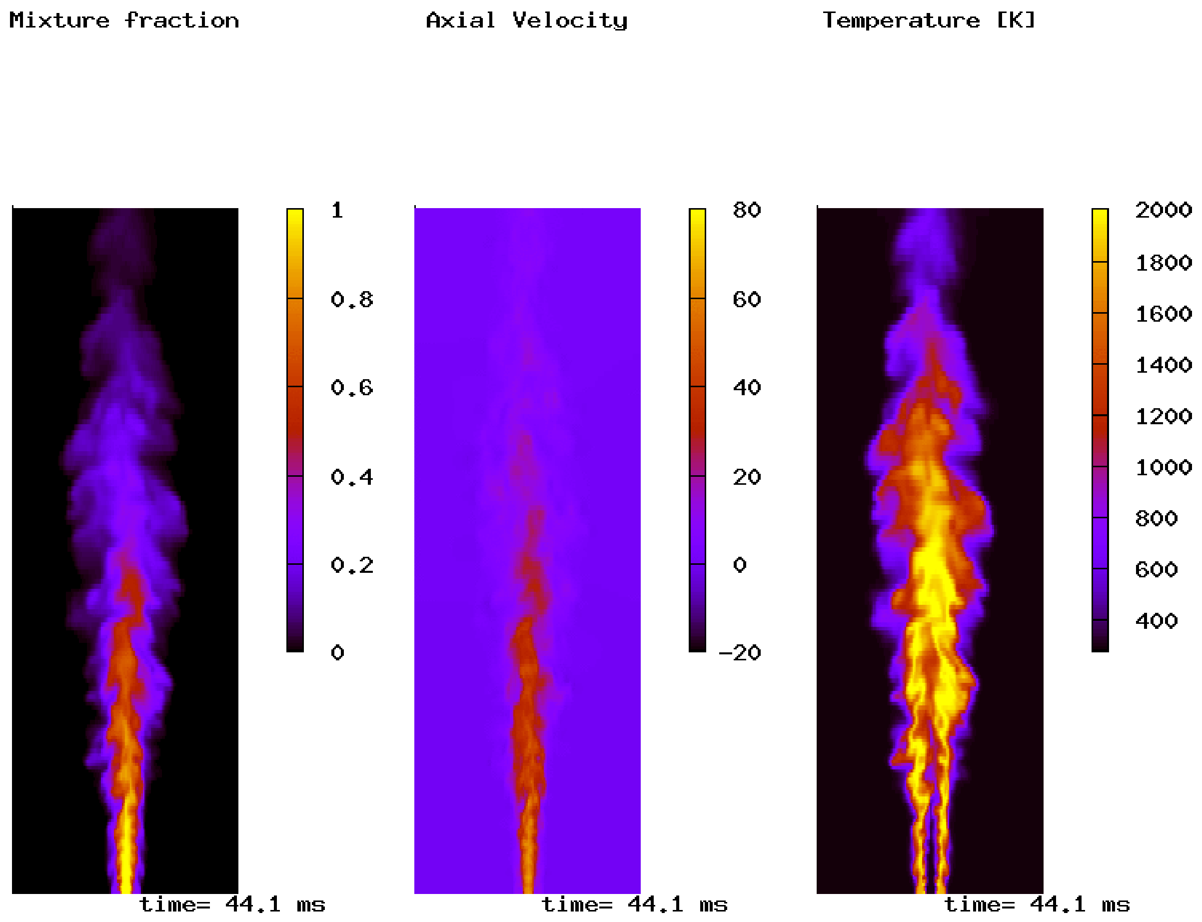
Basic combustion types- Diffusion (non-premixed) flame

Turbulent Jet Diffusion Flames

- Fuel enters into the combustion chamber as a round jet

- Example: Diesel combustion in internal combustion engine

Turbulent convection mixes fuel and air macroscopically, then molecular mixing completes the process so that chemical reaction can take place.



Basic combustion types- premixed flame

Premixed combustion used in combustion devices when high heat release rates are desired

Small devices

Low residence times

- Examples:

SI engine

Stationary gas turbines

- Advantage

Lean combustion possible

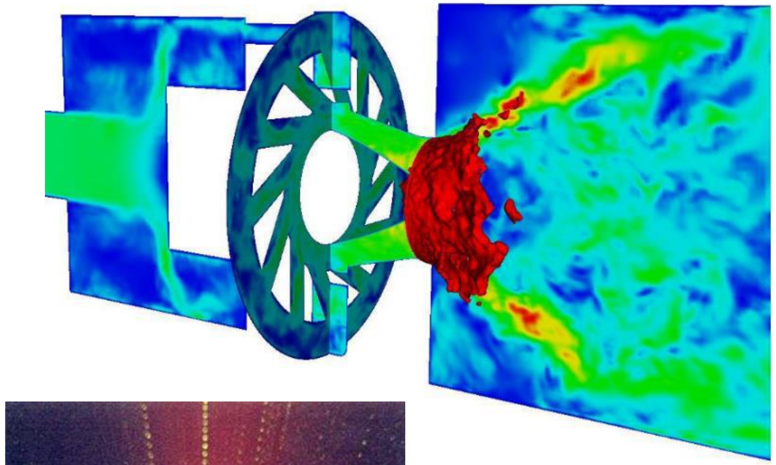
Smoke-free combustion

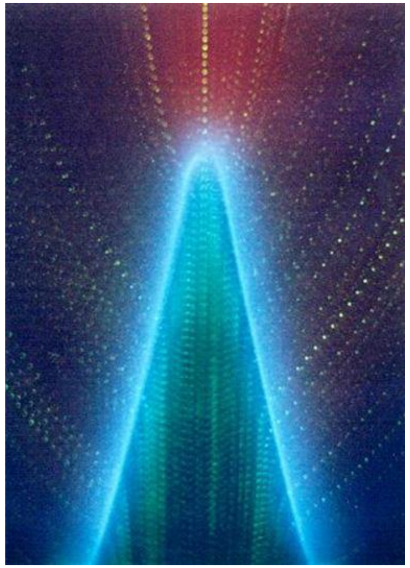
Low NOx

- Disadvantage: Danger of Explosions

Combustion instabilities

Large-scale industrial furnaces and aircraft engines are typically non-premixed





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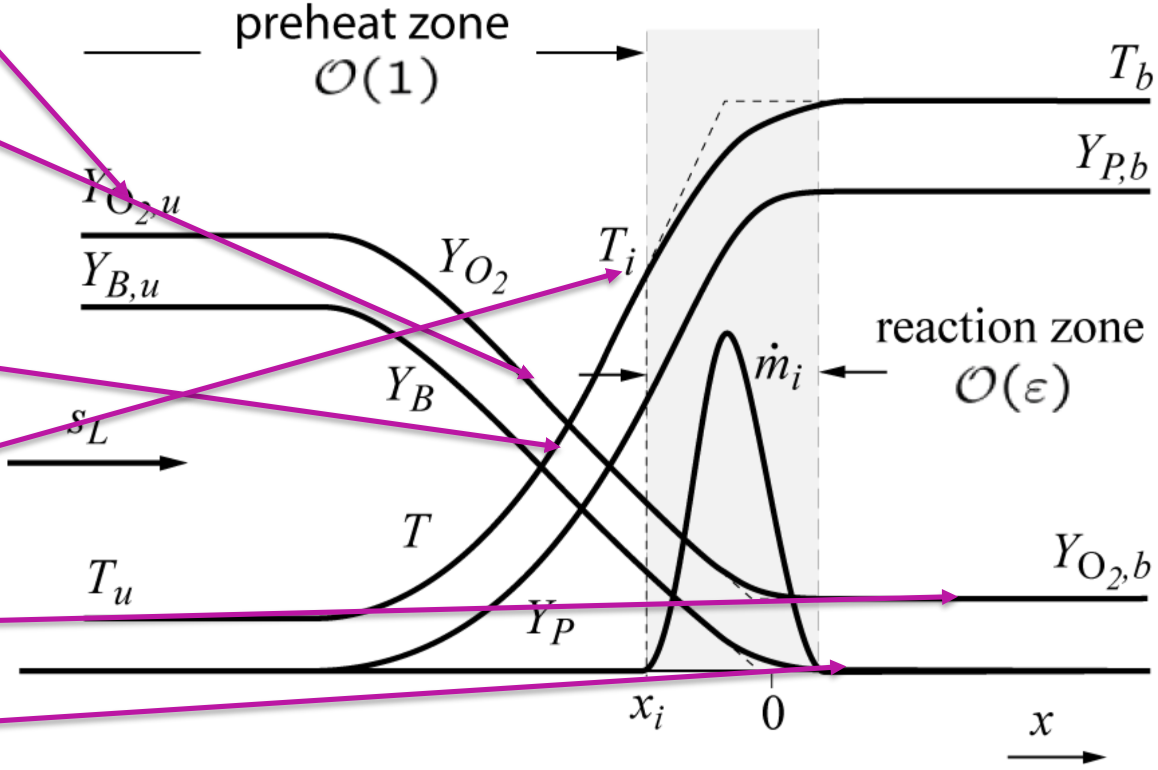
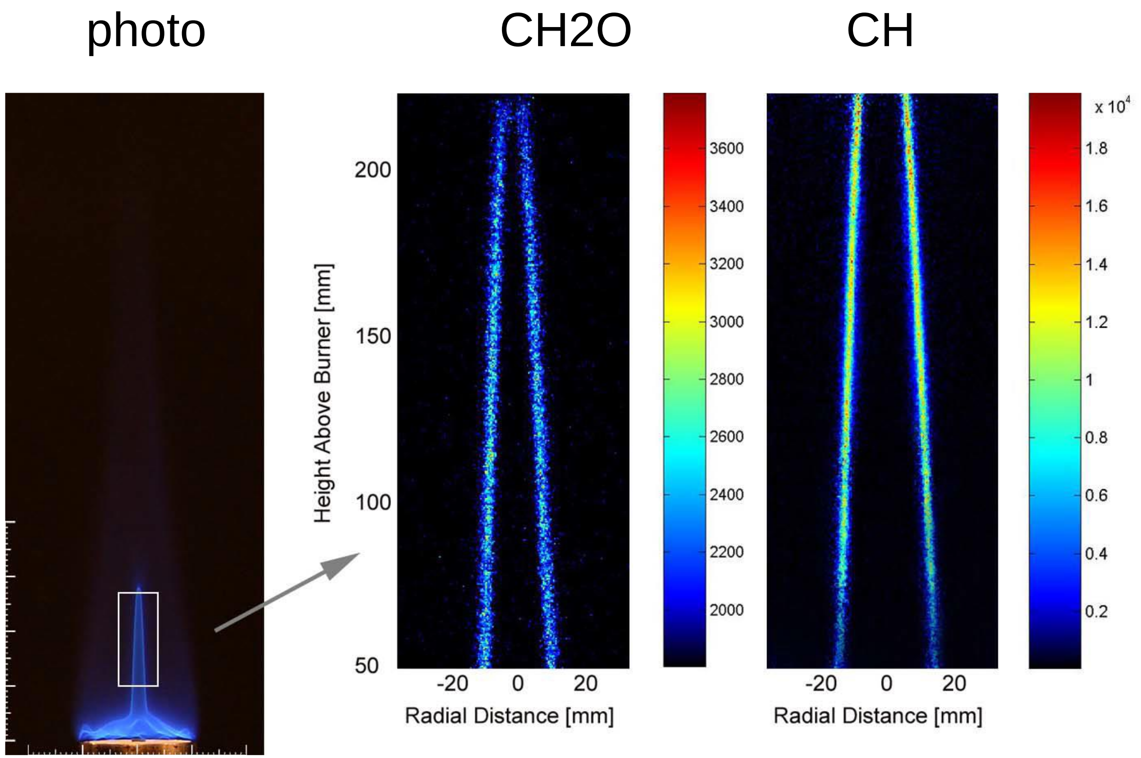
Basic combustion types- premixed flame

Cut through flame

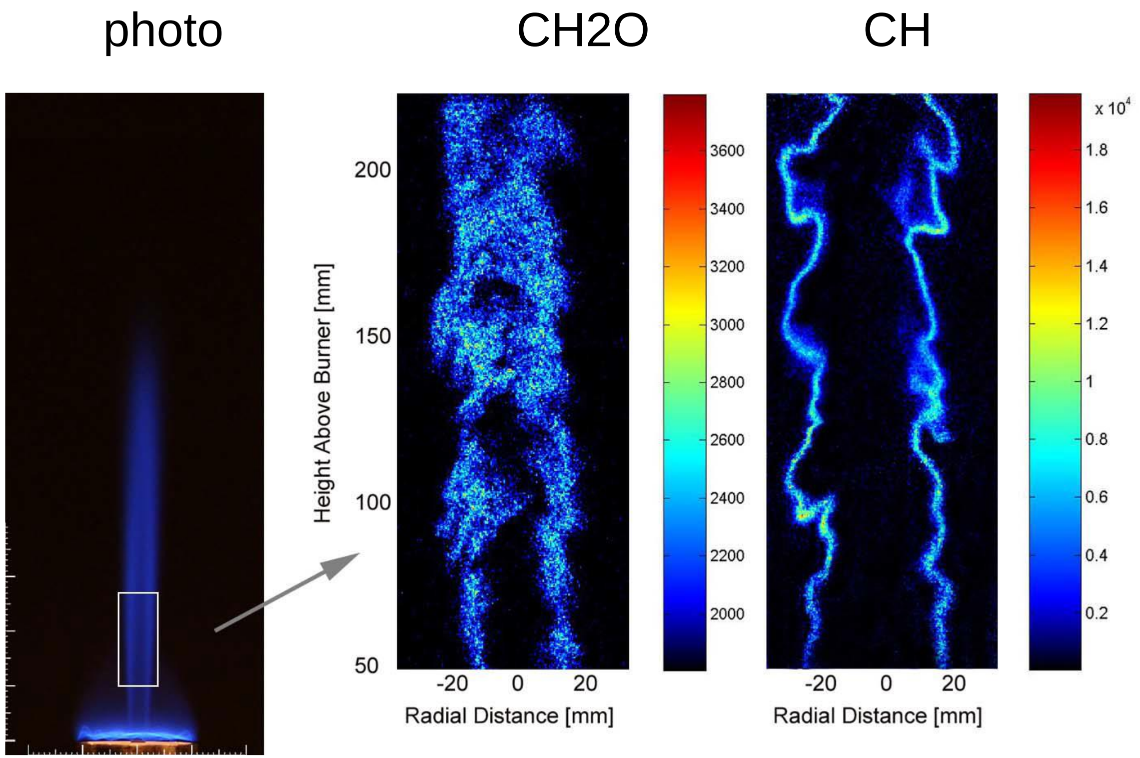
- Fuel and oxidizer are convected from upstream with the burning velocity s_L
- Fuel and air diffuse into the reaction zone
- Mixture heated up by heat conduction from the burnt gases
- Fuel consumption, radical production, and oxidation when inner layer temperature is reached
- Increase temperature and gradients
- Fuel is entirely depleted
- Remaining oxygen is convected downstream



Basic combustion types- premixed flame



Vo=0.45 m/s, phi=1.17; Vin=11m/s, phi=1.1
Lamilar premixed flame



Vo=0.45 m/s, phi=1.17; Vin=120m/s, phi=1.0
Turbulent premixed flame

Combustion basics

- Thermal engines use fuel and oxygen (from air) to produce energy through combustion.
- To guarantee the combustion process, certain quantities of fuel and air need to be supplied in the combustion chamber.
- A complete combustion takes place when all the fuel is burned, in the exhaust gas there will be no quantities of unburned fuel.
- Air-fuel ratio (AF or AFR) is the ratio between the mass of air $\dot{m}_{air}$ and mass fuel $\dot{m}_{fuel}$, used by the engine when running:

$$\frac{A}{F} = \frac{\dot{m}_{air}}{\dot{m}_{fuel}}$$

Stoichiometric (ideal) air-fuel ratio

- Consider the complete combustion of a general hydrocabon fuel of average molecular composition CaHb with air. The overall complete combustion equation is:

$$C_aH_b + \left(a + \frac{b}{4}\right)(O_2 + 3.773N_2)$$

$$= aCO_2 + \frac{b}{2}H_2O + 3.773\left(a + \frac{b}{4}\right)N_2$$

- The stoichiometric air/fuel or fuel/air ratio depend on fuel composition.

$$\left(\frac{A}{F}\right)_s = \left(\frac{A}{F}\right)_s^{-1} = \frac{(1 + y/4)(32 + 3.773 \times 28.16)}{12.011 + 1.008y}$$

- where $y = \frac{b}{a}$.

Combustion basics

- **Because the composition of the combustion products is significantly different for fuel-lean and fuel-rich mixtures, and because the stoichometric fuel/air ratio depends on fuel composition, the ratio of the actual fuel/air ratio to the stoichometric ratio is a more informative parameter for defining mixutre composition. The fuel/air equivalence ratio ∅**

$$\emptyset = \frac{(F/A)_{actual}}{(F/A)_s} = \frac{1}{\lambda}$$

Depending on the value of lambda, the engine is told to work with lean, stoichiometric or rich air-fuel mixture.

Equivalence factor	**Air-fuel mixture type**	**Description**
$\lambda < 1.00$	Rich	There is not enough air to burn completely the amount of fuel; after combustion there is unburnt fuel in the exhaust gases
$\lambda = 1.00$	Stoichiometric (ideal)	The mass of air is exact for a complete combustion of the fuel; after combustion there is no excess oxygen in the exhaust and no unburnt fuel
$\lambda > 1.00$	Lean	There is more oxygen than required to burn completely the amount of fuel; after combustion there is excess oxygen in the exhaust gases

Combustion basics

Example

Considering that gasoline is made up from isooctane (C_8H_{18}), calculate the **stoichiometric air-fuel ratio for gasoline**.

Step 1. Write the chemical reaction (oxidation)

$C8H18+O2\rightarrow CO2+H2O$

Step 2. Balance the equation

$C8H18+12.5\cdot (O2+3.773N2)\rightarrow 8\cdot CO2+9\cdot H2O+47.16N2\cdot$

Step 3. Write down the standard atomic weight for each atom

Hydrogen=1.008 amu

Carbon =12.011amu

Oxygen=15.999 amu

Nitrogen=14.48 amu

Step 4. Calculate the mass of fuel, which is 1 mol of isooctane, made up from 8 atoms of carbon and 18 atoms of hydrogen.

$mf=8\cdot12.011+18\cdot1.008=114.232$ g

Step 5. Calculate the mass of oxygen, which consists of 12.5 moles, each mol made up from 2 atoms of oxygen.

$mo=12.5\cdot15.999\cdot2=399.975$ g

Step 6. Calculate the mass of nitrogen,which contains 12.5× 3.773 moles, each mole made up from 2 atoms of nitrogen.

$mn=12.5\cdot3.773\cdot14.48\cdot 2=1365.826$ g

$Ma=mo+mn=1765.801$g

Step 7. Calculate the air-fuel ratio using equation (1)

$AFR=ma/mf=1765.801/114.232=15.458$

Again, the calculated stoichimetric air-fuel ratio for gasoline is slightly different that the one provided in literature. Thus, the result is acceptable since we made a lot of assumptions (gasoline contains only isooctane, air contains only oxygen in proportion of 21 %, the only products of combustion are carbon dioxide and water, the combustion is ideal).

Chemistry in combustion and ignition

- An *elementary* reaction is one that occurs on a molecular level exactly in the way which is described by the reaction equation.
- $OH + H_2 \rightarrow H_2O + H$
- The equation above is an elementary reaction. On the contrary, the following is not an elementary reaction:
- $2H_2 + O_2 \rightarrow 2H_2O$
- Above reaction is *global* or *overall* reaction.
- A general *global reaction mechanism* involving overall reaction of a moles of oxidizer with one mole of fuel to form b moles of products:
- $F + aOx \rightarrow bPr$
- Experimental observations yield the rate at which fuel is consumed as

$$\frac{d[F]}{dt} = -k_G(T)[F]^n[O_x]^m$$

- [X] denotes molar concentration of X, e.g. $kmol/m^3$.
- $k_G(T)$ is the global rate coefficient.
- n and m relate to the *reaction order*.
- According to Eqn 2.2, reaction is

- nth order with respect to fuel,
- mth order with respect to oxidant, and
- (m+ n)th order overall.

- m and n are determined from experimental data and are not necessarily integers.

Chemistry in combustion and ignition

- Use of global reactions to express chemistry is usually a *black box* approach and has limited use in combustion.
- It does not provide a basis for understanding what is actually happening.
- Let's consider the following global reaction:

  $2H_2 + O_2 \rightarrow 2H_2O$
- It implies that two moles of hydrogen molecule react with one mole of oxygen to form one mole of water, which is not strictly true.
- In reality many sequential processes occur that involve several intermediate species. Following elementary reactions, among others, are important in conversion of H2 and O2 to water:

$$\mathrm{H_2 + O_2 \rightarrow HO_2 + H}$$

$$\mathrm{H + O_2 \rightarrow OH + O}$$

$$\mathrm{OH + H_2 \rightarrow H_2O + H}$$

$$\mathrm{H + O_2 + M \rightarrow HO_2 + M}$$

Chemistry in combustion and ignition

- Chemical reaction kinetics deals with the rates of chemical processes. Any chemical process may be broken down into a sequence of one or more single-step processes known either as *elementary processes*, *elementary reactions*, or *elementary steps*
- The rate law is an expression relating the rate of a reaction to the concentrations of the chemical species present, which may include reactants, products, and catalysts. Many reactions follow a simple rate law, which takes the form

$$\nu = \boldsymbol{k}[\boldsymbol{A}]^{\boldsymbol{a}}[\boldsymbol{B}]^{\boldsymbol{b}}[\boldsymbol{C}]^{\boldsymbol{c}}\cdots$$

Example

- Consider some of the reactions in H2-O2 system

$$H_2 + O_2 \underset{k_{r1}}{\overset{k_{f1}}{\rightleftharpoons}} HO_2 + H \qquad (R.1)$$

$$H + O_2 \underset{k_{r2}}{\overset{k_{f2}}{\rightleftharpoons}} OH + O \qquad (R.2)$$

$$OH + H_2 \underset{k_{r3}}{\overset{k_{f3}}{\rightleftharpoons}} H_2O + H \qquad (R.3)$$

$$H + O_2 + M \underset{k_{r4}}{\overset{k_{f4}}{\rightleftharpoons}} HO_2 + M \qquad (R.4)$$

- The net production rate of any species, say X, involved is the sum of all of the individual elementary rates producing X minus all of the rates destroying X.

$$\begin{aligned}\frac{\mathrm{d}[O_2]}{\mathrm{d}t} =& k_{r1}[HO_2][H] + k_{r2}[OH][O] \\ &+ k_{r4}[HO_2][M] - k_{f1}[H_2][O_2] \\ &- k_{f2}[H][O_2] - k_{f4}[H][O_2][M]\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}[H]}{\mathrm{d}t} =& k_{f1}[H_2][O_2] + k_{r2}[OH][O] \\ &+ k_{f3}[OH][H_2] + k_{r4}[HO_2][M] \\ &- k_{r1}[HO_2][H] - k_{f2}[H][O_2] \\ &- k_{r3}[H_2O][H] - k_{f4}[H][O_2][M]\end{aligned}$$

$$\frac{\mathrm{d}[X_i](t)}{\mathrm{d}t} = f_i\{[X_1](t), [X_2](t), \ldots\ldots[X_n](t)\}$$

$$[X_i](0) = [X_i]_0$$

Chemistry in combustion and ignition

Factors affecting reaction rate

Nature of the reactants

The nature and strength of bonds in reactant molecules greatly influence the rate of their transformation into products.

Physical state

When reactants are in the same phase, as in aqueous solution, thermal motion brings them into contact. However, when they are in different phases, the reaction is limited to the interface between the reactants.

Surface area of solids

In a solid, only those particles that are at the surface can be involved in a reaction.

Concentration

The reactions are due to collisions of reactant species. The frequency with which the molecules or ions collide depends upon their concentrations.

Temperature

Molecules at a higher temperature have more thermal energy. Although collision frequency is greater at higher temperatures, this alone contributes only a very small proportion to the increase in rate of reaction. Much more important is the fact that the proportion of reactant molecules with sufficient energy to react (energy greater than activation energy: $E > E_a$) is significantly higher and is explained in detail by the Maxwell–Boltzmann distribution of molecular energies.

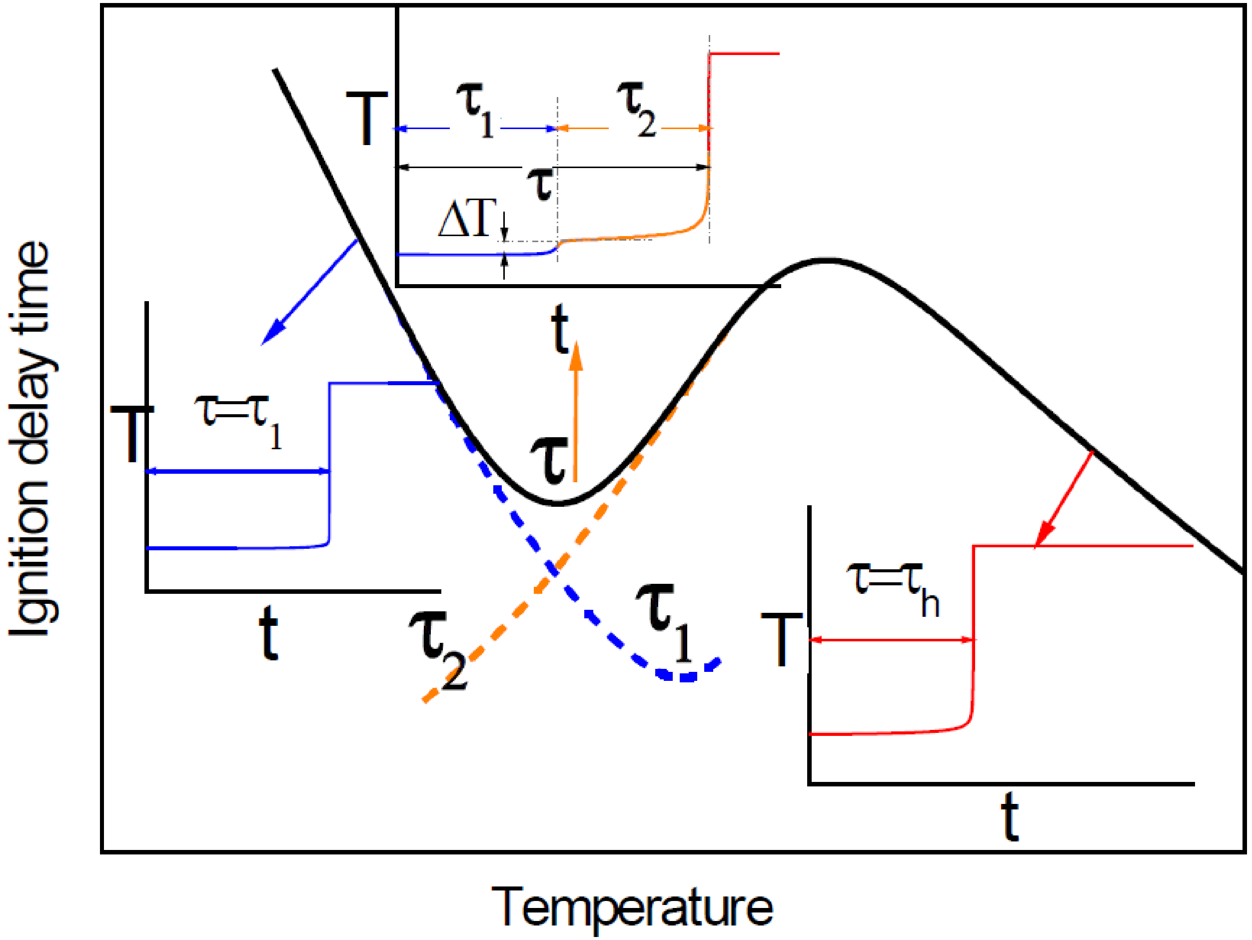
Pressure

Increasing the pressure in a gaseous reaction will increase the number of collisions between reactants, increasing the rate of reaction. This is because the activity of a gas is directly proportional to the partial pressure of the gas. This is similar to the effect of increasing the concentration of a solution.

Chemistry in combustion and ignition

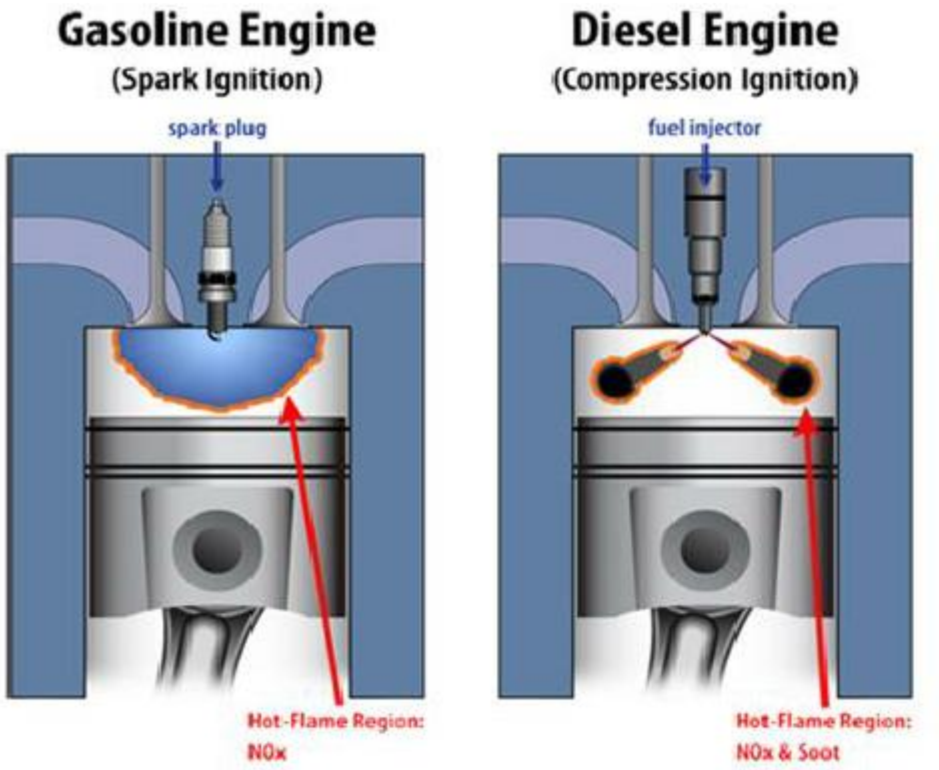
NTC behavior

- Figure at the right shows a schematic of the NTC behavior and ignition histories (i.e., T vs. t) in the low-temperature, NTC and the high-temperature autoignition regimes. It is seen that ignition consists of two stages within the NTC regime in which the ignition delay varies non-monotonically with temperature, with the chemical reactions experiencing distinct



CI and SI combustion processes

Parameter	SI	CI
Fuel	highly volatile fuels with high self ignition temperatures	non volatile fuels whose self ignition temperature is comparatively lower.
Fuel Injection	Port Fuel Injection(PFI), Gasoline Direct injection(GDI)	Common Rial Direct Injection
Injection Pressure	PFI: lower than 10bar GDI:50-600bar	CRI: 800-3000bar
Timing Delay	Depends to the spark timing, Relatively long	Denpends on the fuel properties (e.g. CN, etc.), charge air temeprature, and compression ratio. Relatively short
Method of ignition	Spark ignition	Compressed ignition
Subsequent combustion	Premixed combustion	Diffusion combustion



Problem 5

Engine	Bore D(mm)	Stroke S(mm)	Compression ratio, ε	Maximum Power (kW)/ Engine Speed (r/min)	Weight (kg)
1.9 JTD	82	90,4	18,5:1	85 / 4000	180
F12	94	75	13,5:1	545/ 8250	250
ASP 49 CWA	108	134	17,0:1	206 / 2200	390
W4L20	200,0	280,0	16,0:1	800/1000	7200

- Crank radius R
- Displacement V_H
- Compressed volume Vc
- Torque
- BMEP (max P)
- Power-to-weight ratio

- The stroke and crank radius are related to :

$$S = 2R$$

- The displacement for 4-cylinder engine can be calculated as follows:

$$V_H = 4 \times S \times \frac{D^2}{4} \times \pi$$

- Compressed volume can be calculated by using the compression ratio:

$$V_C = \frac{V_H}{\varepsilon - 1}$$

- Torque can be calculated as follows:

$$M_d = \frac{60 \cdot P_{max}}{2\pi \cdot n}$$

- Brake mean effective pressure is calculated as:

$$p_e = \frac{M_d \cdot 2\pi}{V_H \cdot i}$$

- Power-to-weight ratio is often calculated as:

$$R_e = \frac{P_e}{m_{engine}}$$

Problem 6

Engine	Bore D(mm)	Stroke S(mm)	Compression ratio, ε	Maximum Power (kW)/ Engine Speed (r/min)	Weight (kg)
V6 Twin-Turbo	86,0	86,0	10,3:1	298 / 6400	194

Vol.eff. η_{vol}	Ind. Eff. η_i	Mech.Eff. η_m	Lambda λ	Air Density $\rho(kg/m^3)$	Speed n(r/min)
0,92	0,39	0,86	1	1,2	2000

Step 1: Displacement volume

$$V_H = 4 \times S \times \frac{\pi \cdot D^2}{4}$$

Step 2: Volume of inlet air

$$V_{air} = \eta_{vol} \cdot V_H$$

Step 3: Mass of inlet air

$$m_{air} = \rho_{air} \cdot V_{air}$$

Step 4: Mass of fuel

$$m_{fuel} = \frac{m_{air}}{AFR}$$

Step 5: Energy admitted with fuel

$$E_{fuel} = m_{fuel} \cdot LHV$$

Step 6: Work done by gas

$$W_{gas} = E_{fuel}$$

Step 7: Indicated mean pressure

$$p_{imep} = \frac{W_{gas} \cdot \eta_i}{V_H}$$

Step 8: Indicated power of 4 cylinders

$$P_i = i \cdot n \cdot p_{imep} \cdot V_H$$

Step 9: Effective power of 4 cylinders

$$P_e = \eta_m \cdot P_i$$

Step 10: Torque of the engine

$$M_d = \frac{P_e}{2 \cdot \pi \cdot n}$$

Step 11: Brake mean effective pressure

$$p_{bmep} = \frac{M_d \cdot 2 \cdot \pi}{V_H \cdot}$$

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GOOD LUCK !!!

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