

# STOICHIOMETRY OF COMBUSTION

# FUNDAMENTALS: moles and kilomoles

Atomic unit mass:  $1/12 \text{ }_{12}^{6}\text{C} \sim 1.66 \cdot 10^{-27} \text{ kg}$

Atoms and molecules mass is defined in atomic unit mass: which is defined in relation to the 1/12 of carbon  $_{12}^{6}\text{C}$ .

Mole: (Avogadro number)  $6.022 \cdot 10^{23}$  atoms

Volume of 1 mole (perfect gas)  $22.414 \text{ l}$  (T= 0 °C, p = 1 atm)

Kmole:  $10^3$  moles

Mass of one mole (kmole) is a number of grams (kilograms) equal to the relative atomic mass.

# CHEMICAL REACTIONS

**Consider a simple chemical reaction of two species A and B giving a single product C**



A, B and C are reactants. A and B are substrates. C is a product of reaction.

Stoichiometry of chemical reactions means that species react in exact proportions.

# SPECIE'S CONCENTRATIONS AND FRACTIONS

## Concentration of $i$ specie:

- (moles of  $i$  specie) /volume
- (mass of  $i$  specie)/volume

## Mole fraction:

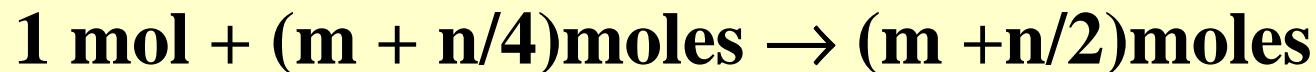
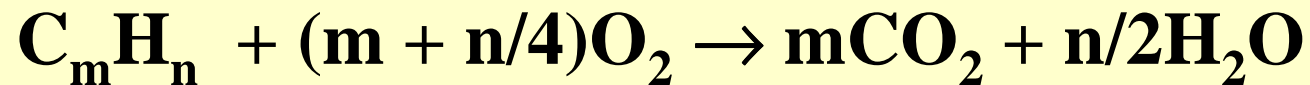
- (moles of  $i$  specie)/(total number of moles of species)

## Mass fraction:

- (mass of  $i$  fraction)/(total mass)

# STOICHIOMETRY OF HYDROCARBONS OXIDATION

Fossil fuels are mainly compounds of carbon and hydrogen (hydrocarbons -  $C_mH_n$ ). The reaction of its oxidation can be written by the equation of stoichiometry:



This is an equation of stoichiometry of combustion.

It is important that for one mole of fuel  $C_mH_n$  there is necessary exactly:

(m + n/4) moles  
of oxygen for complete combustion.

# TYPES OF OXIDIZERS

In combustion processes the oxidizer could be:

- 1. Oxygen ( $O_2$ )**
- 2. Air (21% $O_2$  + 79% $N_2$ )**
- 3. Air enriched with oxygen ( $O_2 > 21\%$ )**
- 4. Some compounds containing oxygen, like nitrogen oxides:  $N_2O$**

# COMPOSITION OF FUEL MIXTURE

When fuel and oxidizer composition in the mixture (fuel and oxidizer) results from the equation of stoichiometry we say that the mixture is **stoichiometric**.

**If combustion of a stoichiometric mixture is complete in flue gas cannot be nor fuel neither oxygen.**

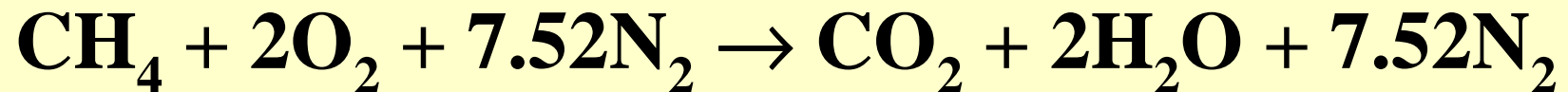
# TYPES OF COMBUSTIBLE MIXTURES

<b>FUEL MIXTURE</b>		
<b>Rich</b>	<b>Stoichiometric</b>	<b>Lean</b>
Excess of fuel	Stoichiometric content of fuel and oxygen	Excess of oxidizer



# BURNING OF STOICHIOMETRIC METHANE MIXTURE IN AIR

Air: 79% N<sub>2</sub> + 21% O<sub>2</sub>



Attention: there is not **fuel** neither **oxygen** in flue gas.

# BURNING OF STOICHIOMETRIC METHANE MIXTURE IN AIR: flue gas composition

A number of moles of flue gas  $N$ :

$$N = 1 \text{ mole CO}_2 + 2 \text{ moles H}_2\text{O} + 7.52 \text{ mole N}_2 = 10.52 \text{ moles}$$

According to the *wet* (water is steam/liquid) analysis of flue gas the concentration of the components is as follows:

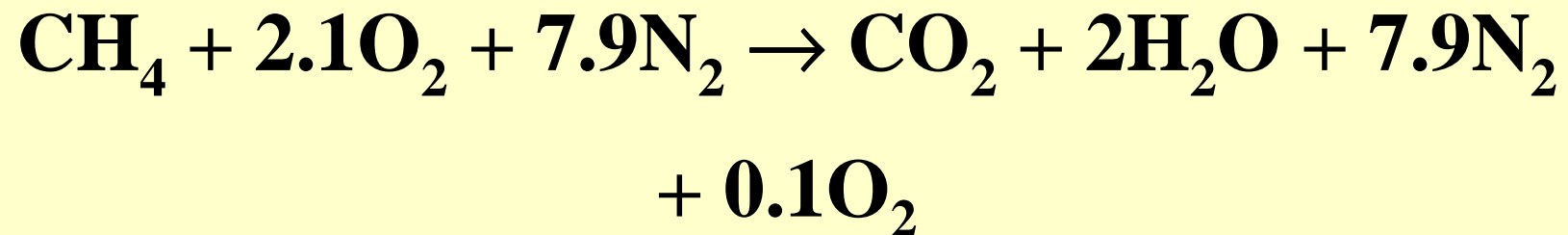
$$[\text{CO}_2] = 1 \text{ mole CO}_2 / 10.52 = 9.5\% \text{ CO}_2 \text{ vol.}$$

$$[\text{H}_2\text{O}] = 2 \text{ moles H}_2\text{O} / 10.52 = 19\% \text{ H}_2\text{O vol.}$$

$$[\text{N}_2] = 7.52 \text{ mole N}_2 / 10.52 = 71.5\% \text{ N}_2 \text{ vol.}$$

# BURNING OF LEAN METHANE MIXTURE IN AIR

Assumption: AIR EXCESS = 5%



Attention: there is **oxygen** in flue gas.

# BURNING OF LEAN METHANE MIXTURE IN AIR: flue gas composition

A number of moles of flue gas  $N$  equals:

$$N = 1 \text{ mole CO}_2 + 2 \text{ moles H}_2\text{O} + 7.9 \text{ mole N}_2 + 0.1 \text{ mole O}_2 = 11 \text{ moles}$$

According to the *wet* (water is liquid) analysis of flue gas the concentration of the components is as follows:

$$[\text{CO}_2] = 1 \text{ mole CO}_2 / 11 = 9.09\% \text{ CO}_2 \text{ vol.}$$

$$[\text{H}_2\text{O}] = 2 \text{ moles H}_2\text{O} / 11 = 18.2\% \text{ H}_2\text{O vol.}$$

$$[\text{O}_2] = 0.1 \text{ mole O}_2 / 11 = 0.91\% \text{ O}_2 \text{ vol.}$$

$$[\text{N}_2] = 7.52 \text{ moles N}_2 / 10.52 = 71.82\% \text{ N}_2 \text{ vol.}$$

# STOICHIOMETRIC AIR

The theoretical air required to complete combustion of fuel results from the equation of stoichiometry of oxygen/fuel reaction. Stoichiometric air means the minimum air in stoichiometric mixture. The stoichiometric air/fuel ratio (AFR) can be calculated from the reaction equation (g/g). For gas AFR is usually determined in  $\text{m}^3/\text{m}^3$ .

**The actual combustion air** depends also on the assumed air excess (equivalence ratio or stoichiometric ratio).

# THE STOICHIOMETRIC RATIO ( $\lambda$ )

(WSPÓŁCZYNNIK NADMIARU POWIETRZA)

$$\lambda = \frac{\text{Actual air}}{\text{Stoichiometric air}}$$

$$\lambda \cong \frac{20.9}{20.9 - [O_2]}$$

# AN EQUIVALENCE RATIO $\phi$

(WSPÓŁCZYNNIK EKWIWALENCJI)

In English more often than stoichiometric ratio  $\lambda$  the equivalence ratio  $\phi$  is in use.

$$\phi = \frac{F/A}{(F/A)_s}$$

$$\phi = \frac{1}{\lambda}$$

F – number of moles of fuel,  
A – number of moles of air.

s - stoichiometric

# AIR/FUEL RATIO (AFR) and FUEL/AIR RATIO (FAR)

Form the practical reasons in aviation (aircrafts) mostly in use is the ratio of air mass-flow to the fuel mass-flow determined as AFR (Air/Fuel Ratio)

$$\text{AFR} = \text{F/A}$$

A – air mass-flow (A – air), kg/s

F – fuel mass-flow (F – fuel), kg/s

In similar way FAR (Fuel/Air Ratio) is defined.



# STOICHIOMETRIC RATIO/EQUIVALENCE RATIO AND TYPE OF MIXTURE

Type of flame/type of mixture		
Rich	Stoichiometric	Lean (weak)
$\lambda < 1$	$\lambda = 1$	$\lambda > 1$
$\phi > 1$	$\phi = 1$	$\phi < 1$

## AIR EXCESS ( $n$ )

$$n = \frac{\text{actual - stoichiometric air}}{\text{stoichiometric air}}$$

The relationship between the stoichiometric ratio  $\lambda$  and air excess  $n$

$$n = (\lambda - 1) * 100\%$$

# STOICHIOMETRIC AIR/FUEL RATIO FOR SELECTED GASES

Gaz	Stoichiometric air/fuel ratio AFR, m <sup>3</sup> /m <sup>3</sup>
CO	2.87
H <sub>2</sub>	2.82
CH <sub>4</sub>	10.42
C <sub>2</sub> H <sub>2</sub>	12.43
C <sub>2</sub> H <sub>6</sub>	18.14
C <sub>3</sub> H <sub>8</sub>	26.11
Natural gas	8.43 (approx. 82% CH <sub>4</sub> )

## EXAMPLE

Stoichiometric air for methane burning ( $\text{CH}_4$ ) is  $10.42 \text{ m}^3 / \text{m}^3$

Assuming:

➤ the rate feeding of methane  $V = 10 \text{ m}^3/\text{h}$

➤ the rate feeding of air  $V = 114.62 \text{ m}^3/\text{h}$

We have:

$$\lambda = 114.62/104.2 = 1.1$$

$$n = (1.1 - 1.0) * 100\% = 10\%$$