STOICHIOMETRY OF COMBUSTION

FUNDAMENTALS: moles and kilomoles

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

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

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

Volume of 1 mole (perfect gas) 22.414 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

$$A + 2B \rightarrow C$$

$$1\ \text{mol} + 2\ \text{moles} \rightarrow 1\ \text{mol}$$

A, B and C are reactants. A and B are substracts. 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 by written by the equation of stoichiometry:

$$\mathbf{C_mH_n + (m + n/4)O_2 \rightarrow mCO_2 + n/2H_2O}$$

$$\mathbf{1\ mol + (m + n/4)moles \rightarrow (m + n/2)moles}$$

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

FUEL MIXTURE		
Rich	**Stoichiometric**	**Lean**
Excess of fuel	Stoichiometric content of fuel and oxygen	Excess of oxidizer

BURNING OF STOICHIOMETRIC METHANE MIXTURE IN AIR

Air: 79% N_2 + 21% O_2

$$\mathbf{CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2}$$

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*:

$$N = 1 \text{ mole } CO_2 + 2 \text{ moles } H_2O + 7.52 \text{ mole } N_2 = 10.52 \text{ moles}$$

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

$[CO_2]$ = 1mole CO_2/10.52 = 9.5% CO_2 vol.

$[H_2O]$ = 2 moles H_2O/10.52 = 19% H_2O vol.

$[N_2]$ = 7.52 mole N_2/10.52 = 71.5% N_2 vol.

BURNING OF LEAN METHANE MIXTURE IN AIR

Assumption: AIR EXCESS = 5%

$$CH_4 + 2.1O_2 + 7.9N_2 \rightarrow CO_2 + 2H_2O + 7.9N_2 + 0.1O_2$$

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:

$$N = 1 \text{ mole } CO_2 + 2 \text{ moles } H_2O + 7.9 \text{ mole } N_2 + 0.1 \text{ mole } O_2 = 11 \text{ moles}$$

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

$[CO_2] = 1\text{mole } CO_2/11 =$ 9.09% CO_2 vol.

$[H_2O] = 2 \text{ moles } H_2O/11 =$ 18.2% H_2O vol.

$[O_2] = 0.1 \text{ mole } O_2/11 =$ 0.91% O_2 vol.

$[N_2] = 7.52 \text{ moles } N_2/10{,}52 =$ 71.82% N_2 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 m^3/m^3.

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

THE STOICHIOMETRIC RATIO (λ)
(WSPÓŁCZYNNIK NADMIARU POWIETRZA)

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

$$\lambda \cong \frac{20.9}{20.9 - [0_2]}$$

AN EQUIVALENCE RATIO ϕ

(WSPÓŁCZYNNIK EKWIWALENCJI)

In English more often than stoichiometric ratio λ the equivalence ratio ϕ 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)

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

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 λ and air excess n

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

STOICHIOMETRIC AIR/FUEL RATIO FOR SELECTED GASES

Gaz	Stoichiometric air/fuel ratio AFR, m^3/m^3
CO	2.87
H_2	2.82
CH_4	10.42
C_2H_2	12.43
C_2H_6	18.14
C_3H_8	26.11
Natural gas	8.43 (approx. 82% CH_4)

EXAMPLE

Stoichiometric air for methane burning (CH_4) is 10.42 m^3 /m^3

Assuming:

- the rate feeding of methane V = 10 m^3/h
- the rate feeding of air V = 114.62 m^3/h

We have:

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

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