Calculation of the main parameters involved in the combustion process of CH$_4$-H$_2$ mixtures at different proportions

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Abstract. By setting clear targets for reducing pollutant emissions, the researchers in the field of combustion are pushed lately to find new alternatives for cleaner combustion. The partial or total transition to other types of fuels, such as hydrogen, involves substantial changes in the combustion process and possible necessary constructive changes. In the study of the combustion of CH$_4$-H$_2$ mixtures, both numerically and experimentally, preliminary calculations are required, which will help to easily establish the parameters and working regimes and then to use for verifying the results. This paper aims to find an easier method of calculating these parameters, depending on the percentage of gas in the fuel mixture. The calculated values resulted this way will lead to some logical estimates of important aspects of combustion, such as flame field and temperature variation, related to the variation of the amount of hydrogen in the mixture. The method can be a useful tool in the preliminary design of a combustion chamber for CH$_4$-H$_2$ mixtures.

1 Introduction

Starting from the environmental problems form the past decades, the scientific world is lately in a constant search for less pollutant and more efficient fuels. Hydrogen is studied as a possible alternative, since new ways for producing and transporting it developed in the past few years [1]. For example, from wind or solar energy, hydrogen can be produced on site by electrolysis and can be transported with the existing natural gas distribution network and then used for different existing or new applications. In the field of energy, it could be interesting to use this new fuel in gas turbines, at industrial level, in order to produce electricity and heat.

The new resulting gas, as a mixture of hydrogen and natural gas, depending on the proportions, can change significantly the combustion parameters of the final application, due to the different mixtures properties. From this perspective, numerical and experimental investigations are needed. Various studies and experiments were made with results pointing

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that above 15-20% H₂, some structural modifications of the equipment are requested [2] [3] [4].

For both numerical simulations and experimental sessions, the preliminary calculations of the input values and nominal regimes are needed. In order to find the main operating parameters of the combustion, formulas and calculations are usually required, based on theory and literature. These calculations and the preliminary results obtained can be later used to define the input and output parameters in the numerical simulations and to establish the operating regimes, air and fuel flows, temperatures, pressures and stability limits in the experiments. The present paper will point below a method to easily calculate the excess air, the calorific value of the fuel mixture, adiabatic temperature and other important parameters in the combustion chamber and the variation of the products in the combustion gases, according to this mixture’s different proportions between methane and hydrogen. Hence, the acquired formulas can be used for obtaining useful values that can be used both as starting data and also for verifying the experimental measured results.

2 Excess air - mixture ratio - gas analysis

The combustion process for a CₙHₘ hydrocarbon fuel, as a global stoichiometric reaction using air as an oxidizer, is written as [5] [6]:

\[
\text{C}_n\text{H}_m + \left( n + \frac{m}{4}\right) (\text{O}_2 + 3.76\text{N}_2) \rightarrow n\text{CO}_2 + \frac{m}{2}\text{H}_2\text{O} + 3.76\left( n + \frac{m}{4}\right)\text{N}_2
\]

(1)

Although the air contains other compounds in small quantities, beside oxygen (20.95%) and nitrogen (78.08%) and other [5], here is simply considered to be composed only of oxygen (21%) and nitrogen (79%). Thus the molar ratio between the two compounds is considered to be 3.76 in the above relationship.

Therefore, for the combustion of each mole of fuel are required \( (n+m/4)(1+3.76) \) moles of air, resulting in \( 4.76(n+m/4)+m/4 \) moles of reaction products.

2.1 Combustion of CH₄

The overall reaction for stoichiometric combustion process in the case of CH₄ is written as follows [7]:

\[
\text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O}
\]

(2)

The molar mass of CH₄ is 16.043 g/mol. Thus, the fuel / stoichiometric air ratio is:

\[
\left( \frac{\dot{m}_a}{\dot{m}_{\text{f(CH₄)}}} \right)_s = \frac{2 \times \left( 32 + \frac{79}{21} \times 28 \right)}{16.043} = 17.16 = L_{0\text{CH₄}}
\]

(3)

To burn 1 kg of CH₄ requires 17.16 kg of air, an amount known in the literature as \( L_{\text{minCH₄}} \) or \( L_{0\text{CH₄}} \).

2.2 Combustion of H₂

The overall reaction for stoichiometric combustion in the case of H₂ is:

\[
\text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O}
\]

(4)

The molar mass of H₂ is 2.016 g/mol. Thus the fuel/stoichiometric air ratio is:
\[
\left( \frac{m_a}{m_f(H_2)} \right)_s = \frac{0.5 \times (32 + \frac{79}{2} \times 28)}{2.016} = 34.32 = L_{0H2} \tag{5}
\]

To burn 1 kg of \( H_2 \) requires 34.32 kg of air, an amount known in the literature as \( L_{minH2} \) or \( L_{0H2} \).

### 2.3 Combustion of \( \text{CH}_4 + \text{H}_2 \) mixtures

The classical stoichiometric method of calculation is adopted, writing the individual equations for \( \text{CH}_4 \) and \( \text{H}_2 \) based on the relation (1): [8]

\[
\text{CH}_4 + 2(\text{O}_2 + 3.76\text{N}_2) \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 2 \times 3.76 \times \text{N}_2 \tag{6}
\]

\[
\text{H}_2 + \frac{1}{2}(\text{O}_2 + 3.76\text{N}_2) \rightarrow \text{H}_2\text{O} + 3.76 \times \frac{1}{2} \times \text{N}_2 \tag{7}
\]

Then the stoichiometric equations are multiplied by the molar fractions of the fuel mixture. For this paper, the following notations and rule are adopted: the molar fraction (or the volume percentage by multiplying by 100) for \( \text{CH}_4 \) is noted with \( x \), and for \( \text{H}_2 \) it is noted with \( y \). The condition is \( x + y = 1 \); \( (1 = 100\% \text{ as percentage}) \). In these conditions:

\[
x \times [\text{CH}_4 + 2(\text{O}_2 + 3.76\text{N}_2)] \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 2 \times 3.76 \times \text{N}_2 \tag{8}
\]

\[
y \times [\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)] \rightarrow \text{H}_2\text{O} + 3.76 \times 0.5 \times \text{N}_2 \tag{9}
\]

By mixing the above results in the stoichiometric equation of combustion for the mixture \( \text{CH}_4 - \text{H}_2 \):

\[
x \times \text{CH}_4 + 2x \times (\text{O}_2 + 3.76\text{N}_2) + y \times \text{H}_2 + 0.5y \times (\text{O}_2 + 3.76\text{N}_2) \rightarrow
\]

\[
\rightarrow x \times (\text{CO}_2 + 2\text{H}_2\text{O} + 2 \times 3.76 \times \text{N}_2) + y \times (\text{H}_2\text{O} + 3.76
\]

\[
\times 0.5 \times \text{N}_2) \tag{10}
\]

By transformations the stoichiometric equation is obtained:

\[
(1 - y) \times \text{CH}_4 + y \times \text{H}_2 + (2 - 1.5 \times y) \times \text{O}_2 + 3.76 \times \text{N}_2
\]

\[
\rightarrow (1 - y) \times \text{CO}_2 + (2 - y) \times \text{H}_2\text{O} + (2 - 1.5 \times y) \times 3.76
\]

\[
\times \text{N}_2 \tag{11}
\]

From the relation (11), depending on the molar (volumetric) participations, the stoichiometric air is further defined – \( L_s [\text{Kmol}_{\text{air}}/\text{Kmol}_{\text{fuel}}] \) \( [\text{m}^3_{\text{N}_{\text{air}}}/\text{m}^3_{\text{N}_{\text{fuel}}}] \)

\[
L_s = \frac{(2 - 1.5y)(1 + 3.76)}{(1 - y) + y} = (2 - 1.5 \times y) \times 4.76 \quad \text{[m}^3_{\text{N}_{\text{air}}} / \text{m}^3_{\text{N}_{\text{fuel}}}] \tag{12}
\]

The minimum theoretical air required [8] \( [\text{Kg}_{\text{air}}/\text{Kg}_{\text{fuel}}] \):

\[
L_0 = L_s \times \frac{\text{Mair}}{\text{M}_{\text{fuel}}} = \frac{4.76 \times (2 - 1.5 \times y) \times \text{Mair}}{\text{M}_{\text{fuel}}} \quad \text{[kg}_{\text{air}}/\text{kg}_{\text{fuel}}] \tag{13}
\]

Where: \( \text{Mair} = 28.84 [\text{kg/kmol}] \) is the molar mass of air;

\( \text{M}_{\text{fuel}} = (1 - y) \times 16 + y \times 2 \) \( [\text{kg/kmol}] \) is the molar mass of the fuel mixture.

It results:
The excess air is further defined by an excess air coefficient, known also as air–fuel equivalence ratio [5] [9]:

$$\lambda = \frac{m_a}{m_{fuel}} = \frac{m_a}{m_{fuel} \cdot L_0} \quad (15)$$

where: $m_a$ - air flow
$m_{fuel}$ - fuel mixture flow

Fuel–air equivalence ratio, is defined as:

$$\phi = \frac{m_{comb}}{m_a} = \frac{1}{\lambda} \quad (16)$$

Thus, for lean fuel combustion ($\phi \leq 1; \lambda \geq 1$) the relation (11), can be redefined, obtaining the global equation in the form:

$$(1 - y) \cdot CH_4 + y \cdot H_2 + \lambda \cdot (2 - 1.5 \cdot y) \cdot (O_2 + 3.76 \cdot N_2) \rightarrow (1 - y) \cdot CO_2 + (2 - y) \cdot H_2O + \lambda \cdot (2 - 1.5 \cdot y) \cdot 3.76 \cdot N_2 + (\lambda - 1) \cdot (2 - 1.5 \cdot y) \cdot O_2 \quad (17)$$

Starting from the above, the excess air and dosage are defined (required for comparisons with data from the literature, where dosage is used as a basis):

Stoichiometric dosage:

$$f_0 = \frac{1}{L_0} \quad [\text{kg}_{fuel}/\text{kg}_{air}] \quad (18)$$

$$\varphi_0 = \frac{1}{L_s} \quad [\text{m}^3_{fuel}/\text{m}^3_{air}] \quad (19)$$

The table below shows the variations of these parameters, depending on the composition of the mixture:

| H$_2$(y) | H$_2$ % mass | M$_{fuel}$ | $f_0$ [kg/kg] | L$_0$ [kg/kg] | $\varphi_0$ [m$^3$/m$^3$] | L$_s$ [m$^3$/m$^3$] |
|---------|-------------|-----------|--------------|--------------|----------------|-----------------|
| 0       | 0.00%       | 16        | 0.058        | 17.160       | 0.105          | 9.520           |
| 0.2     | 3.03%       | 13.2      | 0.057        | 17.680       | 0.124          | 8.092           |
| 0.4     | 7.69%       | 10.4      | 0.054        | 18.480       | 0.150          | 6.664           |
| 0.6     | 15.79%      | 7.6       | 0.050        | 19.869       | 0.191          | 5.236           |
| 0.8     | 33.33%      | 4.8       | 0.044        | 22.880       | 0.263          | 3.808           |
| 1       | 100.00%     | 2         | 0.029        | 34.320       | 0.420          | 2.380           |

The flue gas analysis results from the relation (17), depending on the volume fraction of H$_2$ and on the excess air:

$$CO_2 = \frac{(1 - y)}{(3 - 2y) + \lambda \cdot (2 - 1.5 \cdot y) \cdot 3.76 + (\lambda - 1) \cdot (2 - 1.5 \cdot y)} \quad (20)$$
\[ H_2O = \frac{(2 - y)}{(3 - 2y) + \lambda \ast (2 - 1.5 \ast y) \ast 3.76 + (\lambda - 1) \ast (2 - 1.5 \ast y)} \]  
\[ N_2 = \frac{\lambda \ast (2 - 1.5 \ast y) \ast 3.76}{(3 - 2y) + \lambda \ast (2 - 1.5 \ast y) \ast 3.76 + (\lambda - 1) \ast (2 - 1.5 \ast y)} \]  
\[ O_2 = \frac{(\lambda - 1) \ast (2 - 1.5 \ast y)}{(3 - 2y) + \lambda \ast (2 - 1.5 \ast y) \ast 3.76 + (\lambda - 1) \ast (2 - 1.5 \ast y)} \]  

Considering that in practice, when using the gas analyzer, water is condensed on the well path, or at the inlet through the special installation in the analyzer, the analysis of dry flue gases, respectively CO\(_2\), is considered as the main reference element:

\[ \text{CO}_2 = \frac{(1 - y)}{(1 - y) + \lambda \ast (2 - 1.5 \ast y) \ast 3.76 + (\lambda - 1) \ast (2 - 1.5 \ast y)} \]  

It results:

\[ \lambda = \frac{1 - y + \text{CO}_2 - 0.5 \ast y \ast \text{CO}_2}{4.76 \ast \text{CO}_2 \ast (2 - 1.5y)} \]  

Or by transforming the relationship (24):

\[ \text{CO}_2 = \frac{1}{1 + \lambda \ast (2 + 0.5 \ast \frac{y}{1-y}) \ast 4.76 - (2 + 0.5 \ast \frac{y}{1-y})} \]  

\[ \text{CO}_2 = \frac{1}{4.76 \ast \lambda \ast (2 + 0.5 \ast \xi) + 0.5 \ast \xi - 1} \]  

Where: \( y/(1-y) = \xi \) represents the molar ratio \( \text{H}_2/\text{CH}_4 \)

In this way, it turns out that:

\[ \lambda = \frac{1}{\text{CO}_2} + 1 + 0.5 \ast \xi \]  

\[ 4.76 \ast (2 + 0.5 \ast \xi) \]  

These latter relationships will be used during the experiments to determine the excess air, as an additional, and more accurate, verification of the measured \( \text{CH}_4 \), \( \text{H}_2 \) and air flow ratios. Based on the measurements recorded with the gas analyzers, obtaining values for \( \text{CO}_2 \), \( \text{CO} \), \( \text{O}_2 \), the excess air resulting from the measurements can be calculated and then it can be compared as a verification with the calculated one. There are similar formulas obtained and used by the literature in the calculation of excess air based on the concentrations of the components in the flue gases. [10] [6].

3 Adiabatic temperature - mixture ratio

It starts from the relationship known for defining the efficiency of combustion: [11]

\[ \zeta \ast \text{Hi} = (1 + \lambda \ast L_0) \ast h_3 - \lambda \ast L_0 \ast h_2 \]  

where:
- \( \zeta \) – combustion efficiency [%];
- \( \text{Hi} \) – lower calorific value (fuel) [kJ/kg];
- \( h_3 \) – flue gas enthalpy [kJ/kg];
- \( h_2 \) – enthalpy of the air at the entrance to the combustion chamber [kJ/kg];
The enthalpy can be defined by the following relationship [12]:

$$\Delta h = C_p * (T - T_{ref})$$  \hspace{1cm} (30)$$

It was considered that the reference temperature is $T_{ref} = 0 \, ^\circ C$. So, it can be written:

$$\zeta \ast H_i = (1 + \lambda \ast L_0) \ast C_{p_{flgas}} \ast T_3 - \lambda \ast L_0 \ast C_{p_{air}} \ast T_2$$  \hspace{1cm} (31)$$

It results:

$$T_3 = \frac{\zeta \ast H_i + \lambda \ast L_0 \ast C_{p_{air}} \ast T_2}{(1 + \lambda \ast L_0) \ast C_{p_{flgas}}}$$  \hspace{1cm} (32)$$

where:
- $C_{p_{air}}$ – average specific heat for air [kJ/kg K]; [8]
- $C_{p_{flgas}}$ - average specific heat for flue gases [kJ/kg K];
- $T_3$ – the temperature at the outlet of the combustion chamber (flue gases temperature) [K]
- $T_2$ – the temperature at the inlet of the combustion chamber [K]
- $T_0 = T_{ref}$ – ambient temperature, reference [K]; value is considered $0 \, ^\circ C = 273 \, K$
- $\lambda$ - air–fuel equivalence ratio (equation (15));
- $L_0$ – the minimum theoretical air required [kg air/kg fuel] (capitolul 2);
- $H_i$ – lower calorific value

For the calculation of the calorific value, it is possible to calculate by volume or by mass.

If we start from the calorific value by volume, we can write the relationship [6]:

$$H_v = (1 - y) \ast H_{vCH4} + y \ast H_{vH2} \, \, \, \, \, \, \, [kJ/m^3_N]$$  \hspace{1cm} (33)$$

where: $H_{vCH4}$, $H_{vH2}$ the volumetric calorific values of CH$_4$ respectively H$_2$.

$$H_{v} = \frac{H_{vCH4} \ast (1 - y) + y}{M_{fuel}} \ast V_{mol} \, \, \, \, \, \, \, [kJ/kg]$$  \hspace{1cm} (34)$$

where:
- $V_{mol} = $ Molar volume = 22.4 m$^3_N$/kmol
- $M_{fuel} = (1- y) \ast 16 + y \ast 2$ [kg/kmol] is the molar mass of the fuel mixture

Values considered [13]: $H_{vCH4} = 35800 \, kJ/m^3_N$; $H_{vH2} = 10700 \, kJ/m^3_N$;

It results:

$$H_v = \frac{10700 \ast (3.345 \ast (1 - y) + y)}{M_{fuel}} \ast V_{mol} \, \, \, \, \, \, \, [kJ/kg]$$  \hspace{1cm} (35)$$

After transformations it results:

$$H_v = 239680 \ast \frac{[3.345 \ast (1 - y) + y]}{[(1 - y) \ast 16 + y \ast 2]} \, \, \, \, \, \, \, [kJ/kg]$$  \hspace{1cm} (36)$$

If we start from the calorific value by mass, the mass fractions are taken into account and thus the following relation results. [6]:

$$H_{m} = \frac{(1 - y) \ast 16}{(1 - y) \ast 16 + y \ast 2} \ast H_{mCH4} + \frac{y \ast 2}{(1 - y) \ast 16 + y \ast 2} \ast H_{mH2} \, \, \, \, \, \, \, [kJ/kg]$$  \hspace{1cm} (37)$$
Hi_m = Hi_{mCH4} \times \frac{\left[(1 - y) \times 16 + \frac{Hi_{mCH4}}{Hi_{mH2}} \times y \times 2\right]}{\left[(1 - y) \times 16 + y \times 2\right]} \quad [kJ/kg] \quad (38)

The following values are considered: Hi_{mCH4}=50000 kJ/kg; Hi_{mH2} = 120000 kJ/kg (the values presented in the literature differ by +/- 0.5%, preferring these values to simplify the relationship).

Therefore:

Hi_m = 50000 \times \frac{\left[(1 - y) \times 16 + 2.4 \times y \times 2\right]}{\left[(1 - y) \times 16 + y \times 2\right]} \quad [kJ/kg] \quad (39)

With the two calculation relations for the calorific values by mass, the differences are:

**Table 2.** Comparison between the values obtained for the calorific value by mass

| y        | 0   | 0.1 | 0.2 | 0.4 | 0.6 | 0.8 | 1   |
|----------|-----|-----|-----|-----|-----|-----|-----|
| Rel (36) | 50108 | 51063 | 52221 | 55472 | 61118 | 73352 | 119840 |
| Rel (39) | 50000 | 50959 | 52121 | 55385 | 61053 | 73333 | 120000 |
| Differences [%] | -0.22% | -0.20% | -0.19% | -0.16% | -0.11% | -0.03% | 0.13% |

Relation (39) was chosen, and the calculations are presented in the following table:

**Table 3.** Calculated values of calorific value, for different percentages of H\textsubscript{2} in the mixture

| Y (molar fraction) (H\textsubscript{2} % by vol) | 0  | 0.1 | 0.2 | 0.4 | 0.6 | 0.8 | 0.9 | 1  |
|---------------------------------------------|----|-----|-----|-----|-----|-----|-----|----|
| Hi [kJ/kg]                                  | 50000 | 50959 | 52121 | 55385 | 61053 | 73333 | 87059 | 120000 |
| Mfuel                                      | 16 | 14.6 | 13.2 | 10.4 | 7.6 | 4.8 | 3.4 | 2  |
| Mass fraction                              | 0 | 0.0137 | 0.0303 | 0.0769 | 0.1579 | 0.3333 | 0.5294 | 1  |
| \(H_2\) by mass [%]                        | 0 | 1.37% | 3.03% | 7.69% | 15.79% | 33.33% | 52.94% | 100% |
| Hi increment [%]                           | 0% | 2% | 4% | 11% | 22% | 47% | 74% | 140% |

It can be observed that over 40% \(H_2\) (y=0.4) the rising of the lower calorific value is increasing, which is also observed in the diagram below, in which the slope of the curve changes essentially after this value. This observation correlates with the reports in the literature, in which experiments say that up to 10-15% by volume \(H_2\), there are not special problems for the combustion process [14]. This should be monitored during experiments. In addition to this, the variation of the fuel mixture’s flow for \(CH_4-H_2\) will be considered, which will be adjusted with the change of the percentage of \(H_2\), in order to obtain the same constant thermal power.
Finally, for the calculations, the relation (39), will be preferred, which together with the relation (14), by introduction in the relation (32), results:

$$T_3 = \frac{\zeta \times 50000 \times \left\{ \frac{1}{1-y} \times (16 + 2.4 \times y \times 2) \right\} + \lambda \times \frac{8.5799 \times (2 - 1.5 \times y)}{1 - 0.875 \times y} \times C_{p_{air}} \times T_2}{\left(1 + \lambda \times \frac{8.5799 \times (2 - 1.5 \times y)}{1 - 0.875 \times y}\right) \times C_{p_{fgas}}}. \quad (40)$$

To determine the specific heats, the literature and the common methods indicates various ways, or charts to calculate. One example is presented and used in the program and calculation procedures for combustion chambers used in 1968 by NASA [15]. After transformations, the specific heats can be written:

$$C_{p_{air}} = \left[0.2419 - 0.8181 \times 10^{-5} \times T + 17.91 \times 10^{-9} \times T^2 - 2.743 \times 10^{-12} \times T^3\right] \times 4.186 \quad [\text{kJ/kg K}] \quad (41)$$

$$C_{p_{fgas}} = \frac{(0.431 + 52.558 \times 10^{-5} \times T - 38.24 \times 10^{-9} \times T^2 + 0.25 \times 10^{-12} \times T^3)}{8.5799 \times (2 - 1.5 \times y) \times \lambda} \times \frac{(1 - 0.875 \times y)}{8.5799 \times (2 - 1.5 \times y) \times \lambda} \quad (42)$$

The procedure is iterative (2-3 iterations), in which we start from a specific heat value and depending on the resulting temperature, the calculation is repeated with the value of the specific heat corresponding to the temperature resulting in the first iteration. The method is often used in the field, with different calculation relationships [8] [15] [16].

The presented relations do not take into account the thermal dissociation.

In order to make the dissociation correction, we will start from the correction concept according to which the lower calorific value is diminished by the energy lost by dissociation [15] [16]:

$$H_{i_corrected} = H_i - H_{i_dissociation} \quad [\text{kJ/kg}] \quad (43)$$

where $H_{i_{dissociation}}$ is approximated with the relation [15]:

$$H_{i_dissociation} = \frac{3 \times 10^{-26} \times T_3^{7.5}}{f} \times 2.326 \quad [\text{kJ/kg}] \quad (44)$$

where: $f$ – fuel-air ratio; $T_3$ – flue gases temperature [K];

After transformations and adaptation to the CH\textsubscript{4}-H\textsubscript{2} mixture, the relationship becomes:
\[ H_{\text{dissociation}} = \frac{581 \times 10^{-26} \times T_3^{7.5} \times (1 - 0.875 \times y)}{8.5799 \times (2 - 1.5 \times y) \times \lambda} \] [kJ/kg] \quad (45)

\[ H_{\text{dissociation}} \] is shown graphically in the next figure below, in values [kJ/kg]:

**Fig. 2** Corrections of lower calorific value for different values of \( H_2 \) %

In the end, the dissociation correction is applied. Calculations can also be done directly taking into account the dissociation correction, the final relationship becoming:

\[ T_3 = \frac{\zeta \times (50000 \times \frac{[1 - y] \times 16 + 2.4 \times y \times 2]}{([1 - y] \times 16 + y \times 2]} - \frac{581 \times 10^{-26} \times T_3^{7.5} \times (1 - 0.875 \times y)}{8.5799 \times (2 - 1.5 \times y) \times \lambda}}{1 + \lambda \times \frac{8.5799 \times (2 - 1.5 \times y)}{1 - 0.875 \times y}} \times C_{\text{Pfgas}} \]

\[ + \frac{\lambda \times \frac{8.5799 \times (2 - 1.5 \times y)}{1 - 0.875 \times y}}{1 + \lambda \times \frac{8.5799 \times (2 - 1.5 \times y)}{1 - 0.875 \times y}} \times C_{\text{Pgas}} \times T_2 \] [K] \quad (46)

where: \( T_2 \) – air temperature; \( T_3 \) – adiabatic temperature of combustion (in the equation above, \( T_3 \) is iterative, as in the case of specific heats \( C_{\text{Pfgas}} \).

Results of calculations using these relationships are presented in the following graphs:

**Fig. 3** Corrected combustion temperature

a) for \( \text{CH}_4 \) 100%,  b) for the mixture \( \text{CH}_4-\text{H}_2 \), at various % of \( \text{H}_2 \)
Fig. 3b shows the combustion temperatures for the mixtures at values of interest for the experimental sessions.

Verification was performed with data from the known literature [15] [16] [17] [18] [19] [20]. The error margin $\frac{T_{\text{calc}}-T_{\text{lit}}}{T_{\text{calc}}}$ [%] is in between the limits of 1.32 % and -1.27%, the compared cases being methane and pure hydrogen, at different air temperatures. Some examples are given in the table below.

Table 4. Comparison of calculated values with the literature

|     | y=0     | y=1     | Deviation from the literature |
|-----|---------|---------|-----------------------------|
|     |         |         | $\frac{T_{\text{calc}}-T_{\text{lit}}}{T_{\text{calc}}}$ [%] |
| K   | 2251    | 2494    | -0.69%                      |
| C   | 1978    | 2221    | -1.13%                      |
| C   | 1963    | 2254    | 1.32%                       |
| C   | 2004    | 2210    | -0.44%                      |
| K   | 2225    | -       | -1.18%                      |
| K   | 2223    | 2483    | -1.27%                      |

As it can be seen, the deviations are small and of both positive and negative values, not only in one direction (which would suggest a methodological error).

4 Conclusions

The work here does not aim in this phase to bring special innovations in the field of combustion for $\text{CH}_4$-$\text{H}_2$ mixtures, it starts from known formulas, specific to the physical and chemical processes that take place in the combustion chambers. However, going deeper into the calculation details for the peculiarities of burning $\text{CH}_4$ and $\text{H}_2$ mixtures, new aspects come to light, highlighting specific tendencies that should direct numerical or experimental research for a certain course. For example, a clear picture of the variation in lower calorific value, depending on the variation in the percentage of hydrogen in the fuel mixture, can lead to some logical estimates of important aspects of combustion, such as flame field and temperature variation, related to the variation of the amount of hydrogen.

Moreover, in this paper very useful formulas have been developed for establishing the starting parameters for possible numerical calculations, as well as for establishing operating regimes for experiments. Finally, the data obtained with these calculations can be compared with those obtained by CFD analysis, or from experiments, as a very useful, correct and easy verification.

This work has been funded by the European Social Fund from the Sectorial Operational Programme Human Capital 2014-2020, through the Financial Agreement with the title "Scholarships for entrepreneurial education among doctoral students and postdoctoral researchers (Be Antreprenor)", Contract no. 51680/09.07.2019 - SMIS code: 124539.

5 References

1. E.-I. Koytsoumpa, C. Bergins, B. Buddenberg, S. Wu, O. Sigurbjornsson, K.C. Tran, E. Kakaras, The Challenge of Energy Storage in Europe: Focus on Power to Fuel, ASME J. Energy Resour. Technol., 138(4), p. 042002, 2016
2. M. Aigner, EU-Turbines & GERG Workshop, Brussels, Burning Natural Gas / Hydrogen Mixtures in DLN Gas Turbines October 2011
3. R. Carlanescu, T. Prisecaru, M. Prisecaru, I. Soriga, *Swirl Injector for Premixed Combustion of Hydrogen–Methane Mixtures*, Journal of Energy Resources Technology, **140**(7), 2018. Paper No: JERT-16-1506; doi: 10.1115/1.4039267

4. M. Andersson, J. Larfeldt, A. Larsson, B., *Co-Firing With Hydrogen in Industrial Gas Turbines*, Swedish Gas Technology Centre (SGC), Malmo, Sweden, Report No. 2013:256, 2013

5. A.H. Lefebvre, D.R. Ballal, *Gas Turbine Combustion. Alternative Fuels and Emissions* CRC Press, New York, 2010

6. L. Mihaescu, T. Prisecaru, I. Oprea, *Cazane si Turbine - Notiuni de baza*, Editura MatrixRom Bucuresti, 1999

7. T. Prisecaru, *Simularea Numerica a Proceselor de Arder a Combustibililor Gazosi si Solizi Pulverizati*, Editura Bref, Bucuresti, ISBN 973-8143-76-4, 2001

8. S. McAllister, J-Y. Chen, A. C. Fernandez-Pello, *Fundamentals of Combustion Processes, Chapter 2 - Thermodynamics of Combustion*, Springer, ISBN 978-1-4419-7943-8, 2011

9. C. Carlanescu, I. Manea, C. Ion, S. Sterie, *Turbomotoare - Fenomenologia Producerii Si Controlul Noxelor*, Editura Academiei Tehnice Militare, 1998

10. R. Chiriac, R. Radu, *Cercetarea Experimentala a Masinilor Termice - Indrumar de Laborator*, Universitatea Politehnica Bucuresti, Facultatea de Inginerie Mecanica, Bucuresti, 1997

11. V. Pimsner, C.A. Vasilescu, G.A. Radulescu, *Energetica turbomotoarelor cu ardere interna*, Ed. Academiei Republicii Populare Romania, 1964

12. B. P. Meherwan, *Principles Of Operation And Performance Estimation Of Centrifugal Compressors*, Proceedings of the Twenty-First Turbomachinery Symposium, [Dallas, Texas], 1992

13. M. Fossum, R.V. Beyer, *Co-combustion: Biomass Fuel Gas and Natural Gas*, SINTEF Energy Research, Technical Report TRA **473**, ISBN 82-594-1296-94, 1998

14. R. Carlanescu, T. Prisecaru, R. Kuncser, E. Pop, *The optimization of a swirl injector for combustion of hydrogen fuel mixtures flame temperature of hydrogen in combination with gaseous fuels*, U.P.B. Sci. Bull., Series D, **81**(1), ISSN 1454-2358, 2019

15. NASA report, Northern Research and Engineering Corp., *Computer program for the analysis of annular combustors. Volume I - Calculation procedures*, Cambridge, MA, United State, NAS3-9402, 1968, https://ntrs.nasa.gov/search.jsp?R=19680008088 (accessed: may 2019)

16. J. Hodge, *Cycle and Performance Estimations*, Butterworth Scientific Publications London, England, 1955

17. S.K. Mishra, R.P. Dahiya, *Adiabatic flame temperature of hydrogen in combination with gaseous fuels*, International Journal of Hydrogen Energy, **14**(11), Pages 839-844, 1989

18. B. Lewis, G. von Elbe, *Combustion, Flames and Explosions of Gases - Third Edition*, Academic Press, ISBN: 978-0-12-446751-4, 1987

19. A. M. Helmenstine, ThoughtCo, , https://www.thoughtco.com /flame-temperatures-table-607307 (accessed: may 2019)

20. R. J. Richard, *North American Combustion Handbook: A Basic Reference on the Art and Science of Industrial Heating with Gaseous and Liquid Fuels, Vol. 1*, North Amer Manufacturing Co, Cleveland, Ohio, U.S.A., 1985