

A COMPUTATIONAL SOFTWARE PROGRAM FOR DETERMINING THE COMBUSTION TEMPERATURES OF SOLID FUELS

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ABSTRACT

The combustion temperature is one of parameters influencing the efficiency of combustion process. The analytical, model and design calculations of processes related to fuel combustion and heat exchange intensity require the combustion temperature to be correctly determined. These are, however, complex, and, as a consequence, burdensome and time-consuming requirements. Developing an appropriate software program will considerably streamline the calculation procedure. Based on analytical relationships for the combustion process, a computational software program has been developed within this study, which enables the determination of the calorimetric, theoretical and actual combustion temperatures of solid fuels.

Key words: combustion of solid fuels, combustion temperature, computational software program.

INTRODUCTION

A basic combustion process control parameter, aside from the excess air factor, is temperature. The temperature of combustion is a factor determining the efficiency of heat transfer. Normally, efforts are made to increase the combustion temperature with the aim of increasing the heat transfer efficiency. There are several methods that allow the increase of this parameter, namely [1, 2]:

- heating up the fuel and incoming air,
- enriching the air with oxygen,
- thermal insulation of the combustion chamber,
- assuring the complete and total combustion with the lowest possible value of the excess air factor, α .

The proper selection of the combustion temperature allows the correctness of analytical, and in a particular model and design combustion process-related calculations, to be maintained. Determining the combustion temperatures conditions, *inter alia*, model studies of the combustion of solid

fuels in the context of reducing atmospheric pollutant emissions. Hence, it seems to be of paramount importance to determine this parameter in an efficient and, at the same time, expeditious manner.

COMBUSTION TEMPERATURE

The temperature that combustion gas attains at the end of the combustion process is called combustion temperature. Three combustion temperature types are distinguished [3–6].

The calorimetric combustion temperature is the highest temperature achievable by undissociated combustion gas as a result of the adiabatic and isobaric combustion of fuel with theoretical amount of air [3, 5]:

$$t_{kal} = \frac{i_0 + i_r}{c_{sp}} \quad (1)$$

where: c_{sp} – mean specific heat of combustion gas, $J/(\mu\text{m}^3 \cdot \text{K})$,

i_0 – enthalpy of $1 \mu\text{m}^3$ of wet theoretical combustion gas ($\alpha = 1,0$), $J/\mu\text{m}^3$,

i_r – combustion substrates enthalpy per 1 μm^3 wet theoretical combustion gas, J/ μm^3 .

The enthalpy of wet theoretical combustion gas is expressed by the relationship [3, 5]:

$$i_0 = \frac{Q_d}{V_s''} \quad (2)$$

where: V_s'' – unit of wet combustion gas volume, μm^3 sp. wilg./kg fuel,

Q_d – calorific value, J/kg:

$$Q_d = \left[33900 \cdot c + 144030 \cdot \left(h - \frac{o}{8} \right) + 10400 \cdot s - 2500(w_c - 9h) \right] \cdot 10^3 \quad (3)$$

where: c, s, h, o, w_c – mass fractions of liquid and solid fuel components.

The enthalpy of combustion substrates per 1 μm^3 of theoretical wet combustion gas is determined from the relationship [3]:

$$i_r = \frac{V_{a\min} \cdot c_{pow} \cdot t_p + c_{fuel} \cdot t_{fuel}}{V_s''} \quad (4)$$

where: c_{pow} – mean specific heat capacity of combustion air, J/(μm^3 K),

c_{fuel} – mean specific heat capacity of combustion gas, J/(kg · K),

t_p – combustion air temperature, °C,

t_{fuel} – fuel temperature, °C,

$V_{a\min}$ – minimum combustion air demand, μm^3 pow./ kg_{fuel},

The theoretical (initial) combustion temperature is the highest temperature achievable by dissociated combustion gas [3, 5]:

$$t_{teor} = \frac{i_a + i_r - i_d}{c_p} \quad (5)$$

where: i_a – enthalpy of 1 μm^3 of wet real combustion gas allowing for the value of the excess air factor, J/ μm^3 ,

i_d – enthalpy of dissociation of 1 μm^3 of real combustion gas, J/ μm^3 .

The enthalpy of wet real combustion gas, while allowing for the value of the excess air factor, is expressed by the relationship [3, 5]:

$$i_a = \frac{Q_d}{V_s''} \quad (6)$$

The enthalpy of real combustion gas dissociation is determined from the relationship:

$$i_d = 12470 \cdot \alpha_{CO_2} \cdot r_{CO_2} + 10620 \cdot \alpha_{H_2O} \cdot r_{H_2O} \quad (7)$$

where: r_{CO_2}, r_{H_2O} – volumetric fractions of combustion gas components,

$\alpha_{CO_2}, \alpha_{H_2O}$ – dissociation coefficients.

For combustion temperatures below 1700 °C the enthalpy of dissociation is negligible and its influence on the combustion temperature can be omitted.

The actual combustion temperature is also called flame temperature. This is a temperature at a given moment and in a given location in the flame (furnace). It allows for the effect of heat radiation into the furnace space. It is determined from the relationship [3, 5]:

$$t_{rzecz} = \mu \cdot t_{teor} \quad (8)$$

where: μ – pyrometric combustion factor.

The values of the pyrometric combustion factor is provided in literature [3] for different types of furnace.

COMPUTATION METHODOLOGY

For developing the program, analytical relationships for the combustion temperature were used. The implementation of these relationships in the program required mathematical functions describing the following quantities to be formulated:

- the mean specific heat capacity of the gas, air and combustion gas;
- the coefficients of dissociation of CO_2 and H_2O .

The value of mean specific heat capacity of the solid fuel, expressed in $\text{kJ}/(\text{kg} \cdot \text{K})$, was determined from the relationship:

$$c_{\text{paliwa}} = 0.708 \cdot c + 14.195 \cdot h + 0.915 \cdot o + 1.039 \cdot n + 0.699 \cdot s + 0.795 \cdot p + 4.186 \cdot w_c \quad (9)$$

where: p – ash mass fraction of fuel.

The value of the mean specific heat capacity of air and combustion gas, expressed in $\text{kJ}/(\mu\text{m}^3 \cdot \text{K})$, was determined from the relationship:

$$c = \sum \bar{c}_i \cdot r_i \quad (10)$$

where: \bar{c}_i – mean specific heat capacity of air or combustion gas component, $\text{kJ}/(\mu\text{m}^3 \cdot \text{K})$,

r_i – volumetric fraction of an air or combustion gas component.

Based on the value of mean specific heat capacity for individual air and combustion gas components, mathematical functions describing the effect of temperature on their heat capacities were formulated. The general relationship assumes the form as below:

$$\bar{c}_i = A + B \cdot t + C \cdot t^2 \quad (11)$$

where: A, B, C – constant values,

t – temperature, $^\circ\text{C}$.

The solid values to calculations of average proper warmth for individual components of gas and air and the fumes summarized in Table 1.

The dissociation coefficients represent a function of temperature and partial pressure being dependent on the CO_2 and H_2O contents of combustion gas. The energy balance equation enabling computations to be performed with the method presented herein and the problems related to the dissociation of CO_2 and H_2O are described in a greater detail in references [7–9]. For particular partial pressure ranges, relationships for the dissociation coefficients as a function of temperature were developed. The general relationship adopts the following form:

$$\alpha = A_1 + B_1 \cdot t + C_1 \cdot t^2 + D_1 \cdot t^3 \quad (12)$$

where: A_1, B_1, C_1, D_1 – constant values.

The solid values to calculations of dissociation H_2O coefficients for individual ranges of partial pressure summarized in Table 2.

Table 1. The solid empirical values to calculations of average proper warmth for individual components of gas and air and the fumes

Components	The solid values		
	A	B $\cdot 10^3$	C $\cdot 10^7$
CO_2	1.61957	0.844664	-2.5154100
H_2O	1.48957	0.201901	0.3196780
O_2	1.29731	0.225157	-4.6761200
N_2	1.28986	0.084818	1.7209400
SO_2	1.71520	0.773119	-2.7719800
Air	1.28957	0.113784	0.0353641
CO	1.28882	0.113424	0.0546218

Table 2. The solid empirical values to calculations of dissociation CO₂ coefficients for individual ranges of partial pressure

Partial pressure CO ₂ in fumes, kPa	The solid values			
	A ₁	B ₁ · 10 ³	C ₁ · 10 ⁷	D ₁ · 10 ¹⁰
3	1.0769795	-1.5647	5.62075	0
4	1.2074031	-1.6814	5.83561	0
5	1.2856280	-1.7473	5.93966	0
6	1.3233584	-1.7727	5.94880	0
7	1.3760369	-1.8167	6.01631	0
8	1.3985608	-1.8310	6.01588	0
9	1.4233874	-1.8483	6.02667	0
10	1.4440101	-1.8628	6.03492	0
12	1.4567568	-1.8623	5.98104	0
14	1.4782624	-1.8732	5.96471	0
16	1.4724573	-1.8583	5.89191	0
18	1.4510133	-1.8272	5.78002	0
20	1.4630247	-1.8325	5.76571	0
60	-0.0158115	0.4452	-5.45004	1.72170
100	-0.1273187	0.5825	-5.83210	1.69451

Table 3. The solid values to calculations of dissociation H₂O coefficients for individual ranges of partial pressure

Partial pressure H ₂ O in fumes, kPa	The solid values			
	A ₁	B ₁ · 10 ³	C ₁ · 10 ⁷	D ₁ · 10 ¹⁰
3	-0.7364956	1.4376	-9.62587	2.21989
4	-1.0296681	1.8584	-11.54020	2.48524
5	-0.8522410	1.5838	-10.10520	2.22688
6	-0.6930881	1.3379	-8.82552	1.99883
7	-0.7293497	1.3821	-8.95886	1.99728
8	-0.7181641	1.3609	-8.80892	1.95824
9	-0.7496520	1.4005	-8.94406	1.96426
10	-0.7169212	1.3437	-8.60804	1.89549
12	-0.7338214	1.3595	-8.60589	1.87277
14	-0.7216266	1.3362	-8.44132	1.83081
16	-0.6944776	1.2922	-8.18712	1.77720
18	-0.7296117	1.3336	-8.31393	1.77953
20	-0.7199730	1.3262	-8.29773	1.77486
60	-0.7236804	1.2654	-7.51713	1.52914
100	-0.6085711	1.0674	-6.35763	1.29584

The solid values to calculations of dissociation H₂O coefficients for individual ranges of partial pressure summarized in Table 3.

Using the described mathematical functions allowing for the effect of temperature, the dissociation coefficients were determined from the relationships:

$$\alpha_{CO_2} = \alpha_{(i+1)CO_2} + \{(\alpha_i CO_2 - \alpha_{(i+1)CO_2}) \cdot [p_{(i+1)CO_2} - p_{CO_2}]\} \quad (13)$$

$$\alpha_{H_2O} = \alpha_{(i+1)H_2O} + \{(\alpha_i H_2O - \alpha_{(i+1)H_2O}) \cdot [p_{(i+1)H_2O} - p_{H_2O}]\} \quad (14)$$

where: $\alpha_i CO_2$, $\alpha_i H_2O$ – the coefficients of dissociation of CO₂ and H₂O for the lower partial pressure value from the range under consideration,

$\alpha_{(i+1)CO_2}$, $\alpha_{(i+1)H_2O}$ – the coefficients of dissociation of CO_2 and H_2O for the higher partial pressure value from the range under consideration,
 p_{CO_2} , p_{H_2O} – the actual partial pressure of CO_2 i H_2O , kPa,
 $P_{(i+1)CO_2}$, $P_{(i+1)H_2O}$ – the higher CO_2 and H_2O partial pressure value from the range under consideration, kPa.

COMPUTATIONAL SOFTWARE PROGRAM

For developing the software program, computational procedures were employed, as illustrated in Figure 1. Considering the analytical relationships and the determined mathematical functions, a computational software program has been developed, whose screenshot is shown in Figure 2.

According to the procedures shown in Figure 1, the input data in a form of the oxygen content of combustion air, the excess air factor value, the temperatures of combustion air and fuel as well as fuel composition needs to be entered in the program (Figure 3). The procedure for the calorimetric temperature provides combustion process computation results for $\alpha = 1.0$ and specific heats and enthalpies necessary for determining the temperature sought for (Figure 3). The assumed calorimetric temperature should be selected so that its value be approximate to the obtained result.

The procedure for the theoretical temperature provides combustion process computation results for the actual value of the excess air factor α and specific heats and enthalpies necessary for determining

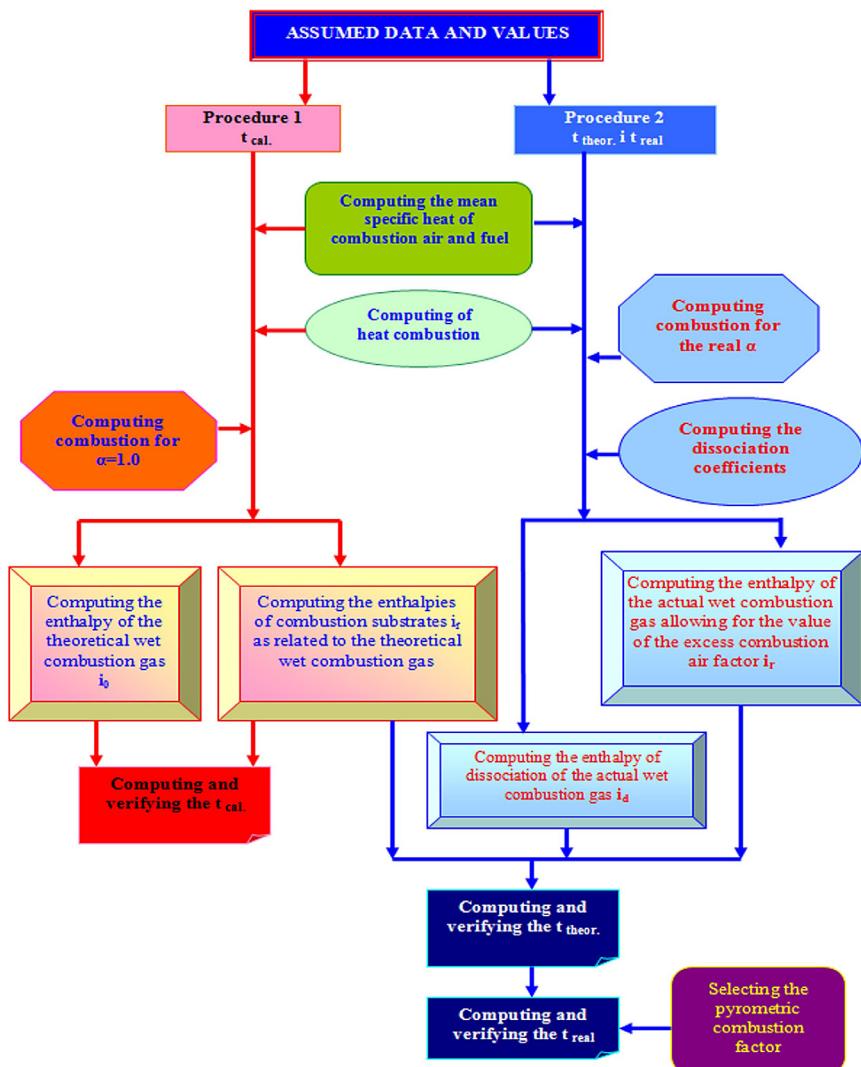


Fig. 1. Computational procedures of program to marking the combustion temperatures of the solid fuels

the temperature sought for (Figure 4). The assumed theoretical temperature must be approximate to the obtained result, whereas the actual temperature results from the theoretical temperature. The design of the program enables fast determination of solid fuel combustion temperatures; however, it requires basic theoretical knowledge of combustion processes.

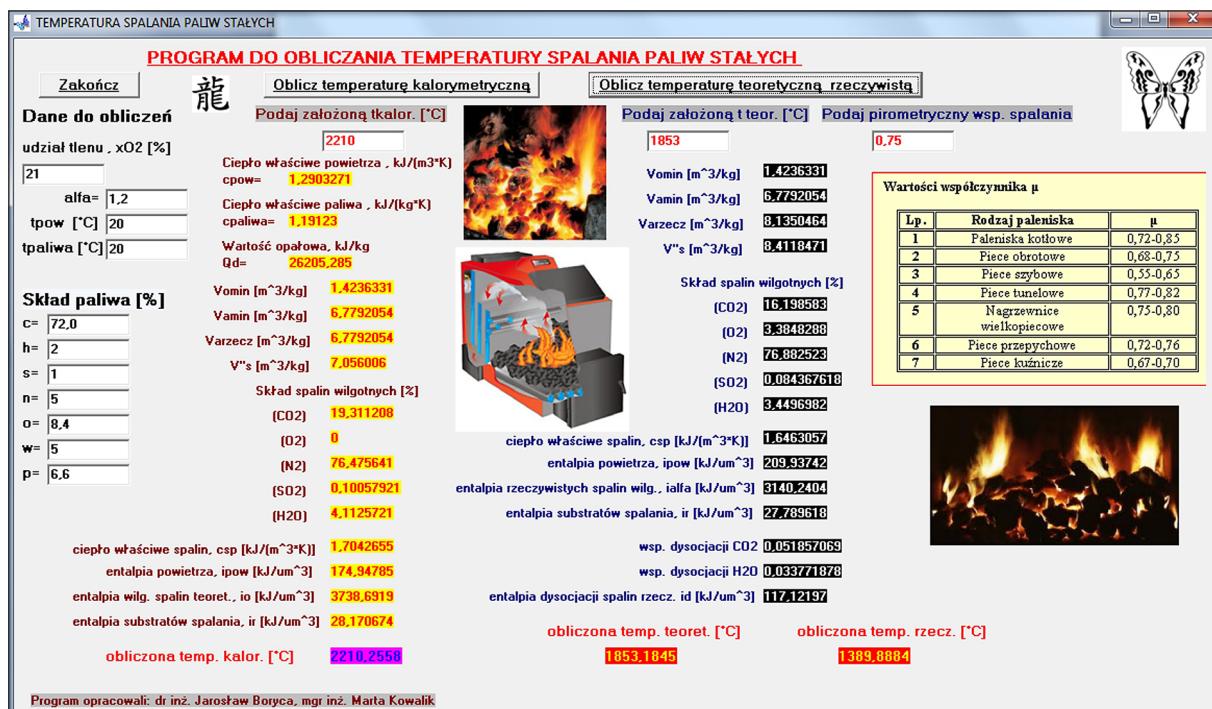


Fig. 2. A screenshot of program for calculations of combustion temperature of the solid fuels

Fig. 3. Part of the program window for input and calorimeter temperature

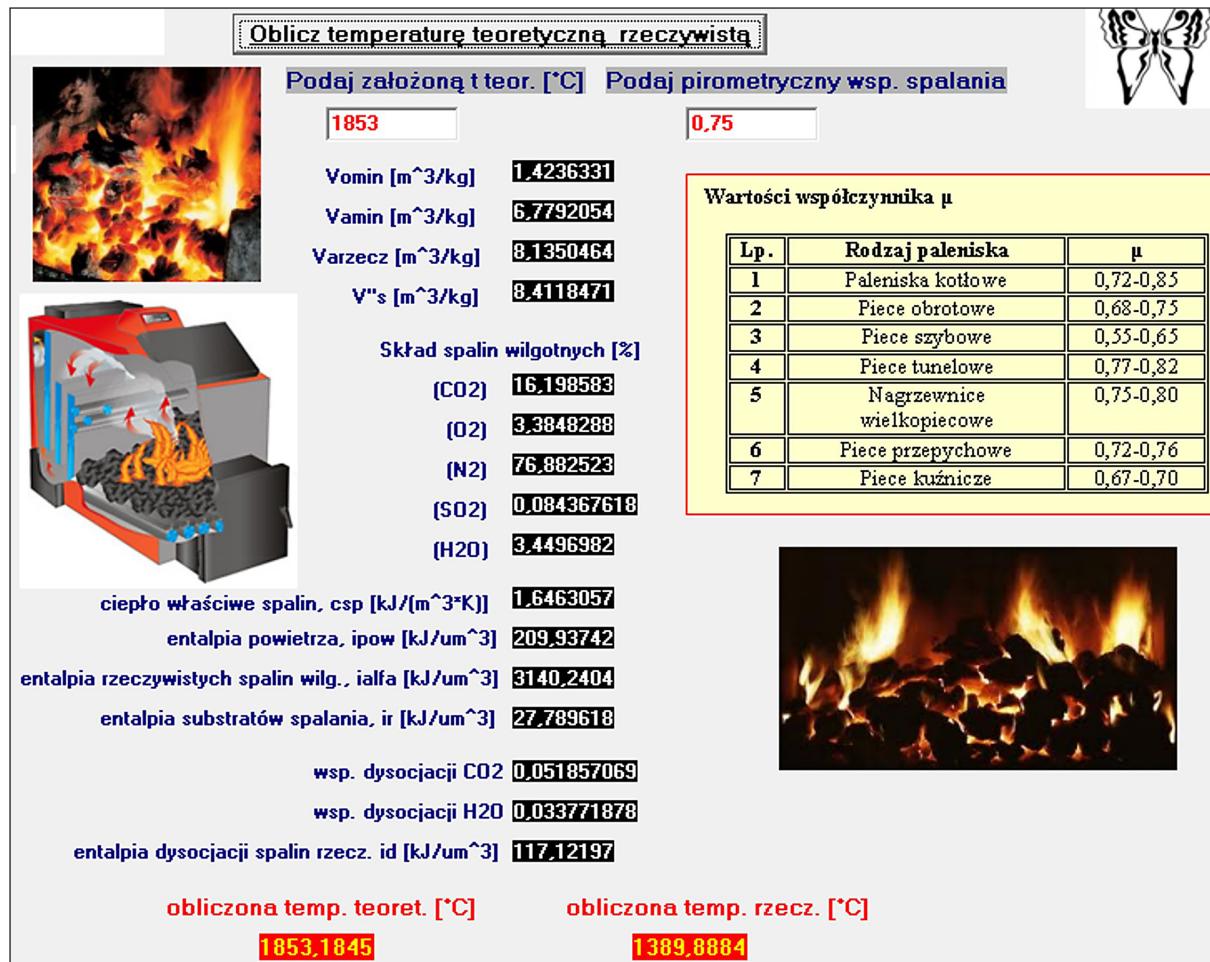


Fig. 4. Part of the program window for theoretical and real temperature

EXAMPLE COMPUTATION RESULTS

For the fuel composition shown in the program window (Figure 3), the theoretical temperature was computed for the variable value of the excess combustion air factor and the calorimetric, theoretical and actual temperatures for the variable combustion air temperature, with an excess combustion air factor of $\alpha = 1.2$.

The computation results are summarized in Figures 5 and 6. By examining Figure 5 it can be stated that with the increase in the excess air factor value, the theoretical combustion temperature decreases, whereas increasing the air temperature (Figure 6) causes an increase in the calorimetric, theoretical and actual combustion temperatures.

SUMMARY

The paper has presented basic assumptions used for the development of a software program that will enable the user to determine the solid

fuel combustion temperature in an easy and expeditious manner. An asset of the program is the fact that, in addition to the ease of operation, provides the capability to readily change the input data in the form of the excess air factor value, combustion substrate temperature, fuel composition and the oxygen fraction of the feed air. The possibility of entering a variable oxygen fraction is extremely important in case of computation concerning combustion in an oxygen-enriched atmosphere. For the actual temperature, it is also possible to select an appropriate pyrometric coefficient.

The presented computation results enable the authors to state that the theoretical and the actual combustion temperatures depend on the value of the excess air factor. With the increase in α , the above-mentioned temperatures decrease. In turn, the increase in substrate temperature causes an increase in combustion temperatures, including also the calorimetric temperature. The results obtained for different fuels are approximate to those provided in the literature, which evidences the correctness of operation of the developed program.

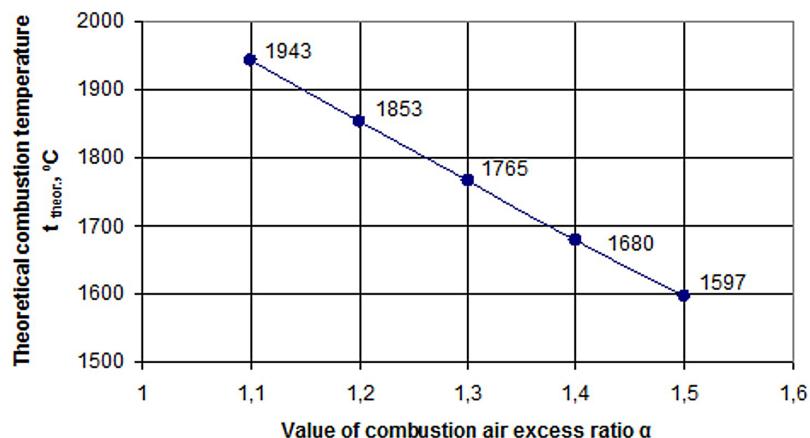


Fig. 5. The results of calculation of the theoretical combustion temperature

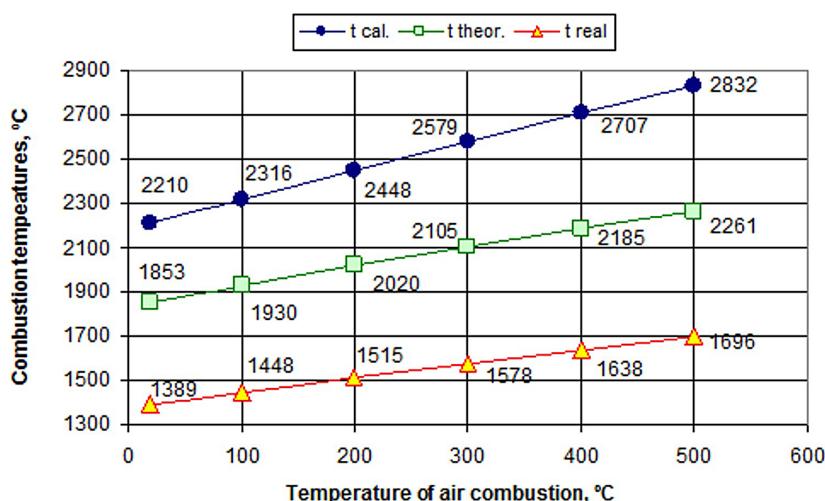


Fig. 6. The results of calculation of the calorimetric, theoretical and real combustion temperatures for variable of air temperature

The presented computational program can provide a useful tool for both teaching and research purposes. Indeed, combustion temperature computation results are an essential input data element in the modelling of combustion processes, as well as in designing combustion chambers.

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