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VALIDATION OF 3-DIMENTIONAL MODELS OF NATURAL GAS COMBUSTION AND TEMPERATURE MEASUREMENTS

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Abstract: *Technological combustion processes present serious environmental problems due to the emission of harmful substances, predominantly in gaseous state. According to the generally accepted view, the nitrogen oxides mostly originate in combustion plants in the high temperature zones. Therefore, determination of such zones within the combustion applications at a stage of design calculations or by means of directs measurements are of a major importance. The problems associated with the thermocouple errors at temperature measurements in the flames and combustion product flows are being dealt with. A model has been derived aimed at the evaluation of correction factors that are to be applied, when processing data of the direct thermocouple readings. The model takes into account convective heat transfer, irradiation from the combustion products on a part of the thermocouple bead. It also takes into consideration that a part of the thermocouple bead irradiates in the direction of the cooled surrounding. As a result, a transcendent fourth order equation has been obtained and solved numerically by MathCad. A set of correction coefficient was obtained which, when added to the direct readings of thermocouples, have shown a close conformity to the results obtained from the 3-D modeling of natural gas combustion in the cylindrical downflow reactor. Thus developed correction methodology may be recommended for use in practice, when temperature measurements are performed by bare thermocouples, when bead sheathing or suction pyrometer can not be used.*

Key words: *thermocouple, heat flux, convection, radiation, flame, reradiation.*

1. Introduction

The problem of flame temperature measurements with bare thermocouples has been dealt with in [1-8, 10, 11]. They mainly address the measurement of temperature in combustion processes within the flame or near it in the vicinity of cooled walls or adversely - temperature measurements of relatively cold gas flows in the presence of high-temperature enclosures that are in direct exposure to the thermocouple.

If a thermocouple measures the temperature of gas flow outside of the radiating flame, it most likely gives too high temperature readings, since the thermocouple bead receives not only the convective heat from the flow itself but irradiative flux from the flame as well. Because the radiant flux is proportional to the 4th temperature degree, it is clear that thermocouple measurements in high temperature processes, particularly in combustion ones, the input of radiant flux will be much more significant than that from convection.

Similarly, when measurements take place in a close vicinity of flame with the enclosure at a lower temperature and with optically transparent medium, the thermocouple readings will be lower than the actual flame temperature. This is due to the effect that the thermocouple bead, being a participant of complex heat transfer, will receive heat as a result of convection from the gas flow and radiation from the flame, will also irradiate towards the cooled enclosure. Shannon and Butler [1] suggested a mathematical model that takes into account the heat balance of the thermocouple bead:

$$(\varepsilon_{fl} 6 T_{fl}^4 - \varepsilon_b 6 T_b^4) F_{fl-b} - (\varepsilon_b 6 T_b^4 - \varepsilon_\infty 6 T_\infty^4)(1 - F_b) = h A_b (T_{fl} - T_b)\,, \quad (1)$$

where F – a function that takes into account the relative exposure according to subscripts flame-bead or bead-surrounding;

h, A - heat transfer coefficient to the thermocouple bead and its surface area, respectively;

ε, б –respective surface emissivity (absorptivity) and Stefan-Boltzmann constant.

In [2] an extremely simplified model was accepted, according to which the thermocouple radiates all the heat, obtained by the convection from the flow:

$$\left(T_{fl} - T_b\right) = \frac{\varepsilon 6}{h}(T_b^4 - T_\infty^4), \quad (2)$$

where h – heat transfer coefficient from the gas flow calculated by:

$$Nu\left[\frac{\frac{1}{2}(T_{fl}-T_b)}{T_b}\right]^{-0.17} = 0.24 + 0.56\left(\frac{wd}{\nu}\right)^{0.45}, \quad (3)$$

Combining (2) and (3) one can approximately determine the thermocouple error from the re-radiation:

$$\left(T_{fl} - T_b\right) \sim \frac{d^{0.55}}{U^{0.45}}(T_b^4 - T_\infty^4). \quad (4)$$

From (4) it follows that the reduction of the error can be achieved by reducing the diameter of the thermocouple bead or by decreasing U - the proportion of radiant heat transfer between the gas flow and the bead.

Walker-Stokes [3] proposed the method of measuring temperature with a thermocouple set, whose diameter is decreased progressively. This method has allowed to reduce inertia of thermocouple readings and to determine the effect of radiation basing upon the expression (4). The method becomes unrealizable due the temperature instability of flows and necessity to install the thermocouple in the same place of a flow.

Most often, the protective screens are used to shield thermocouple beads [1-4]. Protective screens can be accompanied with the suction of flow through a cylindrical screen, which leads to an increase of flow speed around the thermocouple bead and, as a result, increasing convective heat transfer coefficient thus bringing closer bead actual temperature to that of flow. In practice, the speed of sucked flow is limited by the experimental considerations (prevention of significant disturbance in the flow).Comparative results of the temperature measurement in industrial furnaces by means of unprotected thermocouples of different diameters, two types of shielded thermocouples, that differed by the place of suction, were given in [1, 2, 8]. The authors have shown that the greatest error occurs at measuring the temperature of medium with the thermocouple irradiation.

From the data given in [1-8] follows that the error of "cold" flow measurement by bare thermocouple within the radiating environment reaches 250%. Errors of temperature measurements by bare thermocouples in "hot" flows surrounded by cooled walls reach 25%. Installing of a dual screen can reduce the error to 25% and 7%.

The main objective of the work is to derive a method to correct the direct readings obtained when measuring temperatures of hot combustion products by bare thermocouples in the presence of cooled walls

2. Matherials and methods

Experiments have been conducted in the experimental rig designed and erected at the Coal Energy Technology Institute of the NAS of Ukraine. The scope of experimentation covered the following:

- Obtaining experimental data of the direct temperature and components" concentration distribution within the reactor when burning natural gas, which then will be used for the 3-D CFX and FLUENT models validation by the comparison of the measured and modeled data;
- Co-combustion of coal and solid biomass aimed at the determination of the optimal process conditions;
- Combustion of solid biomass at different regime parameters aimed at the determination of the effect of the various types of biomass burning kinetics, its conditions and properties aimed at the determination of the optimal process conditions.

Since the experimental rig closely models the conditions which exist in the lower radiation section of industrial boiler furnaces in the vicinity of burners, the experimental results obtained thus may be applicable for the designing optimal combustors.

The layout of the stand is shown in Figure 1.

Thermal capacity of the unit when burning coal with air as an oxidant reaches 100 KW. The main part of the unit is a down flow test channel with four diagnostic sections in which combustion takes place. Each of three initial sections is 0.6 m long with the internal diameter 0.28m. The last one has the same length and 0.2 m internal diameter. The internal walls of all test sections have a tree layer protective covering consisting of consecutive layers of zircon dioxide, fire clay and asbestos. Each section has a water cooled jacket with the individual supply and water flow measurement, which in turn allows thecalorimetry of each section. The burner head is equipped with two natural gas burners. The main burner has an additional (ground) solid biomass or coal together with NG and initial air.

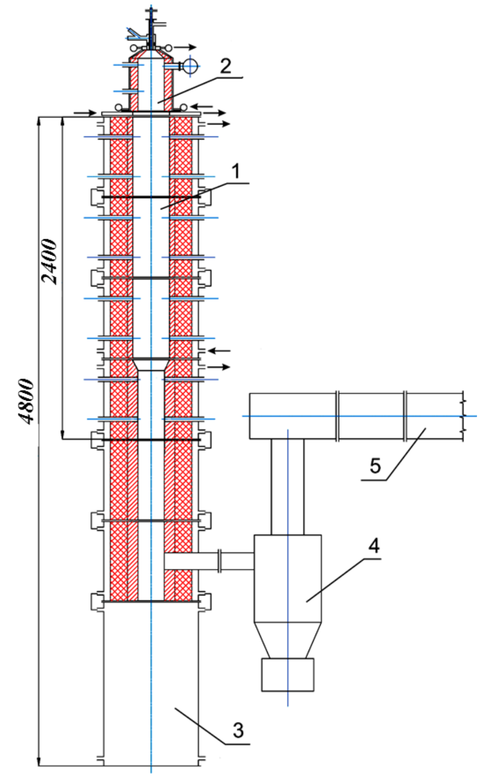


Fig.1. Experimental down flow unit VGP-100 B

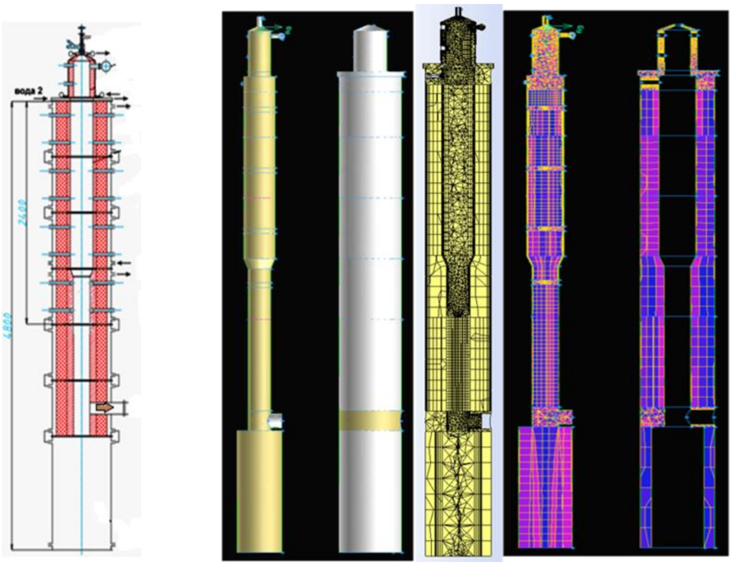
1-experimental sections, water cooled jackets for calorimetry;
2-burner head with multiple air inlets;
3-ash collector;
4-cyclon for fly ash removal;
5-flue gases duct.

The secondary burner is designed to inject natural gas and air only. There are also additional inlets allowing injection of any of the combustion components with the respective measurements of the component's flow rate. Each section also equipped with the inlets allowing inserting probes and thermocouples allowing direct measurements of local temperature and flue gases composition.

The experiments of natural gas combustion were carried out in the down flow cylindrical reactor VGP-100, Figure1. The temperature of test sections' walls was measured by chromel-alumel (type K) thermocouples that were built in the fire proof lining 10 mm deep from the fire layer. Periodical measurements of fire layer of lining were performed with the pyrometer "DPR-1" through the diagnostic openings. The temperature of the gas flow on the axis of the reactor was measured by Platinum-Platinum-Rhodium thermocouples (Type R) with 0.2 mm diameter wires in corundum protective cover with 0.5 mm diameter channels positioned in probes at a midsection of each test section. Hot thermocouple junctions were covered with a layer of corundum making the bead diametr-5 mm.

Thus obtained data related to the combustion of natural gas of a known composition were used for the validation of the developed 3-D CFX model of the process along with the direct temperature measurements which were used as benchmark data for developed model of measured temperatures correction.

In order to carry out the validation, a complex 3-D meshes of the reactor has been developed. The mesh represents the experimental stand VGP in general and in minor details. The main problem of the mesh development consisted in finding an optimum compromise between the number of mesh cells (which eventually determines accuracy and calculations convergence time and, thus, the required computer capacity) on the one hand, and the necessity to represent minor stand details which affect the actual process and are to be represented in the mesh – on the other.



(a) *(b)* *(c)*

Fig.2. Reactor VGP

a - VGP Reactor; b - geometry model with and without insulation;
c - 3-D mesh of the reactor core and insulation

It was found that the gas temperature measured in 4 points in the middle of each diagnostic section on the axis were 120-150^0C lower than respective CFX – FLUENT simulated values.

The difference in the obtained data can be explained by re-radiation of thermocouple beads towards the cooled walls. Thermal balance of thermocouple bead, that considers both convective and radiant flows, can determine the value of error of flow temperature measurement on the axis of the reactor.

It should be noted that the model under consideration becomes significantly complex as a result of taking into account radiant heat transfer between the thermocouple and gas flow, since gases are characterized by selective spectral energy absorption and emission. The absorption and emission of energy by monatomic and diatomic gases, including nitrogen, oxygen, and hydrogen are insignificant and may be neglected. Polyatomic gases, including carbon dioxide CO_2, water vapour H_2O, sulphur dioxide SO_2, ammonia NH_3, and others, have a large capacity for absorption and emission of radiant energy. Carbon monoxide CO also has a significant level of emission and absorption, but this gas occurs only as traces in the products of methane combustion at a proper air – fuel ratio.

The model of radiant heat exchange of bead with the environment has been derived under the assumption that there exists a local thermodynamic equilibrium bead-environment, so we can assume the equality absorption – emission according to the Kirchhoff's law. Flue gas and the walls are considered gray bodies. Radiation of the wall is characterized by a continuous spectrum and the medium (combustion gases) has selective radiation in a form of separate bands.

The results of direct temperature measurements with bare thermocouples during the experimental combustion of natural gas in a vertical reactor VGP-100 (100 KW_{th}) of the Coal Energy Technology Institute were taken as benchmark values for the validation of the model.

The objective of the proposed model is to derive a comparatively simple equation which will allow to calculate the temperature of a hot bead of a thermocouple (T_b) placed into the flow of hot combustion gases at a given (T_{fl}) and being exposed to the relatively cold walls at given T_w. Thus, the correction temperature can be determined which is to be used when direct readings of unsheathed thermocouples which are used for temperature measurements in media with convective-radiative heat transfer.

The equation was derived under the condition of equality of heat supplied to a thermocouple bead and the amount of heat, that thermocouple gave off to the walls as a result of re-radiation. Heat input is realized by means of convective heat transfer, radiation of hot flue gas and by radiation of heated head burner lining towards the bead.

For the approximate estimation of the re-radiation effect it was decided to apply the simplified model of radiant heat transfer between the bead surface and the heated lining surface under the following conditions: a) bead surface and radiating lining surface are plane-parallel; b) the area of bead surface, that receives radiation, is equal to a half of the total area of a thermocouple bead; c) absorbing capacity of corundum is $\varepsilon_{ef} = 0.9$; d) the temperature of the heated lining is taken equal to the temperature of the gas core T_{fl}. Then, the components of a heat balance of the bead will be:

$$\text{Absorbed heat } Q_{abs} = h\left(T_{fl} - T_b\right)A_b + \frac{A_b C_0 \varepsilon_{be}\left[\left(\frac{T_{fl}}{100}\right)^4 - \left(\frac{T_b}{100}\right)^4\right]}{2} + \frac{A_b C_0 \left[\varepsilon_{fl}^{\infty}\left(\frac{T_{fl}}{100}\right)^4 - \varepsilon_{fl,wall}^{\infty}\left(\frac{T_b}{100}\right)^4\right]}{\frac{\varepsilon_{fl}^{\infty}}{\varepsilon_{fl}} + \frac{1}{\varepsilon_{fl,wall}} - 1}, \qquad (5)$$

Heat radiated by the thermocouple bead on the wall

$$Q_{rad} = \varepsilon_{ef}\, C_0\, \frac{A_b}{2}\Big[\Big(\frac{T_b}{100}\Big)^4 - \\ -\Big(\frac{T_{wall}}{100}\Big)^4\Big], \qquad (6)$$

where T_{fl}, T_b, T_{wall} - temperatures of gas flow, thermocouple bead and wall, respectively, $[K]$;

h – heat transfer coefficient from gas environment to the thermocouple bead, *[W/m²K]*;

ε_{ef}, ε_{fl}, $\varepsilon_{fl,wall}$, $\varepsilon^{\infty}_{fl,wall}$ - emission factors taken for bead-lining effective, for gas flow at gas temperature, for gas flow at wall temperature and for gas flow at wall temperature at a infinite beam length, respectively [9, 11, 13, 14];

A_b - thermocouple bead surface area.

The heat transfer coefficient was calculated for the case of an external flow of hot flue gases around a thermocouple taken from [9]; thermophysical properties were calculated by the software EnecCalc3, and checked with the data base [9]:

$$\overline{Nu} = 2 + 0.03\,\mathrm{Re}^{0.54}\,\mathrm{Pr}^{0.33} + 0.35\,\mathrm{Re}^{0.58}\,\mathrm{Pr}^{0.36} \qquad (7)$$

The speed of the flue gases for determining the Reynolds number was calculated on the basis of process modeling CFX 15 Fluent code (Lic.No**1023420)** and conventionally accepted as constant, w=4.5 m/s, the diameter of the thermocouple bead - $d = 0.005$ m.The values of heat transfer coefficients were calculated for three different temperatures of incoming flow – flue gases core.

The calculations were performed with variations of temperatures of the gas core within the limits T_{fl} = 2200 ... 1600 K and with the temperature of cooled walls variation so that the temperature difference between the wall-flow changed recursively 200 ... 400 ... 600 K, which corresponds to the actual conditions of the experiment. Thermophysical properties of combustion products, optical properties of CO_2 and H_2O, both individually and in mixtures were defined as a result of the process modeling). Convective heat transfer coefficients were calculated for each pair of the assumed combustion gas and walls temperatures, accordingly.

Thus derived transcendental equation of 4th degree with nonlinear coefficients was solved in Mathcad software package as the point of intersection of the two functions (5 and 6). The solution was obtained in graphical and numerical forms.

The results of equations solving for different cases of gas stream and wall temperatures are summarized in Table 1 and shown in the graph (Figure 3).

Table 1.

Summary table of thermocouple readings at different temperatures of the gas core and walls

T_z, K	T_c, K	T_m, K
2200	2000	2077
	1800	1986
	1600	1910
	1400	1854
	1200	1814
2000	1800	1880
	1600	1792
	1400	1724
	1200	1677
1800	1600	1686
	1400	1606
	1200	1548

According to the obtained data, shown in the Figure 1, at the actual 2,200 K temperature of the flow and 2000 K temperature of the wall, thermocouples will show the temperature at 123 K less than the actual gas temperature. At the same gas temperature, the difference between actual temperature and measured thermocouple will increase to 386 K at 1200 K temperature of the wall. At 1800 K of core temperature and 1600 K of wall temperature specified difference will be 114 K that is slightly smaller than the measurement of a core temperature.

3. Results and discussion

Analyzing the obtained data, one can conclude that re-radiation plays a significant role in the measurement of temperature at the considered conditions. The graphical interpretation of MathCad solution of the developed model at a flow temperature of 1400 K and variations of wall temperature is presented in Figure 4.

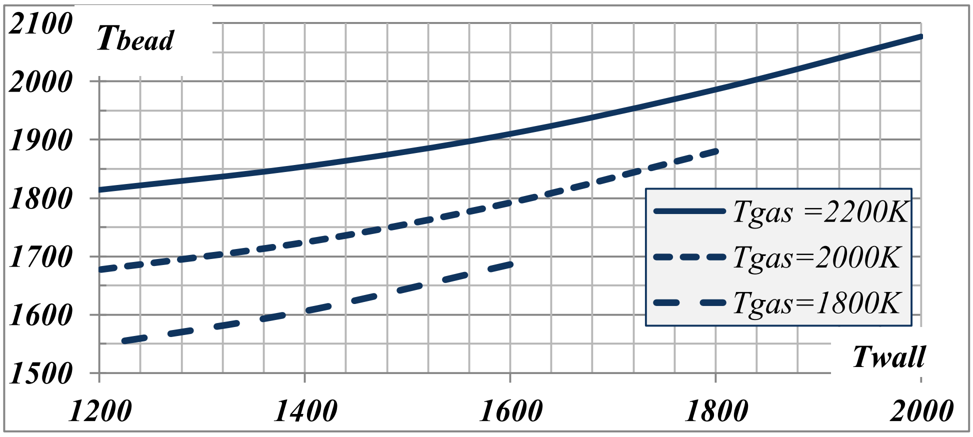


Fig. 3. Calculated readings of a thermocouple installed in the flow of flue gases and emitting radiation on the channel wall (T_{wall}) at different temperatures of a flow

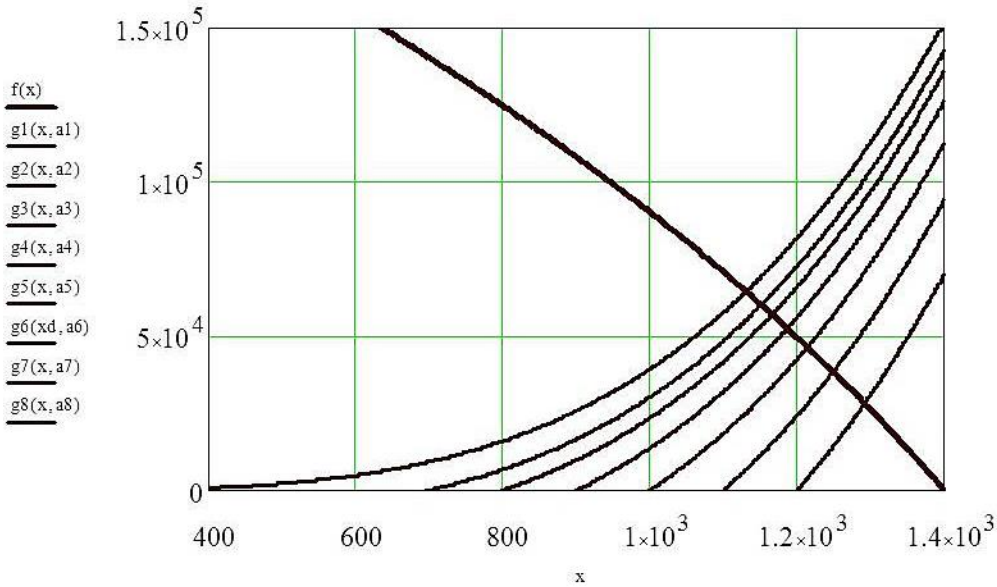


Fig. 4. Calculation by the model for conditions [2, 8]

Each abscissa value of the lines' intersection gives the value of thermocouple bead temperature at the flue gas temperature 1400 K and respective wall temperature. The bigger the wall temperature, the closer to the 1400 K value moves the intersection point, and respectively closer to 1400 K moves the reading of the thermocouple.

To define a degree of reliability of the developed model, the data obtained from the above calculation were displayed in coordinates given in [2, 8] namely, T_{error} - difference between the gas temperature and thermocouple bead temperature as a function of wall temperature T_{wall}. The results are given in of Fig. 5.

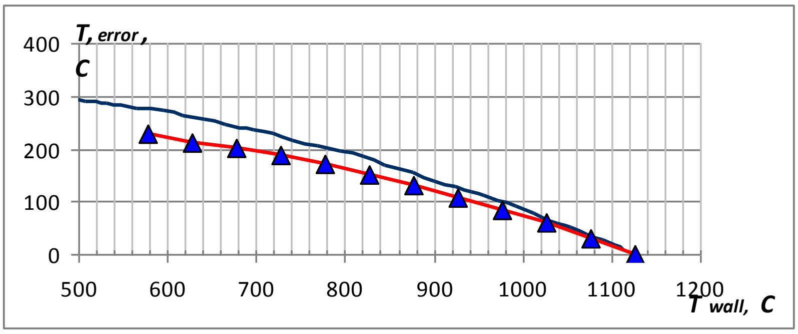


Fig. 5. Comparison of the calculations based upon the developed model and data [2, 8]
The solid line - data [2, 8]. The points – calculation by the model.

Apparently, the data obtained from the proposed model are slightly lower than those given in [2, 8] at wall temperatures below 850^{0}C.
This can be explained by the fact that in our model it is assumed that the bead emits energy by the half of its surface that is directed down towards the ash collector, as the upper part of the bead is directed to head with burners, which emits energy to the bead. In addition, the proposed model takes into account emission and absorption of triatomic gases in the combustion products, whereas the models [2, 8] threat the gas flow as afully transparent medium.
It seems possible to use the obtained data toadjust the results of a direct temperature measurement of the thermocouples located at the middle of each test section and VGP-100D, and to compare them with the calculated data of process modeling by means of FLUENT and CFX packages.

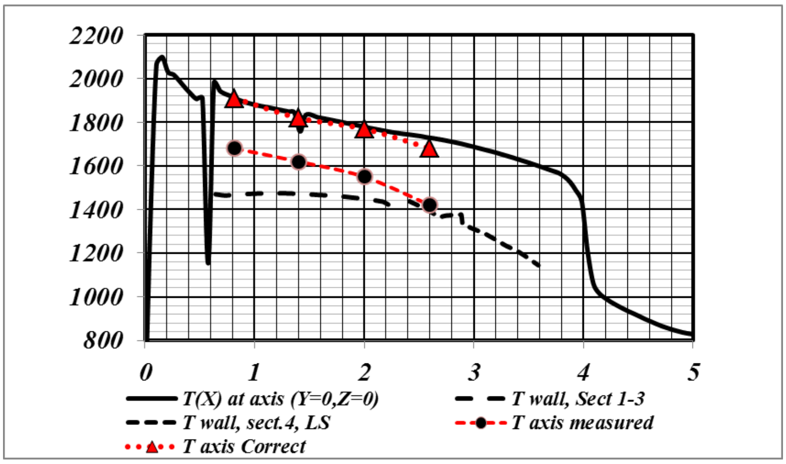


Fig. 6. Comparison of the results of calculation by means of CFX package with the results of measurements with a consistent refinement that based on the model of reradiation

Thus, the calculation of corrective corrections held on stream temperatures according to the model, and the temperature of the wall was taken according to the measurements that were considered reliable because thermocouple of the wall, being embedded in the lining, do not participate in radiation heat transfer. Thus, obtained corrections were added to the thermocouple readings because they reflect the bead temperature and not the temperature of the flow of combustion products that flows around the thermocouple bead. Instead, corrections to the thermocouple readings reflect the temperature of stream that flows around beads, see equation (5, 6).

As it can be seen from Figure 6, based on the readings of thermocouples and proposed model of measuring, the temperature of the flow on VGP channel axis matched with the modeled results close enough (within 5%), which indicates adequacy of the proposed model and accuracy of data obtained by measurements by the thermocouples.
Validation of the developed 3-D model was based also on the comparison of heat losses obtained by the calorimetry of VGP standsections with the respective data calculated within the CFX model. Apparently, there is a close correspondence of the results within 7.5% on sections and 2.2% on stand as a whole.

Table 2.

Comparison of heating losses on the calorimetric VGP stand sections

Part of the experimental set	Heat loss measured on the stand, W	Heat loss of a model, W	Δ, %
Burner	8600	9113	5.9
Flange of a burner	2500	2320	7.2
Diagnostic section	4300	4641	7.3
Total	15400	15738	2.2

4. Conclusion

3-D modeling gives a very powerful tool for the study of combustion processes of different fuels, allowing any variation of operational parameters and flow rates of components of the process. The model simulation allows to study the particulars of harmful substances appearing, and thus to prevend this. A model has been developed which allowed deriving coorection data, which when added to the direct bare thermocouple measurements present data close to those obtained by modeling. The methodology of the calculational mesh development, the set of thermal boundary conditions together with the kinetic sub models may be used for 3-D modeling of gaseous fuels combustion.

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