Simulation gas combustion process in modern heat generators of small and medium power

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Abstract. The paper presents the problems of numerical modelling of burners and fireboxes the heat generators. The designs household generators placed directly on the premises, in the last decades, for the goal of commercial appeal, tend become more and more compact, which leads to a reduction of the firebox to a burn zone's volume ratio. The numerical study of combustion processes using computational fluid dynamics (CFD) was carried out on the Unimat UT-L18 "Bosch" boiler, the gas heating convector "FEG" Beata 2, and the Vitodens 100-W "Viessmann" boiler. Computations were based on a one-stage combustion process of methane, both mixes with air and oxygen. Geometric models of fireboxes were developed by corresponding to their constructive features, the necessary boundary and initial conditions of furnace processes were determined, temperature, aerodynamic and concentration characteristics of gas fuel combustion processes were also presented. The models provided an opportunity for the quantitative analysis of furnace and burner devices of this heat generators degree of perfections. Also, the completeness of the oxidation of combustible components of the fuel-air mixture in fireboxes, differing in the degree close walls to burn zone, was compared. The obtained results allow to perform the improvement of the furnace and burner devices of domestic heat generators for using at design energy-efficient structures of decentralized heat systems, including individual heat supply in the residential and industrial building.

Keywords: computational fluid dynamics, domestic heat generators, energy saving, combustion process natural gas.

1. Introduction
For decentralized (including individuals) heating of buildings and individual premises, modern types of low and medium capacity heat generators of foreign and domestic manufacturers are used widely. In each new series of such devices are introduced constructive innovations, sometimes - outstanding. Manufacturers readily disclose only the parameters that give the commercial attractiveness of products, and the specific features of the innovative components responsible for improving the consumer properties of the product and often protected as intellectual property are not given. For example, the efficiency of the devices of the last decade is always high, for condensing boilers it is
always over 95% (in terms of the highest calorific value). Apparently, according to such information,
it will not be possible to compare objectively the innovations and receive the right directions for the
constructive improvement of the fireboxes and burner devices of modern heat generators of small and
medium power. This problem has become aggravated in the last two decades - during the period of
intensive distribution of condensing-type devices and reducing the size of the boilers in the pursuit of
commercial attractiveness of products at the compactness direction. To dampen the growth of the
constraint by furnace walls of the combustion zone, introduced were different innovations. But the
question of whether innovations have helped to avoid the growth of chemical underburning or not, is
one of the most pressing challenges of our time. It is directly associated with a real reduction in
greenhouse gas emissions due to a decrease in fuel combustion for heating buildings. As is known,
about a third of the global energy generation is spent on heating buildings. Therefore, in the decisions
of the Paris Agreement on climate, the building sector is equated to the main sectors that directly
produce greenhouse gases — production, energy, and transport. Consequently, any innovations that
make even small cuts in fuel costs to the heating of the building sector facilities deserve close
examination.

2. Methods

The boiler designers establish the effectiveness of innovations based on the results of numerical and
experimental studies. Objective test by the consumer of the receive result is really possible only on the
basis of numerical methods. At the same time, numerical simulation of fuel combustion processes,
even in obviously not constrained fireboxes, presents certain difficulties. One of the principal
difficulties is the difficulty of establishing a set of elementary stages of the radical-chain mechanism
of thermal oxidation of combustible gases, which is close to the reactions that take place in real
furnaces of the boilers. In this direction, quite advanced models have recently been implemented, up to
direct modeling with detailed kinetics [1]. However, to perform calculations on a scale larger than the
thickness of the combustion zone, much less scrupulous calculations are used. In [2-4], for example,
discusses the conditions of the numerical simulation of fuel combustion processes, including waste, in
enough large the furnaces and boilers. In our work, we consider methods for constructing numerical
models and their study by computational fluid dynamics (Computational Fluid Dynamics-CFD) of
three heat generators with different burner devices and geometric characteristics of fireboxes: a
Buderus hot water boiler Logano S825L with output 2500 kW, a FEG gas heating Beata 2 with a
hermetic combustion chamber with a heating capacity of 2.2 kW and a wall-mounted condensing
boiler “Viessmann” Vitodens 100-W with a heating capacity of 19 kW. In addition to other
parameters, the presented devices differ in the degree of constraint the flame space by the firebox
walls, and, accordingly, its heat stress \( q_v \), kJ / m³. The studies used Gambit software products with the
Exceed emulation environment (preprocessor), ANSYS Fluent (solver) and Tecplot (post processing).
The fireboxes and burners of each of the devices have a number of their design features, punctual
copying of the geometry of which is possible in the preprocessor, but often not justified, since it does
not always have a positive effect on accuracy. Therefore, furnace and burner devices were modeled
with certain simplifications, which are discussed further.

2.1. Simulation of geometry and combustion processes in the furnace of the boiler Buderus

The furnace volume of the Buderus boiler has a low heat stress \( q_v \), as well as a minimal flame
constraint, which was done in order to reduce the formation of NO\(_x\) and CO during the combustion of
the gas-air mixture. The movement of combustion products is three-pass. The first pass is a
combustion chamber in the form of a horizontal flame tube with a length of 3149 mm and a diameter
of 776 mm, and part of the turn chamber to the second pass. The second and third passages are
composed of three rows of horizontal fire-tube with a diameter of about 40 mm, penetrating the water
volume of the boiler. A two-dimensional model of the first pass and the turn chamber into the second
pass was created. The fluxes in the second and third passages were not modeled, since their effect on
the completeness of fuel combustion is substantially less than in the firebox [5, 6]. The coordinates of
the nodes (vertex) are constructed in accordance with the technical characteristics of the Unimat UT-L hot water boiler. (URL: [https://www.bosch-climate.ru/bosch-products/promyslennye-kotly/utl.html](https://www.bosch-climate.ru/bosch-products/promyslennye-kotly/utl.html)). The model exported to the solver is adapted to eliminate the grid dependence. At the processor, the type of gas-air mixture “Material Type” (air + methane) is set, the initial values and boundary conditions are established. The initial air velocity is \( \nu = 2.18 \text{ m/s} \), the flow rate is \( G = 0.7 \text{ m}^3/\text{s} \), the temperature of the mixture leaving the gas ramp is 292 K. The ratio of the methane and air flows velocities is taken at the rate of 1:10 by volume (air excess factor \( \alpha \) about 1.05). This corresponds to a mass ratio of gas and air of 1:18, and an initial mass concentration of methane in a mixture of 5.25%. The boundary conditions for the fluxes are established in accordance with [7]. Flow in the furnace is turbulent, adopted model of turbulence k-epsilon. The energy equation and equation radiation of Rosseland are added to calculate the radiative-convective heat transfer in addition to the differential equations of motion and continuity. In the beginning of the first pass on outlet the gas-air mixture from the ramp, the condition of constant gauge pressure \( P = 102034 \text{ Pa} \) was accepted since furnace operating in real conditions under a small supercharging. The boundary conditions at the exit of the turn chamber into the second pass are taken as “Outflow” - the outflow of flue gases without specifying the parameters, since the movement of the streams on the following passes was not considered. The combustion process was modeled as a component transfer (Species Transport) with a single-stage reaction of methane oxidation with air to final products without predicting the formation of NOx:

\[
\text{CH}_4 + 2 \text{O}_2 + 7.52 \text{N}_2 = \text{CO}_2 + 2 \text{H}_2\text{O} + 7.52 \text{N}_2
\]  

(1)

For calculations of combustion at processor solver, the model of the eddy-dissipation was adopted.

2.2. Simulation of geometry and combustion processes in the furnace of the gas-fired FEG Beata unit.

The convector FEG Beata is installed directly in a heated room. It is designed with a fence for burning outdoor air and has a compact combustion chamber with a flame more constrained by its walls than the previous device. According to technical data (FEG Konvektor Rt Öcsa, Kiss János [https://docplayer.com/49705331-Feg-konvektor-rt-ocsza-kiss-janos-u-centralnyy-telefon-36-29-faks-36-29.html](https://docplayer.com/49705331-Feg-konvektor-rt-ocsza-kiss-janos-u-centralnyy-telefon-36-29-faks-36-29.html)), with a growth of power on the line of devices FEG BEATA, the efficiency drops from 92% to 86%, which may be due to the cooling effect of the walls of the heat exchanger due to its proximity to the combustion zone. The latter may affect the radical-chain mechanism for the development of oxidation reactions in the flame zone [8-10].

In the preprocessor, a 3D model of the furnace of the FEG Beata 2 was created. The furnace is vertical, of a simplified form, the output of the gas-air mixture is simulated by holes in the hearthstone. The computational grid is tetrahedral-hybrid, with a linear size of the elements of about 0.005 m. The initial number of grid cells is about 50,000. After exporting to the solver, the model is adapted “by region” to practically eliminate the grid dependence. The final number of cells is 400000. Initial characteristics: air-fuel mixture - methane and air; gas flow consumption \( G_g = 0.25 \text{ m}^3/\text{s} (0.178 \text{ kg/s}) \); the initial velocity \( V_g = 5 \text{ m/s} \), the temperature of the mixture at the inlet is 292 K. The volume ratio of gas-air is 1:10, the mass ratio is 1:18. Air consumption \( G_{air} = 2.5 \text{ m}^3/\text{s} (3.219 \text{ kg/s}) \), its velocity at the outlet from the bottom holes \( V_{air} = 1 \text{ m/s} \). For gas, air, and combustion products, the same boundary conditions are set as in the previous case, and the radiant heat transfer was calculated using the discrete ordinate (DO) model.

2.3. Simulation of geometry and combustion processes in the furnace of the boiler Vitodens 100-W

In the Vitodens 100-W series of boilers, a rather original design solution of the burner is provided, excluding the direct contact of the furnace walls with a flame. The gas-air mixture is released through a cylinder from net of heat-resistant steel, and the combustion front is divided into a large number of small flames up to 10 mm high. Therefore, the burner was modeled as a porous body (internal cylinders 2 in Figure 1).
About two dozen coils of the spiral slot for the passage of flue gases with a width of about 1 mm pass through the screen surface of the boiler, which is why the firebox was also modeled as a cylindrical porous zone (external cylinders 1 in Figure 1). The grid of the tetrahedral-hybrid type with a linear size of elements of 0.008 m was generated in the volumes the firebox and burner at the preprocessor. The initial number of cells was 63758.

Figure 1. Calculated grid of the 3d model of the firebox (1) and the burner device (2) with ignition electrodes (3) in the Vitodens 100-W boiler.

Unlike previous models, methane and oxygen were taken as components of a combustible mixture. In recent years, such studies have noticeably intensified around the world due to the possibility of intensification of heat exchange and combustion kinetics, while simultaneously achieving a number of environmental benefits, up to a decrease in the yield of greenhouse gases [11–17]. Gas consumption $G_g = 2 \text{ m}^3/\text{s}$ (1,434 kg/s), initial velocity $V_g = 12 \text{ m/s}$. The temperature of gas and oxygen at the entrance to the inner space of the burner is 452 K. The initial mass concentration of methane is 20.0%, oxygen is 80.0%, and their mass ratio is 1:4. Another difference is the introduction of initial values of viscous and inertial resistance in porous zones. Combustion process was simulated as Species Transport with a single-step reaction of methane oxidation in oxygen:

$$\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O}$$

Unlike the previous ones, a combined Eddy-dissipation / Finite Rate model was adopted for the calculations of combustion. This is necessary for the formation the ignite of the fuel-oxygen mixture at the outlet of the burner. In the geometric model, electrodes were installed above and below the burner to ignite the outgoing mixture (position 3, figure 1). The electrode surface temperature of 3000 K was set in a solver.

3. Results and Discussion

3.1. Discussion of the results of numerical studies of furnace process in the boiler Buderus.

Numerical calculations of the 2D model of the Unimat UT-L18 boiler firebox made it possible to work out options for preparing a geometric model in a solver with setting boundary conditions, turbulence and combustion models to ensure physically correct results with minimal computational resources. Distributions of streamlines, temperature, CH$_4$, O$_2$, CO$_2$, H$_2$O concentrations, pressures and velocities in the firebox and the turning chamber were obtained. The physical adequacy of the streamlines of the combustion products confirmed the correctness of the adopted model and the boundary conditions for hydraulic characteristics. From the velocity field in Figure 2b one can see that the velocity of the combustion products in the radial direction of the furnace falls from the center to the periphery with a velocity gradient of $\nabla v_R = 20 \text{ s}^{-1}$. It can be also seen that the transition from the firebox to the turn chamber has the form of local resistance of the “sudden expansion” type. But the formation of vortex zones in the corners [18], which are common for channels of such a pattern, is not observed here, which can be explained as follows. With the “Outflow” given condition of leaving the combustion products to the left through the upper and lower exits from the chamber, the flow perceives the
obstructive effect of the chamber end face, and the configuration of local resistance changes to “180° turn”. Therefore, the vortex formation passes to the center of the chamber, where the pressure increases, and to the corners adjacent to its end face, where the pressure drops.

Figure 2 a - velocity field, m / s; b - distribution of methane concentrations, % wt.; dimensions of the firebox on coordinate axes are in mm.

Figure 2b shows the distribution of methane concentration in the combustion space. In the cross section, there is an intensive drop in the concentration of methane from the initial value inlet to trace amounts near the walls (2.3 \cdot 10^{-10} \% wt.). A less intense CH4 conversion observed along the flame axis. However, this is can be due to the fact that was simulated separate supply of gas and air. In a real boiler Unimat UT-L18, ensuring complete combustion of methane in the longitudinal direction is not difficult, since gas and air are intensively mixed in the furnace initial part.

3.2. Discussion of the results of numerical studies of furnace process in the FEG Beata heating device

Figure 3 shows the results of calculations performed on the 3D model of the FEG Beata 2 firebox with calculated grid adapted and tested for physical adequacy. Figure 3a shows the temperature distribution in the vertical median plane of the combustion zone. The maximum temperature of 2100 K is reached in the flame core, which is physically correct: the combustion temperature of the methane-air mixture under adiabatic conditions is, as is known, 2200 K. The temperature monotonically decreases from the center to the periphery in all directions of the flame volume, which is also physically correct.

Figure 3b shows the velocity distribution in the same section. The gradient of the speed decrease in the firebox is \( \nabla v_R = 60 \text{ s}^{-1} \), which is 3 times higher than the previous case. Despite the smaller than in the previous case, the velocity of the products of combustion in the flame, the value of the gradient increases. This is due to the approach of the walls of the furnace to the combustion zone. Consequently, the calculated value of \( \nabla v_R \) correlates with the flame zone constraint in in hollow fireboxes and, along with the thermal stress, can be used for a comparative assessment of the perfection their designs according to this factor.

Figure 4 shows the distribution of CH4 concentration in the vertical median section, as well as in the horizontal section at the outlet of the calculated zone. At the periphery of the exit section, the CH4 concentration is mainly 0.4% of the initial amount. Thus, the conversion of methane, after passing through the calculated zone is within 97.9% - 99.6%. Although the percentage of CH4 conversion seems high, the quality side of the process cannot be overlooked. This is especially important when using the single-stage model of thermal oxidation according to the scheme (1). Of the final products, it shows only the products of complete combustion of CO2 and H2O. The presence of methane source reagent in them serves as an indicator of the breakage of radical-chain reactions leading to its complete
oxidation, already at the initial stages. Therefore, chemical underburning will be higher, and it is advisable to make improvements in the organization of the combustion process.

![Image](image.png)

**Figure 3.** Temperature field (a) and distribution of the flow rate of combustion products (b) in the furnace space of the convector Feg Beata 2.

3.3. *Discussion of the results of numerical studies of furnace process in the Vitodens 100-W boiler*

The 3D model of the Vitodens 100-W boiler was tested for physical adequacy and adapted “by region” for the achievement of mesh independence of up to 235,000 cells. The results regarding the methane combustion model in oxygen were validated according to well-known empirical data: the maximum temperature of the combustion zone 3370 K obtained in the work exceeds the temperature of the conical combustion front determined by reversing sodium lines [19] by 11%. Therefore, the validation result is satisfactory.

![Image](image.png)

**Figure 4.** Distribution of methane concentration in the furnace space of the FEG Beata 2.
Figure 5a shows the temperature distribution in a longitudinal vertical section along the axis of the firebox. At the beginning of the furnace, the temperature of the mixed methane and oxygen flows is assumed to be 400 K. The mixture of oxygen and methane is ignited by electrodes with a temperature of 3000 K, after which the temperature of the homogeneous phase reaches a maximum of about 3370 K in the flame zone above the burner surface. In the transverse direction, the temperature slowly decreases and at the screen surfaces remains still quite high - almost 2800 K. In the longitudinal direction along the axis in the space behind the burner, the temperature is in the range of 2800-3000 K, and then decreases to the end of the firebox to 1600 K. Thus, manifestations of physical incorrectness of the results of thermal calculations as a whole in the pattern of the temperature distribution in the furnace are not observed.

Figure 5b shows the velocity distribution in the longitudinal section of the furnace. The velocity gradient $\nabla v_R$ in the transverse direction of the high-temperature zone between the burner and wall the furnace has an order of 12 s$^{-1}$. We note in this case an additional influence on the velocity of the porous zone, the passage of which the flux spends a significant part of the kinetic energy. As the calculations show (Figure 5b), due to the presence of a porous zone, the flow dramatically slows down and reduces speed by 47.5 times at a distance of 0.005 m. At these space, the gradient $\nabla v_R$ is close to 200. You can make an estimate of the upper limit $\nabla v_R$ in the annular space between the burner and the wall of the firebox net the influence of the porous zone. Let us assume that the maximum possible velocity the flux at the surface of the burner does not exceed the initial average flow rate (by mass) of the mixture $v_m = 2.64$ m/s. Then $\nabla v_R$ of expanding combustion products in the annular space will be no higher than 80 s$^{-1}$. Therefore, it can be estimated that the development conditions for the flame in the Vitodens 100-W firebox are similar to that of the Feg Beata 2 convector.

Figure 5c shows the distribution of CH$_4$ concentration in the longitudinal section of the firebox. It can be seen that after ignition of the gas-oxygen mixture, the CH$_4$ concentration in the annular space between the burner and the firebox surface decreases to 0.2%, and with such a concentration goes into the convective part of the boiler, where burnout will stop. Not converted methane in the same quantity will be removed with the flue gases. Consequently, the methane conversion in the boiler will be 99.8%, which is close to the results for the FEG Beata 2 convector. The latter was expected as the velocity gradient values are close, which confirms the validity of the $v_R$ indicator. The presence of unconverted methane in the flue gases also serves as an indication of the breakage of the radical-chain
reactions of methane oxidation in the flame already at the initial stage. Therefore, furnace process is also advisable to improve in order to reduce the proportion of unconverted methane to negligible values.

4. Conclusions

Thus, the methods of modeling the design features of the furnace and burner devices of modern household heat generators used in the work give the correct numerical values of the hydrodynamic, thermal, and concentration parameters of the species. The possibility of using a fairly simple and at the same time fundamental parameter of furnace processes - the radial gradient of the flow velocity in the flame zone $\nabla v_R$, for the estimated of the furnace process perfection is illustrated. It is shown that the value of $\nabla v_R$ correlates with the degree of flame constraint with the firebox walls, which directly affects the completeness of fuel combustion. In the further development of the presented method of modeling through the porous structures the structural features of furnaces and burners with numerous holes and slit, it is necessary to further clarify the values of viscosity and inertial coefficients of hydraulic resistance of specific designs the furnaces and the burners.

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