Numerical modeling of combustion of gaseous and solid fuels in the furnaces of small and large boilers to reduce harmful emissions

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Abstract. The issues of the formation of toxic compounds that enter the air of the residential area during the circulation of household waste and the provision of energy supply services, in particular, during the decentralization of heat supply to residential buildings, are considered. The problems of finding the optimal ways to reduce toxic emissions are solved using a numerical experiment based on computational fluid dynamics. The results of numerical modeling of the corresponding combustion device are compared with the geometry created using the Gambit software and in the Solid Edge 3D design environment. The influence of the pressure in the furnace on the characteristics of fuel combustion during operation in the pressurization mode of the recently widespread condensing boilers is given. Acceptable simplifications for the application of the normative method in the calculations of modern combustion devices with a specific geometry are proposed.

1 Introduction

The multifaceted activity of mankind and its increasing interaction with the environment leads to the pollution of the atmospheric air of the urban area. Of the pollutants, sulfurous anhydride SO_2, nitrogen oxides NO_x and carbon monoxide CO account for up to 80%, and the main sources of their emission are considered to be transport, large energy, industry and housing and communal services with their own infrastructure, including treatment facilities and solid waste landfills. However, in matters of the influence of air purity on the state of national health, the most important factors are not only the mass fraction of atmospheric emissions, but also their toxicity. Taking into account the numerical ratings of the influence of various sources, for example, according to the method [1], shows that the share of the impact of Thermal Power Plants (TPP) and district Boiler Houses (BH) on urban air is currently not so high.

Approaching the problem and making assessments taking into account the toxic effect of pollutants, it can be found that the continuous replacement of large emission sources with a multitude of small dispersed ones, from mini-CHP and block boiler houses to individual heat generators in individual apartments of multi-apartment buildings has led to a decrease in the dominant role of centralized generation in pollution air environment. At the same time, NO_x and CO are moderately hazardous substances in terms of toxicity, which also leads to the equalization of the influence of the centralized and decentralized energy sectors on the formation of urban air pollution. Also, the issues of reducing the emission of nitrogen oxides in large-scale power engineering have been considered for more than half a century, and at present the main methods are quite deeply developed and widely used. The development of individual heat generators, especially the widespread domestic condensing boilers, has recently been proceeding mainly along the line of increasing the fuel utilization factor, which, as is known, is achieved by methods directly opposite to the methods of reducing the formation of nitrogen oxides in the process of gas combustion. In addition, emissions from small boiler houses and individual boilers fall directly into the air of a residential area, and pipes of TPPs and BHs are installed taking into account the wind rose of a given area.

A numerical assessment of the toxicity of emission sources according to the methodology [1] also shows that in terms of air pollution in cities, large and small generating devices do not even collectively outperform housing and communal services enterprises dealing with the circulation of solid and liquid household wastes. The so-called "landfill" gas - a product of decomposition of household waste without oxygen, emitted at solid waste landfills, without taking into account the toxicity of all its components, is considered mainly as an insignificant source of atmospheric emissions. As a rule, only approximate information is available about its quantity and composition. The output of "landfill" gas at large landfills does not exceed 5 thousand m^3/h, which is incomparably less than emissions from thermal power plants. Moreover, it consists of 90% or more of carbon dioxide, ammonia and methane. These are non-toxic and slightly toxic compounds, and the concentration of the

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latter, depending on the stage of decomposition, can exceed 5%, which in the USA and the EU has led to its use for energy generation. However, as individual studies show [2], the rest of its pollutants are represented by a variety of classes of chemical compounds with hundreds of names of substances, including furans and dioxins. Among them there are saturated hydrocarbons, unsaturated, cyclic non-aromatic, aromatic, polycyclic, oxygen-, nitrogen- sulfur- and chlorine-containing, as well as furans and pyrans. The total concentration of the latters reaches 1.2 mg/m^3. This level of concentration of weakly toxic compounds in emissions is insignificant, but furans and pyrans are themselves highly toxic and, in addition, serve as indicators of the presence of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD / F) - chemically persistent highly toxic pollutants that can accumulate in the tissues of organisms [3, 4]. Some of them (for example, 2,3,7,8-tetrachloro-p-dibenzodioxin) are extremely toxic and can cause carcinogenic diseases, hormonal disorders, and defeat to the immune system. Therefore, the maximum permissible concentrations of PCDD / Fs are 7-8 orders of magnitude lower than those of moderately hazardous substances. Consequently, the emission of 10 m^3/h of "landfill" gas with a dioxin concentration of 1.2 mg/m^3 is equivalent in toxicity to the emission of 400 thousand m^3/h of flue gases with a concentration of 300 mg/m^3 NOx, which corresponds to the operating parameters of one TPP boiler.

The transformation of waste in the furnaces of steam generators of "municipal" TPPs (MWIP) takes a place in an oxidizing mode. In this case, sulfur, nitrogen and phosphorus-containing chemical compounds of various toxicity are formed, up to chemical warfare agents and the furans and dioxins, superior their in. Waste incinerators, including the most dangerous of them - medical waste incinerators [5], are the main sources of supply of polychlorinated dibenzo-p-dioxins and dibenzofurans [6] to the atmosphere. In such conditions, in order to reduce damage, it is possible to organize pre-treatment of waste before a high-temperature zone with the removal of chlorine compounds [7]. In order to be principial able to regulate the release of toxic compounds when burning conventional gaseous fuel or garbage, it is necessary to know the sequence of reactions taking place in the thermo-oxidizing zone. Since during waste incineration the specific initial composition of the fuel is unknown, and when using household waste it is unstable, it is possible to establish a set of elementary stages of the radical chain mechanism of thermal oxidation only empirically. The data available in the literature on the kinetics of reactions during waste combustion are insufficiently complete and sometimes contradictory.

At temperatures above 1200-1300 °C, thermal oxidation of organic and organochlorine components of MSW in the presence of metals can occur in conjunction with the reduction of their oxides. In some cases, this can be used for the thermal treatment of toxic compounds, for example, to reduce hexavalent chromium compounds to trivalent [8]. The intermediate products formed in the high-temperature zone react with each other to the final products upon cooling, and PCDD / F are formed in the range from 650 to 250 °C [9]. It is believed that their main part is condensed on ash suspended in combustion products, in connection with which it becomes especially important to use technologies with a high degree of purification of flue gases from suspensions [10]. A number of studies have shown an increase in the yield of PCDD / F in the presence of aromatic hydrocarbons and some metals [11, 12, 13] and a decrease in the yield in the presence of sulfur dioxide SO_2 [14, 15]. A sharp cooling ("quenching") of combustion products from 1300 to 200 °C is proposed [16]. In general, the scheme for the formation of PCDD / Fs is not fully understood [17]. Experimental and numerical studies on the kinetics only of a limited number of initial components [18, 19, 20, 21] carried out.

2 Methods

Numerical modeling of furnaces of a steam boiler E-220/100 (TP-14A, manufactured by JSC TKZ "Krasny Kotelshchik") with a steam capacity of 220 t/h and a gas floor condensing boiler Vitocrossal 200 (manufactured by VIESSMANN Group) with a thermal power/ capacity of 400 kW. Geometric modeling of the TP-14A furnace for studying the combustion of low-grade fuel and waste was carried out using the Gambit software product with the Exceed emulation environment. Firstly, a geometrically accurate 3D model of the furnace with a cold funnel and all burners was performed (Fig.1), but due to difficulties in generating the grid using Gambit software, a simplified model of the combustion chamber was built, in which an unstructured hexahedral grid was generated (Fig.2).

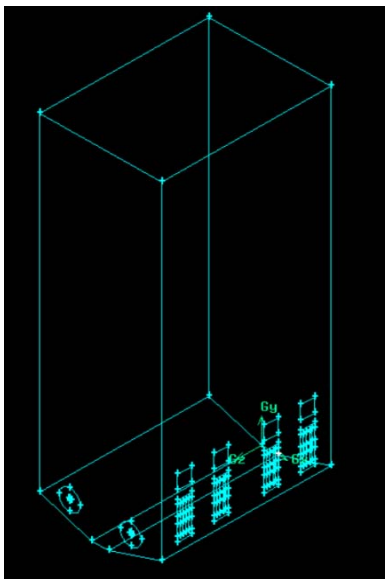

Fig. 1. Construction of a 3D model of the TP-14A boiler combustion chamber in the Gambit program geometrically accurate model of the TP-14A boiler combustion chamber.

The burner device of the Vitocrossal 200 domestic boiler is a perforated cylinder located axially in a water-cooled stainless steel cylindrical firebox. Flue gases leave the furnace through 18 vertical slotted passages at

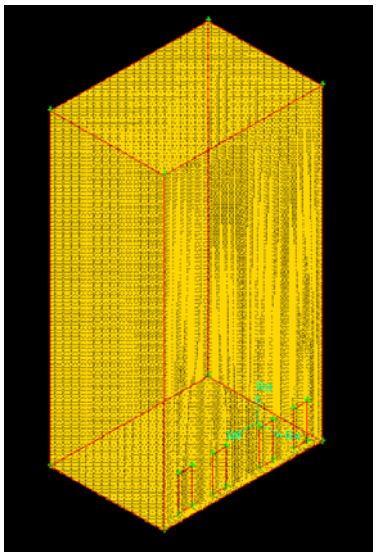

Fig. 2. Construction of a 3D model of the TP-14A boiler combustion chamber in the Gambit program a simplified model with a generated computational grid.

chamber with heat exchange surfaces, after which they are sent to the chimney. The firebox geometry was created in refined and simplified versions using Solid Edge software. Due to the difficulties with mesh generation in the model created in Solid Edge software, a model with simplified geometry has used (Fig. 3), for which it was possible to generate a mesh after transferring it to Gambit program (Fig. 4).

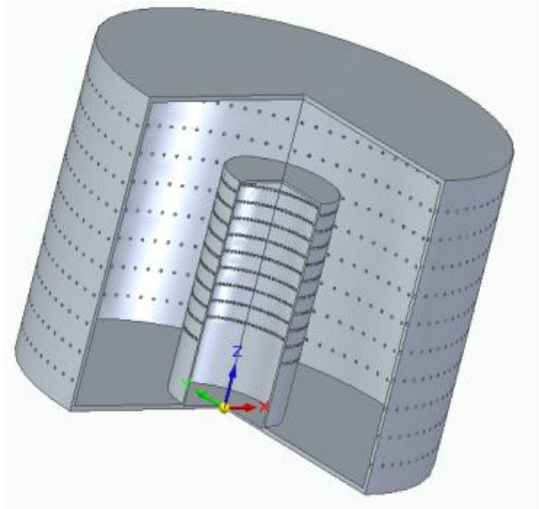

Fig. 3. Construction of a 3D model of the combustion chamber of the Vitocrossal 200 boiler the geometric model of the furnace, built in the Solid Edge system.

The resulting models were transferred to the Ansys Fluent processor. The movement of flows in the furnaces was calculated on the basis of the Navier-Stokes equations (RANS) with closing of their according to the two-parameter k-ε model. Both tasks are non-isothermal, using the energy equation ("EnergyEquation") and the P1 radiation model.

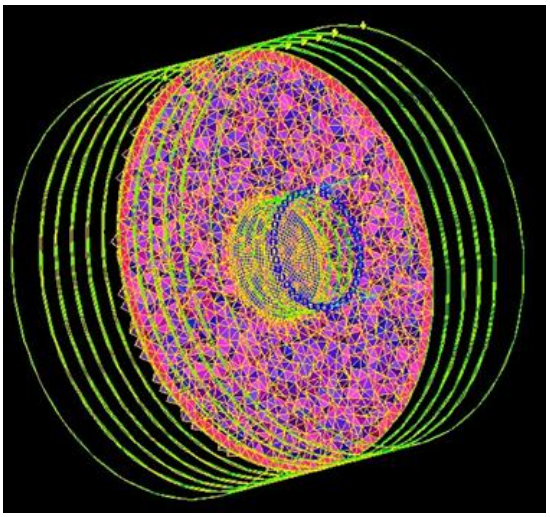

Fig. 4. Construction of a 3D model of the combustion chamber of the Vitocrossal 200 boiler the computational grid on the surface and in the volume of the geometric model of the boiler furnace is generated by the Gambit program.

For combustion of coal dust and garbage particles in the TP 14A furnace, used a compositional transport model based on the probability density function (PDF) - Composition PDF Transport. The average reaction rate is modeled using the Eddy-Dissipation model. The task is loaded with the reaction material - "coal-volatiles-air" (coal-mv-volatiles-air). When specifying the initial and boundary conditions for calculating the combustion process in the furnace of a domestic boiler, a methane-air mixture was adopted (material type "MaterialType" - air + methane). The combustion model is adopted as the transfer of combustible reagents "Species Transport", the model of mixing the reaction components, as for the TP 14A furnace - "Eddy-Dissipation".

3 Results

Numerical modeling, despite its obvious advantages, is based on a significant number of assumptions and empirical constants obtained for specific conditions, and requires comparison with experimental data [22].

The choice of the type of steam generator was dictated by the possibility of verifying the simulation results according to the test data for a similar steam generator at the Kumertau CHP Plant [23]. Verification and validation of the data obtained showed the physical adequacy of the created model. The data of the static pressure in the TP 14A furnace (Fig. 5 a) show that they are close to the atmospheric pressure, set as the initial parameter with the condition that there is no excess pressure at the outlet of the furnace (Gauge Pressure = 0 Pa). Furthermore there are no backflow at the outlet of the furnace. The results of numerical calculations for volatile fuels (Fig. 5 b) and CO_2 (Fig. 5 c) showed that their highs are located above the burners, which can also be considered physically adequate.

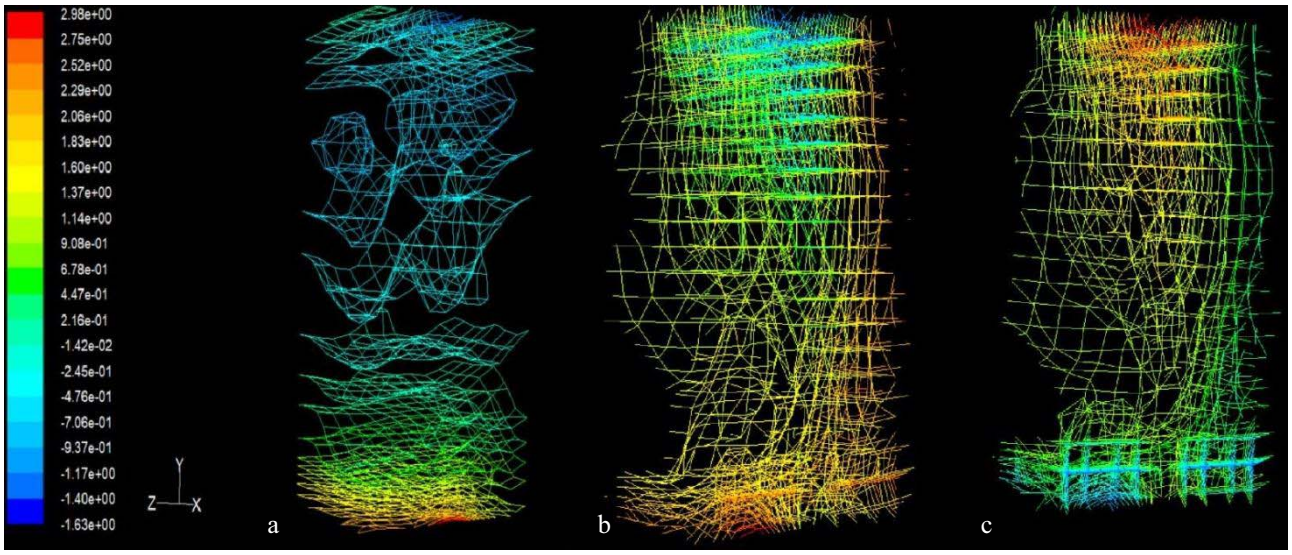

Fig. 5. Distribution of static pressure and content of volatile fuels and CO_2 in the TP-14A furnace: a - calculated data on the distribution of static pressure in the boiler furnace, b - results of calculations on the release of volatile fuels, c - results of calculations on the afterburning of volatile fuels to CO_2.

The sequences of the elementary stages of chemical reactions in the modeling of the processing of unconventional fuels, including garbage, have been recently investigated using the ANSYS Chemkin-Pro software package, which contains a set of kinetic models of pollutant emissions with detailed and exact fuel model. Separate studies using Chemkin-Pro have been performed in the field of dioxin formation during combustion of halogen-containing compounds [24, 25]. They used a 45- and 71-stage model of the formation of 1,3,6,8- and 1,3,7,9-TCDD (tetrachlorodibenzo-p-dioxins) from one initial compound 2,4,6-trichlorophenol.

The primary problem in the study of the calculated model of the Vitocrossal 200 domestic boiler was the ensuring physically adequate characteristics of combustion processes. Figure 6 a, b presents the calculated data on the temperature in the furnace of the Vitocrossal 200 boiler, showing an adequate temperature distribution, both in the volume and in the cross section of the furnace. The distribution of CO_2 concentrations is also adequate to the temperature distribution: the maximum temperature in the center of the furnace section (Fig. 6 b) corresponds to the most intense reaction zone (Fig. 6 c) with a minimum of CO_2 content as the final reaction product.

In recent decades, to study models of the combustion process of domestic boilers working on gas fuel, an algorithm for adaptive tabulation of reactions "in situ" (in the sense of "by moment of their appearance and location in the flame zone") ISAT (in situ Adaptive Tabulation) has been practiced, in which now have been made a number of improvements to increase its stability and speed without reducing the level of accuracy [26, 27, 28]. However, they are adapted to combustion engines and need to be validated in the transition to boilers.

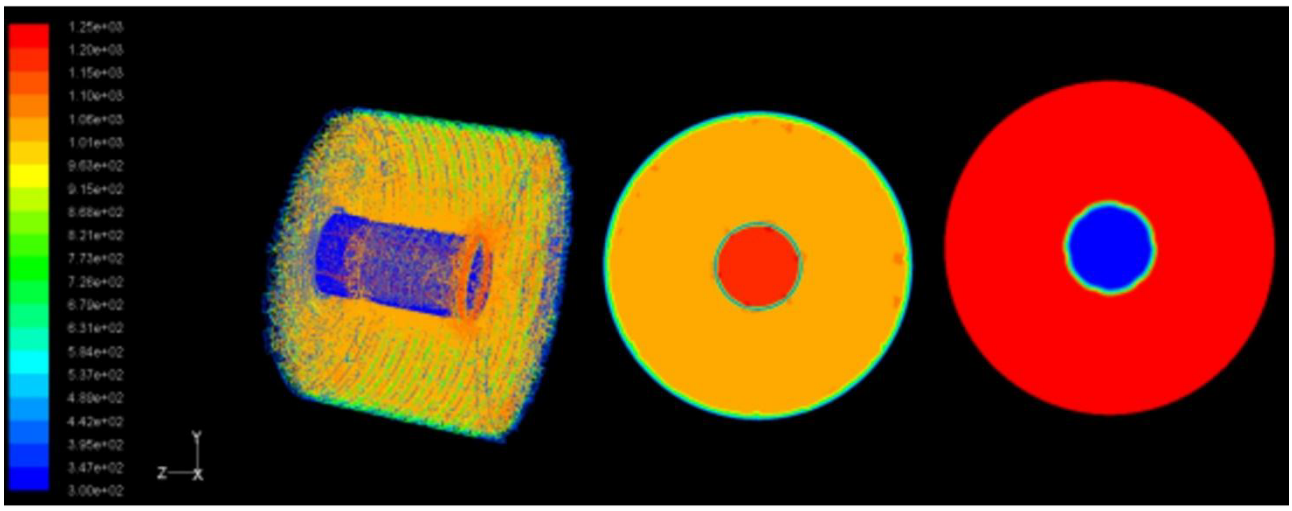

Fig. 6. Distribution of temperature and CO_2 content in the furnace of the Vitocrossal 200 boiler: a, b - temperature distribution in the volume and cross section, c - distribution of CO_2 concentration in the cross section

4 Conclusion

Thus, the results of the study allow us to assert that large energy facilities are not the dominant sources of air pollution even in large cities. Their contribution to the deterioration of the atmosphere in cities is approaching emissions from decentralized energy sources, and their joint contribution with the latter to urban air, taking into account the toxicity of pollutants, is lower than the impact of emissions from household waste. The methods of numerical simulation of fireboxes of energy sources used in centralized and decentralized power supply, considered in the article, provide the physical adequacy of the models. Therefore, they can be used for numerical studies of the furnaces of modern household boilers in order to increase the efficiency of fuel use and reduce the harmful components of fuel combustion products. The presented method for simulating a furnace for heat treatment of non-standard fuels and household waste also allows obtaining physically adequate results on standard fuel. However, today there are no methods that provide the adequacy of the results for the case of heat treatment of waste with any large complete set of reactions in the flame zone. Therefore, at present, adequate solutions can be obtained only for a limited number of initial and final products. The results obtained in this case are not very suitable for practical use, but they should be used to find the most general regularities in the transformation of initial substances and conditions that provide a reduced formation of highly toxic final products.

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