Rocznik Ochrona Środowiska

Volume 23 Year 2021 ISSN 1506-218X pp. 503-512

https://doi.org/10.54740/ros.2021.035 open access

Received: 14 June 2021 Accepted: 30 July 2021 Published: 06 December 2021

Numerical Modeling of Solid and Gaseous Fuel Combustion in the TP-14A Boiler Furnace to Reduce PCDD/F and Greenhouse Gas Emissions

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Abstract: The issues related to the emission of atmospheric pollutants during the provision of energy supply services and the circulation of household waste in settlements are considered. The ways of air pollution by toxic compounds and the formation of greenhouse gases with existing methods of waste heat treatment are analyzed. The issues of reducing the content of toxic emissions in combustion products are studied on the basis of a numerical experiment by means of computational fluid dynamics (CFD). The combustion processes in the power boiler TP-14A (E 220/100) are considered and adequate boundary conditions for the processes of aerodynamics, heat transfer and combustion of gas fuel are determined. The temperature, velocity and concentration fields in the furnace of the investigated boiler have been determined. According to the results of the calculations performed, the formation of chemical underburning and nitrogen oxides is predicted.

Keywords: atmospheric pollution, combustion, nitrogen oxides, dioxins and furans, numerical modeling, computational fluid dynamics, pressurization mode, normative method

1. Introduction

Urban air pollution is a major risk factor for public health. The negative impact on the state of atmospheric air is the result of the constant interaction of people with the environment. A wide variety of sources contributes to the loss of air quality. These are transport, energy, industry and the entire complex of housing and communal services – residential complexes and consumer services for the population, down to the smallest. It is believed that from stationary sources

objects of large energy and municipal infrastructure (sewage treatment plants and MSW landfills) of the given settlement make the largest contribution to urban air pollution. The main pollutants in terms of mass emission (excluding greenhouse gases) are sulfur dioxide SO_2, nitrogen oxides NO_x and carbon monoxide CO. They account for up to 80%, the share of other homogeneous pollutants is less than 10%, the rest is solid suspended particles.

With this traditional approach to considering the problem of cleanliness of the urban air environment, which is most important for the state of national health, the aspect of the toxicity of the pollutants emitted does not fall into the field of vision. Approaching the problem from this position, one can find the exaggeration of the influence of large energy facilities on the city air. The constant replacement of large emission sources with many small-dispersed ones – from mini-CHPs and block boiler houses to individual heat generators in apartment buildings, has led to a decrease in the dominant role of centralized generation in air pollution. Now in Russia, the ratio of centralized and decentralized heat supply can be estimated as 2: 1, and in terms of heat supply to the population, it is approaching parity. Note that NO_x and CO represents toxic compounds of emissions from gas power generation, which belong to the class of moderately hazardous substances. This also leads to the equalization of the influence of the centralized and decentralized energy sectors on the formation of urban air pollution. At the same time, 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 worked out and are widely used. The progress of individual heat generators, especially the widely used condensing household boilers, has recently proceeded 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 generation of nitrogen oxides during gas combustion. In addition, large energy facilities have high-rise pipes designed to dilute pollutants and remove them from the settlement, while emissions from small boiler houses and individual boilers remain in the immediate vicinity of their generating device.

Calculations of the numerical ratings of emission sources, taking into account the toxicity of pollutants (Ziganshin 2019), also allow us to find that in terms of air pollution in cities, centralized and decentralized generating facilities and devices, taken together, are not ahead of housing and communal services enterprises dealing with the circulation of solid and liquid household waste. For example, at landfills of solid waste, the so-called «landfill» gas is formed anaerobically, the composition of which is only very rough information. At a large landfill, its output can be in the range of 2-5 thousand m^3/h, which is 3 orders of magnitude lower than the emission of flue gases from a thermal power plant. The main components (90% and more) of «landfill» gas can be, depending on the storage period of solid waste, carbon dioxide, ammonia, methane. At the

same time, the concentration of the latter can at times exceed the lower flammable limit, which in the USA and the EU has led to its use for power generation. However, the rest of its pollutants are represented by a variety of classes of chemical compounds, including furans and dioxins. For example, the analysis of landfill gas at the Kuchino landfill (Moscow region) made it possible to identify 157 names of substances. Among them there are the following classes of chemical compounds: hydrocarbons (saturated, unsaturated, cyclic non-aromatic, terpene, aromatic, polycyclic aromatic) – 74 names, total concentration from 61 to 80 mg/m^3; oxygen-containing (alcohols, ketones, ethers and esters, organic acids) – 53 items, total concentration from 24 to 44 mg/m^3; sulfur-containing (sulfides, thiols, etc.) – 22 items, total concentration from 6 to 11 mg/m^3; nitrogen-containing – 2 items, total concentration up to 0.6 mg/m^3; chlorine – 3 items, total concentration from 0.18 to 2.1 mg/m^3; furans and piranas – 2 names, total concentration from 0.17 to 1.2 mg/m^3. Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) are chemically stable organic compounds. These are highly toxic pollutants that can accumulate in the tissues of organisms. Some of them (for example, 2,3,7,8-tetrachloro-p-dibenzodioxin) are extremely toxic, carcinogenic, cause hormonal disorders and damage to the immune system, which is especially dangerous in the context of a coronavirus pandemic (Bilalov et al. 2019, Feng et al. 2018, Rigang et al. 2020). Therefore, the MPC for PCDD/F is an order of magnitude lower than the MPC for chemical warfare agents and is 7-8 orders of magnitude lower than the MPC for NO_x and CO, and the emission of 1 mg of dioxin is commensurate with the emission of 10 tons of NO_x.

This means that the emission of 10 m^3/h of «landfill» gas with a dioxin concentration of 1.2 mg/m^3 in toxicity is equivalent to the emission of 400 thousand m^3/h of flue gases with a concentration of 300 mg/m^3 NO_x, which corresponds to the operating parameters of one boiler at a TPP.

The transformation of garbage in the furnaces of the steam generators of «garbage» TPPs takes 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, furans, and dioxins that exceed them in toxicity. Waste incinerators, including the most dangerous of them (medical waste incinerators) are the main sources of supply of polychlorinated dibenzo-n-dioxins and dibenzofurans to the atmosphere. In such conditions, in order to reduce damage, it is possible to organize preliminary waste treatment to the high-temperature zone with the removal of chlorine compounds (Ziganshin et al. 2009).

However, unauthorized fires in the places of collection and storage of solid waste, where preliminary processing is impossible, are also very dangerous sources. At the same time, incinerators and landfills are placed, as a rule, away from housing, while approximately the same set of chemical compounds is emitted directly into the air of a residential area during fires and arson at sites for temporary storage of household waste.

To reduce the formation of toxic compounds both when burning traditional fuel and when burning garbage, it is especially important to establish a sequence of elementary stages of transformation of the initial components in the thermo-oxidizing zone. Since during 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 incineration are insufficiently complete and sometimes contradictory.

Recently, a lot of research has been carried out on the production of hydrogen from recycled plastic. Plastic waste from the city's waste collection system is decomposed by thermal gasification. In this case, the organic part of the waste is converted into hydrogen, and carbon monoxide is also released. Carbon monoxide from this process is used to make carbon-based products. Hydrogen goes to the production of ammonia, goes to hydrogen gas stations, and is also used to generate electricity.

Hydrogen is poised to decarbonize many sectors of our economy. It can be directly used in fuel cells for carbon-free power, or in gas turbines where its high energy density, higher auto-ignition temperatures and ability to lean-burn are favored.

Simulating the combustion of hydrogen fuels with the ANSYS Fluent software can help the energy and aviation sectors achieve the low-carbon faster while saving costs.

When burning waste with a temperature above 1200-1300°C, thermal oxidation of organic and organochlorine components of MSW in the presence of metals can occur together with the reduction of their oxides. In this case, in some cases, it is possible to create conditions for the joint thermal neutralization of toxic compounds, for example, for the reduction of hexavalent chromium compounds to trivalent (Bilalov & Ziganshin 2019). The intermediate products formed in the high-temperature zone react with each other to the final products upon cooling the zone itself, and PCDD/F are formed in the range from 650°C to 250°C (Tugov eta al. 2018). 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 (Belyaeva et al. 2019). In general, the scheme for the formation of PCDD/Fs is not fully known. Full-scale and numerical studies on the kinetics of reactions were carried out for a limited number of starting components (Hongting et al. 2018, Min et al. 2018).

The presence of SO_2 in the high-temperature zone of sulfur dioxide ultimately leads to a decrease in the concentration of PCDD/F in the combustion products. However, on the whole, the picture of their formation is not yet clear enough. Recommendations for reducing the generation of PCDD/F so far boil

down to the following: the temperature in the combustion zone should be above 1200-1300°C, with the residence time of gaseous products of the reactions of thermal destruction and oxidation of solid waste in the high-temperature zone for at least 2-4 s, followed by sharp cooling («Hardening») of combustion products up to 200°C.

2. Methods

The paper considers the results of numerical modeling of the furnaces of a steam boiler E-220/100 (TP-14A, manufactured by JSC TKZ «Krasny Kotelshchik») with a steam capacity of 220 t/h. 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).

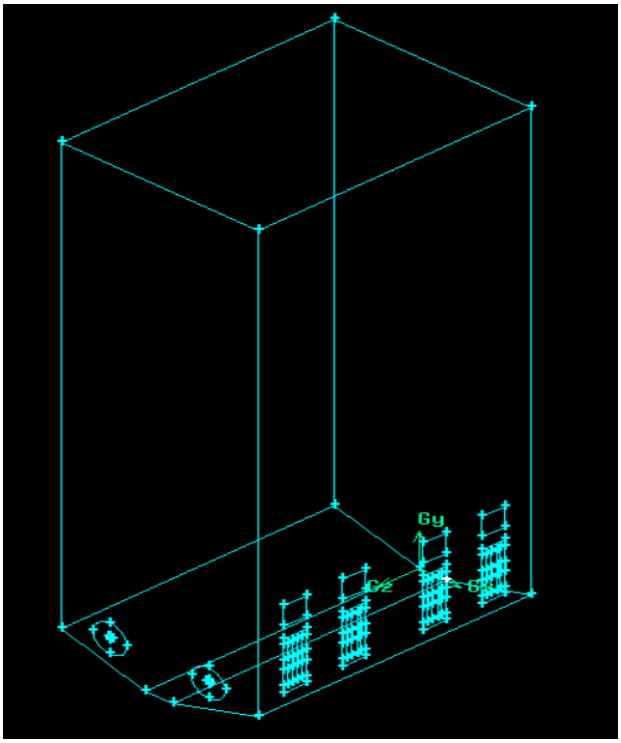

Fig. 1. Construction of a 3D model of the TP-14A boiler combustion chamber in the Gambit program, geometrically accurate model of the TP-14A boiler combustion chamber

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).

The model was transferred to the Ansys Fluent processor. The movement of flows in the furnace was calculated on the basis of the Navier-Stokes relations (RANS), the convergence of the relations according to the two-parameter k-ε model. The task is non-isothermal, using the energy equation («Energy Equation») and the P1 radiation model. For combustion of coal dust and garbage particles in the TP 14A furnace, 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 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 – vortex dissipation «Eddy-Dissipation».

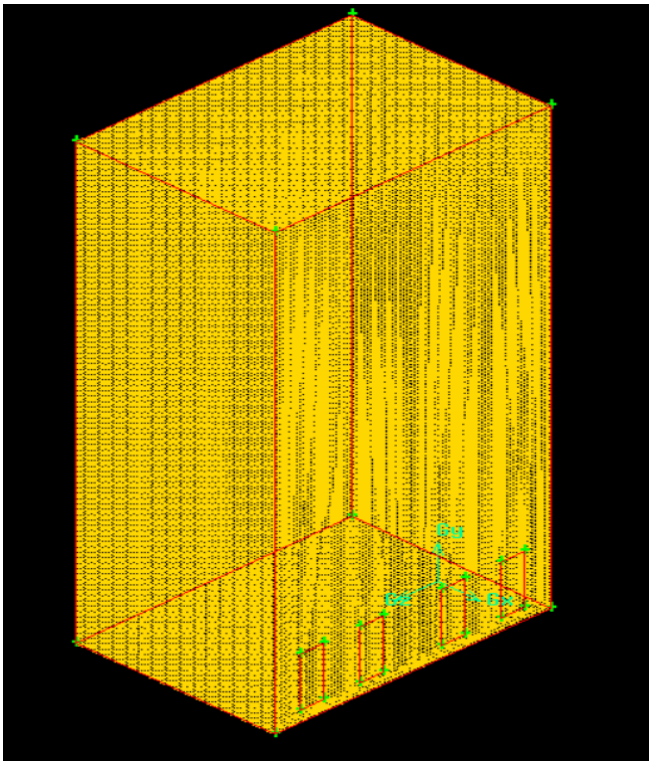

Fig. 2. Construction of a 3D model of the TP-14A boiler combustion chamber in the Gambit program, a simplified model with a generated computational grid

3. Simulation results

Numerical modeling requires verification and validation using reliable experimental data. The type of steam generator for modeling was selected from the condition of the possibility of verifying the results of modeling according to the data of (Kaverin 2017), where the test results of a similar steam generator at the Kumertau CHPP (Kaverin 2017) are considered. The physical adequacy of the created model in hydrodynamics is confirmed by the results of calculations of the pressure in the furnace, the values of which are close to atmospheric (Fig. 3a), and the absence of reverse currents. The adequacy of the calculations of combustion processes is confirmed by the fact that the maximum yield of volatiles and their most complete afterburning to CO_2 occur above the level of the location of the burners (Fig. 3b, 3c).

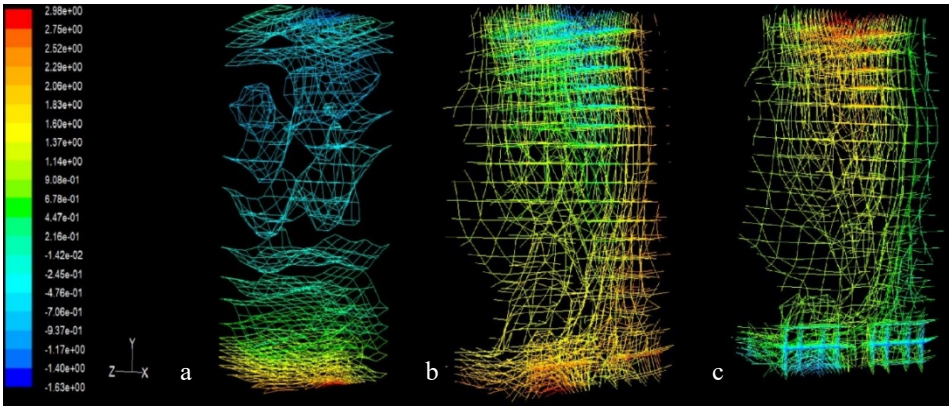

Fig. 3. Distribution of static pressure and content of volatile fuels and CO_2 in the TP-14A boiler furnace: a – calculated data on the distribution of static pressure in the boiler furnace, b – calculation results for the release of volatile fuels, c – the results of calculations on the afterburning of volatile fuels to CO_2

In recent decades, the ISAT (in situ adaptive tabulation) algorithm of adaptive tabulation of reactions has been practiced to study models of the combustion process of domestic boilers operating on gas fuel, which has now been made a number of improvements to increase its stability and speed without reducing the level of accuracy (Xie et al. 2018a, Xie et al. 2018b). However, they are adapted to internal combustion engines and need to be validated in the transition to boilers.

Recent versions of ANSYS include redesigned Chemkin combustion kinetics code in the ANSYS Chemkin-Pro software package to simulate pollutant emissions with detailed and accurate descriptions of combustion processes,

taking into account the various properties of the fuel. Separate studies using Chemkin-Pro are available in the field of dioxin formation during combustion of halogen-containing compounds. They used 45- and 71-stage models of the formation of 1,3,6,8- and 1,3,7,9-TCDD (tetrachlorodibenzo-para-dioxins) from one starting compound 2,4,6-trichlorophenol.

ANSYS Chemkin-Pro software is designed for detailed kinetic modeling of chemical mechanisms. The program is a set of tools for solving a wide range of tasks. With the help of this product, equations of state are solved, thermophysical properties and reaction rates are determined (Recording… 2019).

To gain a deeper understanding of kinetic mechanisms, ANSYS Chemkin provides a Reaction Path Analyzer.

Having a visual display of kinetic mechanisms when using the Reaction Path Analyzer tool gives an accurate understanding of the prevailing pathways of reactions.

The ANSYS Chemkin Extinction Model provides fast and accurate calculations of flame decay rates to determine combustion stability. Attenuation is especially important to consider in premixed and low NO_x combustion systems.

ANSYS Chemkin's innovative particle tracing technology simulates particle nucleation, growth, aggregation and oxidation. Two independent tracing methods predict the average particle size and particle diameter distribution, which in turn can be used to predict the formation of soot or to optimize the particle production process.

Many combustion system designers use combustion models that are based on Flamelet libraries. ANSYS Chemkin provides a robust and fast method for generating Flamelet libraries as input to CFD models.

Combustion chamber modeling requires the resolution of complex geometry, turbulent flow, heat transfer, and detailed chemistry. Typical CFD analysis is used to model chemical kinetics on detailed geometry, but with simplified chemical reaction models that do not accurately predict emissions and product stability. The simplified formulation used in CFD modeling chemical kinetics cannot fully resolve the release of harmful substances such as NO_x, CO and unburned hydrocarbons. To allow the formation of these substances, it is necessary to use detailed kinetic mechanisms with hundreds of components and thousands of reactions.

The Energico software module allows you to superimpose idealized chemical reactors on the flow field, which makes it possible to effectively apply detailed chemistry of combustion processes to accurately determine the formation and destruction of components present in negligible concentrations. The use of equivalent reactor circuits makes it possible to represent the flow field in the form of a set of ideal mixing and ideal displacement reactors with appropriate gas inlets and outlets. Energico directly transmits the results of the gas dy-

namic calculation into an equivalent circuit that describes the prevailing flow distribution and recirculation zones. For each calculation step, Energico contains automated templates, as well as many additional parameters for fine-tuning.

4. Conclusions

Analysis of the ways of air pollution in the residential area shows that the negative role of large-scale energy storage in this issue is exaggerated. In connection with the continuing decentralization of heat supply to the housing stock, the contributions of large-scale energy and decentralized sources to the deterioration of the atmosphere are converging, and in aggregate they do not exceed the impact on the urban air environment of emissions generated during the handling of household waste, due to their toxicity.

The developed numerical model of the combustion device of the TP-14A steam boiler, despite some simplifications of geometry, showed physical adequacy and can be used for numerical studies of furnaces of heat sources with the constructive know-how of modern manufacturers, provided that solid fuel with characteristics close to standard is burned.

With their significant deviation, it is difficult to predict the adequacy of modeling by the kinetics of thermal oxidation reactions, since at present there are no robust algorithms that provide acceptable accuracy of results when processing models with a sufficient number of initial fuel components, and validated for steam generator furnaces.

The use of professional ANSYS Chemkin software tools for solving combustion problems and flows with chemical reactions in the design of boilers allows us to understand and predict the chemical processes occurring in the system, which is of key importance in the development and calculations of thermal power plants. In addition, the emission of pollutants must be minimized. It is very costly to carry out only field tests to accurately assess performance, given the complexity of the structures and the shortened design time. Detailed chemical simulations are often critical to the cost-effective design of low-emission systems.

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