Mathematical Model for Optimizing the Composition and operating Modes of TPP Steam Boilers according to the Environmental Safety Criterion

MS Ivanitckii¹, AA Konstantinov², EV Kuryanova ³ and MM Sultanov ⁴

¹,²,⁴ National Research University «MPEI», Russia, 404110 Volzhsky, Lenina Avenue, 69
³ National Research University «MPEI», Russia, 111250 Moscow, Krasnokazarmennaya, 14

kuryanovaev@yandex.ru

Abstract. This paper deals with the problem of optimizing the composition and operating modes of boilers of thermal power plants according to the criteria of environmental performance in accordance with the main changes made to Federal law № 219-FZ of 21.07.2014 «On amendments to the Federal law «On environmental protection» and certain legislative acts of the Russian Federation» and taking into account the new principles of environmental management of energy enterprises. It is proposed to use the minimum value of the total index of harmful combustion products, depending on the type of fuel being burned, as a criterion for the environmental safety of the gas and oil boiler. The contribution of each individual harmful component of combustion products is taken into account based on the determination of specific indicators of the harmfulness of flue gas components. The proposed approach allows us to take into account the influence of important operational and technological factors on the change in total mass emissions of substances and the formation of a total indicator of the harmfulness of flue gases, including the dynamic nature of changes in the load of TPP boilers.

1. Introduction

The basic basis of the Russian electric power industry is thermal power plants (TPP), including thermal power plants (CHP) that use natural gas, fuel oil and coal as fuel. The installed capacity of Russia's TPP is about 153.5 GW, which provides 66 % of the country's total electricity generation. Operation of steam power plants in various operating modes in conjunction with their individual performance characteristics leads to the need to improve mathematical models and techniques that take into account the parameters of power plants and environmental standards for optimal loading of operating equipment and improving the technical and economic indicators of generating systems, including the use of modern effective mechanisms for managing equipment in a market and digital economy [1].

In accordance with Federal law № 219-FZ of 21.07.2014 «On amendments to the Federal law «On environmental protection» and certain legislative acts of the Russian Federation», new principles of state environmental policy have been established, including [2]: the division of all industrial...
enterprises into 4 categories and the application of differentiated measures of state regulation to each category; the introduction of technological rationing based on the principles of best available technologies (BAT); systematization of environmental information about the enterprise within the framework of state environmental accounting of objects. Consequently, all industrial enterprises are subject to the requirement of Federal law 219-FZ [2, 3] on equipping air pollution sources with systems for automatic continuous monitoring and accounting of harmful emissions (CMAHE) into the environment. Thus, the main tasks are implemented CMAHE [3]: continuous instrumental monitoring and recording of concentrations and mass emissions of harmful substances into the atmosphere; reduction of harmful emissions into the atmosphere due to the control and regulation of combustion of fuel and operation of dust-, gas-cleaning equipment; monitoring compliance with the maximum permissible emissions set for thermal power plants; calculation of fees for emissions based on the results of instrumental measurements; transfer of information on emissions of energy facilities to the data Fund of the state environmental monitoring.

At the request of Federal law № 219-FZ from 01.01.2019, category I enterprises are required to obtain a comprehensive environmental permit (CEP), which will replace the previously existing environmental approval procedures: maximum permissible emissions, permissible discharge standards, waste limits, and a list of environmental protection measures. The CEP will be issued for a separate facility based on an application to oversight of the organization for a period of 7 years and will contain: technological standards; standards for permissible emissions and discharges; limits on the placement of production and consumption waste and requirements for handling them. In addition, when preparing an application for a CEP, standards for permissible emissions of highly toxic substances, substances with carcinogenic or mutagenic properties (substances of hazard classes I and II) calculated for each source of pollutants should be determined [3 – 6].

2. Description of the algorithm flowchart

The mathematical model includes: a block for collecting initial data on the operating modes of boiler equipment (heat capacity, temperature and pressure of the working body, characteristics of heat losses with outgoing gases, with chemical and mechanical underburning of fuel, heat loss from external cooling, energy loss with the physical heat of slags and associated process parameters; calculation block for determining the concentrations of marker harmful (polluting) substances formed as a result of fuel combustion); optimization block for determining the most profitable variant of the composition and operating mode of boiler equipment and ranking fuel-burning plants according to the criteria of environmental safety of the furnace process.

The block diagram of the algorithm for optimizing the composition and operating modes of boilers based on the environmental safety criterion is shown in figure 1.
Launch

Block for collecting initial data on the composition and operating modes of boiler equipment

Block for calculating concentrations markers of harmful (polluting) substances and the total index of harmful emissions

Block of optimization and determination of the most profitable version of the composition and mode of operation boiler equipment according to the environmental safety criterion

Completion

**Figure 1.** Block diagram of the algorithm for optimizing the composition and operating modes of boiler plants based on the environmental safety criterion.

The overall hazard of combustion products of boiler plants reflects the level of ecological safety of TPPs, and within the framework of new environmental legislation can be used as a measure of the efficiency of the process. Mathematical model of optimization of composition and modes of operation, including boilers used at thermal power plants, sufficiently studied and presented in [7, 8], so the work is heavily analyzed approach to the analytical determination of total harm of combustion products for boilers of TPP as criterion of ecological safety taking into account marker substances, represented by oxides of nitrogen \((NO_2)\), sulphur dioxide \((SO_2)\), carbon monoxide \((CO)\), solid particles of ash.

### 3. Mathematical model for the formation of environmental safety criterion

The total harmfulness of the exhaust gases is determined by the contribution of the private harmfulness of the flue gas components due to the influence of \(NO_2, SO_2, CO\), benz(a)pyrene \((BP)\), hydrogen chloride \((HCl)\), vanadium pentoxide \((V_2O_5)\) according to the expression [9]:

\[
I = \sum_{i=1}^{n} I_i ,
\]

where \( I_i \) – indicator of the private harmfulness of each component of flue gases.

Private hazard rate \( I_i \) represents the number of grams of harmful impurities \( m_i \) formed when burning 1 g of fuel is related to the relative heat of combustion of fuel and to the relative toxicity of the contaminants is calculated according to the equation [9]:

\[
I_i = m_i \cdot R_i ,
\]
\[ I_i = \frac{m_i (1 - \eta_i)}{Q_i^{\text{mv}} \cdot \text{MPC}_{m.p.i} \cdot (Q_i')_{e.f.} \cdot \text{MPC}_{m.p.} \cdot \lambda_{\text{ash}}} , \]  

where \( Q_i^{\text{mv}}, (Q_i')_{e.f.} \cdot \text{MPC}_{m.p.} \cdot \lambda_{\text{ash}} \) – the calorific value of the considered and conventional fuel, respectively, MJ/kg (MJ/m\(^3\)); \( \text{MPC}_{m.p.i} \cdot (\text{MPC}_{m.p.} \cdot \lambda_{\text{ash}} \) – maximum single maximum permissible concentration (MPC) for each impurity and ash, mg/m\(^3\); \( \eta_i \) – the degree of purification of the exhaust gases from each impurity before being released into the atmosphere.

The calculated index of the private harmfulness of the second group of substances (nitrogen oxides, carbon monoxide, benz(a)pyrene) is determined by the dependence [9]:

\[ I_i = \frac{1.462 \cdot 10^{-2} V_i C_i (1 - \eta_i)}{Q_i^{\text{mv}} \cdot \text{MPC}_{m.p.i}} , \]  

where \( \eta_i \) – the degree of delay of a toxic substance in the gas treatment system; \( \text{MPC}_{m.p.i} \) – average daily maximum permissible concentration of harmful substance, mg/m\(^3\).

The indicator of private harmfulness of benz(a)pyrene is determined by the dependence [9]:

\[ I_{BP} = \frac{4.387 \cdot 10^{-3} C_{BP} V_i (1 - \eta_{BP})}{Q_i^{\text{mv}} \cdot \text{MPC}_{BP}^{\text{BP}}} , \]  

where \( V_i \) – the volume of flue gases produced by the combustion of 1 m\(^3\) of natural gas under normal conditions, m\(^3\)/kg; \( \text{MPC}_{BP}^{\text{BP}} \) – average daily maximum permissible concentration BP, mg/m\(^3\).

Note that for benz(a)pyrene, only the average daily maximum permissible concentrations are set, so for expression (2) BP is correlated with the value of the MPC of non-toxic dust equal to \( \text{MPC}_{da} \cdot 0.15 \) mg/m\(^3\).

The specific harmfulness of substances of the first hazard group, which includes sulfur oxides \( \text{SO}_2 \), is calculated by the equation [9]:

\[ I_{\text{SO}_2} = \frac{0.1462 C_{\text{SO}_2} V_i (1 - \eta_{\text{SO}_2})}{Q_i^{\text{mv}} \cdot \text{MPC}_{m.p.}^{\text{SO}_2}} , \]  

where \( \text{MPC}_{m.p.}^{\text{SO}_2} = 0.5 \) mg/m\(^3\) – maximum single maximum permissible concentration of sulfur oxides.

The indicator of private harmfulness of vanadium pentoxide is determined by the expression:

\[ I_{\text{V}_{2}O_5} = \frac{1.755 \cdot 10^{-2} A_i^{\text{mv}} F (1 - \eta_{\text{V}_{2}O_5})}{Q_i^{\text{mv}} \cdot \text{MPC}_{m.p.}^{\text{V}_{2}O_5}} , \]  

where \( A_i^{\text{mv}} \) – ash content of fuel per working weight, %; \( F \) – dimensionless coefficient that takes into account the rate of impurity deposition in the atmosphere; \( \eta_{\text{V}_{2}O_5} \) – degree of purification of
combustion products from vanadium pentoxide; \( \text{MPC}_{\text{m.p.}}^{V,O_2} = 0.002 \text{ mg/m}^3 \) – maximum single maximum permissible concentration of vanadium pentoxide.

The concentration of nitrogen oxides, \( C_{\text{NO}_2} \text{ g/m}^3 \), in the combustion products of boilers when burning natural gas and fuel oil is calculated using the expression of the standard method [10]:

\[
C_{\text{NO}_2}^{\text{NG}} = 2.05 \cdot 10^{-3} K_b \left[ 26.0 \cdot \exp \left( 0.26 \cdot \frac{T_{\text{acz}} - 1700}{100} \right) - 4.7 \right] \cdot \left( \exp(q_{\text{ref}}^{\text{acz}}) - 1 \right) \times 
\]

\[
\times \left[ 13.0 - 79.8(\alpha_{\text{acz}} - 1.07)^4 + 18.1(\alpha_{\text{acz}} - 1.07)^3 + 59.4(\alpha_{\text{acz}} - 1.07)^2 + 9.6(\alpha_{\text{acz}} - 1.07) \right] \cdot \tau_{\text{acz}}, 
\]

\[
C_{\text{NO}_2}^{\text{FO}} = 2.05 \cdot 10^{-3} K_b \left[ 24.3 \cdot \exp \left( 0.19 \cdot \frac{T_{\text{acz}} - 1650}{100} \right) - 12.3 \right] \cdot \left( \exp(q_{\text{ref}}^{\text{acz}}) - 1 \right) \times 
\]

\[
\times \left[ 15.1 - 131.7(\alpha_{\text{acz}} - 1.09)^4 + 72.3(\alpha_{\text{acz}} - 1.09)^3 + 73.0(\alpha_{\text{acz}} - 1.09)^2 + 2.8(\alpha_{\text{acz}} - 1.09) \right] \cdot \tau_{\text{acz}} + 
\]

\[ + \Delta \text{NO}_2^{\text{fuel}} \]

\( \tau_{\text{acz}} \) – coefficient that characterizes the design of the burner device; \( T_{\text{acz}} \) – average integral temperature of combustion products in the active combustion zone (ACZ), K; \( q_{\text{ref}}^{\text{acz}} \) – reflected heat flow in the ACZ, MW/m²; \( \alpha_{\text{acz}} \) – coefficient of excess air in the active combustion zone of the combustion chamber; \( \tau_{\text{acz}} \) – residence time of combustion products in the ACZ; \( \Delta \text{NO}_2^{\text{fuel}} \) – a term that takes into account the amount of fuel nitrogen oxides.

The content of sulfur oxides in flue gases during the combustion of fuel oil taking into account the delay in the desulphurization unit is calculated according to:

\[
C_{\text{SO}_2} = 2 \cdot 10^{-2} \cdot S^{\text{w.m.}} \cdot \frac{V_{\text{dry}}}{V_{\text{dry}}} \cdot \left( 1 - \eta_{\text{SO}_2} \right) \cdot \left( 1 - \eta_{\text{SO}_2} \right), 
\]

where \( S^{\text{w.m.}} \) – sulfur content in fuel oil per working mass, %; \( V_{\text{dry}} \) – dry flue gas output per 1 kg of burnt fuel oil, m³/kg; \( \eta_{\text{SO}_2} \) – degree of purification of flue gases from sulfur oxides.

The calculated determination of the concentration of sulfur dioxide was carried out taking into account the 5% \( \text{SO}_2 \) delay on the convective surfaces of the boiler heating and binding with volatile oil ash \( \eta_{\text{SO}_2} \). The concentration of benz(a)pyrene in the flue gases of steam boilers, taking into account the influence of regime and technological factors, is calculated in accordance with the method [11].

The specific yield of dry exhaust gases as a result of burning 1 kg of fuel oil taking into account the influence of their temperature is calculated according to [10]:

\[
V_{\text{dry}} = \left[ V_{g}^{0} + 1.016 \left( \alpha_{\text{acz}} - \beta_{\text{acz}} \right) V_{a}^{0} - V_{w}^{0} \right] \frac{L_{en} + 273}{273}, 
\]

where \( \beta_{\text{acz}} \) – the degree of combustion in the zone of active combustion furnace; \( V_{g}^{0} \) – the theoretical volume of flue gas generated by burning 1 kg of fuel, m³/kg; \( V_{a}^{0} \) – theoretical amount of
air required for burning 1 kg of fuel, m³/kg; $V_{wv}^0$ – the amount of water vapor released in the combustion of 1 kg of fuel, m³/kg; $t_{ex}$ – temperature of exhaust gases, °C.

The concentration of chloride compounds in fuel oil combustion products is determined by the expression:

$$C_{HCl} = \frac{C_{Cl'}}{V_{dg}},$$

where $C_{Cl'}$ – the content of chloride salts in the fuel, mg/kg.

Thus, by applying the equations (1) – (9), the total index of harmful flue gases of TPP boilers is calculated. The lowest value of the criterion $\Sigma I$ is determined by the order of commissioning of the corresponding boiler, which can be used by energy companies to improve the environmental performance of the TPP.

4. Conclusions

In order to provide a comprehensive approach to solving the problem of improving the efficiency of the technological process, the paper offers an analytical description of the formation of an environmental safety criterion as part of a mathematical model for optimizing the composition and operating modes of TPP steam boilers. The results obtained can be used by energy companies of category I and II to improve the environmental performance of boilers of various thermal capacities and develop programs to improve environmental efficiency in the absence of the possibility of meeting technological standards, including the approval of technological indicators, annual gross emissions and specific mass values of emissions, inventory of emissions, preparation and revision of the application for obtaining a CEP in accordance with the requirements of the new environmental legislation of Russia, they can also be used to ensure optimal loading of the boiler equipment of existing thermal power stations and improve the technical, economic and environmental performance of TPP power units.

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