

Application of high optical technologies to determine the temperature field, ingredient composition and microstructure of the dispersed phase of combustion products of energy fuels

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Abstract. Application of high optical technologies for determining the temperature field, ingredient composition and microstructure of the dispersed phase of combustion products of power fuels is considered. The temperature of the combustion products is determined by method of the self-reversal of spectral lines. To determine the ingredient composition, the methods of fine-structure spectroscopy are used, when the absorption spectra of flame radiation are measured with a high spectral resolution. Then the ingredients are identified by the position of the spectral lines, and their concentration - by the intensity of the spectral lines at a fixed temperature. The temperature field in the combustion chambers of power plants is reconstructed by the method of numerical simulation of radiation transfer in combustion products of an inhomogeneous radiation propagation medium. The obtained experimental data on optical characteristics are used to solve problems of radiation heat transfer in combustion chambers of power plants with multi-chamber furnaces. Prospects for the creation of high-temperature atlases of the parameters of spectral lines of the ingredients of the gas phase of combustion products and their application in promising developments of power plants and in rocket technology are considered.

1 Introduction

The problem of radiation heat exchange in the combustion chambers of power generating units is of decisive importance for the development of environmentally friendly technology for the production of heat and electrical energy. Combustion products emitted into the atmosphere have harmful ingredients and carcinogenic components that lead to the formation of tumors. Air pollution leads to a change in the habitats of humans, animals, and also causes climatic changes [1,2]. The scale of atmospheric pollution increases linearly with the growth of the population [2,3]. The spectrum of human activity is expanding over time in the direction of increasing living comfort, which causes an increase in the need for energy and changes in technologies for the exploitation of natural resources in order to minimize environmental damage to the environment. The fundamental basis of the country's socio-economic development is energy, which mainly relies on the use of fossil fuels in the production of heat and electricity. During the production of thermal energy in power units operating on gas fuel, a finely dispersed soot sol is formed from the gas phase of fuel combustion products in the furnaces of power plants [4, 6], the microstructure of the particles of which changes as the combustion products move [7-10]. When burning solid fuel, in addition to soot ash particles, burnt-out particles of the fuel itself are carried out in the form of a fraction of mineral ash particles [11-12]. Thus, radiative heat exchange in

combustion chambers and radiation heat exchangers occurs in a two-phase environment with the transfer of heat from fuel combustion products to the water vapor of the heat exchanger tube system. The present work is devoted to investigations of the optical characteristics of combustion products in combustion chambers and heat exchangers of power plants and of combustion products emitted into the atmosphere.

2 Measuring complexes

To carry out studies of the optical characteristics of combustion products, spectral installations were developed for studying optically active ingredients of combustion products in the temperature range 200-2500 K with middle and high spectral resolution, described in [10, 14, 15, 17, 22, 23]. Changes in the ingredient composition of combustion products emitted into the atmosphere were carried out by sampling with subsequent spectral analysis in an analytical setup based on an upgraded IKS-31 spectrometer and an MHK-1 multi-pass cell with external and internal electric heating. The IKS-31 spectrometer is supplemented with radiation detectors, diffraction gratings and cut-off interference filters to expand the area of its operation from 0.2 μm to 100 μm in order to obtain data on the microstructure of the soot sol by the attenuation spectra of the dispersed phase of combustion products. The spectral resolution $\Delta\nu = 0.2 \text{ cm}^{-1}$ of the spectrum ensured the separation of the spectra of attenuation of radiation by the sol and

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absorption of radiation by spectral lines of the gas phase of combustion products. The ingredients of the gas phase of the combustion products were identified by the position of the spectral lines, and the concentration of the ingredients was determined by the depth of absorption of the spectral lines by the ingredients. Sections of the spectra were chosen so that the bands of different ingredients did not overlap. Samples of combustion products were taken into evacuated samplers along heated stainless steel gas ducts to avoid the effect of condensation processes on the walls of the gas ducts. Before launching into a multi-mode Cell, the samplers were heated to a temperature of $T=150\text{ C}$ and introduced into a MPC heated to a temperature of 150 C using an external heating system. If necessary, the sample in the MPC was diluted with dried nitrogen purified from CO_2 . The purification of nitrogen from H_2O was carried out with phosphorus pentoxide P_2O_5 and zeolites. Purification of N_2 from CO_2 is carried out using caustic potassium KOH. The optical layout of the setup is shown in Fig. 1.

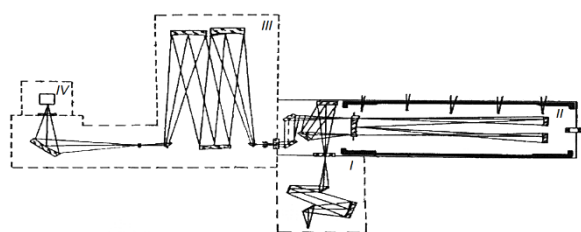


Fig. 1. Optical layout of the spectrometric setup: I - illuminator block; II - multi-pass cuvette; III- monochromator; IV - block of replaceable measurement receivers.

To measure the concentration of small components of combustion products, a spectrophotometric complex based on an IKS-24 spectrophotometer is used; the optical scheme of the installation is shown in Fig. 2.

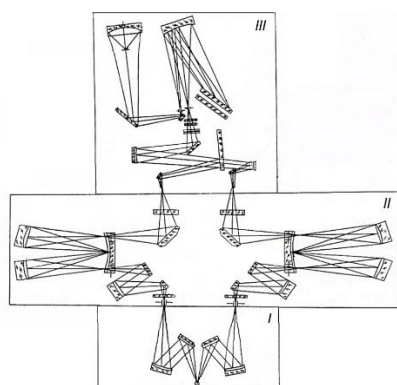


Fig. 2. Optical scheme of the conjugated spectral two-beam complex "IKS-24-MHK-7": I - illuminator unit; II - two-beam multi-pass cell; III - receiving module of the spectrophotometer.

To determine the concentration of ingredients, a dosager with a pure ingredient and a needle leak is used to accurately dose the ingredient into the control measuring channel of the double-beam cell. The test sample of combustion products is introduced into one cell with a given pressure. Nitrogen is introduced into the second cell with an effective pressure in the first cell, and

the investigated ingredient is injected from the dosager until the absorption spectra in both cells are equalized. In this case, the spectrophotometer will record the background noise line. The volume concentration of the ingredient ρ_i is determined by the change in pressure ΔP_{dos} in the dispenser with the number of passes n of the optical path L in the channels of the multi-pass cell and the ratio of volumes V_{dos}/V_c of the dispenser and the cuvette:

$$\rho_i = (\Delta P_{dos} \cdot V_{dos}) / (V_c \cdot n)$$

The pressure in the dosager is measured with a mercury manometer with a vernier scale with an error of 0.1 mm Hg . The use of a double-beam Cell improves the accuracy of measuring the concentration of an ingredient, which is determined by the purity of the ingredients in the dosagers. The optical characteristics of optically active ingredients were measured on flame measuring complexes with middle and high resolution spectrometers. The parametrization of the spectral transmission functions of the average spectral resolution was performed using the two-parameter method of equivalent mass [1, 10]. The temperature of the combustion products was determined by the self-reversal of spectral lines [10]. The complex operates in the modes of absorption of radiation by the flame from standard radiation sources and in the mode of measuring the absolute spectra of flame radiation (combustion products). Calibration of standard radiation sources was performed by the head metrology department of the Ministry of Defense at NPO GIPO (Kazan) on the basis of blackbody radiation. It has been experimentally established that the emission of H_2O in a hydrogen-oxygen flame is equilibrium and the temperature is measured in the bands of 1.37 and $1.87\ \mu\text{m}$. With the use of a SIRSH 8.5-200-1 lamp and a $1.37\ \mu\text{m}$ strip, the maximum measurement temperature is 2400 K . In this case, the lamp radiation is projected by a quartz lens into the center of the optical projection axis "tungsten tape - spectrometer entrance slit". The temperature is calculated using the formula:

$$T_{\lambda}^A = T_{\lambda R}^0 / (1 + \alpha T_{\lambda R}),$$

where $\alpha = 2.303(\lambda \lg \varepsilon_{\lambda} - 0.65 \lg \varepsilon_{\lambda 0}) / C_2$, $\lambda_0 = 0.65\ \mu\text{m}$, $T_{\lambda R}$ - brightness temperature at the wavelength of the EOP-66 pyrometer; C_2 is the second constant in the study of the black body. When determining the flame temperature, the attenuation of radiation by the quartz lens is also taken into account. The change in the temperature of combustion products with height above the cuts of the capillaries of a multi-row gas emitter can be investigated using the "non-uniform gas emitter" setup described in [10] and designed to simulate radiation transfer in media inhomogeneous in temperature.

3 Determination of temperature and ingredient composition

Measurements of the radiation attenuation spectra at high spectral resolution make it possible to separate the radiation attenuation spectra of the dispersed and gas

phases with the smallest errors, which makes it possible to use the data on the radiation attenuation by the dispersed phase to restore the microstructure of the soot sol from the spectral dependences of the radiation attenuation cross section in the spectral range 0.2-25 μm . The microstructure of atmospheric emissions of the discrete phase of combustion products depends on many factors: the elemental composition of the fuel, the residence time of the combustion products in the flame zone, the electrical properties of the combustion products, which determine the rate of coagulation and agglomeration of the primary sol, the modal radius of which is estimated as $r_m=0.003 \mu\text{m}$. Determination of the microstructure of a soot sol is an inverse problem and, for its solution, requires a priori information on the optical (radiation) characteristics of a soot sol of various microstructural formations that cover the entire range of spectral changes in the radiation attenuation coefficients. In this case, the reference wavelengths (measurement channels) are selected in the transparency windows of the gas phase of the combustion products and should include the wavelengths of the UV, visible and IR spectral ranges. Optimization of the solution to the problem of restoring the microstructure of soot sol particles from the radiation attenuation spectra is performed from the condition:

$$\sum_i \frac{(\Delta\sigma_{a\lambda i})}{\sigma_{a\lambda i}} = \min, \quad (1)$$

where $\Delta\sigma_{a\lambda i}$ is the deviation of the calculated spectral dependences of the coefficient $\sigma_{a\lambda i}$ from the measured ones, i is the number of the measurement channel. Table 1 shows the parameters of the models of the microstructures of the soot sol intended to restore the real microstructures of the dispersed phase of combustion products. To select the zero approximation, an additional optical base of the characteristics of "zero approximations" is created. The choice of the zero approximation is determined by the relation (1). Parameters a, b, γ, r_m of modified gamma distributions $f(r)=Ar^a \exp(\gamma r^b)$ (2), where r_m is the modal distribution radius, presented in Table 1.

The electronic database of the optical characteristics of soot sol was prepared for polydisperse particle size distributions [7] under the assumption of a spherical particle shape [15]. The procedure for determining the microstructure of a soot sol is carried out in the following order. The microstructure is set from the database of zero approximations and gamma distributions from Table 1 for the optical density $\tau_0 (\lambda = 0.55 \mu\text{m}) = 1$ and $\sum_i \frac{(\Delta\sigma_{a\lambda i})}{\sigma_{a\lambda i}}$ is calculated for the selected microstructure $N(r)$ from Table 1. Next, the distribution is calculated:

$$N(r) = N_0(r)(1 - \tau_{min}) + N_i(r)\tau_{min}. \quad (3)$$

The obtained value $N(r)$ is assigned a zero approximation and the procedure is repeated for the next sample of the microstructure from Table 1. The procedure for determining $N(r)$ is completed after a complete enumeration of the microstructures of gamma distributions from Table 1. Errors $\Delta\tau/\tau_i$ are 3-4%. In fig. 3 shows the particle size distributions for methane-air, propane-butane-air, acetylene-air flame [16].

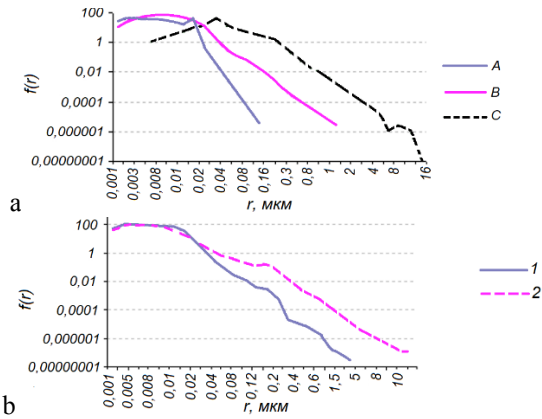


Fig. 3. The distribution function $f(r)$ of the number of particles by size: r is the radius of the particles. Flame: A - methane - air; B - propane - butane - air; C - acetylene - air, in emissions of combustion products: 1 - gasoline engine; 2 - pine timber.

Table 1. Parameters of gamma distributions of microstructure of soot sol

| N | a | b | γ | $r_m, \mu\text{m}$ | N | a | b | γ | $r_m, \mu\text{m}$ |
|-----|-----|-----|----------|---------------------|-----|-----|-----|----------|---------------------|
| 1 | 1 | 50 | 0,5 | $1,6 \cdot 10^{-3}$ | 6 | 1,5 | 6 | 1 | $2,5 \cdot 10^{-1}$ |
| 2 | 0,2 | 6 | 0,5 | $4,4 \cdot 10^{-3}$ | 7 | 0,1 | 0,5 | 2 | $0,3 \cdot 10^{-1}$ |
| 3 | 1 | 9 | 0,5 | $4,9 \cdot 10^{-3}$ | 8 | 1 | 1 | 2 | $0,3 \cdot 10^{-1}$ |
| 4 | 1 | 7,5 | 0,5 | $9 \cdot 10^{-2}$ | 9 | 3 | 6 | 0,5 | $1 \cdot 10^{-1}$ |

The ingredient composition of combustion products was determined by the method of fine-structure spectrometry of high spectral resolution using a priori information on the parameters of spectral lines in the main bands of ingredients. The identification of the ingredient was determined by the position of the spectral lines, and the concentration was measured by the intensity of the lines. The temperature dependence of the intensity of spectral lines is determined by the relation [18, 19]

$$S(T) = S(T_0) \left(\frac{T_0}{T}\right)^{1.5} \frac{\Theta(T)}{\Theta(T_0)} \exp(1.439E'(\frac{1}{T} - \frac{1}{T_0})), \quad (4)$$

where the vibrational partition function $\Theta(T)$ is calculated in the harmonic approximation, E' is the energy of the lower state for the main bands of the vibrational-rotational transition, T is the temperature of the radiation propagation medium, $S(T_0)$ is the measured line intensity at temperature T_0 . The intensity of the spectral lines of combustion products $S(T)$ is measured as follows [10]. The measured spectrum is decomposed into the contours of individual spectral lines by the method of differential moments [21-24]. Further, the profiles obtained in this way are restored to the influence of the instrumental function of the spectrometer. For the number of lines M , the transition to the absorption coefficients

$$K(\nu) = \sum_1^M K_m(\nu - \nu_m^0), \quad (5)$$

where m is the line number, ν_m^0 is the position of the center of the spectral line. The measured half-widths of the spectral lines γ_m of H_2O vapors generally agree with the results of calculations performed at temperatures of 200-3000 K.

Optical density at the center of the spectral line

$$\tau(\nu_m^0) = S_m \rho_i L / \gamma_m, \quad (6)$$

makes it possible to determine the volume concentration ρ_i from the absorption of radiation at the center of the spectral lines, from their intensity S_m , half-width γ_m and the length L of the optical path in the combustion

products. Fig. 4. the decomposition of the measured function $A_{\delta\nu}$ into individual contours is presented.

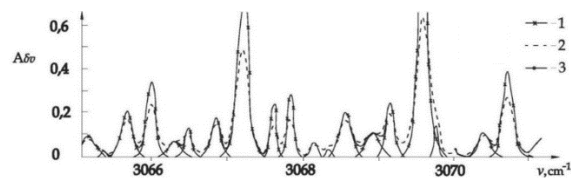


Fig.4. Decomposition of the measured function $A_{\delta\nu}$ into individual contours. 1 - reconstructed decomposition components, 2, 3 - spectral absorption functions of radiation measured and calculated from the reconstructed parameters of spectral lines, respectively.

4 Conclusion

The application of spectral measuring systems for measuring the optical characteristics of the ingredients of the combustion products of fuels is considered. Studies of the fine structure of absorption and emission spectra in flames have been carried out. It was revealed that the emission of H_2O vapors in the combustion products is equilibrium, which makes it possible to determine the gasometric temperature from the absorption lines of H_2O vapors in the combustion products. A self-reversal method for H_2O spectral lines has been implemented for measuring the brightness temperature of the flame. Non-equilibrium of OH , NO_2 radiation in high-temperature flames and the need to take them into account in calculations of radiation heat exchange in combustion chambers are revealed. The application of fine-structure spectrometry for measuring the ingredient composition of combustion products and anthropogenic emissions into the atmosphere is considered. The obtained parameters of the spectral transmission functions are used to calculate the radiation heat transfer in multi-chamber furnaces. The advances in theoretical spectroscopy of the last decade have made it possible to develop an electronic database of spectral line parameters [18, 19, 20, 24] for the ingredients of the gas phase of combustion products, which creates the prospect of their application in the problems of the transfer of selective radiation in the atmosphere [25] and in problems of modeling radiation heat transfer in power plants in order to select optimal design solutions.

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