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Modeling of radiate characteristics of dispersion phase combustion products of energy fuels

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Abatract. The results of an experimental study of the optical characteristics and microstructure of the dispersed phase of the products of combustion of organic fuel in oxygen and atmospheric air are analyzed. For gaseous fuels CmHn, the concentration of soot sol increases with an increase in the ratio of elements Cm / Hn. The microstructure of soot sol strongly depends on the residence time of the combustion products in the flame zone (chemical reaction zone) and the thermodynamic temperature. The maximum ash content is observed at thermodynamic temperatures of 1500-1800K zone of chemical reactions. The minimum ash content is observed when burning fossil fuels in oxygen with a value of the coefficient of excess oxygen $\alpha = 1{,}03$. A technique is proposed for measuring the microstructure of soot sol in atmospheric emissions of the combustion products of turbojet engines, vehicles, and power plants. The results of studies of the microstructure of the dispersed phase of fuel combustion products are used to calculate the light scattering matrices of carbon black sol according to the Mi theory. The radiation characteristics of soot sols are simulated by their superposition for different fractions *i* of the sol microstructure with normalization to optical density $|\tau_i|$ and a wavelength of $\lambda = 0.55$mkm. The optical densities $|\tau_i|$ for $\lambda=0{,}55$mkm for components i are given in numerical form depending on the height z in the combustion chamber. The radiation characteristics (absorption, scattering cross section and scattering indicatrix) are presented in the spectral region of 0.2–40mkm in the form of an electronic computer database for various gamma distributions of the carbon structure of soot sol.

I. Introduction

The problem of radiation heat transfer in the combustion chambers of power units is crucial for the development of environmentally friendly technologies for the production of heat and electric energy. The products of combustion of energy fuels emitted into the atmosphere contain toxic components and carcinogenic components that cause the formation of tumors. Atmospheric pollution leads to a change in environmental conditions of humans and animals, as well as cause climate change [1]. The scale of atmospheric pollution increases linearly with population growth [2,3]. The spectrum of human activity expands over time in the direction of increasing living comfort, which causes an increase in energy demand and changes in the technology of exploitation of natural resources in order to minimize environmental damage to the environment. The control of atmospheric pollution in the production of heat and energy is of paramount importance. 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 thermal and electric energy. During the production of thermal energy in gas-fired power units, finely dispersed soot sol is formed in the fuel combustion products from the gas phase of the combustion products [4-6], the microstructure of which particles in the combustion chamber changes as the combustion products move. When burning solid fuel in the furnaces of power plants, in addition to the particles of soot ash, particles of the fuel itself in the form of a fraction of particles of mineral sol are carried out into the radiation heat exchange chamber [7, 8]. Thus, radiation heat transfer in the combustion chambers and radiation heat transfer in the combustion chambers and radiation heat exchangers occurs in a two-phase medium with heat transfer from the products of fuel combustion to the water vapor of the pipe system of heat exchangers. The present work is devoted to modeling the optical characteristics of the dispersed phase of combustion products in combustion chambers and heat exchangers of power plants.

II. Modeling the microstructure of dispersed and optical characteristics of combustion products in the furnaces of power boilers

To study the effect of the dispersed phase on radiation heat transfer in the combustion chambers of energy units, it is necessary to solve the problem of modeling its optical characteristics taking into account the spatial variability of the microstructure and chemical composition of the sol of the products of combustion of energy fuels. The processes of generation and transformation of sols in the furnaces of power units are insufficiently studied, which causes certain difficulties in modeling the effect of the dispersed phase of the products of fuel combustion on radiation heat transfer in furnaces on radiation heat transfer in furnaces and heat exchangers. In this case, we will rely on modeling optical characteristics in the Earth's atmosphere [12-15].

We assume that the sol of combustion products is multicomponent and polydisperse and its microstructure and optical density τ at a wavelength of $\lambda = 0.55$ μm changes with height in the furnace above the burner devices. As in [7], we will simulate the microstructure of the dispersed phase by a superposition of distributions $n_i(r)$, where r - radius of the particle, i is the number of the fraction of a certain chemical composition and microstructure:

$$N(r) = \sum_i B_i n_i(r), \tag{1}$$

where $n_i(r)$ - defined as a modified gamma distribution

$$n_i(r) = A_i r^{\alpha_i} \exp\left[-b_i r^{c_i}\right]. \tag{2}$$

By setting the vertical profile of the optical and numerical density of the fractions n_i, it is possible to simulate changes in the microstructure and chemical composition of the sol with height in the combustion chambers. The parameters a_i, b_i, c_i are chosen in such a way as to cover the entire region of the observed particle sizes of soot and mineral sols depending on the microstructure and chemical composition of the particles and the type of fuel. Modal radius r_m, in which function (2) has a maximum is determined by the relation:

$$r_m = \left(\frac{a}{cb}\right)^{1/c}. \tag{3}$$

$$A = Ncb^{(a+1)c} / \Gamma\left(\frac{a+1}{c}\right), \tag{4}$$

where $\boldsymbol{N}$ - numerical particle density in cm^3.

The results of calculations of the attenuation coefficients of radiation σ_a are described by the relation

$$\sigma_a = \int n(r)\pi r^2 Q(r)dr. \tag{5}$$

The scattering coefficient σ_a^S is determined by the ratio

$$\sigma_a^S = \int n(r)\pi r^2 Q_S(r)dr. \tag{6}$$

Elements of the scattering matrix are normalized to the probability of quantum survival ϖ_0:

$$2\pi\int M_2\cos\theta d\theta=\varpi_0\,, \tag{7}$$

where

$$\varpi_0=\frac{\sigma_a^S}{\sigma_a}\,, \tag{8}$$

$$M_2(Q)=\int M_2(Q,r)n(r)dr\,. \tag{9}$$

Attenuation $Q(r)$, scattering factors $Q_S(r)$ and matrix elements are calculated using the Mi algorithms [15].

Scattering indicatrix

$$f(Q)=(M_1+M_2)/2\,. \tag{10}$$

The effective cross section of scattering, absorption and the scattering function for soot particles and mineral sols are presented for various gamma distributions in Table 1 in the form of electronic data base of the computer.

Table 1. Microstructure models for carbon black fractions

№	a	b	c	r_m, mkm	№	a	b	c	r_m, mkm
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
3	1	7,5	0,5	$4{,}9{\cdot}10^{-2}$	8	1	1	2	0,3
4	1	7,5	0,5	$9{\cdot}10^{-2}$	9	3	0,5	0,5	1
5	2	12	1,5	$8{,}9{\cdot}10^{-2}$	10	5	0,5	0,5	1,25

Tables 2,3 show the optical characteristics for fractions 2 and 4 (from table 1) of carbon black sol for a humidity of 0%. The coefficients attenuation $\sigma_{\lambda a}$, absorption $\sigma_{\lambda a}^a$, scattering $\sigma_{\lambda a}^S$, scattering indicatrix $f(\theta)$ for different wavelengths λ in the spectral region of 0.2–40 mkm are normalized in such a way that at $\tau_{\lambda a}=\tau_{\lambda a}^S+\tau_{\lambda a}^a=1$ a wavelength of λ = 0.55 mkm.

Table 2. Optical characteristics of smoke black sol (fraction № 2) - normalized spectral coefficients attenuation $\sigma_{\lambda a}$, absorption $\sigma_{\lambda a}^a$, scattering $\sigma_{\lambda a}^S$, scattering indicatrix $f(\theta)$

λ, мкм	0,2	0,55	2	3	5	7	10	14	20
$\sigma_{\lambda a}$	1,71	1	0,354	0,265	0,15	0,096	0,068	0,057	0,051
$\sigma_{\lambda a}^S$	0,619	0,346	0,094	0,056	0,023	0,008	0,002	0	0
$\sigma_{\lambda a}^a$	1,091	0,654	0,26	0,209	0,127	0,088	0,066	0,057	0,051
θ	$f(\theta)$								
0	2100	587	132	65,1	29,9	29,9	4,98	1,84	0,763
0,5	2080	586	132	65	29,9	29,9	4,98	1,84	0,763
1	2030	584	132	65,1	29,9	29,9	4,98	1,84	0,763
2	1840	575	131	65	29,9	29,9	4,98	1,84	0,762
2,5	1720	568	131	64,9	29,9	29,9	4,98	1,84	0,762
3	1580	560	131	64,9	29,8	29,8	4,98	1,83	0,762
3,5	1440	551	131	64,8	29,8	29,8	4,97	1,83	0,762
4	1290	540	131	64,8	29,8	29,8	4,97	1,83	0,761

5	1030	516	130	64,6	29,8	29,8	4,96	1,83	0,76
6	820	489	129	64,3	29,7	29,7	4,95	1,83	0,759
8	566	427	127	63,7	29,5	29,5	4,93	1,82	0,755
10	443	363	124	63	29,3	29,3	4,9	1,81	0,751
20	176	150	104	57	27,6	27,6	4,67	1,72	0,717
30	84,5	86,4	78,4	48,7	24,9	24,9	4,31	1,6	0,666
40	46	53,9	53,9	39,1	21,8	21,8	3,97	1,44	0,602
50	27,3	34,8	35	30	18,4	18,4	3,4	1,28	0,534
60	17	23,3	22,4	22,4	15,2	15,2	2,96	1,12	0,47
70	11,4	16,1	15	16,5	12,4	12,4	2,59	0,988	0,418
80	8,36	11,7	10,8	12,3	10,2	10,2	2,32	0,899	0,382
90	6,58	8,97	8,35	9,56	8,72	8,72	2,18	0,858	0,368
100	5,55	7,33	6,93	7,79	7,81	7,81	2,18	0,87	0,376
110	5,02	6,36	6,12	6,71	7,44	7,44	2,29	0,93	0,404
120	4,79	5,83	5,69	6,09	7,465	7,465	2,5	1,03	0,449
130	4,76	5,58	5,5	5,79	7,76	7,76	2,78	1,15	0,505
140	4,83	5,5	5,46	5,7	8,18	8,18	3,09	1,28	0,566
150	4,95	5,53	5,53	5,74	8,64	8,64	3,37	1,41	0,622
160	5,07	5,62	5,65	5,84	9,03	9,03	3,6	1,51	0,668
170	5,16	5,74	5,77	5,93	9,29	9,29	3,75	1,58	0,698
180	5,21	5,8	5,82	5,97	9,38	9,38	3,81	1,6	0,709

Table 3. Optical characteristics of smoke black sol (fraction № 4) - normalized spectral coefficients attenuation $\sigma_{\lambda a}$, absorption $\sigma^{a}_{\lambda a}$, scattering $\sigma^{S}_{\lambda a}$, scattering indicatrix $f(\theta)$

λ, мкм	0,2	0,55	2	3	5	7	10	14	20
$\sigma_{\lambda a}$	1,157	1	0,569	0,47	0,305	0,271	0,213	0,164	0,111
$\sigma^{S}_{\lambda a}$	0,533	0,445	0,221	0,173	0,122	0,091	0,069	0,051	0,031
$\sigma^{a}_{\lambda a}$	0,624	0,55	0,348	0,297	0,228	0,18	0,144	0,113	0,08
θ	$f(\theta)$								
0	39300	6600	1060	609	325	224	152	109	75,9
0,5	26700	6220	1050	607	324	224	152	109	75,9
1	15300	5290	1040	603	324	223	152	109	75,9
2	6870	3450	980	588	320	222	152	108	75,8
2,5	5190	3860	942	576	318	221	151	108	75,7
3	4090	2400	899	563	315	220	151	108	75,6
3,5	3290	2040	854	548	311	219	150	108	75,5
4	2710	1750	807	532	307	217	150	108	75,4
5	1930	1340	715	497	298	213	148	107	75,1
6	1450	1070	633	460	288	209	147	106	74,8
8	897	746	503	389	264	199	142	104	73,9
10	629	544	410	329	239	187	137	102	72,9
20	200	180	177	460	140	124	105	85,4	64,8
30	80,2	91,5	96,5	90,6	85,8	81,9	74,5	66,2	54,1
40	38,8	55,4	57,2	56,7	55,3	55,2	53,3	49,9	43,3
50	21,5	35	36,1	37,3	37,6	38,1	38,8	37,6	34
60	13,2	22,9	23,9	25,6	26,7	27,3	28,6	28,8	26,7
70	8,71	15,8	16,5	18,4	19,8	20,4	21,7	22,4	21,3
80	6,16	11,6	12,1	13,9	15,2	15,8	17,1	18	17,4
90	4,7	8,99	9,5	10,9	12,3	12,9	14,1	14,9	14,7
100	3,85	7,39	7,9	9,1	10,4	11	12,2	12,9	13
110	3,35	6,41	6,92	7,96	9,34	9,89	11	11,7	12,1
120	3,07	8,8	6,34	7,28	8,73	9,31	10,4	11,1	11,8
130	2,91	5,42	6,02	6,2	8,45	9,07	10,2	11	12
140	2,84	5,2	5,88	6,73	8,41	9,07	10,2	11,2	12,4

150	2,8	5,09	5,86	6,7	8,54	9,25	10,5	11,5	12,9
160	2,79	5,09	5,94	6,77	8,77	9,52	10,9	11,9	13,4
170	2,81	5,15	6,07	6,88	8,99	9,77	11,3	12,2	13,8
180	2,83	5,19	6,13	6,93	9,09	9,87	11,4	12,3	13,9

The use of modeling the optical characteristics of the dispersed phase of fuel combustion products for calculating radiation heat transfer in multi-chamber furnaces of energy units for two-phase media was considered in [10]. In [16], the application of the developed database on optical characteristics for reconstructing the microstructure of the dispersed phase of fuel combustion products was considered.

The primary soot sol formed from the gas phase changes its microstructure as the combustion products move as a result of coagulation of particles. Homogeneous particle coagulation is described by the relation

$$r/r_0 = \left[1+\frac{1}{2}Kn_0\frac{\ln(1+\alpha t)}{\alpha}\right]^{1/3}, \qquad (11)$$

where K - brownian coagulation coefficient, n_0 - number of particles per unit volume; α^{-1} - time during which the particle radius doubles.

For heterogeneous multicomponent coagulation of particles, the distribution of the number of particles *f*[*r(t)*] is determined by the relation [16]:

$$\frac{f[r(t)]}{f_0(r)} = \sum_i\left[1+\frac{1}{2}k_i n_{0i}\ln\left\{\frac{1+\alpha_i t}{\alpha_i}\right\}\right]^{1/3} + \sum_{i\neq k}\left[1+\frac{1}{2}k_{ik}(n_{oi}\cdot n_{ok})^{1/2}\cdot\ln\left\{\frac{1+\alpha_{ik}t}{\alpha_{ik}}\right\}\right]^{1/3}, \qquad (12)$$

where $f_0(r)=\sum_i n_i$, n_i - number of particles with radius r_i per unit volume, *f*[*r(t)*] – temporal dependence of particle size distribution; *i*– fraction number; k_i- brownian coagulation coefficient for component *i*; $k_{i,k}$- brownian interaction coefficient of particles of different fractions *i,k*.

To perform the calculations *f*[*r(t)*] it is possible to use an iterative procedure in time with a step Δ*t*. Experiments show that the coagulation of soot particles is strongly influenced by the electrical properties of the particles. When burning gas fuel, a finely dispersed sol is formed with a modal radius $r_m = 0{,}003$ мкм during methane combustion. With an increase in the C/H ratio of hydrocarbon fuel, the modal radius r_m of soot particles increases. The microstructure of soot sol during the combustion of various hydrocarbons was studied in [16] using measuring complexes [10, 13].

The representation of the sol microstructure in the form of a superposition of individual fractions (1) is used to solve the problem of recovering the microstructure of soot sol in atmospheric emissions of combustion products of automobile and aviation vehicles, in boiler plants. For example, the microstructure of soot sol in atmospheric emissions of the combustion products of turbojet engines P-B, P-27B-300, P-25-300 in the cruiser mode of their operation is described by gamma distributions with parameters $a = 0{,}2$; $b = 6$; $c = 0{,}5$; $r_m = 4{,}4\cdot10^{-3}$ mkm. When turbojet engines operate in the afterburner mode, the microstructure of soot sol is described by a superposition of two distributions with parameters; $a_1 = 0{,}2$; $b_1 = 6$; $c_1 = 0{,}5$; $r_{1m} = 4{,}4\cdot10^{-3}$ mkm, $a_2 = 1$; $b_2 = 9$; $c_2 = 0{,}5$; $r_{2m} = 4{,}9\cdot10^{-3}$ mkm. The weight of each fraction in optical density at λ = 0.55 mkm is $\tau_1 = 0{,}56$, $\tau_2 = 0{,}44$.

Experimental studies on flame measuring complexes showed that the concentration and microstructure of soot sol in the products of the combustion of energy fuels strongly depends on the chemical composition and type of fuel [9-11, 16]. When the combustion products move in the furnaces, the microstructure of the dispersed phase and optical characteristics change: spectral attenuation coefficients of radiation $\sigma_{\lambda a}$, absorption $\sigma^a_{\lambda a}$, scattering $\sigma^S_{\lambda a}$, scattering indicatrix $f(\theta)$, scattering angle θ, which are normalized to the optical density τ_a at a wavelength of λ = 0.55 mkm. If we introduce the optical density for the i-te fraction of the sol $B_i(z) = \left|\frac{\partial \tau_i}{\partial z}\right|$, z is the height in the furnace, then:

$$\sigma_{\lambda a} = \sum_{i=1}^{N} B_i(z)\sigma_{i\lambda a} \ , \tag{13}$$

$$\sigma^{S}_{\lambda a} = \sum_{i=1}^{N} B_i(z)\sigma^{S}_{i\lambda a} \ , \tag{14}$$

$$\sigma^{a}_{\lambda a} = \sum_{i=1}^{N} B_i(z)\sigma^{a}_{i\lambda a} \ , \tag{15}$$

$$f_\lambda(z_i,\theta) = \sum_{i}^{N} B_i(z) f_{i\lambda} / \sum_{i}^{N} B_i(z) , \tag{16}$$

where N - number of fractions.

When modeling a complex refractive index *n* for dry sols of complex chemical composition, the ratio is used:

$$n = \sum_{i=1}^{N} n_i \frac{\delta_i}{\rho_i} / \sum_{i=1}^{N} \frac{\delta_i}{\rho_i} , \tag{17}$$

where n_i, δ_i, ρ_i complex refractive index, weight fraction and density i components respectively.

The soot sol emitted into the atmosphere changes its spectral optical characteristics under the influence of humidity and in connection with a decrease in the temperature of the combustion products as a result of their radiation cooling in the atmosphere. Experimental studies have shown that soot sol of combustion products contains a soluble fraction, which is ≈10% by mass in the products of combustion of gas fuel and ≈20% when burning wood. As a result of condensation processes of moisture on the particles, their complex refractive index, the microstructure of the dispersed phase and its optical characteristics change. The microstructure of soot sol in atmospheric emissions strongly depends on the residence time of the primary sol in the flame zone of the furnace, and the mass concentration of particles of soot sol in atmospheric emissions increases with an increase in the elemental composition C_m/H_n of organic fuel.

III. Conclusion

A system has been developed for numerically modeling the spectral radiation characteristics of the dispersed phase of the combustion products of organic fuels. Numerical modeling of the microstructure of a polydispersed soot sol is performed by superposition of the microstructures of its individual fractions in the form of Gamma distributions with modal radii from 0.016 to 1.5 mkm. The effective cross sections for attenuation of radiation $\sigma_{i\lambda a}$, absorption $\sigma^{a}_{i\lambda a}$, scattering $\sigma^{S}_{i\lambda a}$ and scattering indicatrix $f_{i\lambda}(\theta)$ for fractions of the *i* dispersed phase are calculated for spherical particles according to the Mi theory with normalization to optical density (τ_λ) for the wavelength λ = 0.55 μm and are presented in the form of an electronic database for calculating radiation heat transfer in cameras combustion and heat exchangers of power plants.

To identify the influence of anthropogenic emissions into the atmosphere on radiation heat transfer, it is recommended to use an extended electronic database of optical characteristics obtained for soot sol at a relative humidity of the radiation propagation medium $f \in \{0,1\}$ and normalized to the optical density $|\ln \tau|$ at λ = 0.55 mkm of fractions of gamma distributions of table 1 at relative humidity of the medium. The influence of relative humidity f on the optical characteristics of soot sol was calculated through the refractive index of radiation *n* according to the relation [16].

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