14. Yu. K. Lingart and V. A. Petrov, "Approximation method of calculating the true temperature from infrared pyrometer readings in the presence of a radiation background," Teplofiz. Vys. Temp., 16, No. 5, 1046-1053 (1978).

SOLUTION OF INVERSE PROBLEMS OF RADIATIVE TRANSPORT BY SOOT PARTICLES OF COMPLEX SHAPES

F. G. Bakirov, G. N. Zverev, R. S. Kashapov, and Z. G. Shaikhutdinov

UDC 536.3:621.43.019.7

We work out a method of determining the effective parameters of soot particles from their radiation characteristics. The method is based on the measurements of the spectral transmission coefficient in the infrared region of the spectrum.

It is known that the radiative properties of hydrocarbon flames are determined mainly by a polydisperse system of soot particles with complicated shapes and with a wide spectrum of sizes (from 0.02 to 5 μm) [1]. The current methods of calculating the radiative characteristics are based on the representation of the soot particles as spheres or ellipsoids of the same volume as the actual aggregate. Also the effect of the sizes, shapes, and orientations of the particles in space on the radiative characteristics of the flame are not taken into account. The data from optical measurements cannot be used to establish the concentration of soot in the combustion products because of the unsatisfactory agreement with measurements by contact methods [1, 2].

The refinement and development of optical diagnostics of hydrocarbon propellant flames in the presence of a dust of soot particles requires 1) quantitative relations between the effective parameters of the soot particles which determine their radiative characteristics, and the sizes, shapes, and orientations of the particles in space, and 2) solution of the inverse problem of radiative transport by particles of complicated shapes, i.e., the determination of these parameters from measurements of attenuation or angular scattering upon probing the medium by sources of radiative energy.

The solution of the first problem reduces to the choice of an optical model of the soot particles which would give the dependence of the radiative spectral characteristics of the particles on their sizes, shapes, and orientations in space on the basis of the Mie theory of the interaction of a flux of radiation with a spherical particle.

In [3] this problem was studied analytically and an optical model of the soot particles was worked out for the interpretation of attenuation measurements of the radiation flux by the soot particles. The model uses the following assumptions:

1) the soot particles are represented as clusters of elementary spheres of diameter d_0, and the number of spheres and their relative positions determines the size and shape of the aggregates;

2) the spectral attenuation coefficient of the soot particles $k_\lambda(D^*)$ is determined by the effective size D^*, which is the diameter of a circle with an area equal to the cross-sectional area of the aggregate $F_i = \pi D_i{}^{*2}/4 = \pi d_0^2 m_i/4$, where m_i is the number of elementary particles whose areas projected onto a plane perpendicular to the direction of the flux makes up the area of the irradiated surface;

3) the distribution function of the parameter m for soot particles consisting of n_j elementary particles obeys a normal distribution;

4) the soot particles are oriented randomly in space.

The quantitative relation between the effective parameters of the soot particles and their mass concentrations by size is given in terms of equations which were obtained with the

Sergo Ordzhonikidze Aviation Institute, Ufimsk. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 49, No. 6, pp. 921-925, December, 1985. Original article submitted May 17, 1985.

 0022-0841/85/4906-1408$09.50

use of the properties of the optical model

$$\mu_c = \rho_c \frac{\pi}{6} d_0^3 \sum_{j=k}^{n} n_j N(n_j), \quad N(m_i) = \sum_{j=k}^{n} N(n_j)\,\eta_j(m_i), \; k \geqslant i, \tag{1}$$

where $N(m_i) = N_\Sigma^* f(D_i^*)\Delta D$ is the number of soot aggregates having an irradiated surface area given by $F_i = \pi D_i^*/4$; $N(n_j)$ is the number of soot aggregates with n_j elementary particles, $\eta_j(m_i) = f_j(m_i)\Delta m$ is the relative fraction of soot particles with effective sizes $D_i^* \ldots D_i^* + \Delta D^* (D_i^* = d_0\sqrt{m_i})$ and consisting of n_j elementary particles; $f_j(m) = (\sigma_j\sqrt{2\pi})^{-1}\exp\,[-(m - m_{mj})^2/2\sigma_j^2]$. The parameters of the model m_{mj} and σ_j and their dependence on n_j are found from equations which were obtained from computer simulation of the shapes of the soot particles:

$$m_{m_j} = \frac{1}{3}\left[(2n_j)^{2/3} + \frac{4}{9}n_j + \frac{16}{3\pi}\left(\frac{2}{3}n_j\right)^{1/2} + n_j^{2/3}\right], \tag{2}$$

$$\sigma_j = \frac{1}{6}\left[\frac{2}{3}n_j - \left(\frac{1}{2}n_j\right)^{2/3}\right], \; n \leqslant 27,$$
$$\sigma_j = \frac{1}{6}\left[\left(\frac{1}{2}n_j\right)^{2/3} + \frac{1}{3}n_j\right], \; n_j > 27. \tag{3}$$

The determination of the effective parameters of the soot particles from measurements of the spectral transmission coefficient is based on the solution of the integral equation [4]

$$\sigma(\lambda) = -\frac{\ln t(\lambda)}{l} = \frac{\pi}{4} N^* \int_{D_1^*}^{D_n^*} k_\lambda(D^*)\,D^* f(D^*)\,dD^*. \tag{4}$$

Numerous attempts to solve (4) directly have shown that the solution is quite unstable and the problem belongs to the class of incorrectly posed problems. In order to make the problem a correctly posed one, we apply an information model used in geophysics [5]. In this approach we first carry out a comprehensive normalization of the processes of measurement of the characteristics of the phenomena and an analysis of observations. We thus obtain a set of information models, which, independently of the measurement processes and data analysis, describe the process of constructing *a priori* data and the resulting errors.

In order to construct correct solutions of (4), the observation model describes the experimental dependence $\sigma(\lambda)$ in the form

$$\hat{y} = Az + \Delta Az + \Delta y, \tag{5}$$

where A is a finite-dimensional approximation of the operator (4), ΔAz is an internal disturbance of the direct model, due to noise and the inexact determination of the optical properties of the soot, Δy is the error in the measurement of $\sigma(\lambda)$; $\hat{y} = [\sigma(\lambda_1), \sigma(\lambda_2), \ldots, \sigma(\lambda_n)]$ is the observation vector (the measurements of the spectral transmission coefficient for $\lambda = \lambda_1\lambda_2, \ldots, \lambda_n$; $z = [N(D_1^*), N(D_2^*), \ldots, N(D_n^*)]$ is the vector of unknowns, $N(D_i^*) = N_\Sigma^* f(D_i^*) - dD_i^*$ is the number of soot particles with effective sizes $D_i^* \ldots D_i^* + dD^*$ per unit volume of the gas.

We look for a solution of (5) in the form

$$\hat{z} = z_0 + B_0(\hat{y} - y_0), \tag{6}$$

where $y_0 = Az_0$, and $z_0 = [\bar{N}(D_1^*), \bar{N}(D_2^*), \ldots, N(D_n^*)]$ is an estimate of the required z chosen from the *a priori* information (the *a priori* mean), $B_0 = \mathrm{Cov}(z)A^T[\mathrm{Cov}(z)A\mathrm{Cov}(z)^T + \mathrm{Cov}(\Delta Az + \Delta y)]^{-1}$, Cov(z) is the covariance matrix of the vector z, $\mathrm{Cov}(\Delta Az + \Delta y)$ is the covariance matrix of the errors of the direct model and the measurements.

The accuracy of the solution of the inverse problem for the case where the *a priori* information is specified exactly is characterized by a zero value of the systematic component

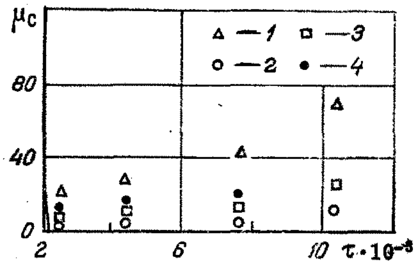

Fig. 1

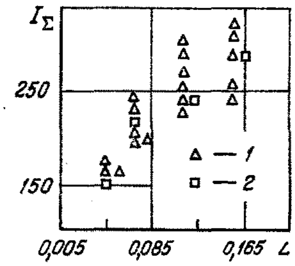

Fig. 2

Fig. 1. Effect of the time duration on the mass concentration of soot particles in flames of homogeneous kerosene—air mixtures for P = 1.5 MPa, α = 0.4: 1) apparent μ_c determined from the condition $D^* = D_{sph}$ (the spherical model); 2) determined with the formula of Medalla and Heckman [6]; 3) determined with the optical model discussed here; 4) measurements by the filtration method based on the sampling of soot from flames. μ_c, g/m³; τ, sec.

Fig. 2. Intensity of radiation of flames of a homogeneous kerosene-air mixture as a function of the reaction length of the chamber for P = 1.5 MPa and α = 0.4: 1) measurements of the radiation intensity by thermoradiometry; 2) calculated results with the use of effective parameters of the soot particles. I_Σ, kW/m²·sr; L, m.

of the error $\Delta z = \hat{z} - z$ and a minimum for the random components of the error

$$\mathrm{Cov}(\Delta z) = \mathrm{Cov}(z) - B_0 A\,\mathrm{Cov}(z). \quad (7)$$

In order to carry out this computational scheme, information is necessary on the elementary covariance matrices Cov(ΔAz + Δy) and Cov(z). The error matrix Cov(ΔAz + Δy) can be written in the form Cov(ΔAz + Δy) = Cov(ΔAz) + Cov(Δy) in the absence of coupling between the errors in the measurements and in the determination of the complex index of refraction.

The diagonal elements of the matrix Cov(ΔAz) represent the dispersion of $\sigma(\lambda)$ caused by the error in the determination of the complex index of refraction of the soot $m(\lambda) = n(\lambda) - i\chi(\lambda)$; where $n(\lambda)$ is the index of refraction, $\chi(\lambda)$ is the absorption coefficient. The absence of a common error in $n(\lambda_i)$ and $n(\lambda_{i+1})$, and $\chi(\lambda_i)$ and $\chi(\lambda_{i+1})$ implies that the nondiagonal elements of this matrix are zero. As *a priori* information, for an estimate of the dispersion of $\sigma(\lambda)$ as a function of the error in $m(\lambda)$, we chose results from the equation

$$D[\sigma(\lambda_i)] = [\sigma_{\max}(\lambda_i) - \sigma_{\min}(\lambda_i)]^2/4f_1^2\left[\frac{\hat{\sigma}(\lambda_i)}{\sigma_0(\lambda_i)}\right]^2, \quad (8)$$

where $\sigma_{max}(\lambda_i)$ is the effective spectral attenuation cross section of the particles with $m(\lambda)$ for amorphous carbon, $\sigma_{min}(\lambda_i)$, $\sigma_0(\lambda_i)$ are the effective spectral attenuation cross sections of particles with $m(\lambda)$ for propanic soot and for soot in the diffusion flame, and $\hat{\sigma}(\lambda_i)$ represents the optical measurements.

The diagonal elements of the covariance matrix Cov(Δy) give the dispersion of $\sigma(\lambda)$ due to inaccuracies of the measurements, and are determined from a statistical analysis of the measurements $D[\hat{\sigma}(\lambda_i)] = \sum_{k=1}^{n}[\sigma_k(\lambda_i) - \tilde{\sigma}(\lambda_i)]^2/n-1$, where $\tilde{\sigma}(\lambda_i) = \sum_{k=1}^{n}\sigma_k(\lambda_i)/n$. In the absence of coupling between the errors in $\sigma(\lambda_i)$ and $\sigma(\lambda_{i+1})$, the nondiagonal elements of the covariance matrix Cov(Δy) are equal to zero.

The estimate of the elements of the covariance matrix Cov(z) and the variation of the required value of z are based on *a priori* information on the parameters of the soot particles and use of the formula of Medalla and Heckman [6]

$$F_j(m_i) = \frac{\pi}{4} d_0^2 n_j^{0.87} = \frac{\pi}{4} d_0^2 m_i. \quad (9)$$

Using the methodology described above, we wrote a program for the ES-1033 computer and applied it to the combustion conditions of a homogeneous kerosene—air mixture. The mass concentration of soot particles was determined from measurements of the spectral transmission coefficient in the region of wavelengths $\lambda = 1.5\text{-}4.0$ μm (with the exclusion of the absorption bands of the triatomic gases (CO_2, H_2O) and gases with hydrocarbon bonds (CH, CH_2, CH_3)). The results are shown in Table 1.

The computed results with our model show a satisfactory agreement with the experimental data. Calculations according to the previous methods predict the mass concentration of soot in the combustion products with acceptable accuracy only in the region $\tau = 2.0 \cdot 10^{-3}$ to $3.0 \cdot 10^{-3}$ sec, since in the initial stage the shape of the soot particles does not deviate significantly from spherical and the effect of coagulation is insignificant.

Our assumption on the important effect of the irradiation surface of the soot particles on the transport of radiation is supported experimentally. In Fig. 2 we show the results of calculations for the radiation intensity of flames with the use of effective parameters of the soot particles from the optical model presented here. A satisfactory agreement between the direct measurements of the radiative energy flux with the help of thermoradiometry and the calculated values is observed. The use of information only on the specific surfaces and mass concentration of soot particles leads to significant errors.

Finally we note that the methodology given here for solving inverse problems of radiative transport can be used to find the mass concentration and effective parameters of the soot particles when the errors in the optical measurements are as large as 20%.

NOTATION

λ, wavelength of the radiation, μm; $t(\lambda)$, spectral transmission coefficient; σ_λ, spectral effective attenuation cross section, μm^{-1}; $k_\lambda(D^*)$, spectral attenuation coefficient of a particle of size D^*; μ_C, mass concentration of soot particles, g/m^3; $N_\Sigma^*(D^*)$, effective total number of particles per unit volume of gas, m^{-3}; D^*, effective size of the particles, μm; $f(D^*)$, distribution function of the soot particles with respect to the diameter D^*, μm^{-1}; $m(\lambda)$, complex index of refraction of the particles; τ, time duration in the flame, sec; L, reaction length of the chamber, m; I_Σ, integral intensity of radiation, $kW/m^2 \cdot sr$; α, excess coefficient of air; f_p, probable rise coefficient; l, effective thickness of the probed volume of the combustion products.

LITERATURE CITED

1. R. S. Kashapov and F. G. Bakirov, "Determination of the dispersion of soot particles in flames by measurements of the spectral transmission," Symp. "On the Theory and Calculation of Processes in Heat Engines" [in Russian], No. 6, Ufa: Ufimsk. Aviation Inst., pp. 110-122 (1982).
2. A. D'Alessio, "Laser light scattering and fluorescence diagnostics of rich flames produced by gaseous and liquid fuels," Particulate Carbon: Formation during Combustion, GMR Symp. (1980), pp. 207-259.
3. R. S. Kashapov, F. G. Bakirov, and G. N. Zverev, "Solution of inverse problems of radiative transport in hydrocarbon propellant flames," in: Methods and Consequences of Computer Diagnostics of Gas Turbine Engines and Their Elements [in Russian], Proc. All-Union Conf., Kharkov Aviation Inst., Vol. 2 (1983), pp. 65-66.
4. K. S. Shifrin, "Study of the properties of matter from single scattering," in: Theoretical and Practical Foundations of Light Scattering Problems [Russian translation], Mir, Moscow (1971), pp. 228-244.
5. G. N. Zverev and S. N. Dembitskii, Analysis of the Geophysical Research on Rifts [in Russian], Nedra, Moscow (1982).
6. A. J. Medalla and F. A. Heckman, "Morphology of aggregates size and shapes factors of carbon black aggregates from electron microscopy," Carbon, 7, 567-582 (1969).